AN ABSTRACT OF THE DISERTATION OF

Thomas J. L. Mustard for the degree of Doctor of Philosophy in Chemistry presented on April, 15, 2015.

Title: Computational Investigations of Transition Metal Catalyses and Amorphous Metal Oxides: Accelerating Scientific Discovery Through Automation.

Abstract approved:

_____

Paul Ha-Yeon Cheong

Automation of computational chemistry, while only an engineering feat, has the potential to accelerating computational research be removing all by the science. The work in this thesis mainly discusses fundamental understanding of complex chemical systems. What is not obvious are the numerous tasks necessary for this fundamental understanding. Under the surface automation and acceleration of many tedious and otherwise intractable tasks has made the research possible.

Density functional theory computations of the Cu-catalyzed ring expansion of vinyloxiranes is mediated by a trace less dual Cu(I)-catalyst mechanism. Overall, the reaction involves a monomeric Cu(I)-catalyst, but a single key step, the Cu migration, requires two Cu(I)-catalysts for the transformation. This dual-Cu step is found to be a true double Cu(I) transition state rather than a single Cu(I) transition state in the presence of an adventitious, spectator Cu(I). Both Cu(I) catalysts are involved in the bond forming and breaking process. The single Cu(I) transition state is not a stationary point on the potential energy surface. Interestingly, the reductive elimination is rate-

determining for the major diastereomeric product, while the Cu(I) migration step is rate-determining for the minor. Thus, while the reaction requires dual Cu(I) activation to proceed, kinetically, the presence of the dual-Cu(I) step is untraceable. The diastereospecificity of this reaction is controlled by the Cu migration step. Suprafacial migration is favored over antarafacial migration due to the distorted Cu π-allyl in the latter.

The origins of differential catalytic reactivities of four Rh(I) catalysts and their derivatives in the (5 + 2) cycloaddition reaction were elucidated using density functional theory. Computed free energy spans are in excellent agreement with known experimental rates. For every catalyst, the substrate geometries in the transition state remained constant (<0.1 Å RMSD for atoms involved in bond-making and -breaking processes). Catalytic efficiency is shown to be a function of how well the catalyst accommodates the substrate transition state geometry and electronics. This shows that the induced fit model for explaining biological catalysis may be relevant to transition metal catalysis. This could serve as a general model for understanding the origins of efficiencies of catalytic reactions.

The cross-coupling of allylzinc halides with aryl and vinyl electrophiles provides an effective means to access a wide range of prenylated arenes and “skipped dienes” in a completely linear-selective fashion, as demonstrated by a concise synthesis of the anti-HIV natural product siamenol. DFT calculations shed light on the origin of the excellent regioselectivity observed with the current Pd-based catalyst system.

We computed band gaps of amorphous oxides within the In-Ga-Zn triad. These included ZnO, Ga_2O_3, In_2O_3, Ga_2ZnO_4, $Ga_2Zn_8O_{11}$, In_2ZnO_4, $InGaZnO_4$, and $InGaO_3$. Comparing the computed band gap to experimental measurements, the results were promising with a mean unsigned error of 0.28 eV and an unsigned standard deviation of 0.28 eV. Unfortunately drastic over prediction of the band gap for ZnO and $InGaZnO_4$ was observed.

The ever acceleration of computational speed and efficiency is allowing for accurate computations of large and complex chemical systems. As these systems grow in size and complexity the number of data points grow exponentially. Traditionally computational chemists would do the tedious work of manually creating, submitting, examining and parsing all files and data points. With the use of both GPU acceleration and ηScripts, a library of tools, we have changed the intractable into the achievable and tedious into the pleasant.

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Computational Investigations of Transition Metal Catalyses and Amorphous Metal Oxides: Accelerating Scientific Discovery Through Automation

by
Thomas J. L. Mustard

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APPROVED:

Major Professor, representing Chemistry

Chair of the Department of Chemistry

Dean of the Graduate School

I understand that my dissertation will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my dissertation to any reader upon request.

Thomas J. L. Mustard, Author

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CONTRIBUTION OF AUTHORS

Chapter 2. Dr. Daniel J. Mack conducted the synthesis and experiments for this project. Jon T. Njardarson, and Paul Ha-Yeon Cheong contributed in part to the preparation and review of this manuscript.

Chapter 3. Paul A. Wender, and Paul Ha-Yeon Cheong contributed in part to the preparation and review of this manuscript.

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Chapter 5. Geneva Laurita-Plankis, Dylan B. Fast, and Prof. Michelle R. Dolgos conducted the experimental PDF study for this project. Benjamin E. Hankin, and Paul Ha-Yeon Cheong contributed in part to the preparation and review of this manuscript.

Chapter 6. O. Maduka Ogba assisted in the creation and validation of several functions. Paul Ha-Yeon Cheong contributed in part to the preparation and review of this manuscript.

Chapter 7. Paul Ha-Yeon Cheong contributed in part to the preparation and review of this manuscript.

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Dedicated to
Erin, Henry,
my loving parents,
family, mentors,
and teachers.

Chapter 1.

Introduction

1.1 Homogeneous Organometallic Catalysis:

Transition metal-catalyzed reactions are of preeminent importance to the practical syntheses of materials, pharmaceuticals and feed stock compounds.[1–3] Organometallic catalysts are among the most reactive and selective forms of catalysis available to man. Furthermore, previously unattainable reaction pathways and products can be accessed with transition metals, providing unique chemistry not found in purely organic reactions from the s and p-blocks of the periodic table. .[4]

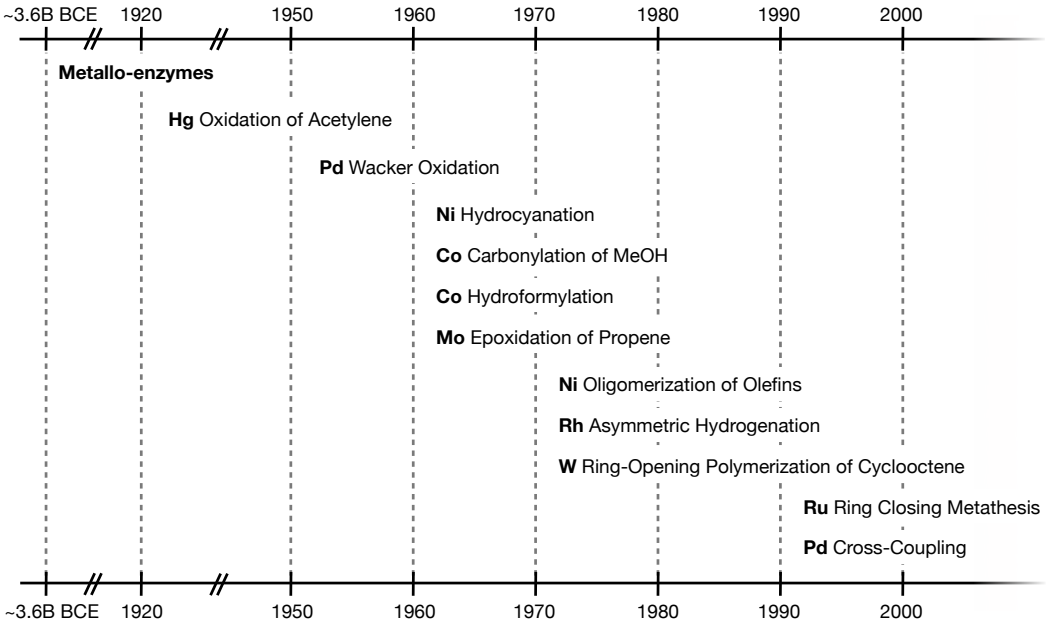
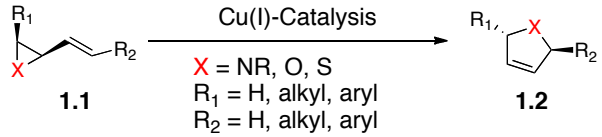


Figure 1.1. Brief history of the industrial use of organometallic catalysts.

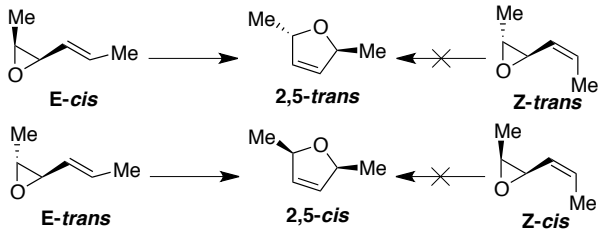
The use of homogeneous transition metal catalysis on planet earth began millions of years ago with nature's metallo-enzymes (Figure 1.1). In today's androsphere, organometallic catalysis accounts for at least $4.7B of the $20.6B catalyst market.[2,5] From mercuric sulfate catalyzed acetylene oxidation in the 1920s to the asymmetric hydrogenation of L-DOPA, organometallic catalysts have come to occupy a critical corner of the chemical industry, academic research, and human existence.

1.1.1 Copper Heterocycle Ring Expansion:

Copper catalyzed ring expansions of vinyloxiranes, -thiiranes, and -aziridines to their respective dihydrofuran, -thiophene, and -pyrrole products, is a relatively new methodology.[6,7] The methodology reported by Njardarson (Scheme 1.1), is exceptionally high yielding, stereoselective (Scheme 1.2), and includes a wide substrate scope, applicable to vinyloxiranes, -thiiranes, and -aziridines.



Scheme 1.1 Model catalytic cycle for the Cu(I) ring expansion of a vinyloxirane.

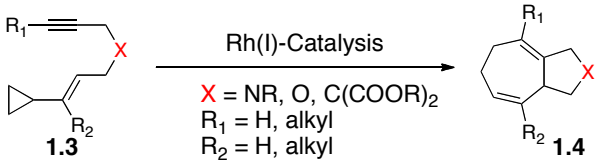


Scheme 1.2 Diasterospecificity and reactivity of the Copper mediated ring expansion of vinyloxiranes.

The complete mechanism for the stereoselective ring expansion of vinyloxiranes was studied using density functional theory. Our computations of the Cu-catalyzed ring expansion showed that vinyloxiranes are mediated by a traceless dual Cu(I)-catalyst mechanism. Overall, the reaction involves a monomeric Cu(I)-catalyst, but a single key step, the Cu migration, requires two Cu(I)-catalysts for the transformation. This dual-Cu step is found to be a true double Cu(I) transition state rather than a single Cu(I) transition state in the presence of an adventitious, spectator Cu(I). Both Cu(I) catalysts are involved in the bond forming and breaking process. The single Cu(I) transition state is not a stationary point on the potential energy surface. Interestingly, the reductive elimination is rate-determining for the major diastereomeric product, while the Cu(I) migration step is rate-determining for the minor. Thus, while the reaction requires dual Cu(I) activation to proceed, kinetically, the presence of the dual-Cu(I) step is untraceable. The diastereospecificity of this reaction is controlled by the Cu migration step. Suprafacial migration is favored over antarafacial migration due to the distorted Cu π-allyl in the latter.

1.1.2 Rhodium [5+2] Cycloaddition:

Rhodium catalyzed [5+2] cycloaddition was first reported by Wender.[8,9] This was the first synthetically viable [5+2] homologue to the Diels-Alder, enabling the facile construction of seven membered rings with two new stereocenters, in the same way Diels-Alder revolutionized organic chemistry by providing a facile way of constructing six membered rings with two new stereocenters. More recently, new catalysts have been introduced that greatly increase the reactivity.[10]

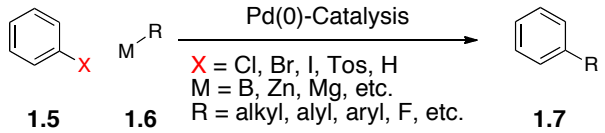


Scheme 1.3 Model catalytic cycle of the Rh(I) [5+2] cycloaddition of **1.5**.

Our research into the origins of differential catalytic reactivities of four Rh(I) catalysts and their derivatives in the (5 + 2) cycloaddition reaction (Scheme 1.3) were elucidated using density functional theory. We have discovered a consistent pattern in the computed transition state structures across the different catalysts. Specifically, for every catalyst, the substrate geometries in the transition state remained constant (<0.1 Å RMSD for atoms involved in bond-making and -breaking processes). Catalytic efficiency is shown to be a function of how well the catalyst accommodates the substrate transition state geometry and electronics. This shows that the induced fit model for explaining biological catalysis may be relevant to transition metal catalysis. This could serve as a general model for understanding the origins of efficiencies of catalytic reactions.

1.1.3 Palladium Cross-Coupling:

The first cross-coupling processes discovered in the 19th century were limited to homocoupling.[11] In the mid- and late-1970s, Negishi, Suzuki & Miyaura, and Heck & Mizoroki created the modern palladium cross-coupling as we know today, and has irreversibly changed organometallic chemistry. For their contribution to science, Suzuki and Heck were awarded the Nobel Prize in 2010.



Scheme 1.4 Model example of Pd Cross-Coupling.

The title reaction provides an effective means to access a wide range of prenylated arenes and "skipped dienes" in a completely linear-selective fashion (Scheme 1.4). Our computations shed light on the origin of the excellent regioselectivity observed. While α-transmetallation is preferred over γ, reductive elimination of the α product is rate and therefore stereodetermining.

1.2 Amorphous Metal Oxides:

Amorphous metal oxides are key components in a wide range of electronics, e.g. LCDs, plasma displays, solar cells, and organic light emitting diodes. For decades hydrogenated amorphous silicon (α-Si:H) has been the material of choice for thin-film transistors (TFT) devices. Amorphous metal oxides, specifically $InGaZnO_4$ (IGZO), is replacing α-Si:H for four main reasons: (1) lower power consumption due to lower current leakage; (2) smaller TFTs due to higher electron mobility; (3) low absorption in the visible spectrum; and (4) a substantial structural bias to maintain an amorphous phase.[12–20] While there are materials that outperform IGZO in one or more aspects, IGZO has many manufacturing advantages as well. IGZO backplanes in excess of $5m^3$ are regularly produced for the LCD industry. Crystalline structures are known to perform better than their amorphous counterparts, yet producing a flawless crystal on this scale and processing it for production has proven difficult and expensive.

The ability to predict the structures and electronic properties of amorphous metal oxides will have a huge impact in the directed synthesis of novel

materials for electronic devices. In the past, these predictions have not been possible. We present here a computational method that can generate atomistic structures of amorphous solids as well as predict their band gap. Amorphous solids discussed explicitly in this work are: ZnO, Ga2O3, In2O3, Ga2ZnO4, Ga2Zn8O11, In2ZnO4, InGaZnO4, and InGaO3. The methodology does not rely on previously know crystal structure data, and thus unknown compositions can be produced. Band gaps calculated have a mean unsigned error of 0.28 eV and standard deviation of 0.28 eV.

1.3 Acceleration and Automation of Computational Research:

The acceleration and automation of computational chemistry can be as simple as the implementation of a loop for iterating through a list of instructions to advanced algorithms capable of sorting millions of objects based on dynamic variables. Many accelerants are hidden in the background behind exceptionally optimized libraries and compilers, while others are more advertised, such as commercialization of the latest hardware. If implemented correctly, both can drastically accelerate computational chemistry research.

1.3.1 Acceleration via Architecture:

Every year or so, new processing units hit the market with incremental increases in processing power. Occasionally, as in the case of general purpose graphics processing units (GPGPUs) and many integrated core (MIC) or new instruction extensions, a leap is introduced. GPGPUs and MICs possess hundreds to thousands of distinct computing cores. This allows them to process orders of magnitude more operations per clock cycle compared to their CPU counterparts. A small GPU cluster was built to take advantage of the accelerations available to harnessing thousands of cores originally intended for video games.

1.3.2 Automated Workflow:

Efficiency in computational chemistry can be increased without changing the software suite, architecture of processing unit, or the compiler and libraries used. Tools for managing, generating, and analyzing the data generated are often underdeveloped or severely inefficient. Efficiency is now strongly dependent on these tools. To this end, we have built a library of tools that accelerate the human aspect of computational chemistry. It is now trivial to create, disseminate, and group thousands of files at a time with unprecedented precision. This acceleration through automation allows the chemist to drive the chemistry rather than tackle the job of manually maintaining and disseminating the ever-increasing data sets.

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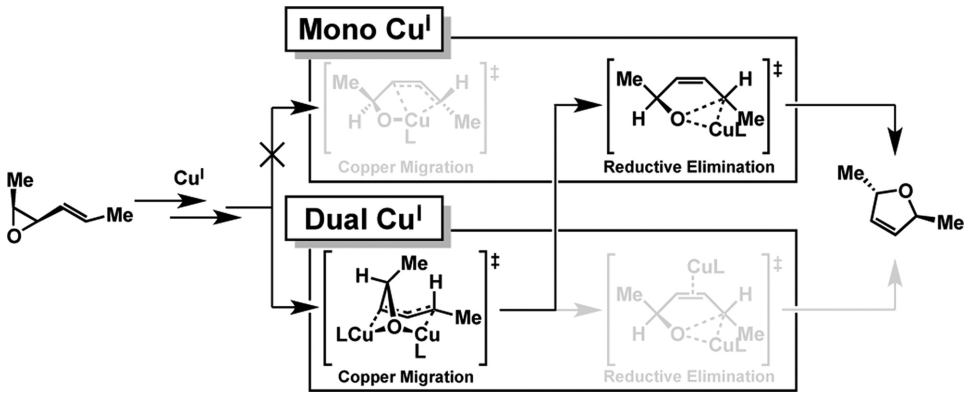
Chapter 2.

Mechanism and the Origins of Stereospecificity in Copper-Catalyzed Ring Expansion of Vinyl Oxiranes: A Traceless Dual Transition-Metal-Mediated Process

Thomas J. L. Mustard, Dr. Daniel J. Mack, Prof. Jon T. Njardarson, and Prof. Paul Ha-Yeon Cheong

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2.1 ABSTRACT:

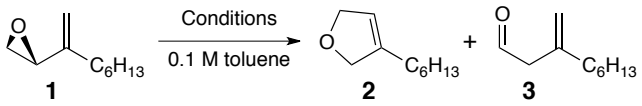


Density functional theory computations of the Cu-catalyzed ring expansion of vinyloxiranes is mediated by a trace less dual Cu(I)-catalyst mechanism. Overall, the reaction involves a monomeric Cu(I)-catalyst, but a single key step, the Cu migration, requires two Cu(I)-catalysts for the transformation. This dual-Cu step is found to be a true double Cu(I) transition state rather than a single Cu(I) transition state in the presence of an adventitious, spectator Cu(I). Both Cu(I) catalysts are involved in the bond forming and breaking process. The single Cu(I) transition state is not a stationary point on the potential energy surface. Interestingly, the reductive elimination is rate-determining for the major diastereomeric product, while the Cu(I) migration step is rate-determining for the minor. Thus, while the reaction requires dual Cu(I) activation to proceed, kinetically, the presence of the dual-Cu(I) step is untraceable. The diastereospecificity of this reaction is controlled by the Cu migration step. Suprafacial migration is favored over antarafacial migration due to the distorted Cu π-allyl in the latter.

2.2 INTRODUCTION:

Cooperative or dual catalysis has become popular in recent literature; dual organocatalyzed,[1] organo- and transition-metal-catalyzed,[2] homobimetallic transition-metal-catalyzed,[3] and even heterobimetallic-catalyzed[4] processes are known.[5] We have previously reported a simple and scalable Cu(II)-catalyzed synthetic method for the preparation of dihydrofurans (DHFs) from vinyloxiranes (VOs)[6a,6b] (Table 2-1),[7] key structural components found in natural products, bulk commodity chemicals, and pharmaceuticals. Herein, we report the complete mechanism and the origins of diastereospecificity for this transformation. Specifically, we propose an unusual, traceless dual catalysis motif. A key step in this reaction requires two Cu(I)-catalysts, but the rate-determining step only requires a single catalyst. Ultimately, this renders the dual catalysis motif kinetically undetectable but crucial for the chemistry.

Table 2.1 Copper-Catalyzed Rearrangement of Vinyloxirane **1**[a]



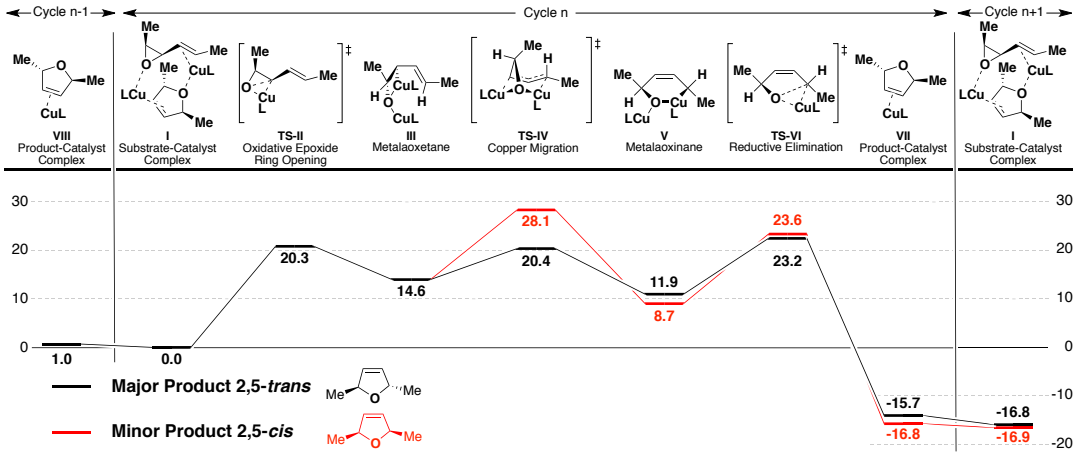
1 **2** **3**

Entry	Conditions	Temp (ºC)	Time (h)	Conv. (%)	DHF:H-shift
1	A	150	0.25	100	13:1
2	B	150	0.25	100	17:1
3	C	150	0.25	100	15:1
4	A	100	4	No rxn	N/A
5	B	100	4	84	>20 : 1
6	C	100	4	65	>20 : 1
7	A	80	10	No rxn	N/A
8	B	80	10	89	>20 : 1
9	C	80	10	70	>20 : 1

[a]Conditions: **A** 5 mol% $Cu(hfacac)_2$**; B** 5 mol% $Cu(hfacac)_2$ + 5 mol% Sn(2-ethylhexanoate)$_2$**; C** 5 mol% Cu(hfacac)(COD)

2.3 Experimental Section:

As previously reported,[6] $Cu(hfacac)_2$ catalyzes the transformation of vinyloxirane **1** to dihydrofuran **2**. In these reactions, a significant initial induction period was observed, suggesting that a more active catalyst was being formed in situ. Njardarson et al. has since discovered that this ring expansion reaction is significantly accelerated by the use of Cu(I) catalysts.[10] This was accomplished using reducing agents such as Sn(II)-2-ethylhexanoate[11a] and cobaltocene,[8b] or alternatively by using preformed Cu(I) catalysts such as Cu(hfacac)(cod).[12] Employing either one of these conditions, significant reaction acceleration was observed, and ring expansions could be run at lower temperatures (Table 2-1). All conditions perform similarly at 150 °C (entries 1–3), but at 100 or 80 °C the Cu(II) conditions (A) fail (entries 4 and 7), while the new Cu(I) catalyzed conditions successfully ring expand **1** to selectively form **2** (entries 5–6 and 8–9). Equally important evidence in favor of Cu(I)-catalysis was the absence of the initial induction period previously observed in all $Cu(hfacac)_2$ kinetic traces.[6a,7,8a,9] Similar Cu(I) supportive insights were also observed for the analogous vinylaziridine expansion.[9]



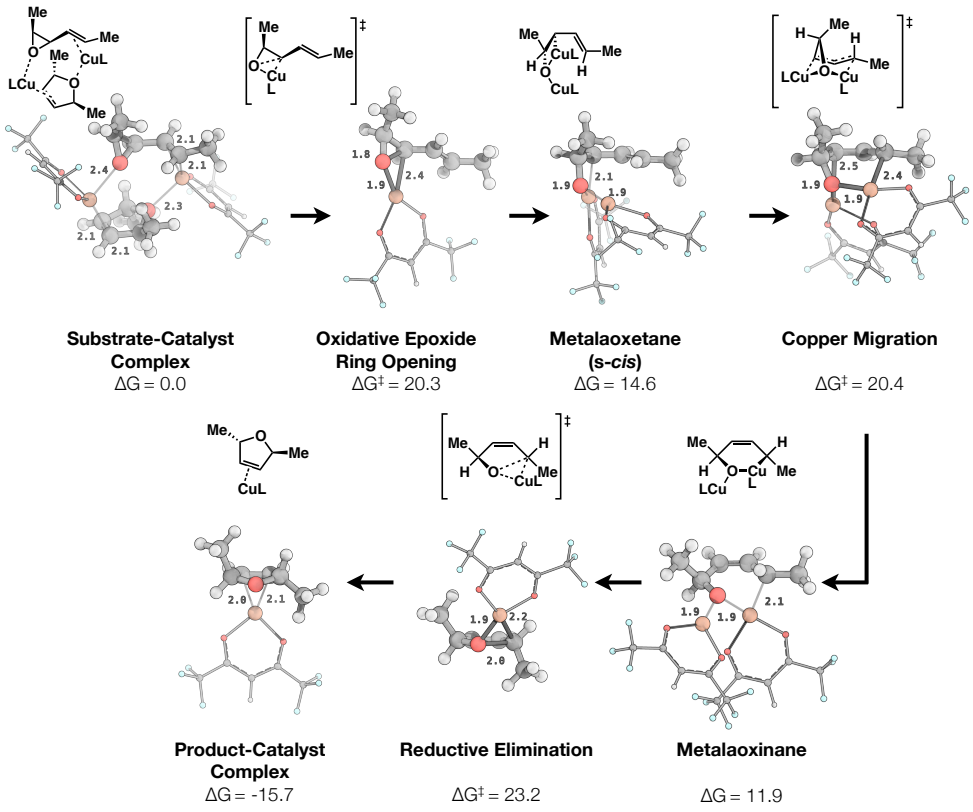


Figure 2.1 Reaction coordinate of Cu(I)-catalyzed ring expansion of *cis*-2,3-epoxy-*trans*-4-hexene (*cis*-2-methyl-*trans*-*3*-propenoxirane) (above) and structures of stationary points along the reaction coordinate for the formation of the major products (below).[7] All structures, energies, and free energy corrections computed at the B3LYP/def2-SVP level of theory, as implemented in Turbomole.[xiiia-xiiid] Energies displayed in kcal/mol, and distances in Å. Computed structures rendered using Pymol.[xiiie]

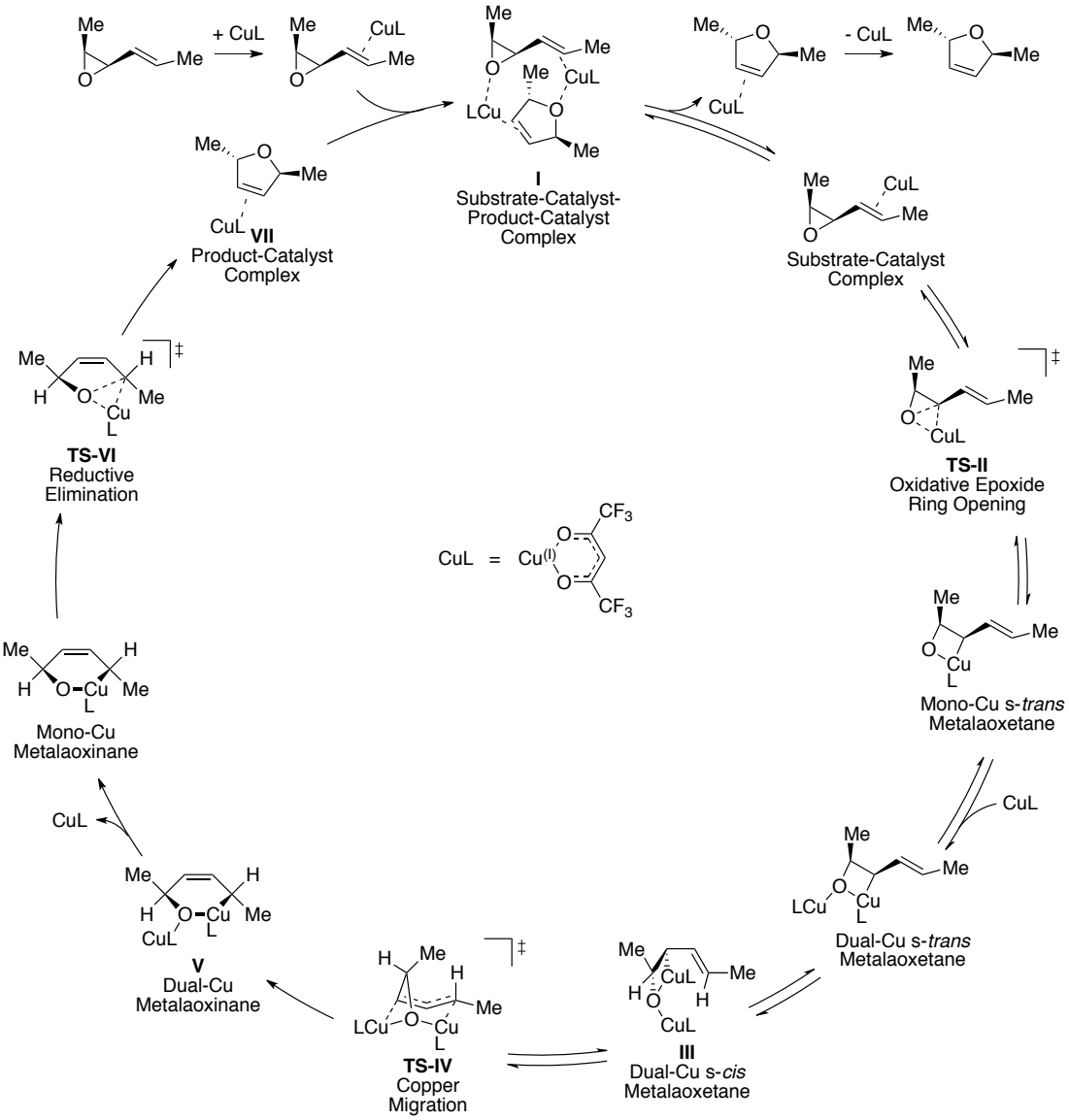


Figure 2.2 Complete catalytic cycle for the Cu(I)-catalyzed stereospecific rearrangement of vinyloxiranes to dihydrofurans.

2.4 COMPUTATIONAL METHODS:

The geometries and thermal corrections for all stationary points along the reaction coordinate were computed with the B3LYP and the def2-SVP basis set, as implemented in the Turbomole suite of programs.[xiii] Manual, exhaustive conformational searches, including all possible single or dual Cu ligation isomers, were performed for all species reported. Stationary points were verified by frequency calculations and wave function stability tests.

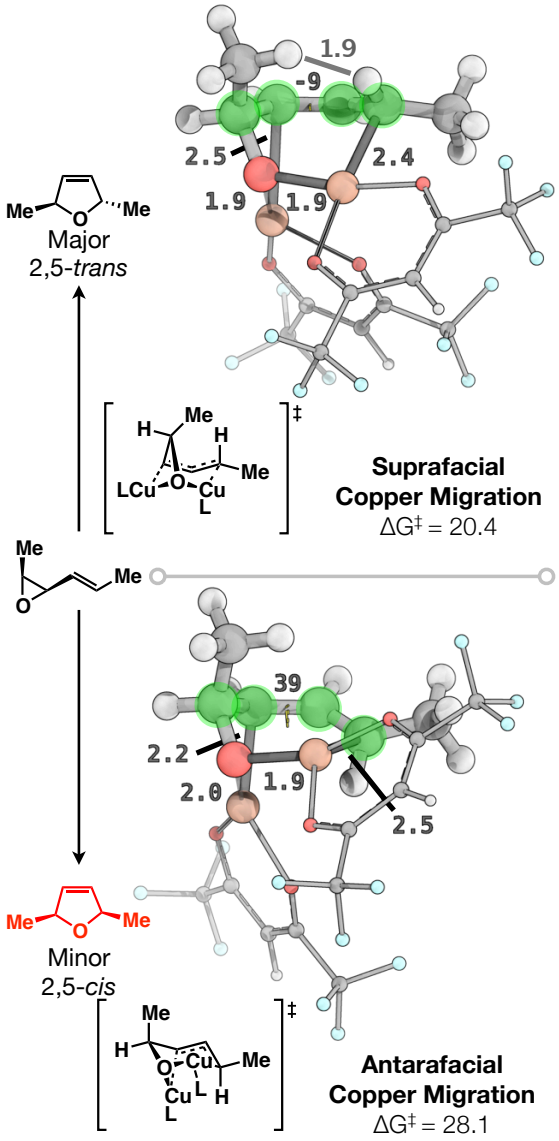


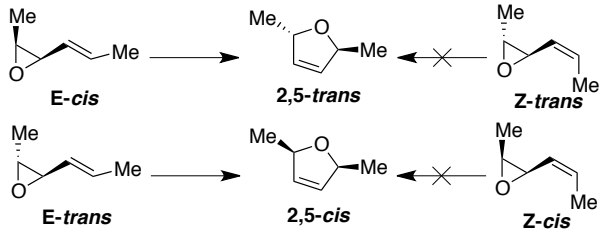
Figure 2.3 Dual Cu(I) migration transition structures leading to the major and minor products, computed at the B3LYP/def2-SVP level of theory, as implemented in Turbomole.[xiii a-xiii d] π-allyl atoms are highlighted in green. Energies displayed in kcal/mol, distances in Å, and dihedrals in degrees. Computed structures rendered using Pymol.[xiii e]

2.5 Results and Discussion:

Initially, the entire reaction coordinate involving a single Cu(I)-catalyst was computed. The catalytic cycle begins with the initial exothermic complexation

of a free Cu(I) catalyst with a substrate alkene. Oxidative epoxide ring opening affords the s-*trans*-metalaoxetane. Upon isomerization to s-*cis*-metalaoxetane, the copper is poised for migration to the distal olefin carbon. However, computations showed that this key Cu(I)-migration step to form the metalaoxinane is not a stationary point on the potential energy surface with a single Cu(I) catalyst. If the metalaoxinane could be produced, the system would undergo reductive elimination to afford the dihydrofuran product.

In the monocopper migration process, the endocyclic Cu(III) migrates to the distal olefin carbon to form the metalaoxinane directly. However, shortening the Cu–C bond along the expected reaction coordinate results in the reformation of the oxirane ring, reverting back to the starting VO–Cu complex. This is presumably due to the large strain in the four membered metalaoxetane during mono copper migration. In sharp contrast, a dual Cu(I)-catalyzed migration step to form the metalaoxinane was a true stationary point along the reaction coordinate. Use of a second copper removes the strain in the metalaoxetane. In the dual-copper process, the exocyclic Cu(I) migrates to the distal olefin carbon forming the metalaoxinane. These computational evidence collectively suggest that this dual Cu step is distinctly different from a single Cu mechanism in the presence of an adventitious, spectator Cu(I); the second Cu(I) is essential for this transformation.



Scheme 2.1. Diastereospecificity of the Title Reaction. *E-cis* and *Z-cis* yield the *trans*-DHP product, whereas the *E-trans* and *Z-trans* yield the *cis*.[6a,xiv]

This reaction involves both single and dual copper intermediates and transition states (Figures A and B).[xv] The reaction coordinate diagram as well

as the computed structures for the formation of the major product is shown in Figure 2.1. The complete detailed catalytic cycle is shown in Figure 2.2. The resting state of the catalytic process is the cyclic substrate–catalyst–product–catalyst complex **I**. Both Cu(I) catalysts are found to be square pyramidal, coordinating to the π-systems of a substrate or product and an oxygen of another substrate or product. The dissociation of this complex to the monocopper vinyl oxirane complex is endothermic by 2.3 kcal/mol. In the oxidative epoxide ring opening **TS-II**, the Cu(I)-hfacac inserts into the epoxide C–O bond. The metalaoxetane Cu(III) is also in a square planar configuration, with the coordinating C, O, and the hfacac in the plane. Upon complexation of a free Cu(I) catalyst to the metalaoxetane oxygen, the s-*trans*/s-*cis* isomerization of this species affords the dual-copper s-*cis*-metalaoxetane **III**. In the following copper migration **TS-IV**, the exocyclic Cu(I) migrates to the distal olefin carbon, forming the metalaoxinane, while simultaneously breaking the metalaoxetane C–Cu bond.[xvi] This metalaoxinane **V** is in an envelope conformation with the newly formed metalaoxinane endocyclic Cu(III) puckered. The dissociation of the exocyclic oxygen bound Cu(I) leads to the reductive elimination of **TS-VI**, closing the ring to produce the DHF product and regenerating the Cu(I) catalyst.

The title reaction is diastereospecific: *E-cis* and *Z-trans* yield the *trans*-DHF product, whereas the *E-trans* and *Z-cis* yield the *cis*-DHF product (Scheme 2.1).[6a,xiv] The complete reaction coordinate of the Cu(I)-catalyzed rearrangement involving all VOs shown in Scheme 2.1 were computed and are included in Appendix 1. In all cases, computations reproduce the experimental diastereoselectivities.

Diastereodifferentiation arises at the copper migration (Figure 2.3). The migration of the exocyclic Cu(I) to the olefin can be either suprafacial or antarafacial to the breaking endocyclic Cu(III)–C bond. The major pathway proceeds through the energetically preferred suprafacial copper migration,

while the minor pathway proceeds through the disfavored antarafacial migration. In all cases, suprafacial rearrangements were energetically more favorable than the antarafacial. In the case shown in Figure 2.3, the preference for the suprafacial migration was 7.7 kcal/mol. This is because (1) the antarafacial transition structure is destabilized by the loss of conjugation in the nonplanar π-allyl. This distortion (39° from planarity) is necessary to realize Cu(I)-catalyst migration to the distal prochiral face of the π-allyl (Figure 2.3, highlighted in green). Analogous distortion from planarity in the parent allyl anion corresponds to 4.6 kcal/mol of destabilization. (2) The rest of the selectivity most likely arises from the strains in the Cu bonds.

Interestingly, the rate-determining steps are different for the formation of the major and minor diastereomeric products. The computed barriers suggest that the dual-Cu(I) migration step is not rate determining for the formation of the major product (i.e., the necessity of two Cu(I)-catalysts for this transformation is kinetically traceless), but it is in the minor product pathway.

While the existence of d-orbitals and the possibility of other intervening mechanisms complicate the extension of Woodward–Hoffmann rules to transition-metal-catalyzed reactions,[xvii] the failure of the monomeric Cu(I)-catalyzed process is conspicuously in line with Woodward–Hoffmann rules which predict a forbidden concerted 1,3-suprafacial sigmatropic shift.[xviii] We hypothesize that the presence of the second intervening Cu(I) circumvents the cyclic π-orbital alignment restrictions of a concerted, thermal pericyclic process and allows the reaction to proceed.

2.6 Conclusion:

In summary, we have used computations and experiments to elucidate the complete mechanism and origins of the diastereospecificity of a Cu(I)-catalyzed rearrangement of vinyloxiranes to dihydrofurans. DFT computations reveal that an unusual, traceless dual transition-metal-mediated process is

operative. Efforts are underway to capitalize on this milder synthetic procedure and for the design of new synthetic processes with improved selectivities based on these discoveries.

2.7 ACKNOWLEDGEMENTS:

We thank Oregon State University (P.H.Y.C.) for financial support.

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(14) The Z-cis/trans substrates afford ketones as the major product, as a result of a competing hydride shift mechanism.

(15) Conversion between mono- and dual-copper species is shown in the Appendix I.

(16) For the unsubstituted VO the suprafacial Cu migration is stepwise. Cu attacks the allyl, forming a tricyclic intermediate followed by Cu-allyl dissociation to form the metalaoxinane intermediate. In contrast, the anta-rafacial copper migration is concerted. See Appendix I.

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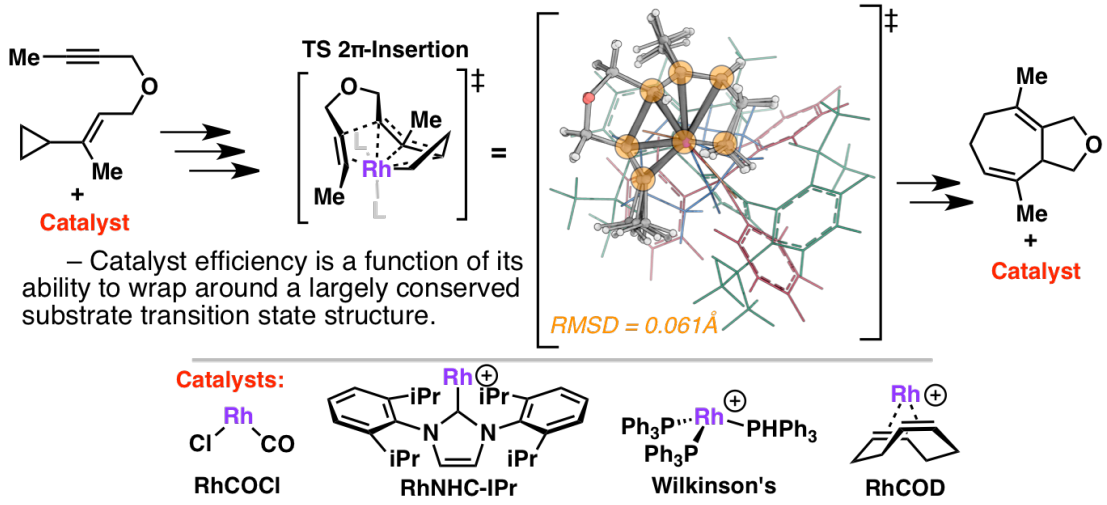
Chapter 3.

Catalytic Efficiency is a Function of How Rhodium(I) (5 + 2) Catalysts Accommodate a Conserved Substrate Transition State Geometry: Induced Fit Model for Explaining Transition Metal Catalysis

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3.1 ABSTRACT:



The origins of differential catalytic reactivities of four Rh(I) catalysts and their derivatives in the (5 + 2) cycloaddition reaction were elucidated using density functional theory. Computed free energy spans are in excellent agreement with known experimental rates. For every catalyst, the substrate geometries in the transition state remained constant (<0.1 Å RMSD for atoms involved in bond-making and -breaking processes). Catalytic efficiency is shown to be a function of how well the catalyst accommodates the substrate transition state geometry and electronics. This shows that the induced fit model for explaining biological catalysis may be relevant to transition metal catalysis. This could serve as a general model for understanding the origins of efficiencies of catalytic reactions.

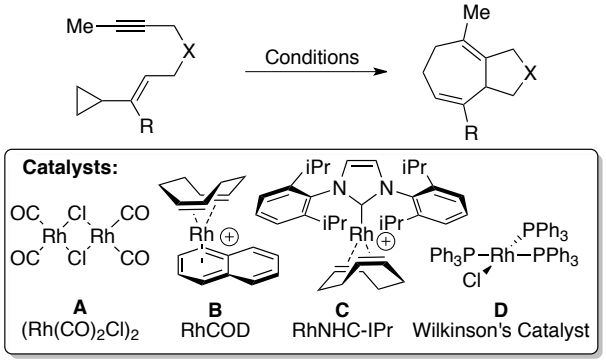
3.2 INTRODUCTION:

The design or discovery of new transition metal-catalyzed cycloaddition reactions is of preeminent importance to the realization of practical, atom-[1] and step-economical,[2] and green syntheses of compounds that exhibit significant biological activity and therapeutic potential;[3] however, the specific origins of different efficiencies of various transition metal cycloaddition catalysts remain elusive. For example, various Rh(I) catalysts are known to catalyze the (5 + 2) cycloaddition of vinylcyclopropanes (VCPs) to π-systems with a wide range of efficiencies (Table 3.1), but their differential reactivities remain poorly understood.[4,5] Herein, we disclose that the catalytic barriers for these (5 + 2) reactions are almost entirely dictated by the ability of the catalysts to geometrically and electronically conform around a conserved, rigid substrate transition state geometry. The surprising extent to which the substrate transition structure (TS) geometry is invariant to widely differing catalyst electronic and steric factors has direct practical implications on how catalysis can be understood and improved through rational design.

3.3 METHOD:

All intermediates and transition states along the reaction coordinates for all four catalysts and derivatives were computed with density functional theory, M06//B3LYP, and the 6-31G* and LANL2DZ basis sets.[6] Interestingly, geometry optimizations with dispersion corrections (B3LYP-D3) or single points with triple-ζ basis sets (M06/def2-TZVP) led to erratic and uniformly worse agreements with experimental barriers.[7] Distortion-interaction energies[8] were computed for all structures. The distortion energies quantify the energetic penalty of distorting the catalyst and substrate to reach the transition state geometry. Interaction energies quantify the electronic stabilization between the catalyst and substrate in the transition state.

Table 3.1 Catalytic Efficiencies of Four Rh (5 + 2) Catalysts

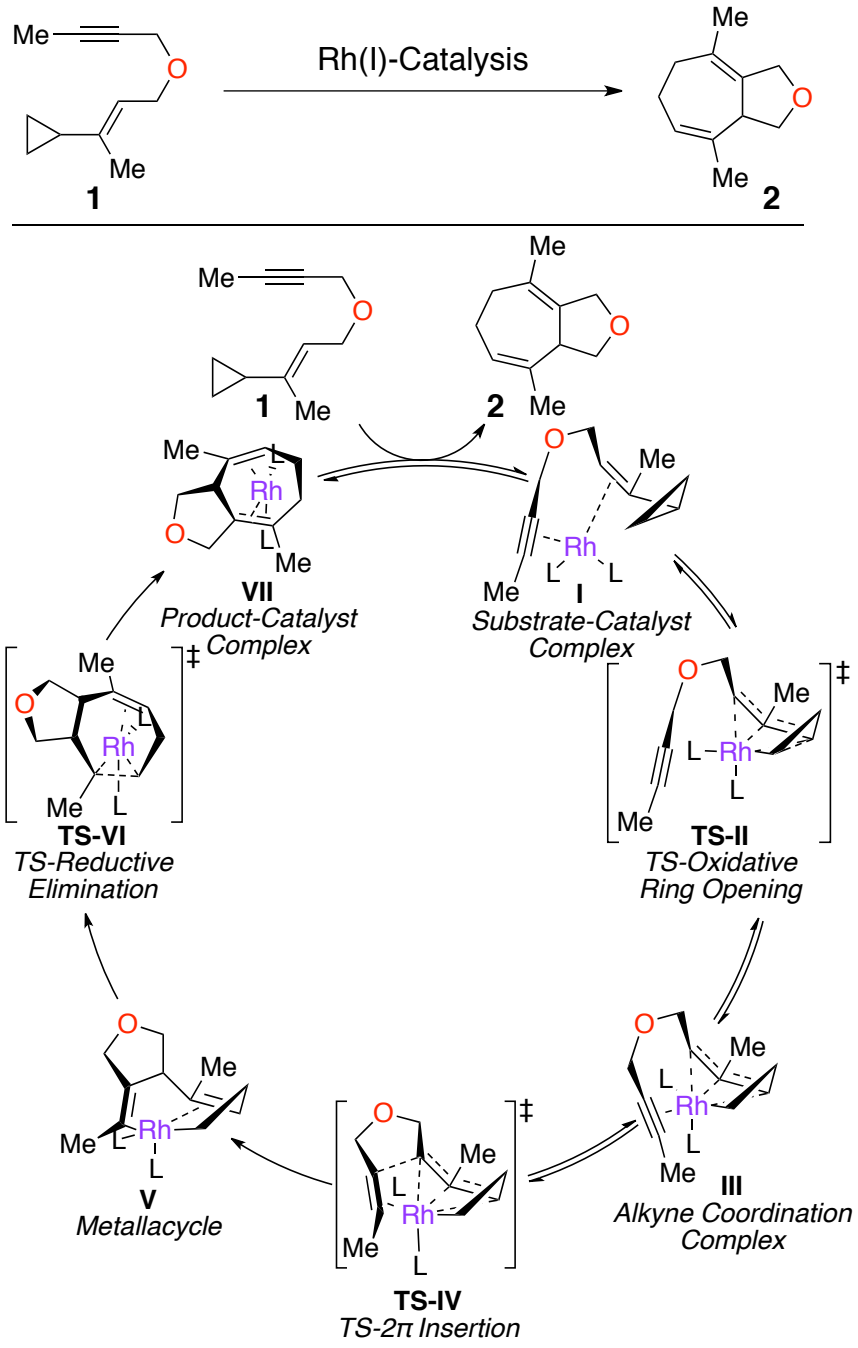


X	R	Catalyst	Conditions	TOF[¶]	ΔG_{FES}
$C(CO_2Et)_2$	H	5 mol% **A**	110°C, 20 min., 82%	1.0	26.5
$C(CO_2Et)_2$	H	2 mol% **B**	rt, 15 min., >99%	4.1	20.8
NTs	H	5 mol% **B**	rt, 65 min., 90%	1.0	20.8
NTs	H	2 mol% **C**	rt, 10 min., 93%	16.8	19.5
O	Me	10 mol% **D**	110°C, 1020 min., 78%	1.0	38.5
O	Me	5 mol% **A**	110°C, 20 min., 78%	102.0	26.5

[¶]TOF = relative catalytic turnover over frequency

3.4 Results and Discussion:

The complete reaction coordinates for the (5 + 2) cycloaddition of four archetypal Rh(I) catalysts were computed (Scheme 3.1): **A**, $(Rh(CO)_2Cl)_2$; **B**, $Rh(COD)Naph^+$ (COD = cyclooctadiene); **C**, Rh bis(2,6-diisopropylphenyl)-N-heterocyclic carbene (RhNHC-IPr; NHC-IPr = *N,N′*-(2,6-diisopropylphenyl)dihydroimidazolium); **D**, Wilkinson's catalyst. The mechanism of Rh (5 + 2) cycloaddition involving an alkyne and vinyl cyclopropane has been studied computationally (Scheme 3.1).[9] The catalytic cycle begins with the substrate–catalyst complex I, followed by oxidative ring opening of the VCP **TS-II**. The coordination of the 2π-alkyne **III** and subsequent 2π-insertion of **TS-IV** lead to the metallacycle intermediate **V**. Reductive elimination **TS-VI** forms the second C–C bond and leads to the product–catalyst complex **VII**. Transfer of the catalyst to another substrate



Scheme 3.1. Mechanism of the Rh (5 + 2) Cycloaddition

releases the product and regenerates the catalyst.

The computed reaction coordinate diagram for all catalysts is shown in Figure 1. The catalytic efficiency is directly proportional to the free energy span (FES) in the computed reaction coordinate with tethered vinylcyclopropane–alkyne **1**.[9b] The computed relative free energy spans and the observed

relative catalytic efficiencies of four Rh (5 + 2) catalysts are in good agreement (Table 3.1). The RhCOD and RhNHC-IPr catalysts are the fastest, with a FES of 20.8 and 19.5 kcal/mol, respectively. The $(Rh(CO)_2Cl)_2$ catalyst with a FES of 26.5 is much slower, and Wilkinson's catalyst with a FES of 38.5 kcal/mol trails behind even more significantly.

The 2π-insertion and reductive elimination steps are of key interest in this reaction; the oxidative ring opening is known to be facile.[9a] The computed transition structures (TSs) involving all four catalysts for these two steps are shown in Figure 2. The geometries of the substrate are indistinguishable from each other: the atoms involved in the bond-forming and -breaking processes of 2π-insertion and reductive elimination transition states (highlighted in orange) share a root-mean-square deviation (RMSD) of 0.061 and 0.056 Å, respectively. The remarkable conservation of the substrate geometry in the transition states strongly suggests that the onus of reaching the transition state falls on the catalyst's ability to mitigate the electronic and steric effects presented by the substrate transition state geometry. This further suggests that the orbital geometries and preferences in the bond-breaking and -forming processes do not change between catalysts. These observations are consistent with the induced fit model for explaining biological catalysis. Similarly, all the catalysts appear to share the same behaviors in ligation preferences. A remarkably strong trans effect is seen in all key TSs. These preferences facilitate the reactivity of the metal center by either donating or removing electron density trans to the bond-forming or -breaking process as needed.

3.4.1 Catalyst A: $(Rh(CO)_2Cl)_2$

This neutral catalyst is an effective catalyst for the Rh (5 + 2) cycloaddition (ΔGFES = 26.5 kcal/mol) (Figure 3.1). The minimal steric encumbrance of this catalyst all but eliminates catalyst distortion, and this correspondingly leads to

low barriers for all key transition states (Figure 3.3); however, the transfer of catalyst from product to the next substrate is significantly endergonic (6.4 kcal/mol). We hypothesize that steric encumbrance in other catalysts typically aids in product release from the catalyst via a strain release.[10] Because the steric encumbrance of this catalyst is minimal, this process is more difficult.

3.4.2 Catalyst B: RhCOD

The cationic RhCOD has a significantly lower FES of 20.8 kcal/mol (Figure 3.1). The cyclooctadiene (COD) ligand stays in the twist-boat configuration throughout the catalytic cycle in order to maintain double ligation to Rh (Figure 3). The greater steric encumbrance of the COD ligand (in comparison with catalyst **A**) increases the catalyst distortion throughout the catalytic cycle. Despite this, the RhCOD maintains excellent catalysis as a result of two effects: (i) the product inhibition for RhCOD is significantly smaller than $(Rh(CO)_2Cl)_2$ (2.4 kcal/mol vs 6.4 kcal/mol, respectively), and (ii) strong stabilizing electronic interactions provided by the COD ligand mitigates the energetic penalty from distortions.[11]

The increased magnitude of electronic stabilization provided by the RhCOD catalyst is surprising. We believe this stabilization occurs from the hemilability[12] of the COD ligand, allowing it to adjust ligand ligation to maximize stabilizing electronic interactions and minimize destabilization. For an example, during the 2π-insertion, the ethylene cis to the forming bond partially dissociates (Rh-$(C{=}C)_{cis}$ 2.8 Å vs Rh-$(C{=}C)_{trans}$ 2.2 Å), suggesting that coordination to the cis position in the 2π-insertion is not stabilizing, but also that the ligand in the trans position is critically important to catalysis of this step. Hemilability allows the catalyst to dynamically tune the electronics to best catalyze the step at hand.

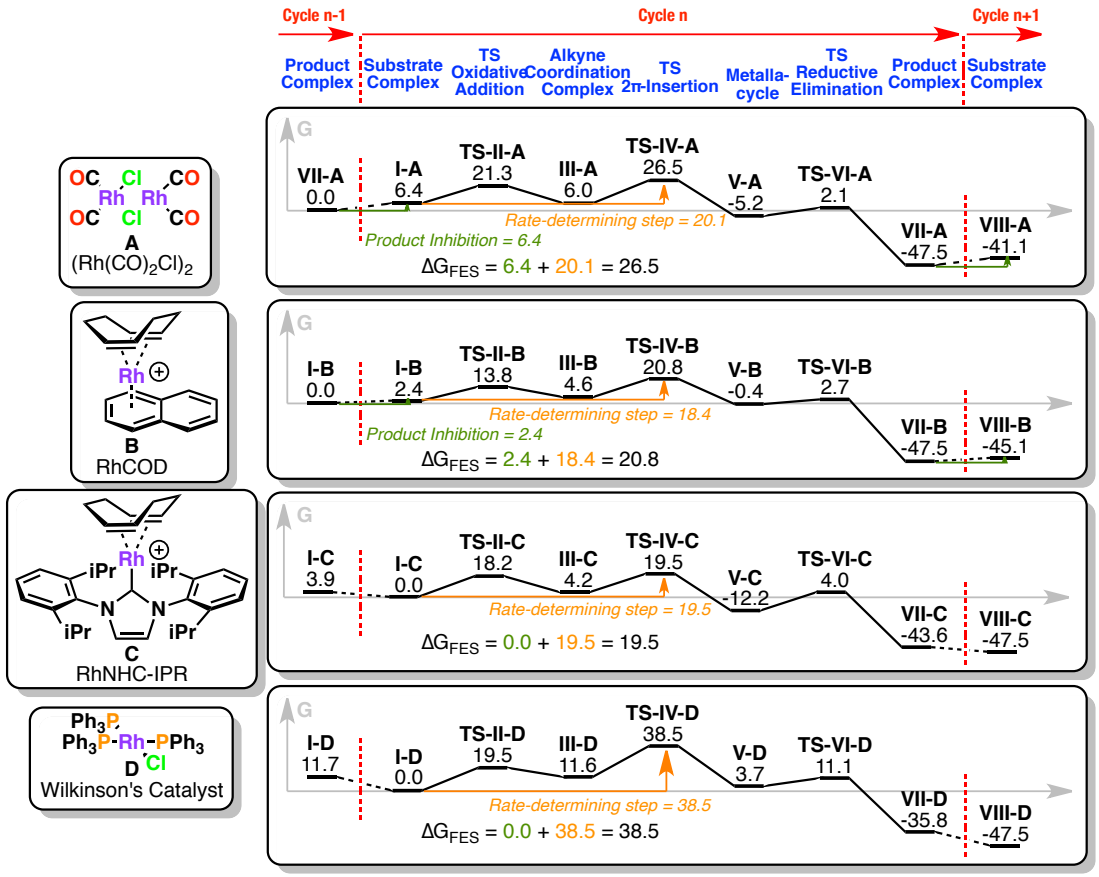


Figure 3.1. Computed reaction coordinate diagram involving substrate **1** and catalysts **A**, **B**, **C**, and **D** corresponding to Scheme 1.

To estimate the steric contributions to catalysis of the COD ligand, the reaction coordinate involving the smaller, untethered double diene catalyst, Rh diethylene (RhDiEt; DiEt = diethylene) (**E**, Figure 3.4.), was computed.[11] Three observations are substantive. First, the FES dropped to 14.6 kcal/mol as a result of the significantly increased stabilizing electronic interaction in the 2π-insertion step (116.9 vs 98.7 kcal/mol in the RhCOD). We attribute this to the greater flexibility with which the RhDiEt catalyst can further accommodate the electronic preferences of the substrate transition state. Second, the loss of the cis olefin amounts to negligible change in the 2π-insertion barrier (ΔΔG‡ = 0.2 kcal/mol), reaffirming our hypothesis that the trans, not the cis geometry, is important for the stabilization of the 2π-insertion step. Last, the product inhibition of RhDiEt was found to be equivalent to RhCOD (2.2 vs 2.4

kcal/mol, respectively). The distortions in the product–catalyst complex were also similar (27.9 vs 28.7 kcal/mol for the RhCOD), stemming from the steric interactions between the olefin hydrogens and the substrate/product. This increased steric encumbrance of the COD ligand as compared with the Rh dimer catalyst **A** aids in product extrusion to the tune of 4 kcal/mol; however, this does not completely eliminate product inhibition.

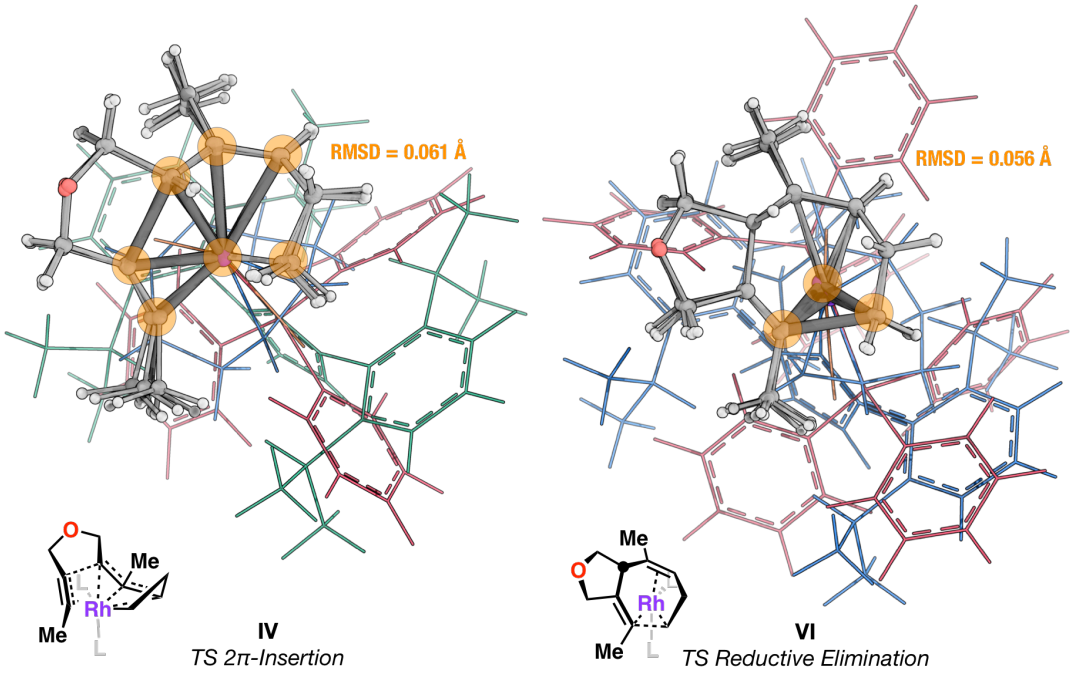


Figure 3.2. An overlay of four Rh(I)-catalysts. The substrate geometries in the transition structures are indistinguishable.[13] The atoms involved in the bond-forming and -breaking processes of 2π-insertion and reductive elimination transition state (highlighted in orange) share RMSDs of 0.061 and 0.056 Å, respectively.

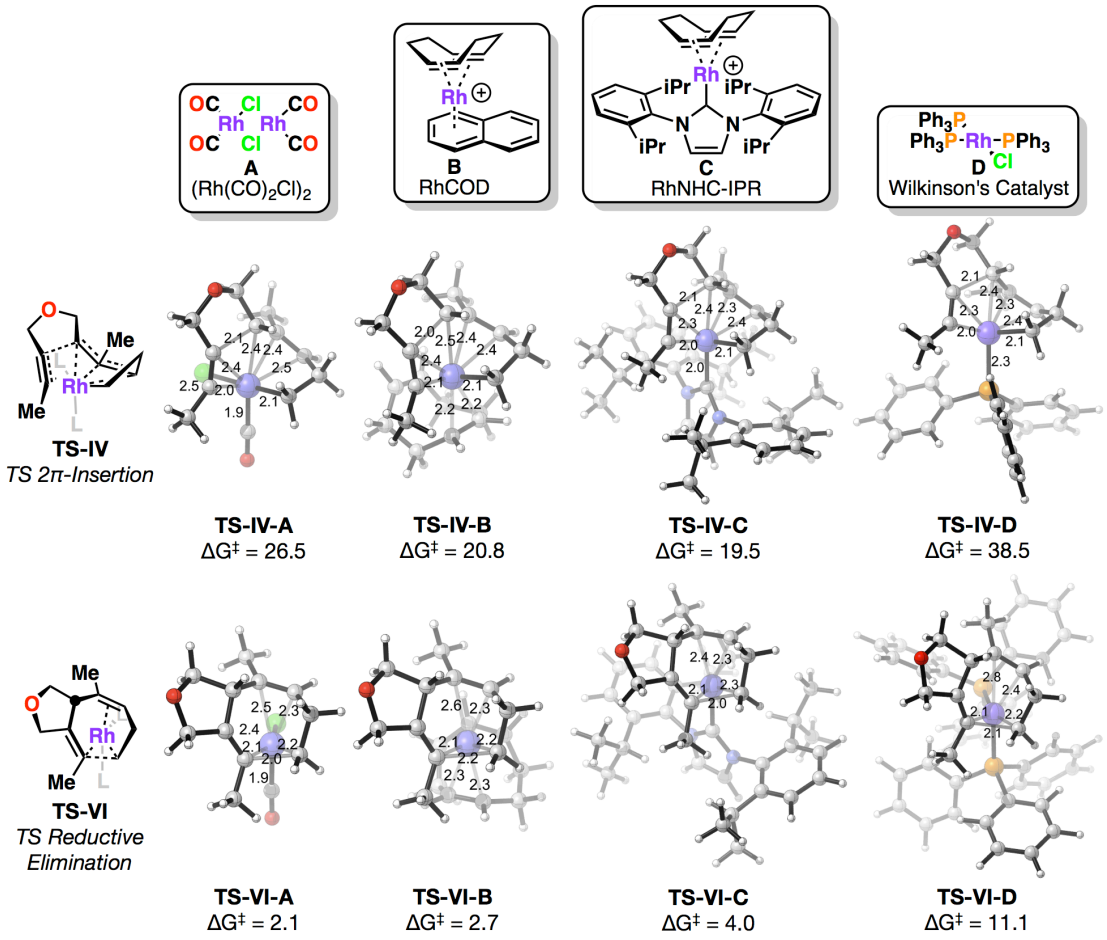


Figure 3.3. 2π-Insertion and reductive elimination transition structure involving substrate **1** and catalysts **A**, **B**, **C**, and **D**.[14]

The electronic contributions of the tether were also studied for the Rh cyclooctatetraene (RhCOT; COT = 1,3,5,7-cyclooctatetraene) (**F**, Figure 3.4.) and Rh dinaphthylcyclooctatetraene (RhdnCOT; dnCOT = dinaphthyl-1,3,5,7-cyclooctatetraene) (**G**, Figure 3.4.) catalysts.[11] The increased interaction energy from the conjugated ligand system (as compared with RhCOD) lowered the energies for each state along the reaction coordinate. The FES of RhCOT and RhdnCOT dropped to 18.6 and 17.4 kcal/mol respectively (from 20.8 kcal/mol for RhCOD, **B**), yet product inhibition increased to 2.5 and 3.2 kcal/mol, respectively. We hypothesize that the change in hybridization of the tether from sp^3 to sp^2 leads to an increase in electronegativity, strengthening the electron-withdrawing abilities of the catalyst. These subtle but substantive

changes for the RhCOD family of catalysts suggest that select perturbation of the tether geometry could lead to substantive increase in the catalytic efficiency of the Rh (5 + 2) process by eliminating product inhibition due to increasing steric bulk and increasing electronic stabilization by adding electron-withdrawing groups.

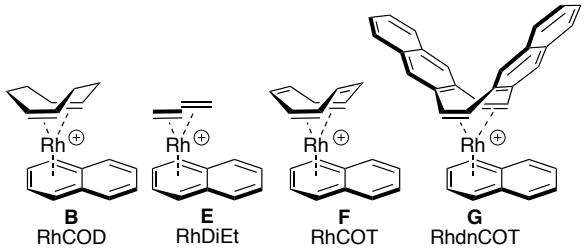


Figure 3.4. Rh cyclooctadiene (RhCOD) and derivatives: Rh diethylene (RhDiEt), Rh cyclooctatetraene (RhCOT), and Rh dinaphthylcyclooctatetraene (RhdnCOT).

3.4.3 Catalyst C: RhNHC-IPr

The RhNHC catalyst exhibited the lowest FES of 19.5 kcal/mol (Figure 3.1). There are three origins for the notable efficacy of this catalyst. First, key agostic interactions between the Rh and the hydrogens of the diisopropyl groups on the bis-2,6-diisopropyl-N-heterocyclic carbene are found in transition structures (the oxidative addition and the reductive elimination), as well as intermediates, along the reaction coordinate and are critical for the electronic stabilization of these structures (Figure 3).[11] Second, the catalyst distortion is surprisingly small; in fact, 2.4 kcal/mol lower for the rate-determining 2π-insertion step compared with RhCOD. Third, unlike the previous Rh (5 + 2) catalysts discussed, the RhNHC-IPr exhibits no product inhibition.

To quantify the effects of the NHC substituents on catalysis, the reaction coordinate involving the unsubstituted parent RhNHC-H_2 (NHC-H_2 = dihydroimidazolium) was also computed (**H**, Figure 3.5).[11] Three observations are substantive: first, the catalyst distortion of the small RhNHC-H_2 is nearly

identical to the significantly larger RhNHC-IPr. This suggests that any distortion in the NHC-IPr is inherent within the NHC ligand, not with the substrate or Rh metal. Second, RhNHC-H_2 also shows no product inhibition. This strongly suggests that the lack of product inhibition in the RhNHC-IPr is not related to the steric repulsion between the large NHC-IPr ligand and the product. Third, the interaction energies between the catalyst and substrate were significantly different between the two ligands. The catalytic ability of NHC-IPr stems from its ability to manifest hemilability during the transition states. Agostic interactions in the NHC-IPr involving the aryl isopropyl C-Hs stabilized all transition structures where these interactions were geometrically possible and stabilizing. Notably, the oxidative addition and reductive elimination transition states were higher for the NHC-H_2 than the NHC-IPr (oxidative addition, 26.3 vs 18.2 kcal/mol; reductive elimination, 9.0 vs 4.0 kcal/mol, respectively). In the 2π-insertion transition step, there were no agostic interactions in RhNHC-IPr, presumably because of the steric congestion around the Rh center. In this case alone, RhNHC-H_2 had a lower barrier compared with the RhNHC-IPr (14.9 kcal/mol vs 19.5 kcal/mol).

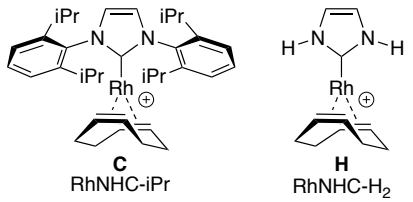


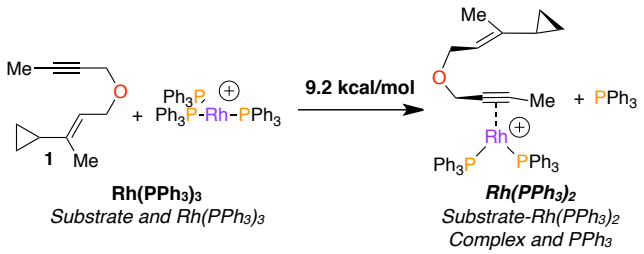
Figure 3.5. Rh *N,N′*-(2,6-Diisopropylphenyl)dihydroimidazolium (RhNHC-IPr) and Rh dihydroimidazolium (RhNHC-H_2).

3.4.4 Catalyst D: Wilkinson's Catalyst

The Wilkinson's catalyst, that is, tris-triphenylphosphine rhodium chloride (ClRhTPPh_3), has the highest FES of 38.5 kcal/mol (Figure 3.1). The ClRhTPPh_3 reaction is heterolobal. The catalytic cycles for the mono-, bis-, and tris-PPh_3 rhodium catalysts were computed. They differ considerably. The

tris-PPh_3 Rh complex was found to be the resting state of the catalytic cycle and is catalytically inactive as a result of severe steric congestion (Figure 3.3). The steady state of this reaction begins with the unfavorable exchange of one of the triphenylphosphine (PPh_3) ligands with the substrate. The cycle continues in the bis-PPh_3 form through the oxidative addition to the 2π-complex. Another PPh_3 dissociates before the sterically congested 2π-insertion of TS. The subsequent metallacycle intermediate is most stable in the bis-PPh_3 form, and the reaction continues in this form through the reductive elimination and the product–catalyst complex. The product is released from the catalyst via the association of another PPh_3.

The 2π-insertion transition structure is the most sterically congested and electronically saturated (18-electron) structure along the reaction coordinate. In this transition state, the catalyst is in the mono-PPh_3 form, and the catalyst distortion is minimal. The energetic penalty of associating another PPh_3 is significant (38.5 vs 39.9 kcal/mol, respectively, for the mono and the bis).



Scheme 3.2. Energetic Penalty of Dissociating PPh_3 to Associate Substrate is 9.2 kcal/mol

It is critical to note that the reactivity in purely the bis- or mono-PPh_3 forms exhibits FESs of 30 and 16.9 kcal/mol, respectively.[11] The penalty for ligand exchange contributes significantly to the overall barrier for Wilkinson's catalyst. Dissociation of PPh_3 from the tris-PPh_3 resting state and substrate association is endergonic by 9.2 kcal/mol (Scheme 3.2). Thus, it would be

entirely possible for less coordinationally saturated phosphine rhodium catalysts to be extremely reactive.[5k]

3.5 Conclusion:

In conclusion, we have discovered that substrates in the transition states for Rh(I) catalyzed (5 + 2) cycloadditions are remarkably invariant with respect to structurally and electronically different catalysts. This suggests that the reactivities of Rh(I) catalysts are almost entirely dictated by the ability of the catalysts to geometrically and electronically conform around a conserved, rigid substrate, transition state geometry. This shows that the induced fit model for explaining biological catalysis may be relevant to transition metal catalysis. We suspect that this theme may be much more prevalent than previously suspected. Work is under way to identify if similar effects are present in other catalytic reactions. Last, our analysis of the four Rh (5 + 2) catalysts reveals the specific requirements to enhance each of these catalysts and lays the foundation for how transition metal catalysis can be improved through rational design.

3.6 Acknowledgment:

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Research Fellowship. T.J.L.M. and P.H.-Y.C. also acknowledge Ryne C. Johnston for assistance with the manuscript.

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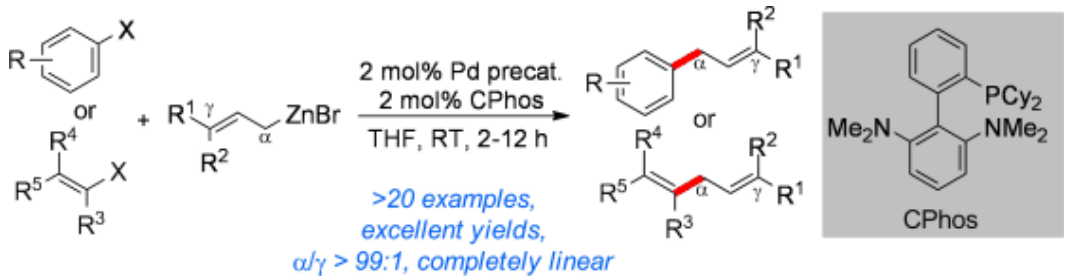
Chapter 4.

Palladium-Catalyzed Completely Linear-Selective Negishi Cross-Coupling of Allylzinc Halides with Aryl and Vinyl Electrophiles

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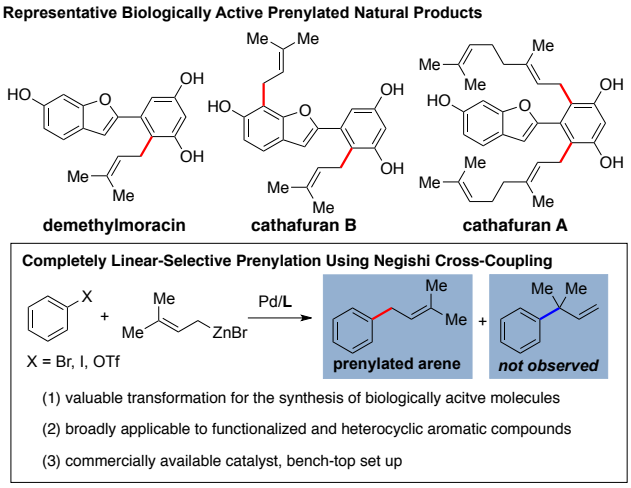
4.1 ABSTRACT:



Completely linear: The title reaction provides an effective means to access a wide range of prenylated arenes and “skipped dienes” in a completely linear-selective fashion, as demonstrated by a concise synthesis of the anti-HIV natural product siamenol. DFT calculations shed light on the origin of the excellent regioselectivity observed with the current Pd-based catalyst system.

4.2 INTRODUCTION:

Prenylated arenes are found in a broad spectrum of naturally occurring bioactive compounds (Scheme 4.1).[1] Studies have revealed that the inclusion of the prenyl side chain could enhance both the bioactivity and bioavailability of natural products, in part due to the increased protein binding affinity and membrane permeability caused by the lipophilicity of the prenyl group.[2] In nature, prenylation processes usually involve enzymatic reactions mediated by a range of substrate-specific prenyltransferases (PTases),[3] giving rise to the corresponding prenylated natural products in a highly selective fashion. However, the ability of synthetic chemists to directly introduce prenyl and related 3,3-disubstituted allyl groups onto functionalized aromatic compounds is generally hampered by poor regioselectivity with respect to the unsymmetrical allyl nucleophile.[4,5] Therefore, a general, reliable, and practical method for regioselective prenylation that emulates the efficiency of nature's biosynthetic machinery is highly desirable.[6]



Scheme 4.1 Top: Representative biologically active prenylated natural products. Bottom: Regioselective Negishi cross-coupling: rapid access to prenylated compounds.

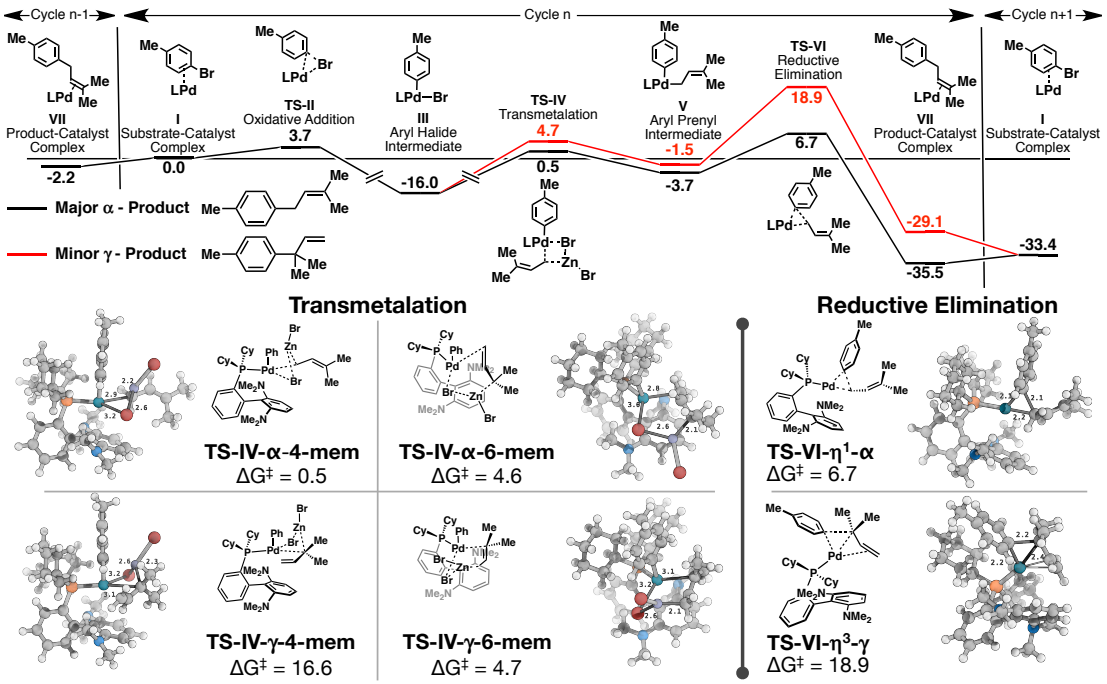


Figure 4.1 Top: Reaction coordinate of the Pd^0-catalyzed cross-coupling of prenylZnBr (**3**) with *p*-bromotoluene. Bottom: Transition structures for and transmetalation and reductive elimination transition structures.[7] Energies are given in kcal mol^{-1} and distances in Å. Computed structures are rendered in Pymol.[8]

Recently, Organ et al.[4] and Buckwald et al.[5] have developed conditions for the linear-selective Suzuki–Miyaura coupling of 3,3-disubstituted allylboronates using N-heterocyclic carbene (NHC)- and phosphine-based catalysts, respectively. While both methods were highly selective, relatively high temperatures and extended reaction times were required, and the yields of the desired prenylated products were moderate due to the inevitable formation of homocoupling products.[4,5] In an effort to develop milder and more efficient prenylation methods, Buckwald et al. sought to utilize alternative prenyl nucleophiles. Prenyl-type organozinc reagents were his first choice, as they had previously demonstrated the high reactivity as well as functional group compatibility of organozinc reagents in a variety of Negishi coupling processes.[9,10] To date, the cross-coupling of 3,3-disubstituted allylzinc reagents with aryl halides remains rare, presumably due to issues of

regioselectivity often experienced with this class of nucleophile.[4,5,11] Buchwald et al. reported the first general and completely linear-selective conditions for the Negishi coupling of 3,3-disubstituted allylzinc reagents with aryl halides and the application of this methodology in the concise and convergent synthesis of anti-HIV natural product siamenol.[12] Computational studies were also carried out to gain a deeper insight into the high level of selectivity observed with the current catalyst system.[13,14]

4.3 COMPUTATIONAL WORK:

To gain further understanding into the regiocontrol of this reaction, we analyzed the reaction coordinate by computation of intermediates and transition state structures (Figure 4.1). [8,15] The catalytic cycle begins with the initial complexation of the Pd^0 catalyst with the aryl bromide (**I**). Oxidative addition into the C–Br bond (**TS-II**) affords the resting state intermediate **III**. The two possible transmetalation processes involving α-prenylzinc were next investigated, namely a four-membered transition state (**TS-IV-α-4-mem**) and a six-membered transition state (**TS-IV-γ-6-mem**) leading to α- and γ-prenyl palladium intermediates **V**, respectively. Given that the prenylzinc species undergoes rapid 1,3-shift at room temperature,[7] we also evaluated two additional mechanisms utilizing γ-prenylzinc bromide as the transmetalating agent (Figure 4.1, **TS-IV-γ-4-mem** and **TS-IV-α-6-mem**, respectively). We found that there is an energetic preference for the α-4-membered transition state over the α-6, but this was reversed in the γ case presumably due to the steric bulk around the forming Pd–C bond in **TS-IV-γ-4-mem**. The minimum-energy pathway involves the **TS-IV-α-4-mem**, generating the α-prenyl palladium intermediate **V**, which then undergoes product-determining η^1-α reductive elimination (**TS-VI**) to afford the product–catalyst complex **VII**. We also investigated γ reductive elimination leading to the γ-isomer and found that the η^3-γ elimination was preferred over the η^1-γ. The η^3-γ process was

found to be disfavored by 12.2 kcal mol^{-Y}. In a model system in which the prenyl substrate is replaced with an allyl, the η^1 reductive elimination is preferred over η^3 by 2.2 kcal mol^{-1}.[16] In the prenyl case, the steric bulk around the forming C–C bond precludes the γ reductive elimination from achieving the more stable η^1 geometry. The α isomer is favored universally for all steps, including the α-4-mem transmetalation. The high level of linear-selectivity observed with the current catalyst system is controlled by the preference for the α-isomer-forming reductive elimination via **TS-VI-η^1-α**.

4.4 Conclusion:

In summary, Buchwald et al. has developed the first general, practical, and completely linear-selective Negishi coupling of 3,3-disubstituted allyl organozinc reagents with aryl, heteroaryl, and vinyl halides. This reaction features exceptionally mild reaction conditions and is broad in scope with respect to both aryl/vinyl halide and allylzinc coupling partners. This linear-selective allylation methodology provides an effective means for accessing highly functionalized aromatic and heteroaromatic compounds bearing prenyl-type side chains. Finally, theoretical calculations provided insights into the regiochemical-controlling parameters of these coupling processes, demonstrating the critical choice of the catalyst and the transmetalating reagent in achieving good selectivity for coupling reactions involving 3,3-disubstituted allyl nucleophiles.

4.5 Acknowledgements:

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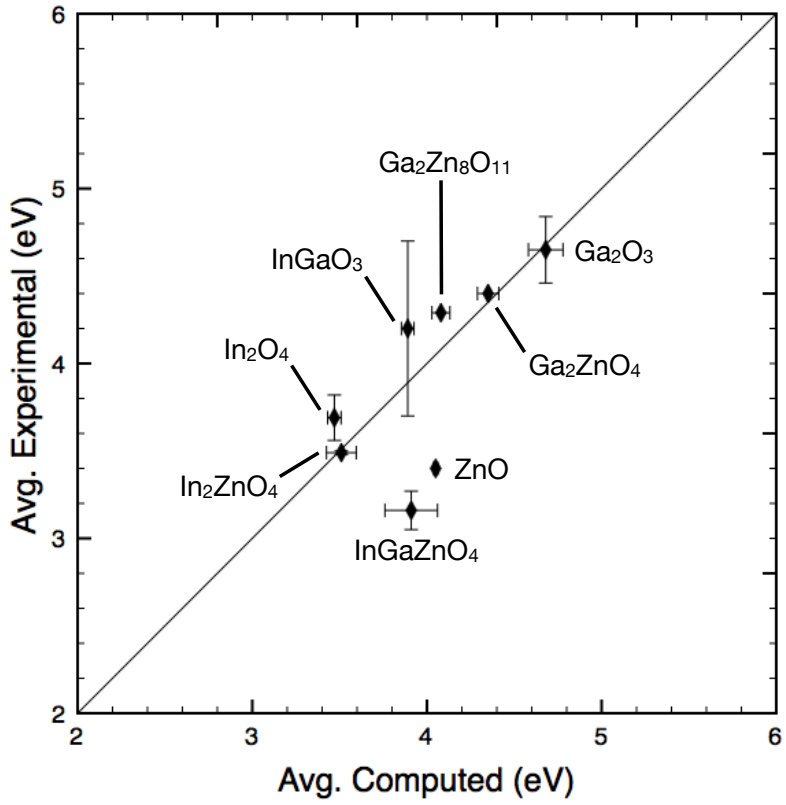
Chapter 5.

Predicting Amorphous Metal Oxide Band Gaps Rapid Band Gap Prediction of Amorphous Metal Oxides

Thomas J. L. Mustard, Benjamin E. Hanken, Geneva Laurita-Plankis, Dylan B. Fast, Prof. Michelle R. Dolgos, Prof. James R. Rustad, Prof. Douglas A. Keszler, and Prof. Paul Ha-Yeon Cheong

Manuscript in Preparation

5.1 ABSTRACT:



We computed band gaps of amorphous oxides within the In-Ga-Zn triad. These included ZnO, Ga_2O_3, In_2O_3, Ga_2ZnO_4, $Ga_2Zn_8O_{11}$, In_2ZnO_4, $InGaZnO_4$, and $InGaO_3$. Comparing the computed band gap to experimental measurements, the results were promising with a mean unsigned error of 0.28 eV and an unsigned standard deviation of 0.28 eV. Unfortunately drastic over prediction of the band gap for ZnO and $InGaZnO_4$ was observed.

5.2 INTRODUCTION:

Amorphous metal oxides are key components in a wide range of electronics, e.g. LCDs, plasma displays, solar cells, and organic light emitting diodes. The ability to predict the structures and electronic properties of amorphous metal oxides will have a huge impact in the directed synthesis of novel materials for electronic devices. In the past, these predictions have not been possible. We present here a computational method that can generate atomistic structures of amorphous solid as well as predict the band gap. Amorphous solids discussed explicitly in this work are: ZnO, Ga_2O_3, In_2O_3, Ga_2ZnO_4, $Ga_2Zn_8O_{11}$, In_2ZnO_4, $InGaZnO_4$, and $InGaO_3$.

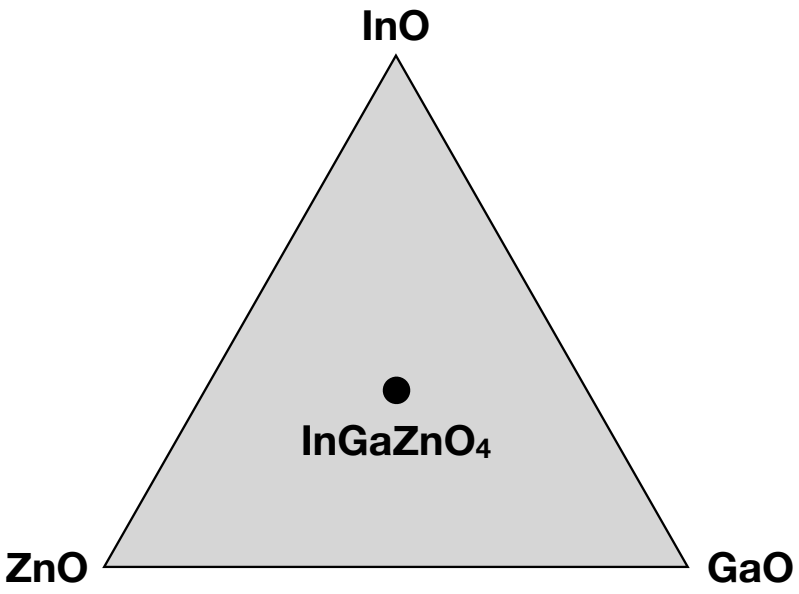


Figure 5.1. The IGZO triad with $InGaZnO_4$ shown in the center. There are infinite stoichiometric combinations.

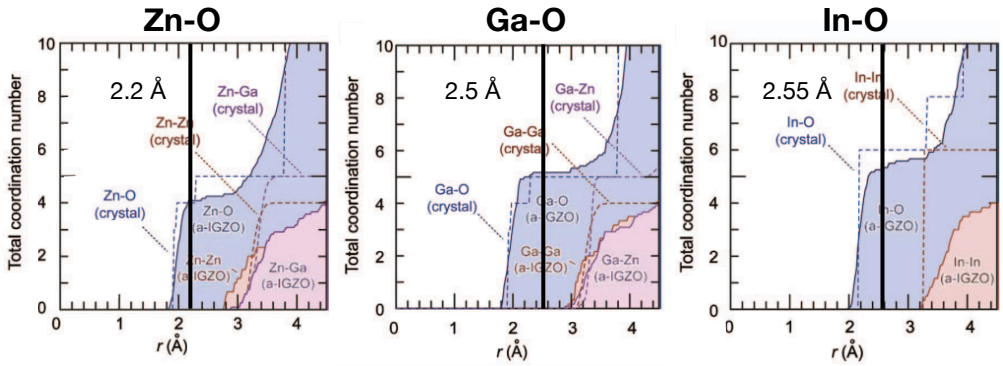
The number of metal oxide and dopant combinations is infinite. Consider the In-Ga-Zn triad (Figure 5.1). For industrial thin film production, deposition is done from prefabricated metal oxide targets. To experimentally produce the ideal target for a given application from every stoichiometric combination in

the IGZO triad is impossible. Computationally we can predict structural and electronic properties of any combination in this triad within days. Our research here can be a powerful tool for directed synthesis.

5.3 Computational Method:

Stoichiometries of interest were submitted to a random cell generation script.[1] All monte carlo and molecular dynamic simulations used GULP 4.0.3.[2] Forcefield parameters used are listed in the SI.[1] Quantum energies were calculated using Quantum Espresso 5.1.[3] Band gap predictions were calculated using the method developed by Chan and Ceder.[4]

Randomized cubes of metal oxides were submitted to a monte carlo equilibration at 4000K for 4 million steps with a acceptance ratio of 20%. These structures were subsequently annealed under molecular dynamics (MD) cooling at a rate of 10K/ps from 4000K to 300K while allowing for isotropic cell expansion and contraction. An additional MD equilibration was



Coordination Radii	Zn-O	Ga-O	In-O
Crystal$_{(exp)}$	~2.2 Å	~2.4 Å	~2.2 Å
Amorphous$_{(comp)}$	~2.2 - 2.8 Å	~2.0 - 2.8 Å	~2.3 - 2.8 Å

Figure 5.2. IGZO experimental and amorphous coordination numbers denoted by dashed lines and filled area respectfully.[5] Approximate radii for amorphous coordinate saturation denoted by thick vertical black lines.

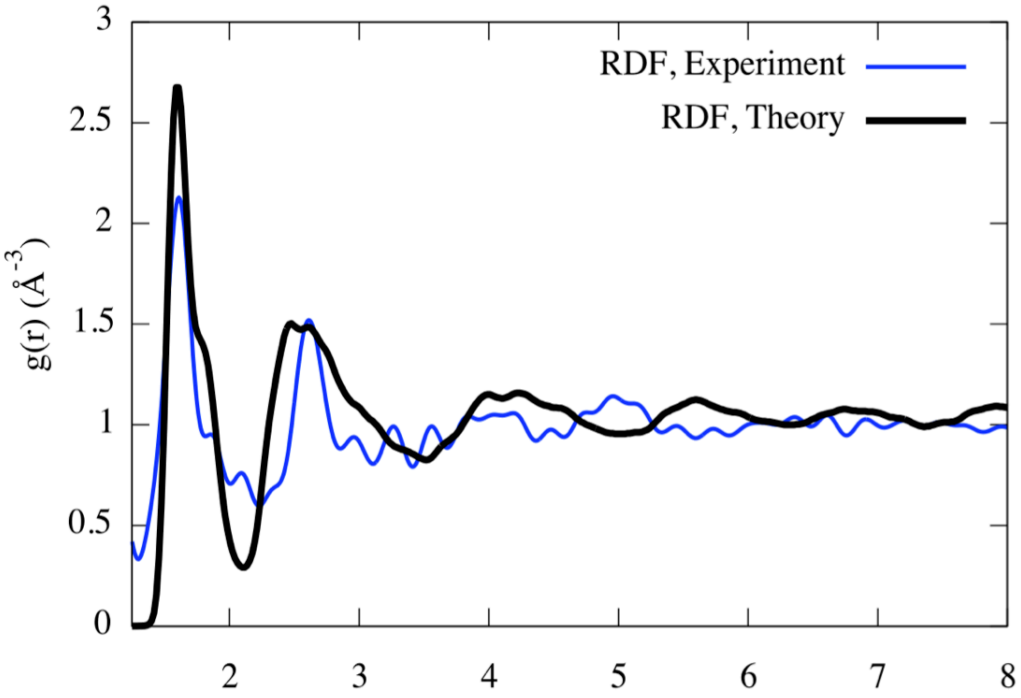


Figure 5.3. Comparison of computed and experimental PDF data for $InGaZnO_4$.

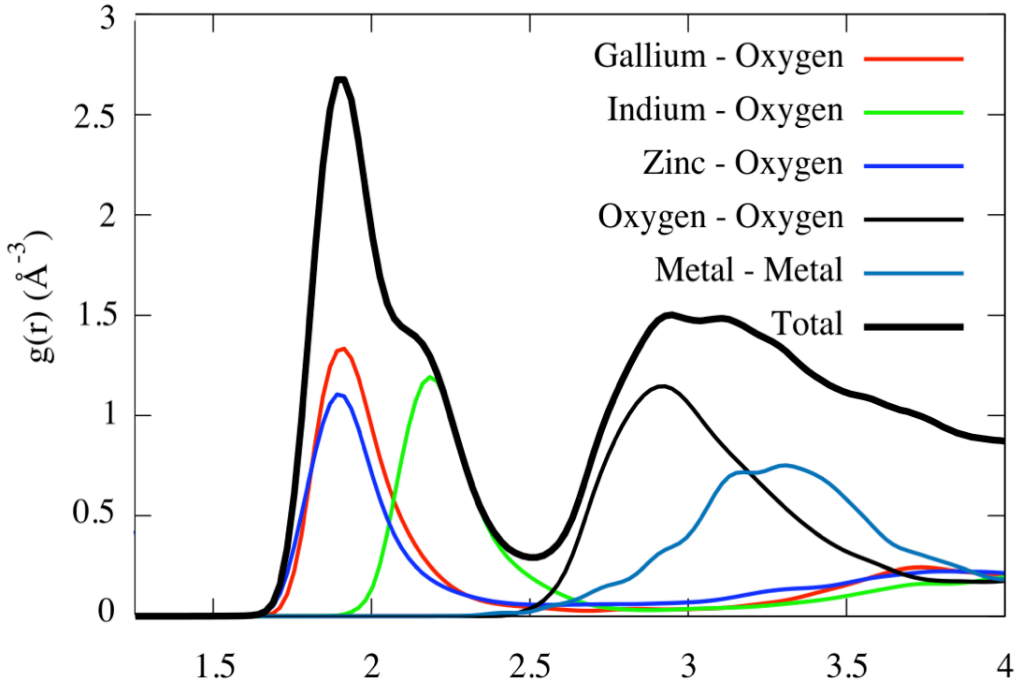


Figure 5.4. A deconstructed computational PDF showing the different components contributing to the major feature shapes.

then ran at 300K for 500ps.[1] Annealed cells were then directly submitted to Cedar's method for band gap prediction. Further QM geometry refinement was found to have no effect on the calculated band gap.

5.4 Results and Discussion:

5.4.1 Structural Predictions:

To compare structural similarities with experimental measurements several metrics were evaluated. Average coordination number and PDF were selected as comparative metrics due to the availability of experimental data for each.

Hosono et al. has shown that, due to the inherent disorder in amorphous solids, equivalent coordination numbers occur at longer radii than their crystal structure radii (Figure 5.2).[5] Within 0.5Å of the crystalline first coordination radii the computed amorphous cells fulfill coordination saturation. In addition, almost all are slightly under coordinated at the denoted amorphous coordination radii's of 2.2Å, 2.5Å, and 2.55Å for ZnO, GaO, and InO respectfully (Figure 5.2).[1]

Experimental data for a PDF comparison was unavailable for the amorphous solids of interest. In colaboration with the Dolgos group we were able to obtain a PDF spectra for $InGaZnO_4$ (Figure 5.3.). Our computed PDF was in agreement with the experimental major features. Both show a large peak, denoting the first coordination sphere, just below 2Å with a shoulder just above the major peak. A deconstructed PDF was computed to elucidate the components contributing to the feature shapes (Figure 5.4.). The major peak consists of GaO and ZnO while the shoulder is of InO. The second coordination sphere consists of O-O and metal-metal interactions.

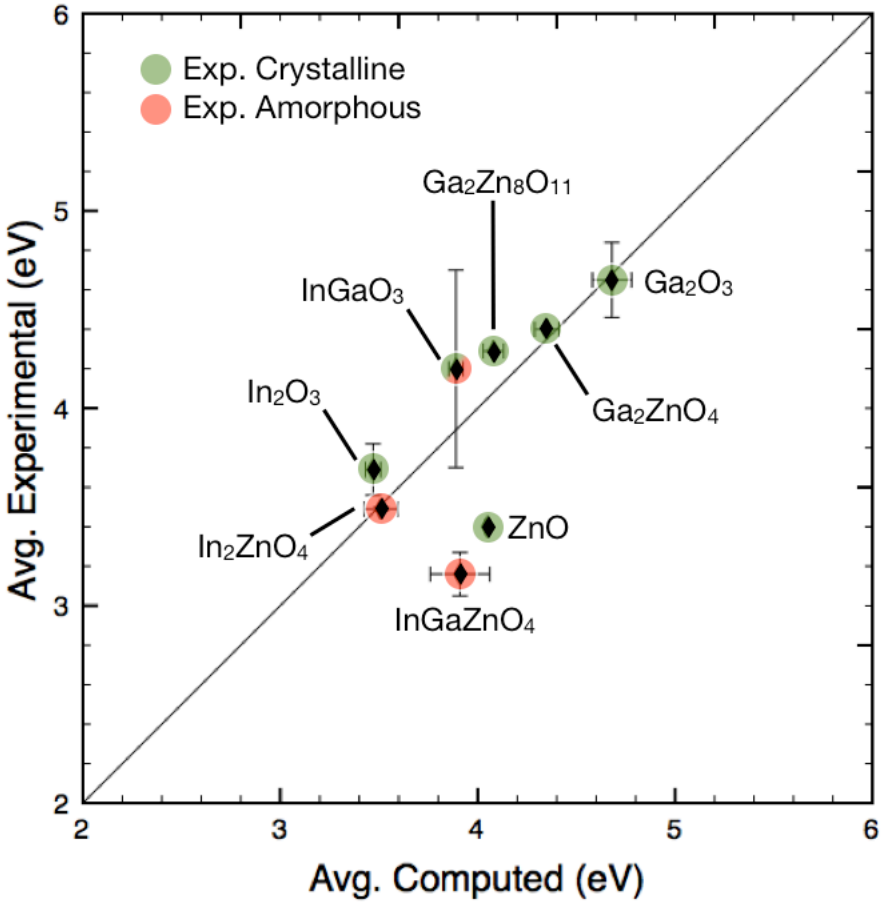


Figure 5.5. Average computed verse average experimental band gaps. Error bars denote one standard deviation.

Table 5.1. Average experimental and computed band gaps for the test set of In-Ga-Zn Oxides.[6]

Stoiciometry	Exp. Band Gap	Comp. Band Gap	Error†
ZnO	4.05	3.40	0.65
Ga_2O_3	4.68	4.65	0.03
In_2O_3	3.47	3.69	-0.22
Ga_2ZnO_4	4.35	4.40	-0.05
$Ga_2Zn_8O_{11}$	4.08	4.29	-0.21
In_2ZnO_4	3.51	3.49	0.02
$InGaZnO_4$	3.16	3.91	-0.75
$InGaO_3$	3.89	4.20	-0.31

†Absolute error in eV. Mean unsigned error: 0.28eV Standard deviation: 0.28eV

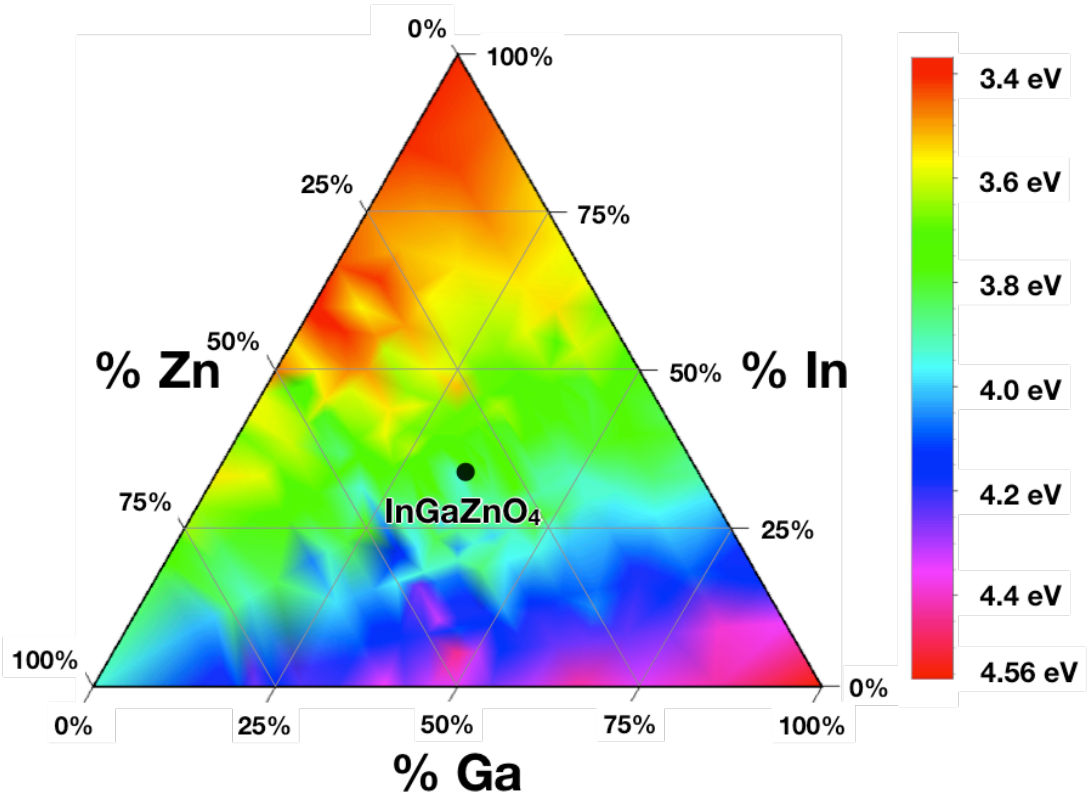


Figure 5.6. Computed band gap heat map using 250 stoichiometries. $InGaZnO_4$ is shown in the center of the In-Ga-Zn Oxide triad.

5.4.2 Electronic Predictions:

To assess the utility of this methodology, we computed band gaps of amorphous ZnO, Ga_2O_3, In_2O_3, Ga_2ZnO_4, $Ga_2Zn_8O_{11}$, In_2ZnO_4, $InGaZnO_4$, and $InGaO_3$ (Figure 5.5). Comparing the computed band gap to experimental measurements, the results were promising with a mean unsigned error of 0.28 eV and an unsigned standard deviation of 0.28 eV (Table 5.1.). Unfortunately, over prediction of the band gap for ZnO and $InGaZnO_4$ were observed. We attribute the ZnO over prediction to its strong crystalline nature.

To test for the size dependency on band gap predictions of the randomized cells, several cell sizes were built and tested. Initially cells of up to 125 atoms (5x5x5) were computed, cells with a maximum atom count of 343 (7x7x7) and 729 (9x9x9) were then built and had no effect to the computed band gap.[1]

Further quantum optimization of the 5x5x5 cells did not lead to more accurate band gap predictions.

Although quantitative agreement was not met in the test set, we generated amorphous cells for 250 stoichiometries in the IGZO triad (Figure 5.6).[7] Qualitatively the band gap has the strongest correlation with Indium content. Gallium and Zinc content have less influence respectfully.

5.5 Conclusion:

The accuracy of the computed band gaps and average coordination numbers imply that the atomistic structure of the generated amorphous solids are chemically realistic. Additional work towards structural refinement is necessary for further agreement with the experimental PDF data. This would also more accurately predict band gaps for all amorphous metal oxides.

5.6 Acknowledgements:

We thank the Center for Sustainable Materials Chemistry, which is supported by the U.S. National Science Foundation under Grant CHE-1102637 and Oregon State University (PHYC) for financial support.

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Chapter 6.

Accelerating and Automating Computational Chemistry through GPU Acceleration and nScripts, a Toolkit of Scripts and Programs

Thomas J. L. Mustard, O. Maduka Ogba and Prof. Paul Ha-Yeon Cheong

Manuscript in Preparation

6.1 Abstract:

The continuing growth of computational speed and efficiency is allowing for accurate computations of large and complex chemical systems. As these systems grow in size and complexity, the numbers of data points grow exponentially. Traditionally, computational chemists would do the tedious work of manually creating, submitting, examining and parsing all files and data points. With the use of both GPU acceleration and ηScripts, a library of tools, all these can be achieved with ease and virtually instantaneously.

6.2 Introduction:

Every 18 months, the transistor count on microelectronics doubles, and for various reasons so do the floating operations per second (FLOPs) (Figure 6.1).[1] Growing gaming and mobile electronics markets are creating market demand and industry pressure for faster, cheaper, and most importantly, efficient computers. This will ensure continued acceleration of computations for the foreseeable future.

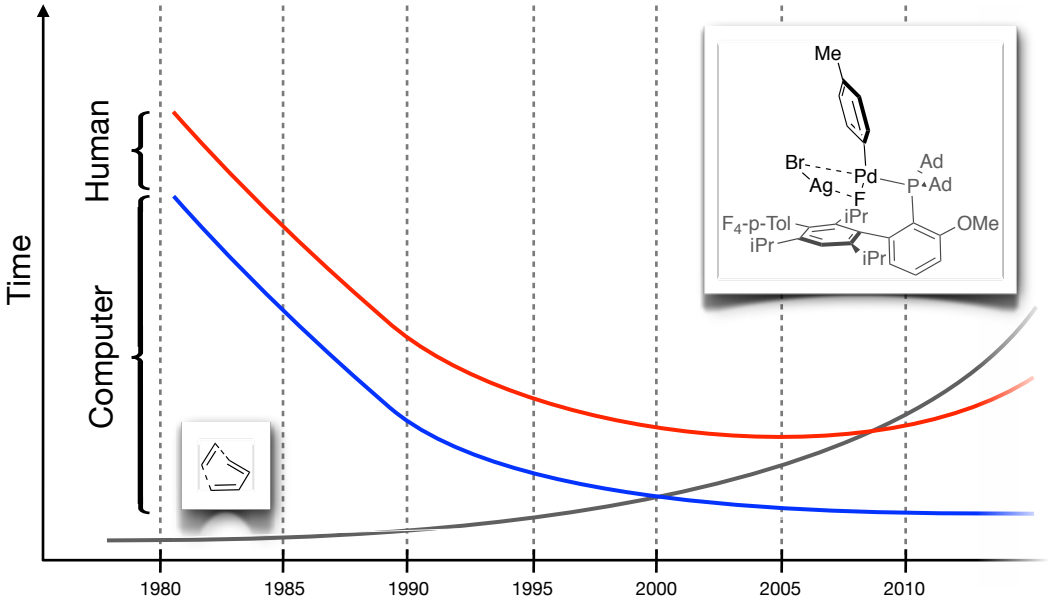


Figure 6.1. Acceleration of computational research as the available computational power increased.[2] The top line in red denotes the total time it takes to complete a computational research project. The difference between the red and blue lines denotes the time it takes the operator to create, maintain, and decipher computations. The gray line denotes the complexity of the chemical system.

Simple systems have one or two variables of chemical interest. As the systems increase in size and complexity, the increased number of chemically meaningful variables implies larger and more complex data sets (Figure 6.1). In addition, as the size and complexity of a chemical system increase, the number of possible conformations such a system can adopt scales at 6*N*. Traditionally, this is where the chemist would manually prune all degenerate

and chemically irrelevant conformations. Once pruning is complete, these geometries are converted into input files for further theoretical refinement. However, this manual process quickly becomes intractable for a large dataset.

For example, a polypeptide of 30 residues will easily have hundreds of thousands of conformations generated by an exhaustive molecular mechanics conformational search. Initial pruning by geometric similarity of heavy atoms and removal of conformations within a conservative 100 kcal/mol window of the global minimum, still leaves you with tens of thousands of structures. Manually pruning through this many structures is practically intractable and quite frankly a waste of resources as the time of a computational chemist is best suited doing science (elucidating reaction mechanisms, ligand binding affinities, and physical-electronic structure relationships).

In the past, it was typical for a graduate student in computational chemistry to compute fewer than 100 structures to acquire a PhD. This was considered state-of-the-art at the time, considering the computational resources available then. We are entering a time when computers are generating results faster than we can interpret the data. Success in computational chemistry will soon switch from about who has the faster computer, to who has the most efficient computational chemistry tools.

6.3 GPU Acceleration Cluster:

Parallelization can dramatically accelerate computations. Parallelization can be implemented in a multitude of ways, but it always boils down to increasing the number of processing units. One possible solution is to combine many computers' processing power by giving each computer a smaller piece of the problem to solve. While this is a much more efficient route, the hardware necessary to complete this task has been limited to supercomputers.

Supercomputers appeared in the 1960s with the Cray machines. In the 1990s, Beowulf clusters, which utilize multiple commodity hardware nodes for parallel computations, appeared. Beowulf clusters are commonplace now, but the cost-efficiency and the performance of an aggregate sum of cheaper and slower machines stunned the scientific computing world, ultimately replacing monolithic computers like the Cray. Recently, computers equipped with multiple physical CPUs and more processing cores (theoretical cores) per physical CPU have emerged, taking this paradigm of parallelization a step further. Today the key challenge to acceleration, apart from cost of the machines, is now the physical size, energy requirement, heat output, and interconnect speed between machines. While miniaturization of electronics has helped, bleeding edge computational projects have always pushed the limits of the powers of the best computers and the best facilities. In the last decade, a number of new revolutionary solutions have been made public, all due to video games.

To quickly draw each frame of the newest and highest resolution video games, an immense number of polygons must be calculated. Due to the desire for higher frames per second on larger resolution screens, graphics processing unit (GPU) companies have been innovating to push the boundaries of how much RAM (random access memory) and computing cores that can be crammed into a single PCI expansion card. This is fortunate for computational chemistry, as high-resolution video gaming and computational chemistry research share a common challenge – they both require an immense number of computations. The gaming industries' solution, GPUs with thousands of energy efficient processing units with interconnect speeds at least twice as fast as comparable CPUs.

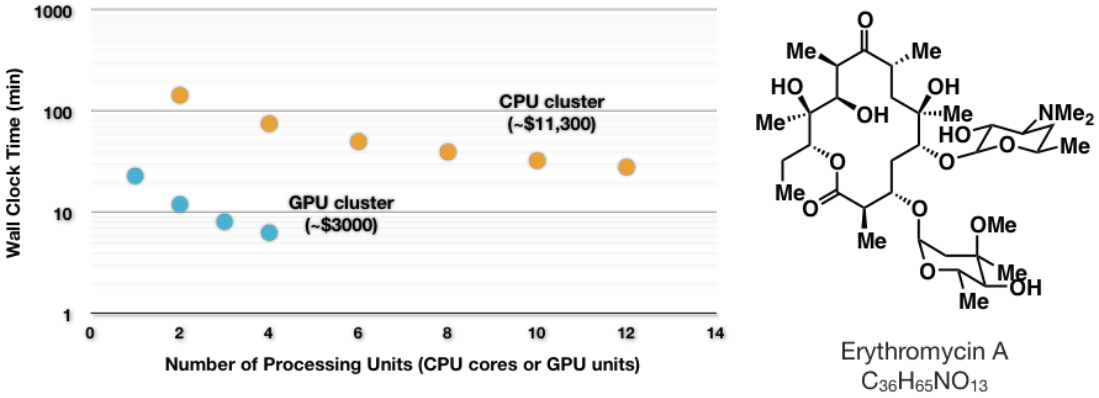


Figure 6.2. Comparison of computational time to compute the energy of Erythromycin A for a range of GPU units and CPU cores. The B3LYP/6-31G* method and basis set was employed on nVidia 480 GTX GPUs and AMD 6300 CPUs using Terachem and Q-Chem respectfully.

In the spring of 2011, I built a $3000 prototype GPU machine using consumer grade components. Using Terachem,[3] I discovered that a single GPU was faster than a 12-core server grade node (Figure 6.2). This success led to building the Fermi cluster, comprised of both GPU and CPU machines. At it's peak 18 computing nodes comprising of 6 GPU nodes with 4 GPUs each and another 12 CPU nodes. This machine assisted in the computations for many projects in the PHYC group. This includes but are not limited to: amorphous metal oxide band gap predictions,[4] aqeous aluminum hydroxo and oxo cluster protonation states, copper mediated ring expansion mechanistic investigation,[5] and gold mediated hydroalkoxylation mechanistic investigation.

6.4 ηSCRIPTS (ETA_SCRIPTS):

The automation of computational workflow can best be seen in computational drug discovery. Here hundreds to thousands of compounds are scrutinized for biological and medicinal properties (binding affinity, solubility, permeability, possible metabolites, etc.). To do this efficiently and effectively, large and

expensive software packages have been created for the pharmaceutical market.

In the realm of materials and catalysis, several tools and workflows to accelerate computational chemistry have recently been released. Several notable examples are: (1) The Alloy-Theoretic Automated Toolkit (ATAT), created by Axel van de Walle, assists in generating *ab initio* phase diagrams.[2] (2) Zimmerman, et al. has developed an automated discovery algorithm for locating reaction steps.[6,7] (3) Wheeler, et al. outlined AARON, Automated Alkylation Reaction Optimizer for N-oxides, which automates the computational workflow to predict enantioselectivity for asymmetric propargylation reactions employing *N,N'*-Dioxide Catalysts.[8] It does so by mapping axially chiral bipyridine *N,N'*-dioxide catalysts onto an existing library of stereodetermining TSs. Once mapped AARON automates the necessary steps to determine relative reaction barriers.

Our group created many of our own in-house tools to fit the needs of our research mission. While not directly changing the chemistry of projects, by removing the tedious work, these tools help computational chemists focus on the science. These scripts and programs described below, in many cases, build on previous work by Cheong, Ogba, and Rajski.

6.4.1 ηSCRIPTS DATA CONTAINERS:

To ensure compatibility and minimize maintenance, sets of standard data containers were built. Transferring molecular geometry data between functions is a simple task as long as no new variables are introduced or frame of reference changed. These data containers were engineered to hold molecular or configuration information in a predictable and flexible way.

Molecular coordinate data is saved in the data type *Atom class*. By becoming a class, a variable assigned to have the *Atom class* now has sub-variables

that can be accessed. These sub-variables are set with a default value and then can be recalled and set at any time. This allows for the *Atom class* to be changed without reconfiguring all the functions that use variables that are assigned the *Atom class*. One can then add a new variable to be stored without breaking the rest of the code base.

Configuration data is stored in snippet files. Snippets are text files holding configuration information with a set style and layout that allows the user to quickly add and edit snippets to fit their current need. In the case of input file generation, snippets hold the method and basis information, solvation, optimization settings, geometric restraints, etc. For submission scripts the snippet file holds particular scripting steps necessary for proper submission.

6.4.2 ηTranslate Scripts:

Most of ηScripts is composed of ηTranslate scripts that by name translate one file or object to another. They come in three major sectors: (1) xyz coordinate file conversion; (2) output file parsing and conversion; (3) archiving.

nTranslate-XYZ-DihAngDist.py: reads a XYZ geometry file and two to four atom numbers to print the distance, angle, or dihedral for those atoms.

nTranslate-XYZ-Remove_Atom.py: reads a XYZ geometry file and removes the atom number specified.

nTranslate-XYZ-Renumber.py: this script will renumber all the XYZ files within the current directory to a specified key structure based on nearest neighbor. If any of the structures within the directory are larger than the specified key file, any unmatched atoms will be appended to the end of the file. All renumbered files are saved in the folder "RENUMBERED" including the key structure. If you do not specify a structure the smallest one will be chosen for you.

nTranslate-New-Second-Line.py: reads a XYZ geometry file and replaces the second line with the name of the file. It can also take all the XYZ files in the current directory.

nTranslate-Change-Geom-XYZ.py: reads a XYZ geometry file and changes a specified bond, angle, or dihedral to the specified distance or angle.

nTranslate-XYZ-XXInput.py: parses a XYZ geometry file and a snippet file to create an input file.
Examples:
nTranslate-XYZ-G09Input.py
nTranslate-XYZ-JaguarInput.py
nTranslate-XYZ-TCInput.py
nTranslate-XYZ-TMInput.py

nTranslate-XXOutput-XXInput.py: parses a output file and a snippet file to create an input file.
Examples:
nTranslate-G0XOutput-G0XInput.py
nTranslate-JaguarOutput-JaguarInput.py

nTranslate-XXOutput-SCREWER-XYZ.py: parses an output file and will output a XYZ geometry that
Examples:
nTranslate-G0XOutput-SCREWER-XYZ.py
nTranslate-TMOutput-SCREWER-XYZ.py

nXT.py: parses output files for rapid interpretation of job progress and answers.
Examples:
nGT.py
nJT.py
nTCT.py
nTMT.py

nXList.py: parses all output files in a folder for rapid interpretation of job progress and answers.
Examples:
nGList.py
nJList.py
nTCList.py
nTMList.py

nXArchive.py: create the ARCHIVE folder and several sub folders that hold a variety of data for long term storage.
Examples:
nGArchive.py
nJArchive.py
nTCArchive.py
nTMArchive.py

6.4.3 Psientific Scripts:

Scripts and programs employing advanced transformations and algorithms are classed into the Psientific section. These scripts do more than a simple task; they complete tasks that cannot be automated with any available tools.

nDeprotonate.py: will deprotonate molecular files into all the combinations possible, for all deprotonation levels of interest. In addition, it removes degenerate geometries by: (1) only creating unique deprotonated states based on user input; and (2) comparing its deprotonated geometry to all other generated geometries.

nDist-Int-Splitter.py: will split molecular files into discrete parts. These separated geometries can then be submitted for distortion interaction analysis to better understand the electronic and steric forces influencing a system.

nTranslate-Change-Geom-XYZ.py: is a command line solution to quickly making minor geometric changes to a molecular file without the need for a GUI interface.

nMAP.py: will map one set of molecules onto another with high selectivity and precision. The mapping replaces one section of a molecule with another section of interest. It does this by first aligning the two sections, then removing any atoms that are unwanted and inserting the new atoms. This is very useful for accelerated QM optimizations, transition state searches and ligand design.

nPersistentOTS.py: wraps around your QM code to add functionality and accelerate OPTs, SCANs, and TS-SCANs. TS-SCANs are dynamic SCANs that will continue to search up a positionally restrained optimization scan to locate an input geometry for further transition state search.

6.4.4 ηSubmit Scripts:

These scripts were written to quickly create submission files and allow for easy cluster migration. They rely on submission script snippets that are specific to both the cluster they are installed on and the type of job they are submitting. These snippets are then dynamically edited to replace set keywords with variables that are necessary for successful job completion. The use of snippets allows for a large number of submission scripts to be updated quickly by editing one snippet all the scripts are affected. Migration is also made easy; you need only update the machine specific snippets. As new software is released, new protocols are adopted, and accelerations are implemented the submission scripts can be quickly and painlessly updated.

nSubmit.All.G09.Core=2.py: creates submission files for all Gaussian input files in a directory and then submits them to the queue.

6.4.5 ηVISUALIZE SCRIPTS:

These scripts were written to accelerate the creation of visually appealing graphics. These scripts create a Pymol script based on the files with in the current directory and runs the created script within Pymol.

nVisualize-Pymol-XYZ.py: creates Pymol script for all the XYZ files in the current directory.
Examples:
nVisualize-Pymol-PDB.py

6.5 CONCLUSION:

Right now the available and affordable computational power allows scientists to ask big questions with exceptionally accuracy. What we get is a mountain of answers and the important ones are hidden like needles in that mountain of needles. To stay at the apex of fundamental understanding and chemical discovery we need not only the computational power but the tools at hand to find that needle. Our tools and the GPU accelerated cluster have proven to accelerate our computational research. As the complexity and size of our chemical systems rise, the flexibility built into *η*Scripts will allow for continued acceleration and automation of building, maintaining, and comprehending the ever-larger datasets.

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Chapter 7.

Conclusion

Organometallic catalysis is of preeminent importance to the practical syntheses of materials, pharmaceuticals and feed stock compounds. They provide unique and predictable chemistry not accessible within the s and p-block elements. Vinyloxirane ring expansions, which are thermally Woodward-Hoffman forbidden, are facile and stereoselective with Cu(I) catalysts. Within the Rh(I) mediated (5 + 2) cycloaddition reaction of vinylcyclopropanes with tethered alkynes, every atom involved in bond-making and -breaking processes remains constant in each TS for every catalyst studied. Palladium mediated cross-coupling of allylzinc halides with aryl and vinyl electrophiles is highly α-selective, with regioselectivity controlled by steric interactions within the reductive elimination TS. These transformations would not be possible or as selective with out the use of transition metal based catalysts.

Amorphous metal oxides are used in key components for a wide range of electronics, e.g. LCDs, plasma displays, solar cells, and organic light emitting diodes. Accurate prediction of structural and electronic properties will allow for the computational design of materials. Towards this goal the In-Ga-Zn Oxide triad was investigated to better predict both structural and electronic properties. The accuracy of the computed band gaps, average coordination numbers, and agreement with experimental PDF imply that the atomistic structure of the generated amorphous solids are chemically realistic. The accuracy of predicting band gaps for ZnO, Ga_2O_3, In_2O_3, Ga_2ZnO_4, $Ga_2Zn_8O_{11}$, In_2ZnO_4, $InGaZnO_4$, and $InGaO_3$ was a promising mean unsigned error of 0.28 eV and standard deviation of 0.28 eV.

The fundamental understanding of complex chemical systems from a computational approach is both daunting and tedious. Automation of computational chemistry, while only an engineering feat, has the potential to accelerating computational research be removing all but the science. What is not immediately obvious are the numerous tasks necessary. Under the surface, automation and acceleration of many tedious and otherwise intractable tasks has made this research possible. Both GPU acceleration and ηScripts, a new suite of tools, has allowed for the timely and accurate study of these phenomena.

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Appendices

Appendix I.

Computational Data for Chapter 2

Mechanism and the Origins of Stereospecificity in Copper-Catalyzed Ring Expansion of Vinyl Oxiranes: A Traceless Dual Transition-Metal-Mediated Process

1. Cu(I)-catalyzed rearrangement of E-Cis dimethylvinyloxiranes

1.a. Additional Figures

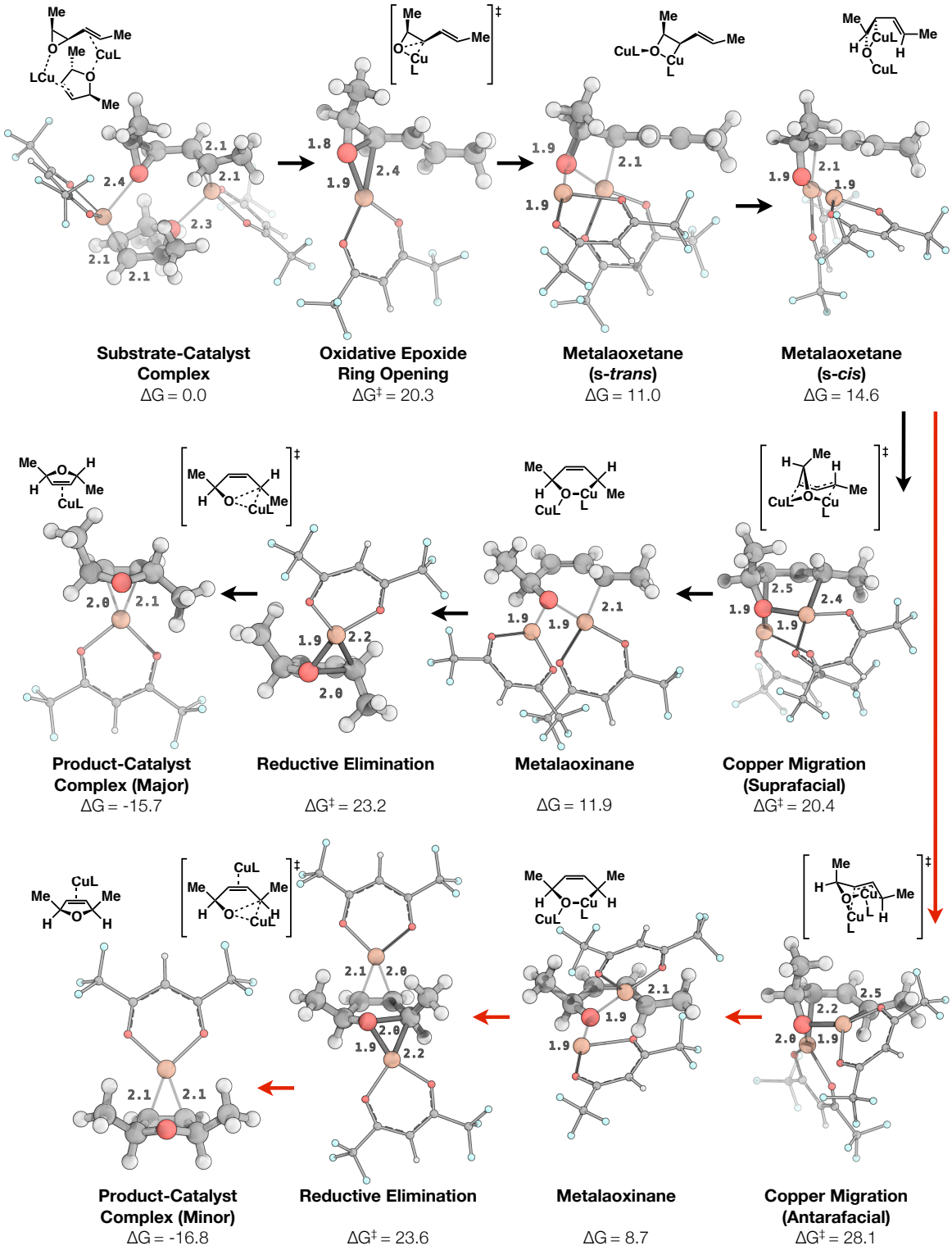


Figure 1. Structures of stationary points for both major and minor pathways for E-Cis VO. All structures, energies, and free energy corrections computed

at the B3LYP/def2-SVP level of theory, as implemented in Turbomole. Figures rendered using Pymol.

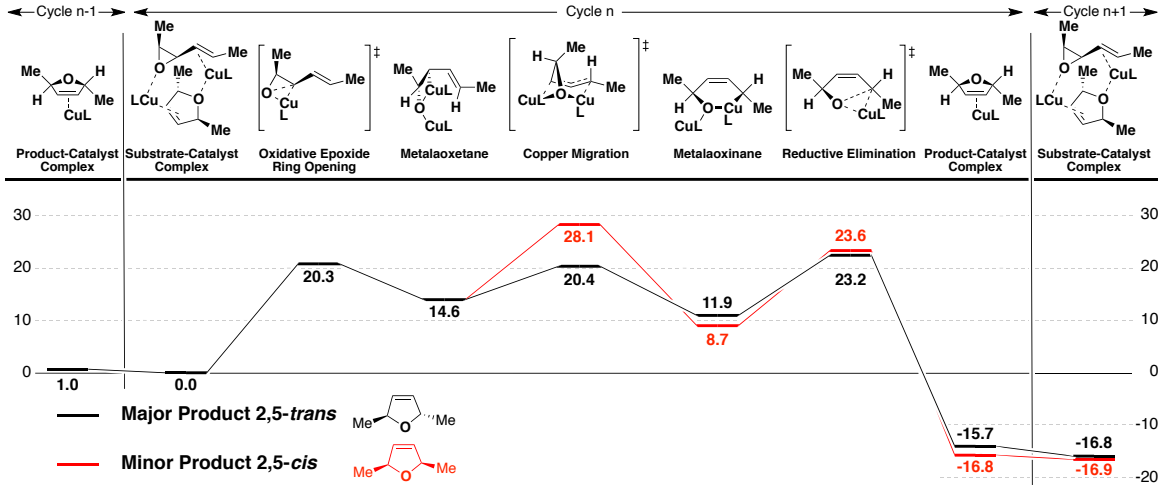


Figure 2. Reaction coordinate of Cu(I)-catalyzed ring expansion of E-Cis VO.

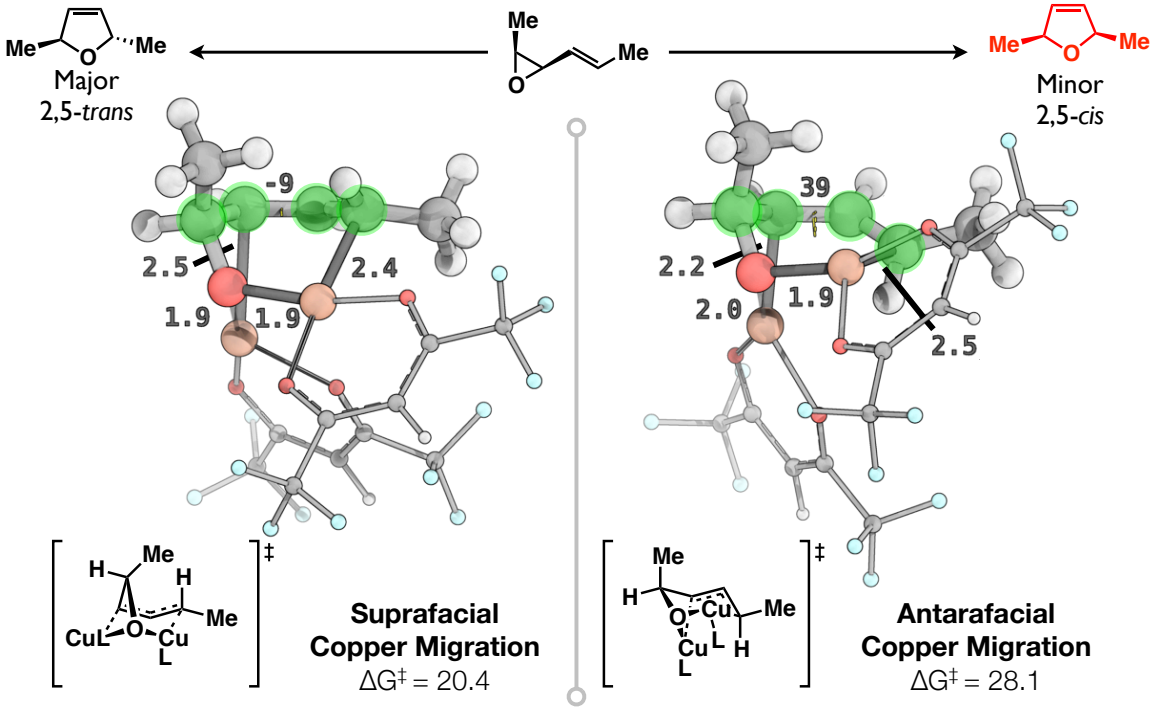


Figure 3. Stereoselective copper migration of E-Cis VO showing π-allyl distortion (green highlight with dihedral), and TS bond distances.

1.b. Geometries, Energies, and Thermal Corrections
Mono Cu(I) DiMeDHF-E-Cis Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp		Basis: def2-SVP		Atoms: 32			
Charge: 0	Spin: 1			Basis Functions: 366			

Energy = -2889.24320988463

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0005840	0.0010000	yes	0.0001035	0.0005000	yes
Grad	0.0000477	0.0010000	yes	0.0000090	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.98135	3.06873	-0.18113
C	-1.70125	1.55383	-0.07311
C	-2.78266	0.69199	0.17751
H	-3.77114	1.12330	0.30986
C	-2.64074	-0.70548	0.25793
O	-1.59750	-1.39396	0.13189
C	-3.90112	-1.55008	0.54799
F	-4.05912	-2.48594	-0.39581
F	-5.02317	-0.81605	0.58864
F	-3.77346	-2.16937	1.72907
O	-0.49233	1.25634	-0.24628
F	-1.73335	3.48925	-1.43029
F	-1.18239	3.75004	0.64918
F	-3.24966	3.38780	0.11428
Cu	0.19901	-0.60987	-0.17144
C	2.88091	-0.60376	0.81997
H	3.58766	-1.37702	1.15889
C	2.21821	-0.90950	-0.49365
H	2.49210	-0.29756	-1.36336
C	1.53805	-2.10170	-0.68296
H	1.48755	-2.80210	0.16261
C	3.05914	0.75525	1.36629
H	3.89919	0.87434	2.06786
O	2.03820	-0.11066	1.87461
C	1.13384	-2.66387	-2.02147
H	1.80710	-3.49462	-2.30043
H	0.11227	-3.07516	-1.99231

H	1.18380	-1.90722	-2.82000
C	2.64008	2.02626	0.67657
H	2.34803	2.77892	1.42677
H	3.48432	2.44102	0.10055
H	1.77979	1.87685	0.01173

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.24320988463

Zero-point correction (ZPE) = -2889.028431 .21477816858

Internal Energy (U) = -2889.163877 .07933255385

Enthalpy (H) = -2889.005068 .238140943579765

Gibbs Free Energy (G) = -2889.084402 .15880786910

Frequencies -- 12.03 20.64 28.17 35.89 45.46 60.61

Dual Cu(I) DiMeDHF-E-Cis Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 64
Charge: 0 | Spin: 1 | Basis Functions: 732

Energy = -5778.54340696243

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000010	yes			
Step	0.0006607	0.0010000	yes	0.0000679	0.0005000	yes
Grad	0.0004977	0.0010000	yes	0.0000456	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.56102	-0.23556	2.31349
H	-1.06062	0.26801	3.15120
C	0.65398	0.46637	1.80809
H	0.52045	1.54774	1.66119
C	2.05579	0.02778	2.05041
H	2.80356	0.83213	2.02301
C	-0.91130	-1.53258	1.98900
H	-0.27094	-2.06420	1.27665
O	1.41220	-0.17142	0.77834
C	5.35190	2.51457	0.56737
C	4.60649	1.37425	-0.16032
C	5.23436	0.11826	-0.23304
H	6.23778	0.01647	0.17233
C	4.60672	-1.02462	-0.76679
O	3.47554	-1.12359	-1.29730
Cu	2.18038	0.40450	-1.41361
C	5.35193	-2.37253	-0.63540
F	5.27694	-3.07674	-1.76563
F	4.77755	-3.09855	0.34466
F	6.64810	-2.22807	-0.32248
O	3.46524	1.70576	-0.56344
F	4.71975	2.78620	1.72719
F	5.35192	3.62814	-0.16889
F	6.62375	2.21313	0.86321
C	-5.54865	-1.94815	-0.90133
C	-4.59639	-0.88263	-0.31443
C	-5.09676	0.41859	-0.12196
C	-4.33114	1.47196	0.41226

C	-5.01183	2.85059	0.57226
O	-3.13518	1.46412	0.79241
O	-3.45031	-1.32762	-0.06260
Cu	-1.99891	-0.21110	0.78723
F	-4.35064	3.77662	-0.14428
F	-4.98541	3.23235	1.85518
F	-6.28962	2.86258	0.16708
F	-5.67497	-2.97072	-0.04406
F	-5.04922	-2.43044	-2.04799
F	-6.77757	-1.47531	-1.15775
H	-6.12929	0.61884	-0.39520
C	0.67897	0.18159	-2.85053
H	1.19862	-0.20336	-3.73241
C	0.72611	1.48003	-2.38672
H	1.28774	2.30336	-2.83694
C	-0.47600	1.72731	-1.49301
H	-0.19863	2.16166	-0.51899
O	-0.97153	0.39613	-1.23597
C	-0.55366	-0.50046	-2.28771
H	-1.33141	-0.50755	-3.08155
C	2.46497	-1.19937	2.81573
H	3.28480	-1.71378	2.28936
H	2.83151	-0.91135	3.81422
H	1.63615	-1.91051	2.93756
C	-1.90858	-2.36972	2.74777
H	-2.52001	-1.76241	3.43298
H	-2.58496	-2.90497	2.06276
H	-1.38302	-3.13381	3.34872
C	-0.38853	-1.91602	-1.76376
H	-1.33766	-2.27677	-1.34024
H	-0.10722	-2.58447	-2.59301
H	0.40366	-1.95882	-1.00186
C	-1.52495	2.61953	-2.15676
H	-1.87421	2.18539	-3.10695
H	-2.38311	2.76238	-1.48698
H	-1.09362	3.61086	-2.37180

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5778.54340696243

Zero-point correction (ZPE) = -5778.110346 .43306043213

Internal Energy (U) = -5778.407871 .13553534165

Enthalpy (H) = -5778.063666 .479740673843675

Gibbs Free Energy (G) = -5778.199201 .34420496316

Frequencies -- 3.83 10.82 14.96 18.96 23.55 27.84

Mono Cu(I) DiMeDHF-E-Cis Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.21141806957

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000008	0.0000010	yes			
Step	0.0005353	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0006634	0.0010000	yes	0.0001125	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.05700	-1.13001	-0.39687
C	-2.27411	-0.23834	0.72307
C	-2.21429	1.10604	0.58765
C	-2.24302	-2.59047	-0.38401
C	-3.00193	-3.29885	0.71668
C	-2.44656	2.10097	1.67240
O	-0.85837	-2.46946	-0.15889
H	-1.91440	-0.67038	-1.38034
H	-2.51760	-0.68075	1.69381
H	-1.93129	1.51668	-0.38789
H	-2.47769	-3.02102	-1.37497
H	-4.08919	-3.23091	0.54857
H	-2.72167	-4.36380	0.71969
H	-2.76272	-2.88784	1.70767
H	-3.26724	2.79146	1.40814
H	-2.68053	1.62844	2.63811
H	-1.54368	2.72673	1.78838
C	4.65315	-0.85878	-0.89478
C	3.19487	-0.36225	-0.75363
C	2.97070	1.03422	-0.72500
C	1.69169	1.59115	-0.60440
C	1.56396	3.12490	-0.49936
O	0.58023	0.99964	-0.54733
O	2.35630	-1.28411	-0.67328
Cu	0.34149	-0.97187	-0.45688
F	1.08804	3.46130	0.71561
F	0.69784	3.58864	-1.41123
F	2.72577	3.76865	-0.67073

F	4.99648	-1.59153	0.17249
F	5.54308	0.14145	-1.00633
F	4.77070	-1.63079	-1.98281
H	3.82700	1.70093	-0.78354

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.21141806957

Zero-point correction (ZPE) = -2888.998734 .21268332920

Internal Energy (U) = -2889.130848 .08056921505

Enthalpy (H) = -2888.975055 .236362234504956

Gibbs Free Energy (G) = -2889.055626 .15579130040

Frequencies -- i268.69 13.03 24.58 25.71 30.71 35.45

Dual Cu(I) DiMeDHF-E-Cis Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05266000319

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000008	0.0000010	yes			
Step	0.0003891	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0005375	0.0010000	yes	0.0001153	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-5.15362	-2.36677	-0.65252
C	-4.40584	-1.04810	-0.35757
C	-5.10137	0.16193	-0.51229
C	-4.49521	1.42047	-0.34139
C	-5.35367	2.68504	-0.56735
C	0.22716	-1.27842	-0.21990
H	0.36946	-0.85943	-1.22226
C	-0.07868	-0.33916	0.86101
C	-0.07060	1.04507	0.69550
C	0.03440	-2.73368	-0.14252
O	-3.30463	1.67811	-0.02690
O	-3.20088	-1.21775	-0.03134
O	1.41505	-2.56359	0.11481
Cu	-1.96279	0.28377	0.31892
F	-5.34509	3.44630	0.53209
F	-6.62935	2.39844	-0.86207
F	-4.84801	3.40320	-1.57733
F	-4.90880	-3.26783	0.30551
F	-4.72228	-2.87315	-1.81726
F	-6.47949	-2.20296	-0.73889
H	-6.15183	0.12501	-0.78860
H	-0.16374	-0.75820	1.86984
H	0.24173	1.44001	-0.27924
H	-0.15453	-3.21145	-1.11971
C	6.84556	-0.92955	-0.70980
C	5.39666	-0.42745	-0.50508
C	5.17737	0.97034	-0.45817
H	6.03152	1.63472	-0.55957

C	3.90906	1.53193	-0.28026
O	2.79724	0.94447	-0.15953
Cu	2.55511	-1.01551	-0.13294
C	3.78674	3.06758	-0.20625
F	3.28905	3.43088	0.99153
F	2.93974	3.51257	-1.14539
F	4.95380	3.70131	-0.36874
O	4.55798	-1.34545	-0.39407
F	7.22548	-1.67040	0.33866
F	7.73314	0.06796	-0.85021
F	6.91345	-1.69403	-1.80628
C	-0.75845	-3.39320	0.96221
H	-1.83689	-3.28774	0.76722
H	-0.50758	-4.46459	0.99796
H	-0.52337	-2.96307	1.94659
C	-0.07418	2.03845	1.82061
H	-0.74991	2.88251	1.61035
H	-0.36218	1.58539	2.78150
H	0.94326	2.45600	1.91909

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05266000319

Zero-point correction (ZPE) = -5468.770694 .28196538074

Internal Energy (U) = -5468.935999 .11666064400

Enthalpy (H) = -5468.732759 .319900620238945

Gibbs Free Energy (G) = -5468.849418 .20324131678

Frequencies -- i274.82 7.43 11.98 14.64 20.93 26.10

Mono Cu(I) DiMeDHF-E-Cis Metalaoxetane (s-*trans*)

Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22520770332

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0005303	0.0010000	yes	0.0001067	0.0005000	yes
Grad	0.0001085	0.0010000	yes	0.0000172	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.12794	-0.03752	-0.47859
C	-1.99762	-0.28976	0.93685
C	-1.74771	0.68720	1.84593
C	-2.61271	-1.05688	-1.48976
C	3.94915	-0.90212	-2.21856
C	2.71223	-0.28392	-1.52513
C	2.92023	0.72581	-0.55679
C	1.85038	1.33616	0.09965
C	2.14224	2.44469	1.13064
C	-3.32495	-2.29564	-0.96885
C	-1.61358	0.48646	3.31613
O	-1.35208	-1.36763	-2.04510
O	0.61340	1.10970	-0.03570
O	1.62334	-0.75712	-1.91005
Cu	-0.19611	-0.26561	-1.14654
F	1.54855	2.15558	2.30093
F	1.64939	3.61322	0.70071
F	3.44962	2.60822	1.36469
F	3.96261	-2.22653	-2.03839
F	5.10478	-0.41003	-1.74489
F	3.90658	-0.65638	-3.53257
H	-2.19330	1.01445	-0.78502
H	-2.11374	-1.32167	1.28493
H	-1.61161	1.71095	1.47883
H	-3.26528	-0.55953	-2.23716
H	3.93445	1.03408	-0.31833
H	-4.28748	-2.04245	-0.49315
H	-3.52332	-2.97351	-1.81374

H	-2.69679	-2.84330	-0.24945
H	-2.33862	1.10800	3.87179
H	-1.75193	-0.56433	3.61209
H	-0.61221	0.81940	3.64461

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22520770332

Zero-point correction (ZPE) = -2889.010810 .21439728869

Internal Energy (U) = -2889.146882 .07832528252

Enthalpy (H) = -2888.987523 .237683887714718

Gibbs Free Energy (G) = -2889.065847 .15936014494

Frequencies -- 16.67 24.88 28.86 32.35 52.81 73.97

Dual Cu(I) DiMeDHF-E-Cis Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07226382278

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000100	yes			
Step	0.0007131	0.0010000	yes	0.0000966	0.0005000	yes
Grad	0.0000367	0.0010000	yes	0.0000074	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.71239	1.23997	-0.55359
H	-2.83759	2.28452	-0.86795
C	-2.54980	1.00457	0.84895
C	-2.33301	2.01088	1.74376
C	-3.14533	0.18992	-1.57014
O	-1.89418	-0.06996	-2.22201
H	-2.54874	-0.02806	1.20660
H	-2.29602	3.03975	1.36659
H	-3.82866	0.65563	-2.30450
C	3.33817	0.35431	-2.28600
C	2.11148	1.04183	-1.64504
C	2.32319	1.98255	-0.61554
H	3.34082	2.21945	-0.31734
C	1.26349	2.60782	0.04671
O	0.01906	2.45735	-0.12774
Cu	-0.76303	1.07822	-1.23589
C	1.58315	3.64171	1.14546
F	0.93431	3.32866	2.27770
F	1.17153	4.85714	0.76073
F	2.88814	3.71540	1.42608
O	1.01379	0.66197	-2.11273
F	3.30103	-0.95934	-2.02562
F	4.49916	0.83479	-1.81911
F	3.32334	0.52073	-3.61080
C	-3.78985	-1.07509	-1.03114
H	-4.74837	-0.85355	-0.53303
H	-3.99036	-1.76131	-1.86914
H	-3.12753	-1.59057	-0.31890

C	-2.10333	1.82307	3.19968
H	-2.82275	2.41117	3.79735
H	-2.15256	0.76750	3.50092
H	-1.10107	2.21193	3.45651
Cu	-0.79584	-1.65218	-1.94072
O	0.35826	-3.16978	-1.83548
O	-0.26058	-1.04050	0.15538
C	1.15647	-3.44575	-0.90519
C	0.63136	-1.67574	0.76549
C	1.34047	-2.81371	0.34074
C	2.05467	-4.66039	-1.23309
C	0.95597	-1.10054	2.16399
H	2.08874	-3.22969	1.01084
F	2.84124	-4.37609	-2.27840
F	2.84658	-5.01867	-0.20965
F	1.30295	-5.71998	-1.55562
F	1.35951	0.17962	2.06082
F	1.90692	-1.77255	2.82197
F	-0.15279	-1.10702	2.92812

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07226382278

Zero-point correction (ZPE) = -5468.789384 .28287949247

Internal Energy (U) = -5468.957677 .11458591488

Enthalpy (H) = -5468.751285 .320978510320681

Gibbs Free Energy (G) = -5468.865872 .20639119345

Frequencies -- 8.53 14.46 23.65 25.55 29.43 32.31

Mono Cu(I) DiMeDHF-E-Cis Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  32
Charge: 0     | Spin: 1                         | Basis Functions:   366
----------------------------------------------------------------------------------------------------
Energy =    -2889.21784321466
----------------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000009  || 0.0000010   yes
Step      0.0008858  || 0.0010000   yes  |  0.0001914  || 0.0005000   yes
Grad      0.0001207  || 0.0010000   yes  |  0.0000273  || 0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
----------------------------------------------------------------------------------------------------
C        0.03836      -1.94836      -0.84037
C        0.16155      -2.05695       0.60789
C        1.27185      -1.86287       1.36234
C        1.16889      -2.06024      -1.84533
C        0.35019       4.35130      -0.61060
C       -0.25458       2.92985      -0.55192
C       -1.55744       2.77810      -0.03046
C       -2.16907       1.52555       0.07076
C       -3.58976       1.44239       0.66642
C        1.31914      -1.99531       2.84844
C        2.32094      -3.02222      -1.60368
O        1.54187      -0.69763      -1.80125
O       -1.70890       0.39701      -0.26345
O        0.50850       2.03680      -0.98046
Cu       0.06815       0.07268      -0.98785
F       -3.58975       0.63750       1.73728
F       -4.43935       0.93416      -0.23430
F       -4.06091       2.63632       1.05057
F        1.46265       4.40175       0.13066
F       -0.49325       5.28910      -0.15184
F        0.66925       4.66519      -1.86972
H       -0.97591      -2.10178      -1.22823
H       -0.78108      -2.26617       1.12875
H        2.19571      -1.54551       0.86714
H       -2.09768       3.65812       0.30713
H        2.08054      -2.73683       3.15079
H        1.62243      -1.04179       3.31786
H        0.34949      -2.29931       3.27082
```

H 0.72777 -2.31267 -2.83320
H 2.80640 -2.87703 -0.62905
H 1.97543 -4.06766 -1.66760
H 3.07858 -2.86350 -2.38752
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.21784321466
Zero-point correction (ZPE) = -2889.003369 .21447346467
Internal Energy (U) = -2889.139432 .07841045202
Enthalpy (H) = -2888.980052 .237790534083229
Gibbs Free Energy (G) = -2889.058464 .15937918894

Frequencies -- 15.46 25.42 29.51 35.34 58.94 72.23

Dual Cu(I) DiMeDHF-E-Cis Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.06543408791

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0004991	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0001509	0.0010000	yes	0.0000238	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.63267	-2.42848	-1.09154
C	-1.53792	-2.45085	0.34586
C	-0.40849	-2.36875	1.11018
C	-0.48355	-2.45667	-2.08578
O	-0.09329	-1.07378	-2.03183
C	-1.32674	3.90387	-0.82476
C	-1.94728	2.48871	-0.79373
C	-3.25112	2.33661	-0.27740
C	-3.88631	1.09317	-0.20083
O	-3.45527	-0.03947	-0.56480
Cu	-1.67466	-0.35757	-1.25615
C	-5.30202	1.02273	0.40953
F	-5.29513	0.21287	1.47640
F	-6.16442	0.52607	-0.48432
F	-5.75567	2.21908	0.80307
O	-1.19542	1.59415	-1.24603
F	-0.20987	3.92592	-0.09149
F	-2.15883	4.83866	-0.34356
F	-1.01337	4.23604	-2.08093
C	5.36351	1.01232	-1.30918
C	3.99782	0.68335	-0.66368
C	3.82090	0.98931	0.70203
C	2.62507	0.74223	1.39108
C	2.54589	1.14480	2.87925
O	1.56051	0.22446	0.96059
O	3.17877	0.16918	-1.45981
Cu	1.30841	-0.33010	-0.94024
F	2.19698	0.08030	3.62667

F	1.61184	2.08699	3.05593
F	3.70268	1.61442	3.36276
F	5.89701	-0.09311	-1.84469
F	6.24991	1.51036	-0.43275
F	5.20463	1.91328	-2.28606
H	-2.63007	-2.63178	-1.49847
H	-2.50257	-2.46008	0.86699
H	0.56813	-2.31325	0.62313
H	-3.77724	3.21592	0.08397
H	4.64781	1.44184	1.24284
C	-0.38664	-2.29492	2.59431
H	0.19587	-3.13352	3.01833
H	0.14557	-1.37747	2.90394
H	-1.39421	-2.30295	3.03571
H	-0.91805	-2.63663	-3.08668
C	0.67129	-3.42942	-1.91717
H	1.19688	-3.32172	-0.95854
H	0.31254	-4.46878	-1.99623
H	1.39877	-3.25734	-2.72593

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.06543408791

Zero-point correction (ZPE) = -5468.782326 .28310802040

Internal Energy (U) = -5468.949446 .11598723712

Enthalpy (H) = -5468.744154 .321279405431837

Gibbs Free Energy (G) = -5468.860139 .20529425938

Frequencies -- 7.80 9.99 12.75 28.32 29.30 34.55

Dual Cu(I) DiMeDHF-E-Cis Suprafacial Copper Migration (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05473197598

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0005066	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0009925	0.0010000	yes	0.0002355	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.63351	-2.97785	0.00554
C	-1.09700	-2.46057	1.17381
C	0.26175	-2.14204	1.40607
C	-0.83837	-3.09395	-1.28027
O	-0.44465	-1.73795	-1.51107
C	-0.57388	2.82039	1.26489
C	-1.50295	1.82930	0.52778
C	-2.88352	2.11573	0.48953
C	-3.84193	1.25005	-0.06192
O	-3.68467	0.11725	-0.59348
Cu	-1.99650	-0.73174	-0.94656
C	-5.32289	1.68894	-0.03045
F	-6.05794	0.77498	0.61644
F	-5.79611	1.79501	-1.27817
F	-5.50554	2.86909	0.57964
O	-0.91605	0.82687	0.06229
F	-0.17382	2.27292	2.42822
F	-1.16347	3.98909	1.54573
F	0.51978	3.07203	0.53631
C	2.45705	2.21861	-3.15006
C	2.34286	1.28636	-1.92177
C	3.23190	1.49203	-0.84220
C	3.21981	0.67921	0.28978
C	4.31597	0.89192	1.35365
O	2.44241	-0.28109	0.57010
O	1.45962	0.41229	-2.02987
Cu	0.93796	-0.84019	-0.50332
F	5.24439	-0.07059	1.23954

F	3.80096	0.82139	2.58722
F	4.93206	2.07360	1.22947
F	2.78199	1.50631	-4.23536
F	3.38706	3.17211	-2.99005
F	1.28533	2.82021	-3.37898
H	-2.69515	-3.24621	-0.00829
H	-1.80532	-2.16719	1.95848
H	1.03587	-2.73909	0.91735
H	-3.22795	3.05251	0.91989
H	3.95930	2.29675	-0.90399
C	0.65966	-1.41785	2.65130
H	0.64292	-2.12977	3.50062
H	1.67378	-1.00763	2.57874
H	-0.04022	-0.60171	2.88818
H	-1.54706	-3.37767	-2.08157
C	0.31846	-4.08614	-1.36183
H	1.11271	-3.90348	-0.62453
H	-0.04508	-5.11742	-1.22294
H	0.76998	-4.01482	-2.36390

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05473197598

Zero-point correction (ZPE) = -5468.772957 .28177494080

Internal Energy (U) = -5468.939267 .11546486416

Enthalpy (H) = -5468.735269 .319462608368275

Gibbs Free Energy (G) = -5468.850732 .20399926776

Frequencies -- i59.27 4.42 13.42 16.01 20.88 26.77

Dual Cu(I) DiMeDHF-E-Cis Antarafacial Copper Migration (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04335220336

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0004390	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0009796	0.0010000	yes	0.0001604	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.31088	-2.49660	-0.81072
C	-0.85111	-2.39428	0.52904
H	-1.21860	-3.19324	1.19092
C	-0.01698	-1.46508	1.13924
H	-0.03372	-0.41725	0.80807
C	-0.44133	-2.19132	-2.01546
H	-1.07171	-2.30449	-2.91926
O	-0.12810	-0.81342	-1.88031
C	-2.33130	3.31468	1.10183
C	-2.68775	2.00257	0.36701
C	-4.03806	1.59644	0.33547
C	-4.45542	0.39060	-0.24246
O	-3.76052	-0.50472	-0.80162
Cu	-1.84012	-0.40863	-1.00255
C	-5.96028	0.04511	-0.21623
F	-6.15054	-1.11960	0.41639
F	-6.42351	-0.07923	-1.46516
F	-6.69388	0.97755	0.40601
O	-1.69572	1.40707	-0.11441
F	-1.64796	3.02185	2.21972
F	-3.41531	4.01964	1.45615
F	-1.56511	4.08775	0.33398
C	4.97412	-0.49420	1.54322
C	3.90818	0.04412	0.56840
C	4.10708	1.29709	-0.00968
C	3.15873	1.89819	-0.87650
C	3.47147	3.31591	-1.41488
O	2.06988	1.43232	-1.25871

O	2.93890	-0.75837	0.42074
Cu	1.36139	-0.45012	-0.67563
F	2.55243	4.18395	-0.97631
F	3.44448	3.31761	-2.75242
F	4.67675	3.76507	-1.02813
F	4.40993	-0.76105	2.73458
F	5.97797	0.36646	1.75298
F	5.49857	-1.63429	1.07594
H	-2.16954	-3.15895	-0.97256
H	-4.78717	2.24456	0.78210
H	5.01239	1.84604	0.23526
C	0.63046	-1.69461	2.46272
H	0.47804	-2.71979	2.83095
H	1.71515	-1.51111	2.37047
H	0.25566	-0.97714	3.21488
C	0.78124	-3.08999	-2.17833
H	1.42520	-3.05009	-1.28444
H	0.48411	-4.13743	-2.35010
H	1.36248	-2.74955	-3.05021

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04335220336

Zero-point correction (ZPE) = -5468.761767 .28158450085

Internal Energy (U) = -5468.929064 .11428725382

Enthalpy (H) = -5468.724331 .319020787698729

Gibbs Free Energy (G) = -5468.838617 .20473436594

Frequencies -- i54.56 9.28 10.55 17.86 19.31 23.25

Mono Cu(I) DiMeDHF-E-Cis Metalaoxinane (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22295336064

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0007866	0.0010000	yes	0.0000929	0.0005000	yes
Grad	0.0000316	0.0010000	yes	0.0000068	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.21735	2.98629	0.62596
C	-0.80815	2.62002	-0.18255
C	-0.71547	1.69877	-1.31154
C	1.55874	2.30871	0.58839
C	1.62882	-3.16723	2.08521
C	0.78407	-2.38359	1.05345
C	-0.36057	-3.01277	0.51211
C	-1.19250	-2.35170	-0.38993
C	-2.44588	-3.07552	-0.91959
C	-1.99508	1.25652	-1.96700
C	2.69367	3.34841	0.39886
O	1.66604	1.36669	-0.40612
O	-1.07606	-1.18268	-0.86236
O	1.20084	-1.23200	0.81476
Cu	0.29759	0.10369	-0.44868
F	-2.38927	-3.18185	-2.25282
F	-3.54308	-2.37265	-0.60646
F	-2.58628	-4.30683	-0.41164
F	1.24238	-4.44744	2.19921
F	1.51161	-2.59507	3.29117
F	2.91745	-3.15465	1.73862
H	0.05875	3.75469	1.39074
H	-1.80826	3.01620	0.03765
H	0.11363	1.88956	-1.99943
H	-0.60475	-4.02776	0.81283
H	-2.41701	2.12162	-2.51543
H	-1.83142	0.44991	-2.69307
H	-2.74741	0.91630	-1.24037

H 1.70771 1.87605 1.61087
H 2.58802 3.84768 -0.57621
H 2.67456 4.10474 1.19944
H 3.65994 2.82592 0.42392
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22295336064
Zero-point correction (ZPE) = -2889.008327 .21462581662
Internal Energy (U) = -2889.145914 .07703865521
Enthalpy (H) = -2888.985539 .237413462994565
Gibbs Free Energy (G) = -2889.062580 .16037328544

Frequencies -- 15.01 21.59 28.37 35.35 52.73 80.92

Dual Cu(I) DiMeDHF-E-Cis Metalaoxinane (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07083784262

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008422	0.0010000	yes	0.0000932	0.0005000	yes
Grad	0.0000878	0.0010000	yes	0.0000150	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.36950	3.69401	0.85493
C	-2.43255	3.33311	0.08621
C	-2.42846	2.37882	-1.01127
C	-0.04004	3.00389	0.84768
O	-0.01034	1.93223	-0.05025
C	2.12705	-3.46118	-1.18766
C	2.41672	-1.99036	-0.81778
C	3.75036	-1.60926	-0.58810
C	4.12427	-0.30863	-0.19897
O	3.39397	0.69206	0.00623
Cu	1.41266	0.63269	-0.16101
C	5.62479	-0.02684	0.03724
F	5.83945	0.28296	1.32384
F	6.02149	1.01262	-0.70842
F	6.41023	-1.07175	-0.26706
O	1.38081	-1.28263	-0.76313
F	1.24013	-3.98211	-0.32367
F	3.21923	-4.23753	-1.16989
F	1.59231	-3.53640	-2.41462
C	-0.08923	-2.47992	2.39784
C	-0.96388	-1.69200	1.39672
C	-1.99221	-2.37761	0.71564
C	-2.87652	-1.72048	-0.13828
C	-4.02221	-2.52307	-0.78722
O	-2.90208	-0.49549	-0.47244
O	-0.69467	-0.47059	1.32599
Cu	-1.54017	0.78084	-0.03083
F	-3.98947	-2.37881	-2.11690

F	-5.20138	-2.06216	-0.34853
F	-3.95985	-3.82990	-0.50789
F	-0.23986	-3.80343	2.27886
F	-0.43713	-2.13594	3.64803
F	1.20234	-2.18572	2.23376
H	-1.49727	4.48707	1.59924
H	-3.40640	3.77567	0.33379
H	-1.57489	2.44360	-1.69456
H	4.52884	-2.35945	-0.69804
H	-2.10548	-3.44740	0.86880
C	-3.73355	2.00790	-1.65170
H	-4.05349	2.84299	-2.30593
H	-3.64319	1.11136	-2.27900
H	-4.52904	1.83334	-0.91205
H	0.13071	2.65886	1.89382
C	1.11396	3.97034	0.50310
H	0.98439	4.37135	-0.51341
H	1.15516	4.80583	1.21871
H	2.06401	3.41711	0.54820

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07083784262

Zero-point correction (ZPE) = -5468.787767 .28306993241

Internal Energy (U) = -5468.956447 .11439059282

Enthalpy (H) = -5468.749996 .320841393561167

Gibbs Free Energy (G) = -5468.864385 .20645213424

Frequencies -- 6.02 12.20 21.46 26.41 29.49 32.87

Mono Cu(I) DiMeDHF-E-Cis Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22503182874

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0008714	0.0010000	yes	0.0002089	0.0005000	yes
Grad	0.0000734	0.0010000	yes	0.0000139	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.34794	3.08394	-0.94369
C	-0.27253	2.27142	-1.83629
C	0.20068	0.96286	-2.26728
C	1.52239	2.63264	-0.12207
C	0.61204	-1.76305	3.50618
C	0.26561	-1.54877	2.01407
C	-0.64231	-2.43912	1.39702
C	-0.98599	-2.30130	0.05228
C	-1.97010	-3.30609	-0.57864
C	1.29782	2.89410	1.38062
C	-0.71178	0.12691	-3.12334
O	1.93802	1.35539	-0.41049
O	-0.58795	-1.43405	-0.77877
O	0.84607	-0.57501	1.49131
Cu	0.61269	0.04077	-0.44927
F	-1.36247	-3.98419	-1.56065
F	-3.01368	-2.65559	-1.11071
F	-2.44408	-4.19292	0.30566
F	-0.03295	-2.81106	4.04144
F	0.28237	-0.67467	4.21155
F	1.92476	-1.97191	3.64698
H	-0.03768	4.09354	-0.76621
H	-1.23069	2.60411	-2.25657
H	1.25905	0.92278	-2.54470
H	2.35108	3.31141	-0.45363
H	-1.07816	-3.24772	1.97749
H	2.20252	2.59999	1.93287
H	1.08254	3.95558	1.58748

H	0.46096	2.28460	1.75708
H	-0.77468	0.60038	-4.12270
H	-0.33083	-0.89305	-3.26242
H	-1.73064	0.05808	-2.71462

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22503182874

Zero-point correction (ZPE) = -2889.010786 .21424493674

Internal Energy (U) = -2889.148030 .07700118063

Enthalpy (H) = -2888.988014 .237017347911524

Gibbs Free Energy (G) = -2889.065012 .16001906715

Frequencies -- 13.78 23.84 27.57 33.52 61.28 76.29

Dual Cu(I) DiMeDHF-E-Cis Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07611703167

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000006	0.0000010	yes			
Step	0.0007590	0.0010000	yes	0.0001492	0.0005000	yes
Grad	0.0000826	0.0010000	yes	0.0000201	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.19722	3.73214	-0.62909
C	-1.74286	2.88716	-1.54717
C	-1.14242	1.66997	-2.06241
C	0.05701	3.44769	0.14393
O	0.54278	2.17203	-0.12790
C	5.36536	-1.46057	0.51559
C	3.95623	-0.96014	0.12353
C	3.11961	-1.84527	-0.58528
C	1.80510	-1.55054	-0.99238
O	1.17182	-0.48016	-0.83774
Cu	2.14458	1.21785	0.25842
C	1.00125	-2.66031	-1.70821
F	0.48566	-2.19016	-2.85597
F	-0.02553	-3.05234	-0.93246
F	1.72659	-3.74559	-2.00257
O	3.74014	0.21592	0.51308
F	6.29843	-0.64048	0.01572
F	5.62773	-2.69907	0.06871
F	5.49473	-1.47219	1.84826
C	-0.73535	-1.04303	3.67789
C	-1.12396	-0.80264	2.20180
C	-2.06795	-1.66001	1.60294
C	-2.49775	-1.47581	0.28594
C	-3.56351	-2.43080	-0.29104
O	-2.14333	-0.59464	-0.54749
O	-0.54350	0.17762	1.68135
Cu	-0.76080	0.72996	-0.25733
F	-3.08345	-3.06405	-1.36526

F	-4.64079	-1.72716	-0.66888
F	-3.96471	-3.35349	0.59266
F	-1.34614	-2.11216	4.20720
F	-1.06844	0.02696	4.41167
F	0.58433	-1.22629	3.78163
H	-1.71911	4.66500	-0.39105
H	-2.74978	3.12246	-1.91504
H	-0.06584	1.70508	-2.25311
H	0.80604	4.17408	-0.25472
H	3.51572	-2.82964	-0.82057
H	-2.48539	-2.47817	2.18338
C	-0.10751	3.72116	1.64603
H	0.85871	3.55675	2.14725
H	-0.43175	4.75619	1.84065
H	-0.83924	3.02628	2.08612
C	-1.92123	0.79811	-2.99821
H	-1.91518	1.27828	-3.99712
H	-1.45313	-0.18971	-3.10758
H	-2.96597	0.66371	-2.68517

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07611703167

Zero-point correction (ZPE) = -5468.793123 .28299375644

Internal Energy (U) = -5468.961956 .11416006737

Enthalpy (H) = -5468.755355 .320761408784783

Gibbs Free Energy (G) = -5468.869516 .20660067739

Frequencies -- 8.71 16.06 17.58 25.21 27.23 27.42

Mono Cu(I) DiMeDHF-E-Cis Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20994683908

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0008740	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0003448	0.0010000	yes	0.0000407	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.65886	3.01474	1.66687
C	-0.64843	2.75742	1.56246
C	-1.18618	2.07336	0.36434
C	1.51467	2.50103	0.53690
C	2.15281	-3.37741	-1.16956
C	0.96189	-2.44038	-0.85986
C	-0.31587	-3.02268	-0.69297
C	-1.45411	-2.26526	-0.39884
C	-2.80022	-2.99667	-0.21881
C	2.57286	1.49515	1.00056
C	-1.79594	2.87994	-0.74915
O	0.65815	2.00318	-0.45960
O	-1.55015	-1.01464	-0.24831
O	1.27163	-1.23286	-0.79060
Cu	-0.08824	0.27652	-0.35884
F	-3.69775	-2.53052	-1.09737
F	-3.28109	-2.78127	1.01413
F	-2.70393	-4.32218	-0.39431
F	1.80808	-4.67455	-1.19125
F	3.10839	-3.22388	-0.24428
F	2.67844	-3.07443	-2.36356
H	1.10597	3.51516	2.53024
H	-1.35623	2.99489	2.36584
H	-1.82381	1.20947	0.62821
H	2.03089	3.37101	0.07651
H	-0.41710	-4.10053	-0.78716
H	3.12993	1.10736	0.13494
H	3.28561	1.96398	1.69941

H	2.09910	0.64094	1.51130
H	-2.04636	2.24297	-1.61089
H	-2.74299	3.32049	-0.38414
H	-1.12887	3.68968	-1.07222

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20994683908

Zero-point correction (ZPE) = -2888.996387 .21355935294

Internal Energy (U) = -2889.132671 .07727485864

Enthalpy (H) = -2888.973794 .236152750566810

Gibbs Free Energy (G) = -2889.051070 .15887642748

Frequencies -- i327.03 16.65 25.08 28.54 29.75 45.01

Dual Cu(I) DiMeDHF-E-Cis Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

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Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05025436947

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0006532	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0007945	0.0010000	yes	0.0001082	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.87987	0.89515	1.78431
C	-0.48393	0.66914	1.68342
C	-1.00749	-0.30298	0.67644
C	1.70781	0.11434	0.78135
O	0.81276	-0.33849	-0.20369
C	-2.71838	5.15202	-1.04573
C	-1.39134	4.59551	-0.48627
C	-0.22158	5.35231	-0.66529
C	1.03996	4.92979	-0.20888
O	1.33561	3.86642	0.39439
Cu	0.00087	2.48504	0.84809
C	2.24992	5.86265	-0.43677
F	3.22497	5.20827	-1.07596
F	2.72982	6.27784	0.74308
F	1.93854	6.94832	-1.15868
O	-1.52185	3.48106	0.08570
F	-3.22459	4.29738	-1.94433
F	-2.57221	6.34201	-1.64424
F	-3.61184	5.29454	-0.05950
C	2.25446	-5.69750	-1.01625
C	1.06951	-4.76106	-0.68480
C	-0.20973	-5.33765	-0.51275
C	-1.34140	-4.58046	-0.19395
C	-2.69106	-5.30729	-0.01993
O	-1.42823	-3.33196	-0.01314
O	1.38688	-3.55522	-0.60172
Cu	0.04751	-2.06153	-0.12218
F	-3.58291	-4.83398	-0.89973

F	-3.17303	-5.09325	1.21225
F	-2.59770	-6.63174	-0.19969
F	1.90100	-6.99051	-1.06827
F	3.20819	-5.56956	-0.08477
F	2.78298	-5.36783	-2.20078
H	1.34334	1.32961	2.67639
H	-1.15580	0.89552	2.52201
H	-1.46505	-1.16629	1.19488
H	2.39913	0.80682	0.26088
H	-0.29358	6.30513	-1.18248
H	-0.31829	-6.41297	-0.62651
C	2.52874	-0.99433	1.44549
H	3.03404	-1.59763	0.67686
H	3.28962	-0.57247	2.12219
H	1.87904	-1.66287	2.03606
C	-1.84013	0.16384	-0.48379
H	-2.25892	-0.68364	-1.04539
H	-2.68082	0.77178	-0.10197
H	-1.25471	0.80670	-1.15636

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05025436947

Zero-point correction (ZPE) = -5468.767793 .28246052459

Internal Energy (U) = -5468.936179 .11407489786

Enthalpy (H) = -5468.730810 .319443564373898

Gibbs Free Energy (G) = -5468.844883 .20537043536

Frequencies -- i309.36 7.82 10.78 14.78 24.41 25.07

Mono Cu(I) DiMeDHF-E-Cis Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20831476650

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0006465	0.0010000	yes	0.0001068	0.0005000	yes
Grad	0.0007521	0.0010000	yes	0.0001250	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.72451	-0.85796	-1.58598
C	-2.57015	0.46786	-1.52579
C	-1.90448	1.09640	-0.35901
C	-2.15355	-1.63823	-0.42834
C	3.75286	-2.05025	0.51652
C	2.74948	-0.87614	0.41840
C	3.27390	0.43483	0.33469
C	2.46158	1.56427	0.19369
C	3.13845	2.94234	0.04462
C	-2.72993	1.69102	0.74793
C	-3.19253	-2.54664	0.24314
O	-1.69148	-0.71251	0.52607
O	1.20022	1.62770	0.15195
O	1.55182	-1.22793	0.40873
Cu	-0.02504	0.11675	0.28760
F	2.65563	3.79807	0.95379
F	2.88485	3.44769	-1.17210
F	4.46954	2.88993	0.19575
F	5.02206	-1.64183	0.67503
F	3.70022	-2.79129	-0.59972
F	3.44351	-2.83752	1.55187
H	-3.20037	-1.36848	-2.42799
H	-2.88202	1.12987	-2.34284
H	-1.09149	1.78273	-0.66078
H	4.35181	0.56935	0.36214
H	-2.09829	1.98695	1.59911
H	-3.21464	2.61056	0.36840
H	-3.50626	0.99543	1.09155

H -1.32673 -2.28036 -0.80302
H -4.03918 -1.95159 0.61911
H -3.57250 -3.29277 -0.47351
H -2.73274 -3.07824 1.08898
==========

Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20831476650
Zero-point correction (ZPE) = -2888.994755 .21355935294
Internal Energy (U) = -2889.130366 .07794826551
Enthalpy (H) = -2888.972085 .236228926544318
Gibbs Free Energy (G) = -2889.050036 .15827844606

Frequencies -- i326.97 15.14 22.71 24.59 29.19 37.71

Dual Cu(I) DiMeDHF-E-Cis Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04987663737

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0005613	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0002956	0.0010000	yes	0.0000508	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.64698	-0.97745	-1.66946
C	-0.47879	0.39375	-1.56562
C	0.44490	0.95678	-0.53296
C	0.14146	-1.77899	-0.65356
O	0.57406	-0.86918	0.32876
C	-4.98974	2.86724	0.66116
C	-4.46267	1.48038	0.23563
C	-5.30552	0.36654	0.38803
C	-4.91639	-0.93652	0.03223
O	-3.81723	-1.32106	-0.44550
Cu	-2.31841	-0.10067	-0.82792
C	-5.92867	-2.08471	0.23474
F	-5.43927	-2.97643	1.10507
F	-6.14668	-2.71211	-0.92705
F	-7.11033	-1.65803	0.70141
O	-3.29173	1.51443	-0.22452
F	-4.17486	3.40135	1.57993
F	-6.22394	2.81916	1.18037
F	-5.01811	3.68796	-0.39635
C	6.03102	-2.20955	0.50538
C	5.02940	-1.03796	0.37119
C	5.55350	0.27097	0.26222
C	4.74250	1.39651	0.09010
C	5.41634	2.77232	-0.08852
O	3.48039	1.45673	0.03948
O	3.83110	-1.39167	0.35637
Cu	2.26585	-0.06110	0.17287
F	4.94622	3.63928	0.81595

F	5.14157	3.25805	-1.30829
F	6.74885	2.72115	0.04210
F	7.30097	-1.79732	0.63943
F	5.96760	-2.98961	-0.58280
F	5.72622	-2.95649	1.57106
H	-1.03922	-1.45716	-2.57279
H	-0.70973	1.05657	-2.41060
H	1.28462	1.47801	-1.02899
H	-6.30054	0.51847	0.79756
H	6.63122	0.40630	0.29338
C	-0.08108	1.73240	0.64024
H	0.73669	2.17110	1.23013
H	-0.72141	2.55488	0.27209
H	-0.70521	1.09650	1.28405
H	0.99907	-2.23998	-1.19130
C	-0.64564	-2.90309	0.02435
H	-1.51083	-2.50002	0.57190
H	-1.01534	-3.61620	-0.72959
H	0.00477	-3.44152	0.72862

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04987663737

Zero-point correction (ZPE) = -5468.767568 .28230817264

Internal Energy (U) = -5468.934540 .11533654211

Enthalpy (H) = -5468.730425 .319451181971648

Gibbs Free Energy (G) = -5468.845763 .20411353173

Frequencies -- i311.42 7.48 10.03 13.07 18.95 22.27

Mono Cu(I) DiMeDHF-E-Cis Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27588137608

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0008614	0.0010000	yes	0.0001316	0.0005000	yes
Grad	0.0000535	0.0010000	yes	0.0000150	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.29176	-1.71592	0.77557
C	0.34902	-2.24546	-0.08673
C	-0.93422	-2.48974	0.69765
C	0.66799	-1.59705	2.15821
C	-1.79697	1.72374	-3.44786
C	-0.82548	1.53420	-2.26121
C	-0.19853	2.67483	-1.72623
C	0.73929	2.60791	-0.68206
C	1.37799	3.92230	-0.18299
C	-1.18724	-3.97626	0.96461
C	0.91856	-0.31367	2.93383
O	-0.72946	-1.75282	1.90587
O	1.16175	1.58985	-0.07484
O	-0.69129	0.33461	-1.91201
Cu	0.49784	-0.23660	-0.43077
F	1.21234	4.04093	1.13978
F	0.85235	5.01140	-0.76286
F	2.69359	3.91684	-0.43782
F	-2.96604	1.12636	-3.19272
F	-1.27808	1.16686	-4.55150
F	-2.04403	3.01397	-3.71810
H	2.37406	-1.70959	0.61608
H	0.55389	-2.73051	-1.04576
H	-1.81928	-2.05970	0.19745
H	1.04219	-2.45325	2.76453
H	-0.44608	3.64806	-2.14156
H	-2.05688	-4.08984	1.62956
H	-1.39831	-4.51057	0.02390

H -0.31700 -4.45258 1.44409
H 0.34002 -0.32440 3.86986
H 1.98674 -0.22387 3.18861
H 0.62950 0.56998 2.34541
==========

Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27588137608
Zero-point correction (ZPE) = -2889.059084 .21679683198
Internal Energy (U) = -2889.199452 .07642884157
Enthalpy (H) = -2889.036696 .239184554471622
Gibbs Free Energy (G) = -2889.113127 .16275378474

Frequencies -- 20.24 26.77 27.73 34.04 38.60 81.36

Dual Cu(I) DiMeDHF-E-Cis Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11045236287

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0001462	0.0010000	yes	0.0000221	0.0005000	yes
Grad	0.0000997	0.0010000	yes	0.0000190	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.35521	-1.86882	1.23379
C	-1.26585	-2.22836	0.27158
C	-2.66723	-1.97906	0.80496
C	-1.11508	-1.37724	2.45488
O	-2.44154	-1.17614	1.96720
C	5.91579	1.20087	-0.34673
C	4.40454	0.88791	-0.45186
C	4.02724	-0.34722	-1.02340
C	2.70273	-0.78838	-1.15704
O	1.65156	-0.16377	-0.85428
Cu	1.77301	1.80938	0.09405
C	2.46153	-2.21994	-1.68060
F	1.45070	-2.23807	-2.55807
F	2.10881	-3.01744	-0.64803
F	3.53299	-2.76297	-2.26357
O	3.68424	1.80802	0.00785
F	6.21306	2.27650	-1.08507
F	6.68868	0.18756	-0.76726
F	6.24012	1.46403	0.92373
C	-3.59718	1.30293	-2.72615
C	-2.37613	1.31198	-1.77589
C	-2.08098	2.51588	-1.07957
C	-1.00550	2.64260	-0.21214
C	-0.74782	3.99505	0.47279
O	-0.17227	1.73023	0.12017
O	-1.78198	0.22086	-1.71277
Cu	-0.43802	-0.40198	-0.32697
F	-0.86821	3.86727	1.80033

F	-1.58069	4.95667	0.06727
F	0.51094	4.40197	0.21618
F	-4.51612	0.44492	-2.25798
F	-3.23272	0.89976	-3.94588
F	-4.17832	2.50540	-2.84236
H	0.69208	-2.17669	1.26224
H	-1.06208	-2.85736	-0.59978
H	-3.27955	-1.38653	0.10365
H	-1.10458	-2.20570	3.20023
H	4.82034	-1.01068	-1.35884
H	-2.71601	3.38171	-1.24937
C	-3.40832	-3.27717	1.13848
H	-4.36674	-3.04156	1.62575
H	-3.61851	-3.85228	0.22199
H	-2.81866	-3.91354	1.81770
C	-0.61456	-0.11711	3.14334
H	-1.28195	0.14321	3.97900
H	0.39655	-0.28000	3.55048
H	-0.58307	0.73329	2.44598

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11045236287

Zero-point correction (ZPE) = -5468.826049 .28440301202

Internal Energy (U) = -5468.994207 .11624501682

Enthalpy (H) = -5468.788277 .322174473167554

Gibbs Free Energy (G) = -5468.904522 .20593032879

Frequencies -- 7.07 11.35 14.32 16.14 27.12 27.80

Mono Cu(I) DiMeDHF-E-Cis Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27811550316

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0007912	0.0010000	yes	0.0001103	0.0005000	yes
Grad	0.0001598	0.0010000	yes	0.0000337	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.53833	-1.91288	0.64778
C	0.46289	-2.50728	0.01259
C	-0.63717	-2.71532	1.04603
C	1.16736	-1.71493	2.11251
C	-2.39612	1.52627	-2.80908
C	-1.11929	1.30312	-1.96961
C	-0.31472	2.41603	-1.66936
C	0.84721	2.32161	-0.88401
C	1.65270	3.60885	-0.60439
C	-2.06849	-2.43561	0.62152
C	1.57847	-0.41258	2.77760
O	-0.25330	-1.84298	2.10708
O	1.34720	1.29840	-0.35049
O	-0.95111	0.10390	-1.62972
Cu	0.52574	-0.50241	-0.45501
F	1.74772	3.81102	0.71601
F	1.09788	4.70150	-1.14909
F	2.89248	3.48978	-1.09666
F	-3.47531	1.18977	-2.08962
F	-2.37199	0.75780	-3.90402
F	-2.54587	2.79946	-3.20354
H	2.57344	-1.90701	0.29376
H	0.49677	-3.05476	-0.93389
H	-0.56426	-3.77331	1.39205
H	1.61360	-2.56542	2.67985
H	-0.60861	3.39000	-2.05122
H	-2.38545	-3.15703	-0.14828
H	-2.74176	-2.53582	1.48632

H	-2.16933	-1.42211	0.20530
H	1.16691	-0.36698	3.79727
H	2.67604	-0.34802	2.84462
H	1.21805	0.45692	2.20771

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27811550316

Zero-point correction (ZPE) = -2889.061356 .21675874399

Internal Energy (U) = -2889.202280 .07583492623

Enthalpy (H) = -2889.039018 .239096952097488

Gibbs Free Energy (G) = -2889.114855 .16326035499

Frequencies -- 20.80 27.38 32.52 38.29 44.28 84.55

Dual Cu(I) DiMeDHF-E-Cis Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11126364820

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008913	0.0010000	yes	0.0001333	0.0005000	yes
Grad	0.0004689	0.0010000	yes	0.0000810	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.31555	-2.43323	1.09487
C	-1.59054	-2.38782	0.58788
C	-2.53463	-1.93711	1.69032
C	-0.36228	-2.00234	2.55130
O	-1.66115	-1.43548	2.69848
C	5.55039	1.64935	-0.95988
C	4.11072	1.11588	-0.76879
C	3.80849	-0.16040	-1.29472
C	2.55882	-0.78646	-1.20336
O	1.50620	-0.32328	-0.68406
Cu	1.49893	1.70434	0.18273
C	2.43543	-2.22380	-1.75223
F	1.25272	-2.39849	-2.35534
F	2.49762	-3.10238	-0.72766
F	3.39919	-2.54321	-2.61822
O	3.37272	1.91573	-0.14503
F	5.52110	2.81690	-1.61101
F	6.32940	0.80897	-1.65779
F	6.12502	1.84756	0.23202
C	-3.63708	0.83885	-2.74926
C	-2.47523	0.91887	-1.73008
C	-2.30119	2.13520	-1.01946
C	-1.28429	2.33198	-0.09172
C	-1.14928	3.71038	0.58196
O	-0.42454	1.47311	0.29727
O	-1.82102	-0.13505	-1.63083
Cu	-0.49452	-0.78436	-0.23872
F	-1.32943	3.59878	1.90242

F	-2.02027	4.60977	0.11521
F	0.09228	4.19677	0.38031
F	-4.53703	-0.06317	-2.32576
F	-3.18562	0.44626	-3.94297
F	-4.27395	2.00801	-2.90921
H	0.52965	-2.97702	0.66700
H	-1.94015	-2.88009	-0.32407
H	-3.05556	-2.85071	2.06097
H	-0.28273	-2.92646	3.16971
H	4.60660	-0.69551	-1.80364
H	-2.97455	2.96066	-1.23501
C	-3.57904	-0.88777	1.34475
H	-4.22300	-1.22925	0.51916
H	-4.21236	-0.67926	2.22021
H	-3.08772	0.04899	1.04380
C	0.69178	-1.01140	3.01884
H	0.51658	-0.73954	4.07083
H	1.69934	-1.44937	2.93643
H	0.64978	-0.09341	2.41235

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11126364820

Zero-point correction (ZPE) = -5468.827165 .28409830811

Internal Energy (U) = -5468.994959 .11630406768

Enthalpy (H) = -5468.789302 .321961180430532

Gibbs Free Energy (G) = -5468.905607 .20565609527

Frequencies -- 6.38 10.84 18.29 20.48 24.74 26.04

2. Cu(I)-catalyzed rearrangement of E-Trans dimethylvinyloxiranes

2.a. Additional Figures

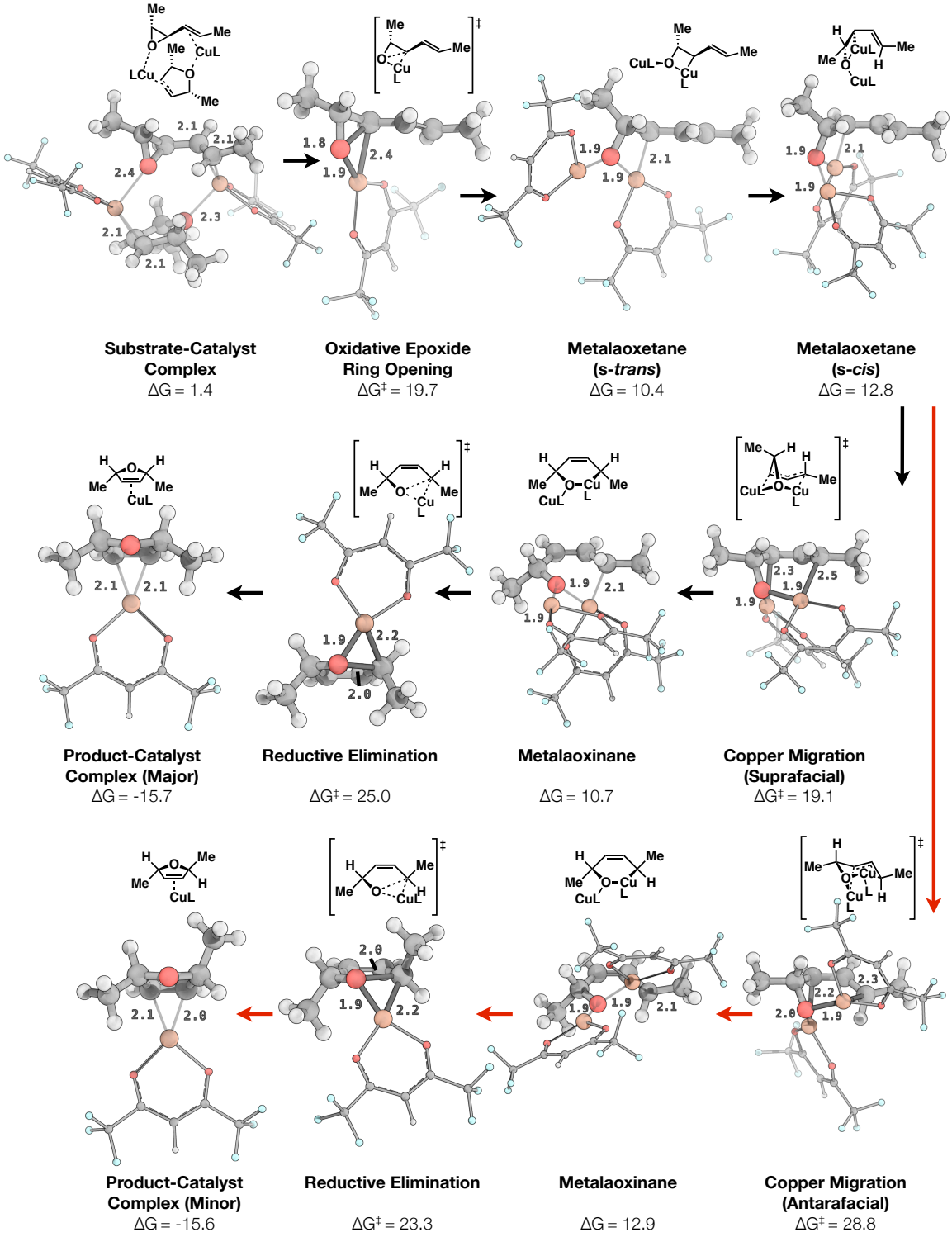


Figure 4. Structures of stationary points for both major and minor pathways for E-Trans VO. All structures, energies, and free energy corrections

computed at the B3LYP/def2-SVP level of theory, as implemented in Turbomole. Figures rendered using Pymol.

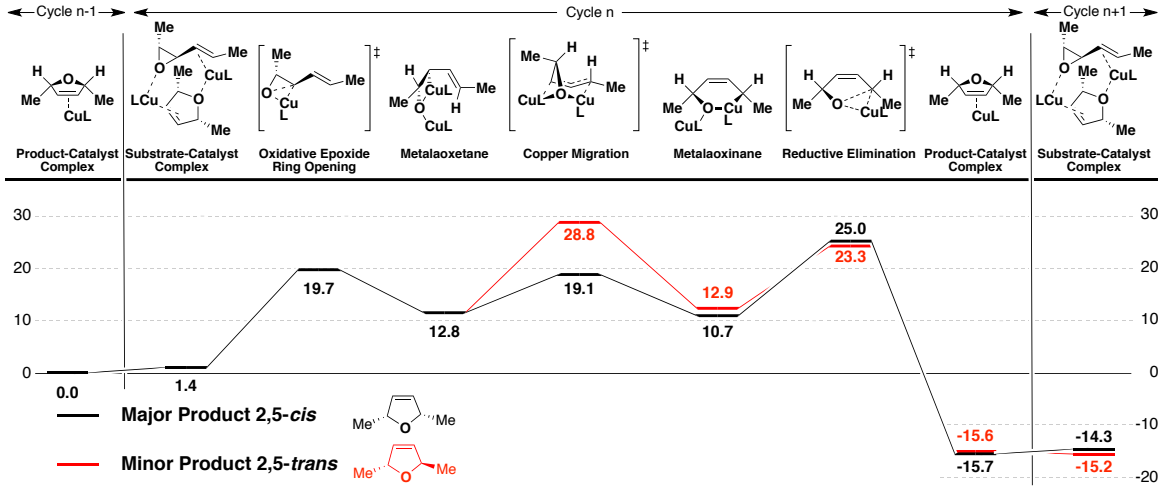


Figure 5. Reaction coordinate of Cu(I)-catalyzed ring expansion of E-Trans VO.

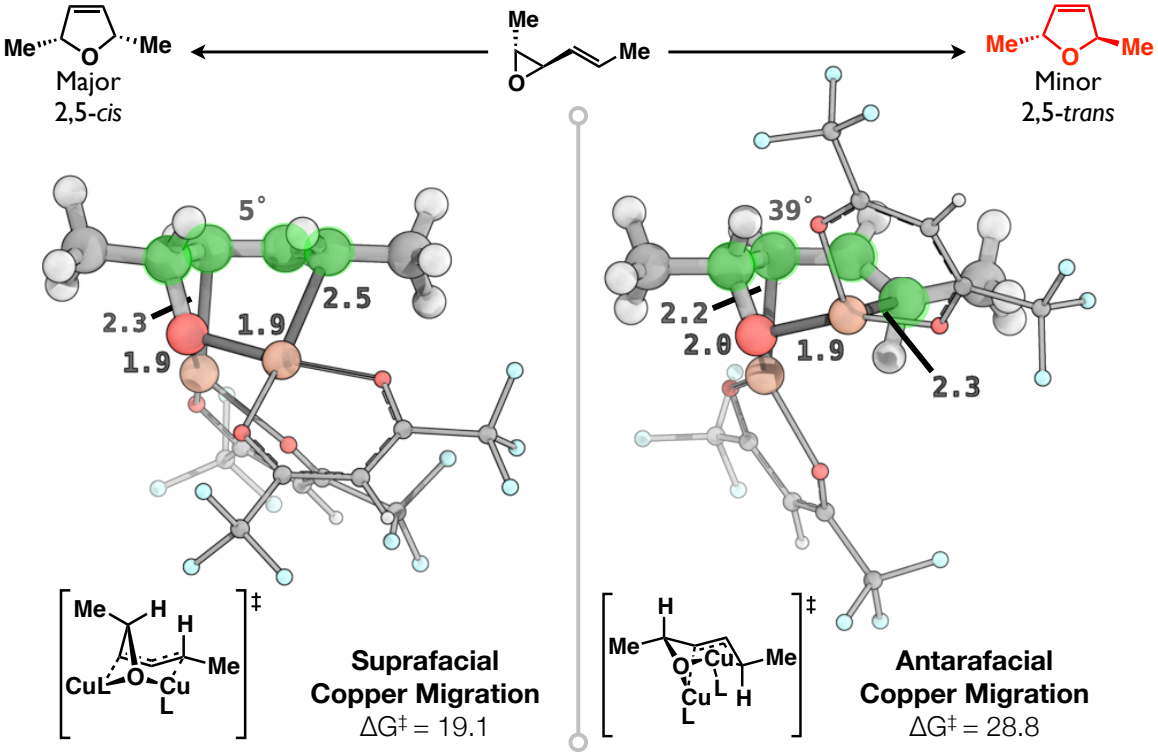


Figure 6. Stereoselective copper migration of E-Trans VO showing π-allyl distortion (green highlight with dihedral), and TS bond distances.

2.b. Geometries, Energies, and Thermal Corrections
Mono Cu(I) DiMeDHF-E-Trans Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp		Basis: def2-SVP			Atoms: 32		
Charge: 0	Spin: 1				Basis Functions: 366		

Energy = -2889.24710933651

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0005072	0.0010000	yes	0.0001215	0.0005000	yes
Grad	0.0000870	0.0010000	yes	0.0000247	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.90914	3.16922	0.04790
C	-1.72260	1.63926	-0.04379
C	-2.85913	0.82164	0.07013
H	-3.82572	1.29419	0.22315
C	-2.80052	-0.58262	-0.01227
O	-1.78940	-1.31195	-0.16174
C	-4.11980	-1.37899	0.09860
F	-4.25347	-2.19341	-0.95540
F	-5.20327	-0.58982	0.14783
F	-4.11029	-2.13211	1.20591
O	-0.52815	1.29432	-0.24047
F	-1.67280	3.73164	-1.14638
F	-1.04326	3.68716	0.92706
F	-3.14500	3.52276	0.42870
Cu	0.05165	-0.59512	-0.36585
C	2.86136	-0.37362	0.32345
H	3.90501	-0.73086	0.34743
C	2.04611	-0.96401	-0.78834
H	2.26484	-0.59241	-1.79935
C	1.34709	-2.15385	-0.64515
H	1.34896	-2.62481	0.34772
C	2.59668	0.93600	0.94680
H	1.72516	1.49901	0.58546
O	2.24510	-0.29488	1.60496
C	0.84954	-3.00826	-1.78276
H	1.49485	-3.89781	-1.89727
H	-0.17236	-3.37257	-1.59163

H	0.85196	-2.46416	-2.74020
C	3.68449	1.75352	1.59052
H	4.06625	2.51109	0.88596
H	3.29377	2.28420	2.47385
H	4.52211	1.11726	1.91515

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.24710933651

Zero-point correction (ZPE) = -2889.032254 .21485434456

Internal Energy (U) = -2889.168484 .07862507917

Enthalpy (H) = -2889.008911 .238198075562896

Gibbs Free Energy (G) = -2889.087535 .15957343768

Frequencies -- 21.16 26.99 30.93 31.83 45.12 53.33

Dual Cu(I) DiMeDHF-E-Trans Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 64
Charge: 0 | Spin: 1 | Basis Functions: 732

Energy = -5778.54436399792

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000005	0.0000010	yes			
Step	0.0009540	0.0010000	yes	0.0000881	0.0005000	yes
Grad	0.0007292	0.0010000	yes	0.0000676	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.80795	-0.49168	2.46634
H	-1.34842	-0.05796	3.31792
C	0.47485	0.19597	2.13650
H	0.43137	1.29393	2.12581
C	1.79273	-0.40882	2.44579
H	1.76606	-1.42393	2.86689
C	-1.14603	-1.75175	2.00786
H	-0.45284	-2.22779	1.30223
O	1.28646	-0.36623	1.09838
C	5.62267	2.56085	0.25574
C	4.81978	1.31235	-0.17121
C	5.49987	0.08434	-0.25535
H	6.56798	0.06771	-0.05542
C	4.85518	-1.12933	-0.56732
O	3.64714	-1.32703	-0.83728
Cu	2.29651	0.15153	-0.99650
C	5.70207	-2.42214	-0.54633
F	5.48093	-3.14510	-1.64845
F	5.35817	-3.16861	0.51584
F	7.02029	-2.18494	-0.46627
O	3.60406	1.55122	-0.37369
F	5.15784	3.01708	1.43164
F	5.48151	3.53682	-0.64794
F	6.93396	2.32232	0.40356
C	-5.73422	-1.82103	-0.97472
C	-4.74949	-0.82107	-0.32915
C	-5.17547	0.50795	-0.15040
C	-4.36327	1.50958	0.41358

C	-4.94152	2.93940	0.50802
O	-3.19183	1.42031	0.85523
O	-3.64353	-1.33594	-0.03563
Cu	-2.16049	-0.31434	0.88676
F	-4.19906	3.77990	-0.23428
F	-4.90826	3.37293	1.77360
F	-6.20752	3.02974	0.07581
F	-5.94192	-2.85829	-0.15281
F	-5.21891	-2.29899	-2.11866
F	-6.92738	-1.27959	-1.26073
H	-6.17828	0.77640	-0.47124
C	0.82660	-0.28948	-2.40818
H	1.39393	-0.79691	-3.19312
C	0.83945	1.06378	-2.14954
H	1.41696	1.81502	-2.69526
C	-0.38157	1.43998	-1.33571
H	-0.10943	1.92396	-0.38122
O	-0.97553	0.16322	-1.01250
C	-0.40464	-0.91498	-1.78622
H	-0.13985	-1.71712	-1.07621
C	3.01686	0.40087	2.76565
H	3.11448	0.51076	3.85831
H	3.92301	-0.10779	2.40002
H	2.97560	1.39907	2.30869
C	-2.18673	-2.64670	2.62924
H	-2.83855	-2.09709	3.32595
H	-2.82224	-3.11591	1.86198
H	-1.69698	-3.46137	3.19298
C	-1.39869	-1.46336	-2.80783
H	-0.96192	-2.32728	-3.33520
H	-2.31587	-1.79656	-2.29960
H	-1.66514	-0.69896	-3.55436
C	-1.34938	2.35168	-2.08659
H	-2.22812	2.56781	-1.46420
H	-0.85715	3.31012	-2.32004
H	-1.67815	1.89147	-3.03116

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5778.54436399792

Zero-point correction (ZPE) = -5778.111684 .43267955224

Internal Energy (U) = -5778.409065 .13529800263

Enthalpy (H) = -5778.064760 .479603557084161

Gibbs Free Energy (G) = -5778.200060 .34430399193

Frequencies -- 7.41 11.44 16.53 19.49 24.47 25.38

Mono Cu(I) DiMeDHF-E-Trans Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.21458997431

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0007264	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0001684	0.0010000	yes	0.0000268	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.20447	-0.53393	-0.22327
C	-2.33844	0.16749	1.03660
C	-1.83525	1.40548	1.24059
C	-2.82153	-1.84095	-0.48913
C	4.29774	-1.69203	0.42731
C	2.97215	-0.99392	0.04172
C	3.02867	0.36038	-0.35897
C	1.89208	1.09025	-0.73348
C	2.06681	2.57067	-1.13266
C	-3.18894	-2.23247	-1.90375
C	-2.00855	2.20714	2.48647
O	-1.53213	-2.22392	-0.06979
O	0.69537	0.70130	-0.79159
O	1.97109	-1.73756	0.13285
Cu	0.07423	-1.13984	-0.24837
F	1.27341	3.34532	-0.37078
F	1.70698	2.75518	-2.41055
F	3.32285	3.01605	-0.99229
F	4.21344	-2.18795	1.66798
F	5.35822	-0.86858	0.38792
F	4.54150	-2.70875	-0.41042
H	-1.78052	0.00644	-1.07651
H	-2.90261	-0.33735	1.82944
H	-1.23576	1.85929	0.44148
H	-3.59117	-2.14076	0.24393
H	3.99374	0.86011	-0.36750
H	-3.26507	-3.32863	-1.97905
H	-4.15969	-1.79807	-2.19412

H	-2.41845	-1.89386	-2.61438
H	-2.51150	3.16587	2.26645
H	-2.59029	1.67398	3.25350
H	-1.02389	2.47361	2.91037

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.21458997431

Zero-point correction (ZPE) = -2889.001982 .21260715322

Internal Energy (U) = -2889.134478 .08011157091

Enthalpy (H) = -2888.978330 .236259396935321

Gibbs Free Energy (G) = -2889.058444 .15614551869

Frequencies -- i267.38 13.08 24.59 31.25 35.92 38.14

Dual Cu(I) DiMeDHF-E-Trans Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05546411806

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0005855	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0003203	0.0010000	yes	0.0000544	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-5.08987	-2.43605	-0.27162
C	-4.37074	-1.08157	-0.09240
C	-5.10313	0.09845	-0.30127
C	-4.54623	1.38254	-0.15207
C	-5.45268	2.60938	-0.39714
C	0.17450	-1.20314	-0.07947
H	0.28086	-0.82990	-1.10424
C	-0.06844	-0.23446	0.99256
C	-0.06885	1.14588	0.80560
C	-0.08125	-2.63566	0.08007
O	-3.36754	1.69210	0.16020
O	-3.16375	-1.20090	0.24795
O	1.32046	-2.51136	0.24083
Cu	-1.97356	0.35701	0.52073
F	-5.48385	3.37697	0.69766
F	-6.71319	2.27028	-0.70114
F	-4.96747	3.34103	-1.40732
F	-5.19439	-3.05753	0.90965
F	-4.38217	-3.22595	-1.09351
F	-6.32010	-2.30897	-0.78339
H	-6.14754	0.01710	-0.59062
H	-0.10667	-0.64638	2.00922
H	0.19797	1.52354	-0.18928
H	-0.58157	-2.90891	1.02417
C	6.82313	-0.95899	-0.14213
C	5.36456	-0.44602	-0.18560
C	5.15381	0.94754	-0.31255
H	6.02029	1.59960	-0.38606

C	3.87945	1.52425	-0.32761
O	2.75466	0.95355	-0.26333
Cu	2.50359	-0.99614	-0.04849
C	3.76968	3.06043	-0.40712
F	3.22023	3.53724	0.72742
F	2.97410	3.42003	-1.42301
F	4.94988	3.66921	-0.57095
O	4.51067	-1.35197	-0.08566
F	7.06607	-1.53722	1.04174
F	7.72884	0.01671	-0.31465
F	7.01899	-1.87255	-1.09922
C	-0.54231	-3.47433	-1.08697
H	-0.29049	-4.53204	-0.91198
H	-1.63455	-3.38918	-1.19898
H	-0.05258	-3.15547	-2.02051
C	-0.02458	2.15698	1.91420
H	-0.71285	2.99542	1.72289
H	-0.26529	1.71797	2.89446
H	0.99388	2.58149	1.95896

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05546411806

Zero-point correction (ZPE) = -5468.773651 .28181302879

Internal Energy (U) = -5468.938592 .11687186437

Enthalpy (H) = -5468.735677 .319786356272683

Gibbs Free Energy (G) = -5468.852550 .20291376008

Frequencies -- i276.72 6.78 10.95 15.98 21.24 24.25

Mono Cu(I) DiMeDHF-E-Trans Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  32
Charge: 0     | Spin: 1                         | Basis Functions:   366
----------------------------------------------------------------------------------------------
Energy =    -2889.22770829877
----------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000003  || 0.0000010   yes
Step      0.0008696  || 0.0010000   yes  |  0.0001616  || 0.0005000   yes
Grad      0.0000910  || 0.0010000   yes  |  0.0000214  || 0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
----------------------------------------------------------------------------------------------
C       -1.73172      -1.12722       0.47370
C       -2.18086       0.20727       0.78150
C       -2.44727       1.14554      -0.16316
C       -1.61436      -2.21857       1.50749
C        4.63329      -0.53438       0.13799
C        3.13108      -0.24075      -0.08632
C        2.78369       0.87273      -0.88740
C        1.45280       1.16715      -1.18294
C        1.13237       2.41071      -2.03473
C       -2.26978      -3.54218       1.15040
C       -2.91321       2.53531       0.10148
O       -0.20593      -2.30397       1.52865
O        0.41205       0.54206      -0.82662
O        2.35997      -1.05501       0.46038
Cu       0.32604      -0.95928       0.40158
F        0.38753       3.27130      -1.31767
F        0.42501       2.06552      -3.11748
F        2.22730       3.06151      -2.44336
F        4.87947      -0.76701       1.42791
F        5.41794       0.48102      -0.25776
F        4.98632      -1.62100      -0.56173
H       -1.80453      -1.45935      -0.57136
H       -2.30229       0.46108       1.84196
H       -2.28751       0.87679      -1.21394
H       -2.00280      -1.86513       2.48604
H        3.56949       1.51233      -1.27998
H       -1.98782      -4.30372       1.89525
H       -3.36978      -3.45850       1.13522
```

H	-1.92066	-3.88932	0.16433
H	-3.85330	2.75119	-0.43705
H	-3.06634	2.73170	1.17329
H	-2.16618	3.25220	-0.28570

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22770829877

Zero-point correction (ZPE) = -2889.013463 .21424493674

Internal Energy (U) = -2889.149294 .07841385880

Enthalpy (H) = -2888.990161 .237546770955203

Gibbs Free Energy (G) = -2889.068572 .15913542581

Frequencies -- 17.32 19.91 26.52 37.11 59.77 75.29

Dual Cu(I) DiMeDHF-E-Trans Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07241112379

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000001	II	0.0000010	yes					
Step	0.0000443	II	0.0001000	yes	I	0.0000072	II	0.0000500	yes
Grad	0.0000501	II	0.0010000	yes	I	0.0000103	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.14188	0.63345	-1.03609
H	-2.25284	0.28447	-2.07271
C	-2.60006	1.95612	-0.72895
C	-2.89305	2.89123	-1.67591
C	-1.97246	-0.44942	0.00892
O	-0.55112	-0.61129	-0.04893
H	-2.69015	2.22418	0.33132
H	-2.76830	2.61202	-2.72890
H	-2.25683	-0.06585	1.00723
C	4.23046	1.23472	-1.34684
C	2.73117	1.52361	-1.59315
C	2.38460	2.66076	-2.35881
H	3.17327	3.31593	-2.71887
C	1.05717	2.96820	-2.66075
O	0.00758	2.33609	-2.34018
Cu	-0.06351	0.80006	-1.17187
C	0.74839	4.23947	-3.47575
F	-0.01951	5.06685	-2.74528
F	0.07000	3.92499	-4.58519
F	1.84750	4.91028	-3.83374
O	1.95492	0.68355	-1.08769
F	4.45269	1.00438	-0.05273
F	5.01448	2.25396	-1.73012
F	4.59480	0.15026	-2.04104
C	-2.71107	-1.74540	-0.26691
H	-2.47709	-2.47715	0.52160
H	-3.80131	-1.57839	-0.27136
H	-2.41194	-2.16020	-1.24351

C	-3.33849	4.28479	-1.40705
H	-4.28394	4.51009	-1.93232
H	-3.47105	4.48648	-0.33367
H	-2.58997	4.99247	-1.80933
Cu	0.51838	-1.77261	1.00320
O	-0.79828	-2.65522	2.32706
O	2.06618	-2.70204	1.69824
C	-0.39918	-3.49344	3.16985
C	2.02220	-3.53113	2.64309
C	0.91296	-3.95172	3.39835
C	-1.53619	-4.07496	4.03934
C	3.39556	-4.16614	2.95290
H	1.07490	-4.68459	4.18423
F	-2.45196	-4.66703	3.25768
F	-1.11094	-4.98189	4.93132
F	-2.14897	-3.09299	4.71509
F	3.78796	-4.92422	1.91857
F	3.37731	-4.94554	4.04564
F	4.31760	-3.21719	3.14404

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07241112379

Zero-point correction (ZPE) = -5468.789760 .28265096454

Internal Energy (U) = -5468.953890 .11852074596

Enthalpy (H) = -5468.751394 .321016598309435

Gibbs Free Energy (G) = -5468.869912 .20249860100

Frequencies -- 4.96 8.17 12.40 18.90 20.97 25.01

Mono Cu(I) DiMeDHF-E-Trans Metalaoxetane (s-*cis*)

Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22503011209

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000010	II	0.0000010	yes					
Step	0.0007519	II	0.0010000	yes	I	0.0001644	II	0.0005000	yes
Grad	0.0000787	II	0.0010000	yes	I	0.0000212	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.02852	1.91220	-0.48410
C	0.04611	2.00307	0.96155
C	-0.95054	2.40339	1.78916
C	-1.23307	2.26018	-1.32090
C	-0.84723	-4.32108	-1.41845
C	-0.21441	-2.99795	-0.92822
C	0.97321	-3.06507	-0.16551
C	1.60384	-1.91441	0.31166
C	2.89223	-2.06357	1.14534
C	-0.94458	3.08707	-2.56370
C	-0.83073	2.50539	3.27333
O	-1.60118	0.93248	-1.62698
O	1.26217	-0.70694	0.15333
O	-0.84779	-1.97591	-1.26665
Cu	-0.31061	-0.08257	-0.80083
F	2.73282	-1.48251	2.34221
F	3.91343	-1.45875	0.52556
F	3.23272	-3.34270	1.35097
F	-2.06646	-4.46801	-0.88766
F	-0.11895	-5.39645	-1.07997
F	-0.96696	-4.30807	-2.74928
H	0.93163	1.90186	-1.01732
H	1.00215	1.70137	1.40385
H	-1.92411	2.67028	1.36118
H	-2.02265	2.76090	-0.72599
H	1.40670	-4.03620	0.05691
H	-1.84618	3.12935	-3.19535
H	-0.65034	4.11830	-2.30463

H -0.13914 2.62240 -3.15583
H -1.05391 3.53206 3.61573
H -1.57180 1.85318 3.77061
H 0.17215 2.22672 3.63000
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22503011209
Zero-point correction (ZPE) = -2889.010594 .21443537668
Internal Energy (U) = -2889.146456 .07857397747
Enthalpy (H) = -2888.987251 .237779107686602
Gibbs Free Energy (G) = -2889.065826 .15920398419

Frequencies -- 16.12 26.40 27.04 35.10 59.68 62.45

Dual Cu(I) DiMeDHF-E-Trans Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

```
============================================================
Method: B3-LYP      |  Basis: def2-SVP            |  Atoms:  47
Charge: 0      |  Spin: *        | Basis Functions:   584
------------------------------------------------------------------------------
Energy =    -5469.07112812233
------------------------------------------------------------------------------
Item      Max Val.     ||  Criteria   Pass? |   RMS Val.  ||  Criteria   Pass?
Energy   0.0000002  ||  0.0000010   yes
Step      0.0003668  ||  0.0010000   yes   |  0.0000861  ||  0.0005000   yes
Grad      0.0004678  ||  0.0010000   yes   |  0.0000915  ||  0.0005000   yes
============================================================
Atomic Coordinates (Angstroms)
Type   X        Y        Z
------------------------------------------------------------------------------
C         1.30405        2.43376       -0.88936
C         1.39630        2.59545        0.53515
C         0.36987        2.92553        1.36636
C         0.09812        2.77236       -1.74212
O        -0.33491        1.45036       -2.08402
C         0.46106       -3.79397       -1.84975
C         1.08870       -2.47068       -1.35656
C         2.28245       -2.52900       -0.60832
C         2.89987       -1.38265       -0.10332
O         2.54409       -0.17341       -0.21756
Cu        0.94034        0.41867       -1.11835
C         4.20344       -1.53935        0.70640
F         4.06525       -0.97916        1.91300
F         5.20884       -0.91917        0.07389
F         4.55358       -2.81983        0.88080
O         0.44155       -1.45077       -1.68566
F        -0.75809       -3.94099       -1.31890
F         1.19096       -4.86698       -1.51368
F         0.34061       -3.77696       -3.18089
C        -0.73615       -1.25254        2.43605
C        -1.59050       -0.74229        1.25316
C        -2.89092       -1.26526        1.11399
C        -3.77168       -0.94078        0.06550
C        -5.17428       -1.59031        0.07495
O        -3.59977       -0.17514       -0.91826
O        -1.01041        0.10753        0.53803
Cu       -1.95504        0.64309       -1.42153
F        -5.40189       -2.21909       -1.08309
```

F	-6.11293	-0.64483	0.22581
F	-5.33402	-2.48284	1.06457
F	0.41666	-1.76948	1.97922
F	-1.33893	-2.18967	3.17669
F	-0.42102	-0.23008	3.25503
H	2.25635	2.37098	-1.43264
H	2.37514	2.38019	0.97666
H	-0.62905	3.07757	0.94270
H	-0.67570	3.29183	-1.15065
H	2.72910	-3.49810	-0.40429
H	-3.23316	-1.98342	1.85450
C	0.40891	3.58047	-2.98806
H	-0.49741	3.67101	-3.60762
H	0.75613	4.59412	-2.72685
H	1.18525	3.08054	-3.58911
C	0.48209	3.04278	2.84417
H	0.04741	3.99210	3.20306
H	-0.10251	2.23288	3.31747
H	1.52224	2.96551	3.19344

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07112812233

Zero-point correction (ZPE) = -5468.788324 .28280331649

Internal Energy (U) = -5468.955076 .11605196594

Enthalpy (H) = -5468.750035 .321092774286943

Gibbs Free Energy (G) = -5468.866085 .20504287865

Frequencies -- 8.69 11.23 21.50 22.89 24.69 27.82

Dual Cu(I) DiMeDHF-E-Trans Suprafacial Copper Migration (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.06164835923

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000007	0.0000010	yes			
Step	0.0003833	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0005651	0.0010000	yes	0.0001241	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.79899	2.11495	1.61842
C	1.33086	0.97140	2.27267
C	-0.02838	0.70624	2.49879
C	0.80257	3.07194	1.01014
O	0.27926	2.24550	-0.04288
C	0.38938	-2.98073	-0.99219
C	1.30592	-1.73579	-1.04858
C	2.69071	-1.94909	-1.22651
C	3.64899	-0.93112	-1.11982
O	3.48942	0.29034	-0.84127
Cu	1.80243	1.13539	-0.44943
C	5.13225	-1.29654	-1.34555
F	5.84900	-0.99560	-0.25438
F	5.62476	-0.59360	-2.37240
F	5.31641	-2.59763	-1.61115
O	0.71945	-0.64549	-0.87055
F	0.14200	-3.28158	0.29606
F	0.94112	-4.05948	-1.56350
F	-0.77947	-2.74411	-1.59245
C	-3.72594	-2.34367	0.75179
C	-3.11515	-1.07583	0.12004
C	-3.66108	-0.58512	-1.06787
C	-3.17980	0.58934	-1.68850
C	-3.87973	1.07745	-2.97855
O	-2.23996	1.32379	-1.31777
O	-2.15634	-0.61416	0.80399
Cu	-1.07031	0.89219	0.28415
F	-2.98304	1.24010	-3.95529

F	-4.47347	2.25746	-2.75540
F	-4.81681	0.22233	-3.41573
F	-2.79743	-3.29867	0.86831
F	-4.74647	-2.84066	0.04094
F	-4.18146	-2.06095	1.98324
H	2.87209	2.32985	1.57774
H	2.05563	0.19787	2.55247
H	-0.72263	1.55600	2.51182
H	-0.00541	3.33610	1.71975
H	3.03553	-2.95887	-1.43484
H	-4.49005	-1.11919	-1.52348
C	1.40386	4.35630	0.45916
H	0.63497	4.92210	-0.08690
H	1.79703	4.98861	1.27190
H	2.22625	4.13227	-0.24002
C	-0.48055	-0.56035	3.15524
H	-0.06608	-0.61370	4.17988
H	-1.57208	-0.63126	3.21203
H	-0.11726	-1.44432	2.60647

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.06164835923

Zero-point correction (ZPE) = -5468.779644 .28200346873

Internal Energy (U) = -5468.947786 .11386140631

Enthalpy (H) = -5468.742200 .319447373172773

Gibbs Free Energy (G) = -5468.856060 .20558753689

Frequencies -- i17.00 5.35 20.03 21.86 22.14 26.28

Dual Cu(I) DiMeDHF-E-Trans Antarafacial Copper Migration (Minor)
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04370044207

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000010	yes			
Step	0.0005559	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0005522	0.0010000	yes	0.0000789	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.61553	-2.04409	0.26077
C	-0.27968	-1.18599	1.33752
H	-0.38810	-1.64760	2.33078
C	0.13675	0.15042	1.35342
H	-0.24428	0.84844	0.59709
C	0.13448	-2.05486	-1.05563
H	1.19549	-2.32466	-0.88349
O	0.02304	-0.70266	-1.50351
C	-3.74473	3.32187	-0.51982
C	-3.54560	1.78880	-0.52163
C	-4.65629	0.96961	-0.23037
C	-4.58144	-0.42884	-0.18864
O	-3.58354	-1.17616	-0.39139
Cu	-1.80294	-0.51736	-0.75964
C	-5.86116	-1.22640	0.14405
F	-5.63946	-2.02786	1.19317
F	-6.20561	-1.99053	-0.89912
F	-6.90253	-0.43764	0.44026
O	-2.37325	1.43237	-0.78631
F	-2.89475	3.88493	0.34796
F	-4.98838	3.68290	-0.17281
F	-3.49436	3.81963	-1.73505
C	5.37678	-1.71988	-0.82859
C	4.30431	-0.62491	-0.61672
C	4.72705	0.61941	-0.08952
C	3.83414	1.64414	0.23254
C	4.39022	2.92468	0.88888
O	2.57760	1.68200	0.09071

O	3.14483	-0.97581	-0.90651
Cu	1.42755	0.27496	-0.57682
F	3.84741	3.07635	2.11024
F	4.07182	3.99991	0.16207
F	5.72162	2.90370	1.03598
F	5.21014	-2.69066	0.08420
F	6.63017	-1.25705	-0.70818
F	5.25369	-2.26726	-2.04093
H	-1.20423	-2.93317	0.51768
H	-5.61148	1.44377	-0.02152
H	5.78517	0.77214	0.10565
C	0.65870	0.80953	2.59169
H	-0.14190	1.40849	3.06512
H	1.03546	0.08411	3.32781
H	1.46249	1.51729	2.33684
C	-0.44354	-3.02290	-2.08413
H	-1.51215	-2.82404	-2.26940
H	0.10273	-2.91719	-3.03224
H	-0.33670	-4.06192	-1.73245

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04370044207

Zero-point correction (ZPE) = -5468.762154 .28154641286

Internal Energy (U) = -5468.929426 .11427362670

Enthalpy (H) = -5468.724630 .319070302084109

Gibbs Free Energy (G) = -5468.838901 .20479911552

Frequencies -- i47.59 9.17 12.56 16.48 21.46 28.24

Mono Cu(I) DiMeDHF-E-Trans Metalaoxinane (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22503182874

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0008714	0.0010000	yes	0.0002089	0.0005000	yes
Grad	0.0000734	0.0010000	yes	0.0000139	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.34794	3.08394	-0.94369
C	-0.27253	2.27142	-1.83629
C	0.20068	0.96286	-2.26728
C	1.52239	2.63264	-0.12207
C	0.61204	-1.76305	3.50618
C	0.26561	-1.54877	2.01407
C	-0.64231	-2.43912	1.39702
C	-0.98599	-2.30130	0.05228
C	-1.97010	-3.30609	-0.57864
C	1.29782	2.89410	1.38062
C	-0.71178	0.12691	-3.12334
O	1.93802	1.35539	-0.41049
O	-0.58795	-1.43405	-0.77877
O	0.84607	-0.57501	1.49131
Cu	0.61269	0.04077	-0.44927
F	-1.36247	-3.98419	-1.56065
F	-3.01368	-2.65559	-1.11071
F	-2.44408	-4.19292	0.30566
F	-0.03295	-2.81106	4.04144
F	0.28237	-0.67467	4.21155
F	1.92476	-1.97191	3.64698
H	-0.03768	4.09354	-0.76621
H	-1.23069	2.60411	-2.25657
H	1.25905	0.92278	-2.54470
H	2.35108	3.31141	-0.45363
H	-1.07816	-3.24772	1.97749
H	2.20252	2.59999	1.93287
H	1.08254	3.95558	1.58748

H	0.46096	2.28460	1.75708
H	-0.77468	0.60038	-4.12270
H	-0.33083	-0.89305	-3.26242
H	-1.73064	0.05808	-2.71462

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22503182874

Zero-point correction (ZPE) = -2889.010786 .21424493674

Internal Energy (U) = -2889.148030 .07700118063

Enthalpy (H) = -2888.988014 .237017347911524

Gibbs Free Energy (G) = -2889.065012 .16001906715

Frequencies -- 13.78 23.84 27.57 33.52 61.28 76.29

Dual Cu(I) DiMeDHF-E-Trans Metalaoxinane (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07611703167

Item	Max Val.	II	Criteria	Pass?	RMS Val.	II	Criteria	Pass?
Energy	0.0000006	II	0.0000010	yes				
Step	0.0007590	II	0.0010000	yes	0.0001492	II	0.0005000	yes
Grad	0.0000826	II	0.0010000	yes	0.0000201	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.19722	3.73214	-0.62909
C	-1.74286	2.88716	-1.54717
C	-1.14242	1.66997	-2.06241
C	0.05701	3.44769	0.14393
O	0.54278	2.17203	-0.12790
C	5.36536	-1.46057	0.51559
C	3.95623	-0.96014	0.12353
C	3.11961	-1.84527	-0.58528
C	1.80510	-1.55054	-0.99238
O	1.17182	-0.48016	-0.83774
Cu	2.14458	1.21785	0.25842
C	1.00125	-2.66031	-1.70821
F	0.48566	-2.19016	-2.85597
F	-0.02553	-3.05234	-0.93246
F	1.72659	-3.74559	-2.00257
O	3.74014	0.21592	0.51308
F	6.29843	-0.64048	0.01572
F	5.62773	-2.69907	0.06871
F	5.49473	-1.47219	1.84826
C	-0.73535	-1.04303	3.67789
C	-1.12396	-0.80264	2.20180
C	-2.06795	-1.66001	1.60294
C	-2.49775	-1.47581	0.28594
C	-3.56351	-2.43080	-0.29104
O	-2.14333	-0.59464	-0.54749
O	-0.54350	0.17762	1.68135
Cu	-0.76080	0.72996	-0.25733
F	-3.08345	-3.06405	-1.36526

F	-4.64079	-1.72716	-0.66888
F	-3.96471	-3.35349	0.59266
F	-1.34614	-2.11216	4.20720
F	-1.06844	0.02696	4.41167
F	0.58433	-1.22629	3.78163
H	-1.71911	4.66500	-0.39105
H	-2.74978	3.12246	-1.91504
H	-0.06584	1.70508	-2.25311
H	0.80604	4.17408	-0.25472
H	3.51572	-2.82964	-0.82057
H	-2.48539	-2.47817	2.18338
C	-0.10751	3.72116	1.64603
H	0.85871	3.55675	2.14725
H	-0.43175	4.75619	1.84065
H	-0.83924	3.02628	2.08612
C	-1.92123	0.79811	-2.99821
H	-1.91518	1.27828	-3.99712
H	-1.45313	-0.18971	-3.10758
H	-2.96597	0.66371	-2.68517

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07611703167

Zero-point correction (ZPE) = -5468.793123 .28299375644

Internal Energy (U) = -5468.961956 .11416006737

Enthalpy (H) = -5468.755355 .320761408784783

Gibbs Free Energy (G) = -5468.869516 .20660067739

Frequencies -- 8.71 16.06 17.58 25.21 27.23 27.42

Mono Cu(I) DiMeDHF-E-Trans Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22295336064

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000001	II	0.0000010	yes					
Step	0.0007866	II	0.0010000	yes	I	0.0000929	II	0.0005000	yes
Grad	0.0000316	II	0.0010000	yes	I	0.0000068	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.21735	2.98629	0.62596
C	-0.80815	2.62002	-0.18255
C	-0.71547	1.69877	-1.31154
C	1.55874	2.30871	0.58839
C	1.62882	-3.16723	2.08521
C	0.78407	-2.38359	1.05345
C	-0.36057	-3.01277	0.51211
C	-1.19250	-2.35170	-0.38993
C	-2.44588	-3.07552	-0.91959
C	-1.99508	1.25652	-1.96700
C	2.69367	3.34841	0.39886
O	1.66604	1.36669	-0.40612
O	-1.07606	-1.18268	-0.86236
O	1.20084	-1.23200	0.81476
Cu	0.29759	0.10369	-0.44868
F	-2.38927	-3.18185	-2.25282
F	-3.54308	-2.37265	-0.60646
F	-2.58628	-4.30683	-0.41164
F	1.24238	-4.44744	2.19921
F	1.51161	-2.59507	3.29117
F	2.91745	-3.15465	1.73862
H	0.05875	3.75469	1.39074
H	-1.80826	3.01620	0.03765
H	0.11363	1.88956	-1.99943
H	-0.60475	-4.02776	0.81283
H	-2.41701	2.12162	-2.51543
H	-1.83142	0.44991	-2.69307
H	-2.74741	0.91630	-1.24037

H	1.70771	1.87605	1.61087
H	2.58802	3.84768	-0.57621
H	2.67456	4.10474	1.19944
H	3.65994	2.82592	0.42392

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22295336064

Zero-point correction (ZPE) = -2889.008327 .21462581662

Internal Energy (U) = -2889.145914 .07703865521

Enthalpy (H) = -2888.985539 .237413462994565

Gibbs Free Energy (G) = -2889.062580 .16037328544

Frequencies -- 15.01 21.59 28.37 35.35 52.73 80.92

Dual Cu(I) DiMeDHF-E-Trans Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07083784262

Item	Max Val.	II	Criteria	Pass?	RMS Val.	II	Criteria	Pass?
Energy	0.0000010	II	0.0000010	yes				
Step	0.0008422	II	0.0010000	yes	0.0000932	II	0.0005000	yes
Grad	0.0000878	II	0.0010000	yes	0.0000150	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.36950	3.69401	0.85493
C	-2.43255	3.33311	0.08621
C	-2.42846	2.37882	-1.01127
C	-0.04004	3.00389	0.84768
O	-0.01034	1.93223	-0.05025
C	2.12705	-3.46118	-1.18766
C	2.41672	-1.99036	-0.81778
C	3.75036	-1.60926	-0.58810
C	4.12427	-0.30863	-0.19897
O	3.39397	0.69206	0.00623
Cu	1.41266	0.63269	-0.16101
C	5.62479	-0.02684	0.03724
F	5.83945	0.28296	1.32384
F	6.02149	1.01262	-0.70842
F	6.41023	-1.07175	-0.26706
O	1.38081	-1.28263	-0.76313
F	1.24013	-3.98211	-0.32367
F	3.21923	-4.23753	-1.16989
F	1.59231	-3.53640	-2.41462
C	-0.08923	-2.47992	2.39784
C	-0.96388	-1.69200	1.39672
C	-1.99221	-2.37761	0.71564
C	-2.87652	-1.72048	-0.13828
C	-4.02221	-2.52307	-0.78722
O	-2.90208	-0.49549	-0.47244
O	-0.69467	-0.47059	1.32599
Cu	-1.54017	0.78084	-0.03083
F	-3.98947	-2.37881	-2.11690

F	-5.20138	-2.06216	-0.34853
F	-3.95985	-3.82990	-0.50789
F	-0.23986	-3.80343	2.27886
F	-0.43713	-2.13594	3.64803
F	1.20234	-2.18572	2.23376
H	-1.49727	4.48707	1.59924
H	-3.40640	3.77567	0.33379
H	-1.57489	2.44360	-1.69456
H	4.52884	-2.35945	-0.69804
H	-2.10548	-3.44740	0.86880
C	-3.73355	2.00790	-1.65170
H	-4.05349	2.84299	-2.30593
H	-3.64319	1.11136	-2.27900
H	-4.52904	1.83334	-0.91205
H	0.13071	2.65886	1.89382
C	1.11396	3.97034	0.50310
H	0.98439	4.37135	-0.51341
H	1.15516	4.80583	1.21871
H	2.06401	3.41711	0.54820

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07083784262

Zero-point correction (ZPE) = -5468.787767 .28306993241

Internal Energy (U) = -5468.956447 .11439059282

Enthalpy (H) = -5468.749996 .320841393561167

Gibbs Free Energy (G) = -5468.864385 .20645213424

Frequencies -- 6.02 12.20 21.46 26.41 29.49 32.87

Mono Cu(I) DiMeDHF-E-Trans Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 32
Charge: 0	Spin: 1	Basis Functions: 366

Energy = -2889.20831476650

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0006465	0.0010000	yes	0.0001068	0.0005000	yes
Grad	0.0007521	0.0010000	yes	0.0001250	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.72451	-0.85796	-1.58598
C	-2.57015	0.46786	-1.52579
C	-1.90448	1.09640	-0.35901
C	-2.15355	-1.63823	-0.42834
C	3.75286	-2.05025	0.51652
C	2.74948	-0.87614	0.41840
C	3.27390	0.43483	0.33469
C	2.46158	1.56427	0.19369
C	3.13845	2.94234	0.04462
C	-2.72993	1.69102	0.74793
C	-3.19253	-2.54664	0.24314
O	-1.69148	-0.71251	0.52607
O	1.20022	1.62770	0.15195
O	1.55182	-1.22793	0.40873
Cu	-0.02504	0.11675	0.28760
F	2.65563	3.79807	0.95379
F	2.88485	3.44769	-1.17210
F	4.46954	2.88993	0.19575
F	5.02206	-1.64183	0.67503
F	3.70022	-2.79129	-0.59972
F	3.44351	-2.83752	1.55187
H	-3.20037	-1.36848	-2.42799
H	-2.88202	1.12987	-2.34284
H	-1.09149	1.78273	-0.66078
H	4.35181	0.56935	0.36214
H	-2.09829	1.98695	1.59911
H	-3.21464	2.61056	0.36840
H	-3.50626	0.99543	1.09155

H	-1.32673	-2.28036	-0.80302
H	-4.03918	-1.95159	0.61911
H	-3.57250	-3.29277	-0.47351
H	-2.73274	-3.07824	1.08898

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20831476650

Zero-point correction (ZPE) = -2888.994755 .21355935294

Internal Energy (U) = -2889.130366 .07794826551

Enthalpy (H) = -2888.972085 .236228926544318

Gibbs Free Energy (G) = -2889.050036 .15827844606

Frequencies -- i326.97 15.14 22.71 24.59 29.19 37.71

Dual Cu(I) DiMeDHF-E-Trans Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04987663737

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0005613	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0002956	0.0010000	yes	0.0000508	0.0005000	yes

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Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.64698	-0.97745	-1.66946
C	-0.47879	0.39375	-1.56562
C	0.44490	0.95678	-0.53296
C	0.14146	-1.77899	-0.65356
O	0.57406	-0.86918	0.32876
C	-4.98974	2.86724	0.66116
C	-4.46267	1.48038	0.23563
C	-5.30552	0.36654	0.38803
C	-4.91639	-0.93652	0.03223
O	-3.81723	-1.32106	-0.44550
Cu	-2.31841	-0.10067	-0.82792
C	-5.92867	-2.08471	0.23474
F	-5.43927	-2.97643	1.10507
F	-6.14668	-2.71211	-0.92705
F	-7.11033	-1.65803	0.70141
O	-3.29173	1.51443	-0.22452
F	-4.17486	3.40135	1.57993
F	-6.22394	2.81916	1.18037
F	-5.01811	3.68796	-0.39635
C	6.03102	-2.20955	0.50538
C	5.02940	-1.03796	0.37119
C	5.55350	0.27097	0.26222
C	4.74250	1.39651	0.09010
C	5.41634	2.77232	-0.08852
O	3.48039	1.45673	0.03948
O	3.83110	-1.39167	0.35637
Cu	2.26585	-0.06110	0.17287
F	4.94622	3.63928	0.81595

F	5.14157	3.25805	-1.30829
F	6.74885	2.72115	0.04210
F	7.30097	-1.79732	0.63943
F	5.96760	-2.98961	-0.58280
F	5.72622	-2.95649	1.57106
H	-1.03922	-1.45716	-2.57279
H	-0.70973	1.05657	-2.41060
H	1.28462	1.47801	-1.02899
H	-6.30054	0.51847	0.79756
H	6.63122	0.40630	0.29338
C	-0.08108	1.73240	0.64024
H	0.73669	2.17110	1.23013
H	-0.72141	2.55488	0.27209
H	-0.70521	1.09650	1.28405
H	0.99907	-2.23998	-1.19130
C	-0.64564	-2.90309	0.02435
H	-1.51083	-2.50002	0.57190
H	-1.01534	-3.61620	-0.72959
H	0.00477	-3.44152	0.72862

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04987663737

Zero-point correction (ZPE) = -5468.767568 .28230817264

Internal Energy (U) = -5468.934540 .11533654211

Enthalpy (H) = -5468.730425 .319451181971648

Gibbs Free Energy (G) = -5468.845763 .20411353173

Frequencies -- i311.42 7.48 10.03 13.07 18.95 22.27

Mono Cu(I) DiMeDHF-E-Trans Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20994683908

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0008740	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0003448	0.0010000	yes	0.0000407	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.65886	3.01474	1.66687
C	-0.64843	2.75742	1.56246
C	-1.18618	2.07336	0.36434
C	1.51467	2.50103	0.53690
C	2.15281	-3.37741	-1.16956
C	0.96189	-2.44038	-0.85986
C	-0.31587	-3.02268	-0.69297
C	-1.45411	-2.26526	-0.39884
C	-2.80022	-2.99667	-0.21881
C	2.57286	1.49515	1.00056
C	-1.79594	2.87994	-0.74915
O	0.65815	2.00318	-0.45960
O	-1.55015	-1.01464	-0.24831
O	1.27163	-1.23286	-0.79060
Cu	-0.08824	0.27652	-0.35884
F	-3.69775	-2.53052	-1.09737
F	-3.28109	-2.78127	1.01413
F	-2.70393	-4.32218	-0.39431
F	1.80808	-4.67455	-1.19125
F	3.10839	-3.22388	-0.24428
F	2.67844	-3.07443	-2.36356
H	1.10597	3.51516	2.53024
H	-1.35623	2.99489	2.36584
H	-1.82381	1.20947	0.62821
H	2.03089	3.37101	0.07651
H	-0.41710	-4.10053	-0.78716
H	3.12993	1.10736	0.13494
H	3.28561	1.96398	1.69941

H	2.09910	0.64094	1.51130
H	-2.04636	2.24297	-1.61089
H	-2.74299	3.32049	-0.38414
H	-1.12887	3.68968	-1.07222

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20994683908

Zero-point correction (ZPE) = -2888.996387 .21355935294

Internal Energy (U) = -2889.132671 .07727485864

Enthalpy (H) = -2888.973794 .236152750566810

Gibbs Free Energy (G) = -2889.051070 .15887642748

Frequencies -- i327.03 16.65 25.08 28.54 29.75 45.01

Dual Cu(I) DiMeDHF-E-Trans Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05025436947

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0006532	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0007945	0.0010000	yes	0.0001082	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.87987	0.89515	1.78431
C	-0.48393	0.66914	1.68342
C	-1.00749	-0.30298	0.67644
C	1.70781	0.11434	0.78135
O	0.81276	-0.33849	-0.20369
C	-2.71838	5.15202	-1.04573
C	-1.39134	4.59551	-0.48627
C	-0.22158	5.35231	-0.66529
C	1.03996	4.92979	-0.20888
O	1.33561	3.86642	0.39439
Cu	0.00087	2.48504	0.84809
C	2.24992	5.86265	-0.43677
F	3.22497	5.20827	-1.07596
F	2.72982	6.27784	0.74308
F	1.93854	6.94832	-1.15868
O	-1.52185	3.48106	0.08570
F	-3.22459	4.29738	-1.94433
F	-2.57221	6.34201	-1.64424
F	-3.61184	5.29454	-0.05950
C	2.25446	-5.69750	-1.01625
C	1.06951	-4.76106	-0.68480
C	-0.20973	-5.33765	-0.51275
C	-1.34140	-4.58046	-0.19395
C	-2.69106	-5.30729	-0.01993
O	-1.42823	-3.33196	-0.01314
O	1.38688	-3.55522	-0.60172
Cu	0.04751	-2.06153	-0.12218
F	-3.58291	-4.83398	-0.89973

F	-3.17303	-5.09325	1.21225
F	-2.59770	-6.63174	-0.19969
F	1.90100	-6.99051	-1.06827
F	3.20819	-5.56956	-0.08477
F	2.78298	-5.36783	-2.20078
H	1.34334	1.32961	2.67639
H	-1.15580	0.89552	2.52201
H	-1.46505	-1.16629	1.19488
H	2.39913	0.80682	0.26088
H	-0.29358	6.30513	-1.18248
H	-0.31829	-6.41297	-0.62651
C	2.52874	-0.99433	1.44549
H	3.03404	-1.59763	0.67686
H	3.28962	-0.57247	2.12219
H	1.87904	-1.66287	2.03606
C	-1.84013	0.16384	-0.48379
H	-2.25892	-0.68364	-1.04539
H	-2.68082	0.77178	-0.10197
H	-1.25471	0.80670	-1.15636

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05025436947

Zero-point correction (ZPE) = -5468.767793 .28246052459

Internal Energy (U) = -5468.936179 .11407489786

Enthalpy (H) = -5468.730810 .319443564373898

Gibbs Free Energy (G) = -5468.844883 .20537043536

Frequencies -- i309.36 7.82 10.78 14.78 24.41 25.07

Mono Cu(I) DiMeDHF-E-Trans Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27811550316

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0007912	0.0010000	yes	0.0001103	0.0005000	yes
Grad	0.0001598	0.0010000	yes	0.0000337	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.53833	-1.91288	0.64778
C	0.46289	-2.50728	0.01259
C	-0.63717	-2.71532	1.04603
C	1.16736	-1.71493	2.11251
C	-2.39612	1.52627	-2.80908
C	-1.11929	1.30312	-1.96961
C	-0.31472	2.41603	-1.66936
C	0.84721	2.32161	-0.88401
C	1.65270	3.60885	-0.60439
C	-2.06849	-2.43561	0.62152
C	1.57847	-0.41258	2.77760
O	-0.25330	-1.84298	2.10708
O	1.34720	1.29840	-0.35049
O	-0.95111	0.10390	-1.62972
Cu	0.52574	-0.50241	-0.45501
F	1.74772	3.81102	0.71601
F	1.09788	4.70150	-1.14909
F	2.89248	3.48978	-1.09666
F	-3.47531	1.18977	-2.08962
F	-2.37199	0.75780	-3.90402
F	-2.54587	2.79946	-3.20354
H	2.57344	-1.90701	0.29376
H	0.49677	-3.05476	-0.93389
H	-0.56426	-3.77331	1.39205
H	1.61360	-2.56542	2.67985
H	-0.60861	3.39000	-2.05122
H	-2.38545	-3.15703	-0.14828
H	-2.74176	-2.53582	1.48632

H	-2.16933	-1.42211	0.20530
H	1.16691	-0.36698	3.79727
H	2.67604	-0.34802	2.84462
H	1.21805	0.45692	2.20771

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27811550316

Zero-point correction (ZPE) = -2889.061356 .21675874399

Internal Energy (U) = -2889.202280 .07583492623

Enthalpy (H) = -2889.039018 .239096952097488

Gibbs Free Energy (G) = -2889.114855 .16326035499

Frequencies -- 20.80 27.38 32.52 38.29 44.28 84.55

Dual Cu(I) DiMeDHF-E-Trans Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11126364820

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008913	0.0010000	yes	0.0001333	0.0005000	yes
Grad	0.0004689	0.0010000	yes	0.0000810	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.31555	-2.43323	1.09487
C	-1.59054	-2.38782	0.58788
C	-2.53463	-1.93711	1.69032
C	-0.36228	-2.00234	2.55130
O	-1.66115	-1.43548	2.69848
C	5.55039	1.64935	-0.95988
C	4.11072	1.11588	-0.76879
C	3.80849	-0.16040	-1.29472
C	2.55882	-0.78646	-1.20336
O	1.50620	-0.32328	-0.68406
Cu	1.49893	1.70434	0.18273
C	2.43543	-2.22380	-1.75223
F	1.25272	-2.39849	-2.35534
F	2.49762	-3.10238	-0.72766
F	3.39919	-2.54321	-2.61822
O	3.37272	1.91573	-0.14503
F	5.52110	2.81690	-1.61101
F	6.32940	0.80897	-1.65779
F	6.12502	1.84756	0.23202
C	-3.63708	0.83885	-2.74926
C	-2.47523	0.91887	-1.73008
C	-2.30119	2.13520	-1.01946
C	-1.28429	2.33198	-0.09172
C	-1.14928	3.71038	0.58196
O	-0.42454	1.47311	0.29727
O	-1.82102	-0.13505	-1.63083
Cu	-0.49452	-0.78436	-0.23872
F	-1.32943	3.59878	1.90242

F	-2.02027	4.60977	0.11521
F	0.09228	4.19677	0.38031
F	-4.53703	-0.06317	-2.32576
F	-3.18562	0.44626	-3.94297
F	-4.27395	2.00801	-2.90921
H	0.52965	-2.97702	0.66700
H	-1.94015	-2.88009	-0.32407
H	-3.05556	-2.85071	2.06097
H	-0.28273	-2.92646	3.16971
H	4.60660	-0.69551	-1.80364
H	-2.97455	2.96066	-1.23501
C	-3.57904	-0.88777	1.34475
H	-4.22300	-1.22925	0.51916
H	-4.21236	-0.67926	2.22021
H	-3.08772	0.04899	1.04380
C	0.69178	-1.01140	3.01884
H	0.51658	-0.73954	4.07083
H	1.69934	-1.44937	2.93643
H	0.64978	-0.09341	2.41235

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11126364820

Zero-point correction (ZPE) = -5468.827165 .28409830811

Internal Energy (U) = -5468.994959 .11630406768

Enthalpy (H) = -5468.789302 .321961180430532

Gibbs Free Energy (G) = -5468.905607 .20565609527

Frequencies -- 6.38 10.84 18.29 20.48 24.74 26.04

Mono Cu(I) DiMeDHF-E-Trans Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27588137608

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0008614	0.0010000	yes	0.0001316	0.0005000	yes
Grad	0.0000535	0.0010000	yes	0.0000150	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.29176	-1.71592	0.77557
C	0.34902	-2.24546	-0.08673
C	-0.93422	-2.48974	0.69765
C	0.66799	-1.59705	2.15821
C	-1.79697	1.72374	-3.44786
C	-0.82548	1.53420	-2.26121
C	-0.19853	2.67483	-1.72623
C	0.73929	2.60791	-0.68206
C	1.37799	3.92230	-0.18299
C	-1.18724	-3.97626	0.96461
C	0.91856	-0.31367	2.93383
O	-0.72946	-1.75282	1.90587
O	1.16175	1.58985	-0.07484
O	-0.69129	0.33461	-1.91201
Cu	0.49784	-0.23660	-0.43077
F	1.21234	4.04093	1.13978
F	0.85235	5.01140	-0.76286
F	2.69359	3.91684	-0.43782
F	-2.96604	1.12636	-3.19272
F	-1.27808	1.16686	-4.55150
F	-2.04403	3.01397	-3.71810
H	2.37406	-1.70959	0.61608
H	0.55389	-2.73051	-1.04576
H	-1.81928	-2.05970	0.19745
H	1.04219	-2.45325	2.76453
H	-0.44608	3.64806	-2.14156
H	-2.05688	-4.08984	1.62956
H	-1.39831	-4.51057	0.02390

H	-0.31700	-4.45258	1.44409
H	0.34002	-0.32440	3.86986
H	1.98674	-0.22387	3.18861
H	0.62950	0.56998	2.34541

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27588137608

Zero-point correction (ZPE) = -2889.059084 .21679683198

Internal Energy (U) = -2889.199452 .07642884157

Enthalpy (H) = -2889.036696 .239184554471622

Gibbs Free Energy (G) = -2889.113127 .16275378474

Frequencies -- 20.24 26.77 27.73 34.04 38.60 81.36

Dual Cu(I) DiMeDHF-E-Trans Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11045236287

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0001462	0.0010000	yes	0.0000221	0.0005000	yes
Grad	0.0000997	0.0010000	yes	0.0000190	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.35521	-1.86882	1.23379
C	-1.26585	-2.22836	0.27158
C	-2.66723	-1.97906	0.80496
C	-1.11508	-1.37724	2.45488
O	-2.44154	-1.17614	1.96720
C	5.91579	1.20087	-0.34673
C	4.40454	0.88791	-0.45186
C	4.02724	-0.34722	-1.02340
C	2.70273	-0.78838	-1.15704
O	1.65156	-0.16377	-0.85428
Cu	1.77301	1.80938	0.09405
C	2.46153	-2.21994	-1.68060
F	1.45070	-2.23807	-2.55807
F	2.10881	-3.01744	-0.64803
F	3.53299	-2.76297	-2.26357
O	3.68424	1.80802	0.00785
F	6.21306	2.27650	-1.08507
F	6.68868	0.18756	-0.76726
F	6.24012	1.46403	0.92373
C	-3.59718	1.30293	-2.72615
C	-2.37613	1.31198	-1.77589
C	-2.08098	2.51588	-1.07957
C	-1.00550	2.64260	-0.21214
C	-0.74782	3.99505	0.47279
O	-0.17227	1.73023	0.12017
O	-1.78198	0.22086	-1.71277
Cu	-0.43802	-0.40198	-0.32697
F	-0.86821	3.86727	1.80033

F	-1.58069	4.95667	0.06727
F	0.51094	4.40197	0.21618
F	-4.51612	0.44492	-2.25798
F	-3.23272	0.89976	-3.94588
F	-4.17832	2.50540	-2.84236
H	0.69208	-2.17669	1.26224
H	-1.06208	-2.85736	-0.59978
H	-3.27955	-1.38653	0.10365
H	-1.10458	-2.20570	3.20023
H	4.82034	-1.01068	-1.35884
H	-2.71601	3.38171	-1.24937
C	-3.40832	-3.27717	1.13848
H	-4.36674	-3.04156	1.62575
H	-3.61851	-3.85228	0.22199
H	-2.81866	-3.91354	1.81770
C	-0.61456	-0.11711	3.14334
H	-1.28195	0.14321	3.97900
H	0.39655	-0.28000	3.55048
H	-0.58307	0.73329	2.44598

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11045236287

Zero-point correction (ZPE) = -5468.826049 .28440301202

Internal Energy (U) = -5468.994207 .11624501682

Enthalpy (H) = -5468.788277 .322174473167554

Gibbs Free Energy (G) = -5468.904522 .20593032879

Frequencies -- 7.07 11.35 14.32 16.14 27.12 27.80

3. Cu(I)-catalyzed rearrangement of Z-Cis dimethylvinyloxiranes

3.a. Additional Figures

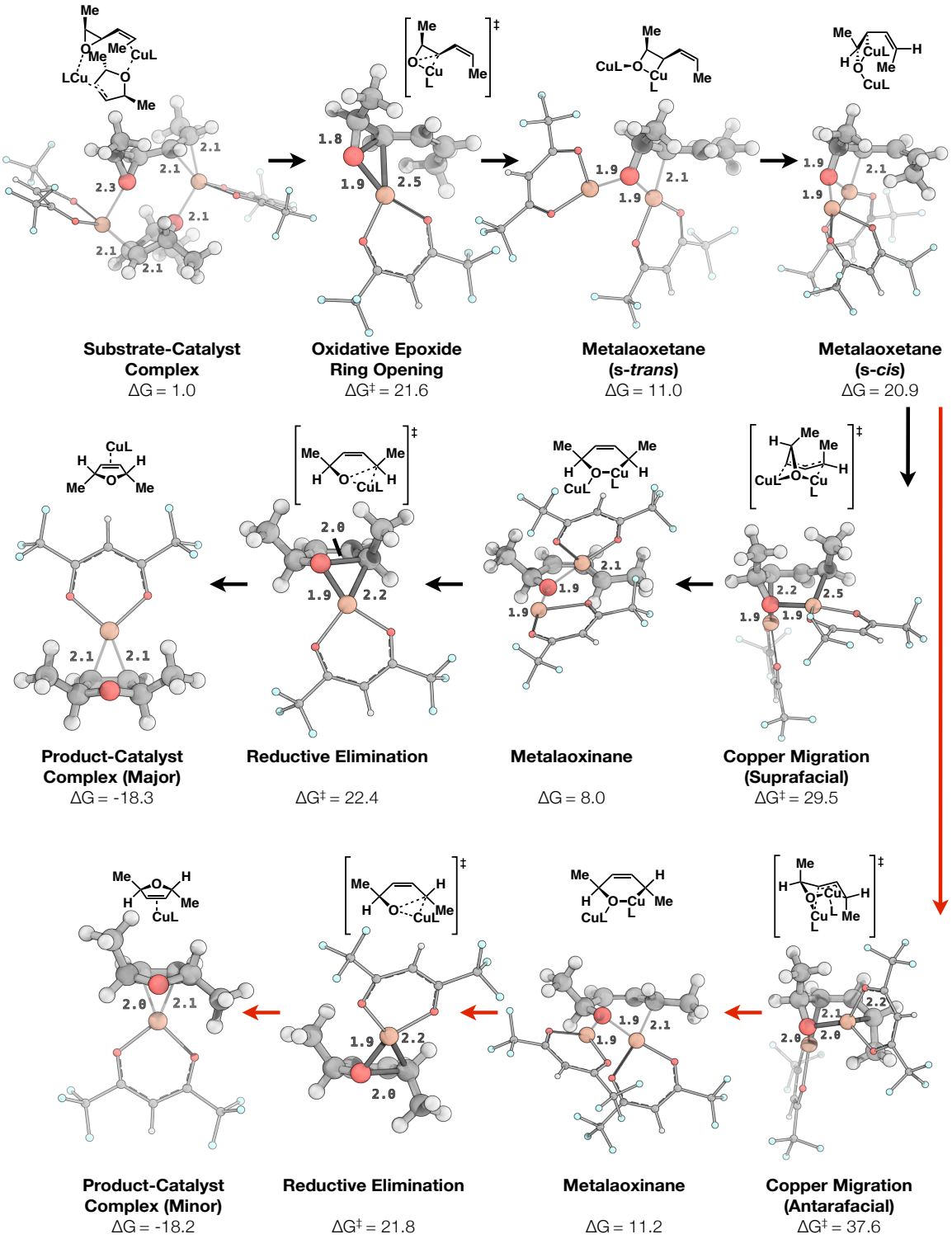


Figure 7. Structures of stationary points for both major and minor pathways for Z-Cis VO. All structures, energies, and free energy corrections computed

at the B3LYP/def2-SVP level of theory, as implemented in Turbomole. Figures rendered using Pymol.

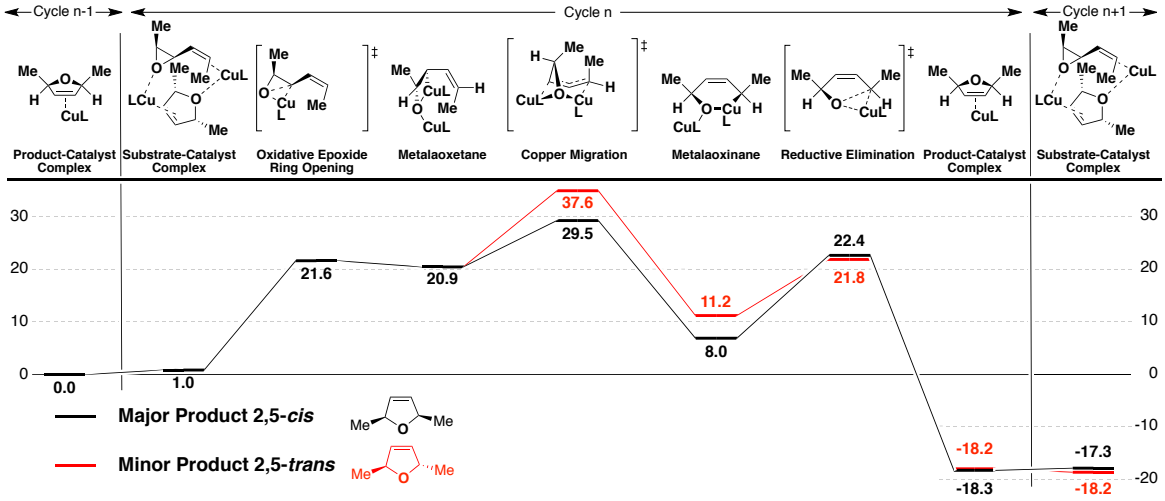


Figure 8. Reaction coordinate of Cu(I)-catalyzed ring expansion of Z-Cis VO.

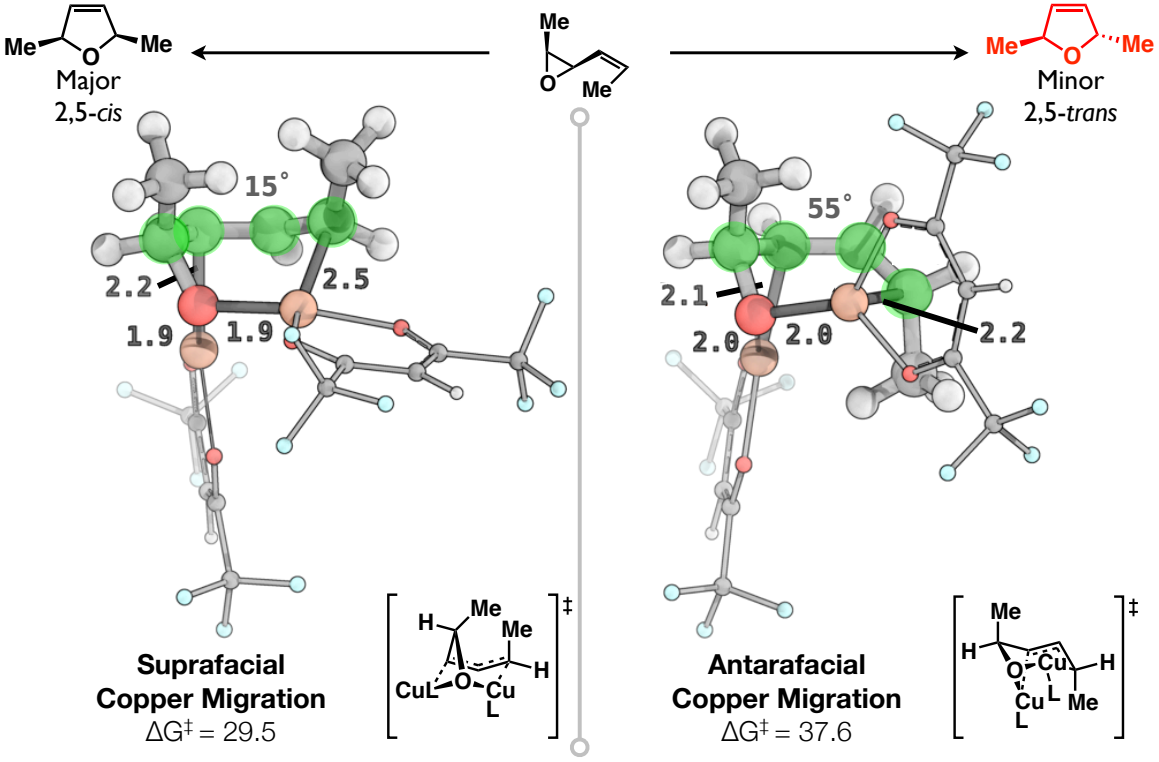


Figure 9. Stereoselective copper migration of Z-Cis VO showing π-allyl distortion (green highlight with dihedral), and TS bond distances.

3.b. Geometries, Energies, and Thermal Corrections
Mono Cu(I) DiMeDHF-Z-Cis Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp		Basis: def2-SVP			Atoms: 32		
Charge: 0	Spin: 1				Basis Functions: 366		
Energy = -2889.24308209800							
Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?	
Energy	0.0000004	0.0000010	yes				
Step	0.0008150	0.0010000	yes	0.0001794	0.0005000	yes	
Grad	0.0002940	0.0010000	yes	0.0000494	0.0005000	yes	

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.99694	3.18163	-0.23761
C	-1.73014	1.66173	-0.28748
C	-2.81144	0.78724	-0.08861
H	-3.79402	1.21010	0.10211
C	-2.67385	-0.61289	-0.11877
O	-1.63574	-1.28983	-0.32257
C	-3.92831	-1.47219	0.15406
F	-4.07858	-2.39642	-0.80074
F	-5.05521	-0.74628	0.20396
F	-3.79696	-2.10608	1.32826
O	-0.52791	1.37442	-0.51868
F	-1.76728	3.72788	-1.44016
F	-1.17492	3.76371	0.64461
F	-3.25614	3.48057	0.11292
Cu	0.16473	-0.48563	-0.58337
C	2.89550	-0.58415	0.46343
H	3.63972	-1.35311	0.72489
C	2.19088	-0.83799	-0.83774
H	2.47277	-0.21597	-1.69627
C	1.46949	-2.00304	-1.06144
H	1.18240	-2.22260	-2.09880
C	3.07044	0.74320	1.08276
H	3.93714	0.83621	1.75546
O	2.08890	-0.17623	1.57804
C	1.29875	-3.14064	-0.08715
H	0.26871	-3.52887	-0.12052
H	1.96985	-3.97531	-0.36089

H	1.51974	-2.84747	0.94907
C	2.60043	2.04626	0.49365
H	2.31290	2.73960	1.30073
H	3.41847	2.51983	-0.07482
H	1.72660	1.92232	-0.15835

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.24308209800

Zero-point correction (ZPE) = -2889.028037 .21504478450

Internal Energy (U) = -2889.164559 .07852287577

Enthalpy (H) = -2889.004765 .238316148328033

Gibbs Free Energy (G) = -2889.083287 .15979434801

Frequencies -- 21.27 25.06 31.13 34.57 44.27 56.26

Dual Cu(I) DiMeDHF-Z-Cis Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 64
Charge: 0 | Spin: 1 | Basis Functions: 732

Energy = -5778.54182464176

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000100	yes			
Step	0.0008992	0.0010000	yes	0.0001408	0.0005000	yes
Grad	0.0003815	0.0010000	yes	0.0000593	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.39063	0.08030	2.24852
C	0.95488	0.38217	1.70050
C	2.18376	-0.38217	2.03427
C	-1.32588	1.03033	2.62136
O	1.50872	-0.58723	0.78520
C	-5.28424	-2.47326	0.44191
C	-4.46196	-1.16378	0.40364
C	-5.13166	0.02304	0.03389
C	-4.48619	1.26406	-0.08651
C	-5.32272	2.48082	-0.53705
O	-3.27885	1.55056	0.11125
O	-3.25859	-1.32329	0.69980
Cu	-1.85950	0.25294	0.74143
F	-4.85314	2.95116	-1.70532
F	-5.22787	3.46629	0.36676
F	-6.62355	2.20330	-0.70583
F	-5.18822	-3.04674	1.64790
F	-4.79942	-3.34085	-0.46412
F	-6.58688	-2.29578	0.17480
H	-0.55539	-0.95457	2.56577
H	1.12214	1.41653	1.37568
H	3.12027	0.18320	1.92794
H	-2.17599	0.66687	3.21192
H	-6.19523	-0.02913	-0.18355
C	5.01697	2.60317	0.09054
C	4.50053	1.23432	-0.40144
C	5.30488	0.10530	-0.16697
C	4.87341	-1.21244	-0.42400

O	3.79250	-1.59727	-0.92522
Cu	2.29214	-0.33203	-1.40608
C	5.79515	-2.37175	0.01877
F	5.95870	-3.25515	-0.96854
F	5.22920	-3.01438	1.05855
F	7.00921	-1.95986	0.41176
O	3.35155	1.29145	-0.90612
F	4.30526	2.96934	1.17560
F	4.85315	3.54251	-0.84297
F	6.31010	2.58771	0.44166
C	0.72395	-1.18994	-2.45524
C	0.75710	0.16669	-2.70060
C	-0.37529	0.85336	-1.96580
O	-0.91656	-0.20317	-1.13589
C	-0.42722	-1.51483	-1.52387
H	6.28791	0.25227	0.27289
H	1.20008	-1.96135	-3.06677
H	1.27141	0.65209	-3.53467
H	-0.00698	1.64142	-1.28544
H	-0.08161	-2.00466	-0.59930
C	-1.18993	2.52918	2.56287
C	2.26932	-1.55813	2.96817
C	-1.51921	-2.35892	-2.17423
C	-1.43549	1.45351	-2.88524
H	-0.37731	2.86733	1.90405
H	-0.99200	2.93043	3.57326
H	-2.12644	2.98534	2.20639
H	1.31768	-2.10195	3.04426
H	2.56847	-1.22258	3.97455
H	3.03869	-2.25715	2.60319
H	-1.89474	-1.88797	-3.09592
H	-2.35543	-2.50001	-1.47511
H	-1.11765	-3.35286	-2.43125
H	-2.26739	1.85588	-2.28938
H	-1.82765	0.70022	-3.58611
H	-1.00031	2.28010	-3.47050

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5778.54182464176

Zero-point correction (ZPE) = -5778.108764 .43306043213

Internal Energy (U) = -5778.407336 .13448832454

Enthalpy (H) = -5778.061965 .479858746608813

Gibbs Free Energy (G) = -5778.196454 .34537045562

Frequencies -- 5.81 11.99 21.15 22.04 26.84 29.11

Mono Cu(I) DiMeDHF-Z-Cis Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20832202525

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0006753	0.0010000	yes	0.0001068	0.0005000	yes
Grad	0.0002068	0.0010000	yes	0.0000324	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.23965	-1.08264	-0.48889
C	-2.42515	-0.04773	0.50452
C	-2.47635	1.28325	0.24145
C	-2.34815	-2.52962	-0.23522
C	-2.84330	-3.07605	1.08735
C	-2.22573	1.98263	-1.05220
O	-0.95393	-2.37099	-0.33887
H	-2.19883	-0.79667	-1.54148
H	-2.60894	-0.37442	1.53124
H	-2.70637	1.93744	1.09046
H	-2.75601	-3.10519	-1.08495
H	-3.94125	-3.00531	1.15714
H	-2.56220	-4.13762	1.16730
H	-2.39251	-2.54640	1.93914
H	-1.31972	2.60397	-0.95032
H	-2.07283	1.30491	-1.90372
H	-3.05784	2.66584	-1.29464
C	4.51754	-1.06008	-0.44991
C	3.10126	-0.47485	-0.23390
C	2.99408	0.91812	-0.00195
C	1.77015	1.54940	0.24185
C	1.76656	3.07140	0.49019
O	0.61598	1.04176	0.29458
O	2.18853	-1.32309	-0.27329
Cu	0.17792	-0.84309	-0.04472
F	1.30123	3.34383	1.71733
F	0.95402	3.68195	-0.39528
F	2.97724	3.63232	0.37618

F	4.86199	-1.81919	0.60081
F	5.46071	-0.11408	-0.59426
F	4.54240	-1.82950	-1.54286
H	3.89913	1.51968	-0.01310

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20832202525

Zero-point correction (ZPE) = -2888.995181 .21314038506

Internal Energy (U) = -2889.128696 .07962553694

Enthalpy (H) = -2888.971681 .236640276822860

Gibbs Free Energy (G) = -2889.051308 .15701392483

Frequencies -- i265.56 19.17 22.22 30.75 36.65 42.53

Dual Cu(I) DiMeDHF-Z-Cis Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04982700409

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0004401	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0001882	0.0010000	yes	0.0000366	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-5.20495	-2.49770	0.06374
C	-4.50146	-1.12287	0.06364
C	-5.28553	0.02881	-0.10542
C	-4.74190	1.32628	-0.15295
C	-5.71091	2.51635	-0.33577
C	0.15569	-1.14183	-0.44522
H	0.20510	-0.85474	-1.49786
C	-0.08557	-0.09717	0.54808
C	-0.19700	1.27157	0.28332
C	0.01783	-2.58330	-0.18384
O	-3.53661	1.67264	-0.05550
O	-3.25146	-1.20086	0.20356
O	1.41939	-2.41158	-0.23059
Cu	-2.07092	0.38491	0.22717
F	-5.67079	3.30409	0.74549
F	-6.98099	2.12638	-0.51482
F	-5.34966	3.24424	-1.39756
F	-4.83494	-3.20485	1.13859
F	-4.84893	-3.18926	-1.02809
F	-6.53989	-2.39839	0.07224
H	-6.36126	-0.08649	-0.20776
H	-0.08726	-0.41482	1.59535
H	-0.23663	1.92380	1.16389
H	-0.34834	-3.15975	-1.05003
C	6.84541	-1.08397	-0.40033
C	5.42834	-0.49650	-0.19447
C	5.32005	0.89619	0.04286
H	6.22649	1.49578	0.04587

C	4.09658	1.53056	0.27054
O	2.93672	1.02734	0.30455
Cu	2.51377	-0.85142	-0.02175
C	4.09215	3.05241	0.51664
F	3.57319	3.32687	1.72133
F	3.32343	3.66364	-0.40550
F	5.31009	3.60354	0.45628
O	4.51312	-1.34145	-0.24570
F	7.18140	-1.83945	0.65485
F	7.78762	-0.13752	-0.54126
F	6.87426	-1.85529	-1.49085
C	-0.54282	-3.11904	1.11488
H	-1.63939	-3.01755	1.12373
H	-0.28640	-4.18569	1.20651
H	-0.11917	-2.59993	1.98745
C	0.08739	1.97382	-1.01507
H	1.10536	2.39639	-0.96700
H	0.03290	1.31684	-1.89546
H	-0.61353	2.80895	-1.16777

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04982700409

Zero-point correction (ZPE) = -5468.767671 .28215582068

Internal Energy (U) = -5468.932869 .11695703387

Enthalpy (H) = -5468.729762 .320064398590587

Gibbs Free Energy (G) = -5468.846718 .20310800882

Frequencies -- i266.21 8.00 9.01 16.66 20.36 23.27

Mono Cu(I) DiMeDHF-Z-Cis Metalaoxetane (s-*trans*)

Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22296671151

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0009484	0.0010000	yes	0.0002158	0.0005000	yes
Grad	0.0000515	0.0010000	yes	0.0000166	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.73992	-1.15261	0.19555
C	-1.94071	-0.33157	1.36905
C	-2.37258	0.95790	1.38690
C	-1.57924	-2.66026	0.26912
C	4.53221	-0.43706	-0.69417
C	3.02707	-0.08602	-0.64062
C	2.63381	1.22793	-0.98357
C	1.29327	1.61476	-0.97193
C	0.93566	3.05964	-1.37409
C	-2.12057	-3.39198	1.48665
C	-2.69544	1.84852	0.23381
O	-0.16833	-2.68239	0.21711
O	0.27708	0.92439	-0.67051
O	2.29309	-1.03634	-0.29993
Cu	0.27038	-0.94251	-0.14303
F	0.29630	3.67528	-0.36522
F	0.11732	3.05365	-2.43396
F	2.00922	3.79509	-1.68530
F	4.94462	-0.88895	0.49376
F	5.29437	0.61862	-1.02108
F	4.74285	-1.39318	-1.60506
H	-2.05065	-0.74250	-0.77198
H	-1.75910	-0.81193	2.33486
H	-2.52320	1.40346	2.37821
H	-2.01696	-3.11887	-0.64186
H	3.39190	1.95283	-1.26619
H	-3.22004	-3.32474	1.54333
H	-1.84226	-4.45522	1.41380

H	-1.68532	-3.00174	2.41914
H	-2.07991	2.76235	0.28452
H	-2.51552	1.38686	-0.74540
H	-3.74941	2.17659	0.28809

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22296671151

Zero-point correction (ZPE) = -2889.008188 .21477816858

Internal Energy (U) = -2889.145568 .07739863832

Enthalpy (H) = -2888.985012 .237954312434870

Gibbs Free Energy (G) = -2889.062410 .16055610779

Frequencies -- 20.13 31.61 34.57 40.11 62.07 79.29

Dual Cu(I) DiMeDHF-Z-Cis Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.06751504721

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000007	0.0000100	yes			
Step	0.0002227	0.0010000	yes	0.0000348	0.0005000	yes
Grad	0.0000456	0.0010000	yes	0.0000105	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.18425	1.13286	0.35787
H	-2.51631	1.46950	-0.63114
C	-2.43496	2.00394	1.47257
C	-2.88832	3.28989	1.40572
C	-1.97032	-0.37030	0.49712
O	-0.55843	-0.42429	0.25307
H	-2.26402	1.58869	2.46998
H	-3.05792	3.79391	2.36510
H	-2.50880	-0.89328	-0.31499
C	4.09831	1.77096	-0.66143
C	2.60534	2.15857	-0.55000
C	2.24857	3.51376	-0.72764
H	3.02691	4.23994	-0.94545
C	0.92425	3.94837	-0.63885
O	-0.11510	3.27158	-0.38660
Cu	-0.15668	1.37312	-0.03473
C	0.61846	5.43759	-0.90416
F	-0.18032	5.92795	0.05585
F	-0.01949	5.56764	-2.07526
F	1.72111	6.19258	-0.94583
O	1.84199	1.19956	-0.29862
F	4.53006	1.29203	0.51003
F	4.87221	2.81580	-0.99145
F	4.25896	0.82673	-1.59017
C	-2.32409	-1.02411	1.82033
H	-3.40167	-0.92650	2.03176
H	-2.07533	-2.09454	1.76432
H	-1.75476	-0.58083	2.65225

C	-3.20728	4.09959	0.19614
H	-2.59315	5.01600	0.19137
H	-3.02694	3.57350	-0.75014
H	-4.26135	4.43053	0.22615
Cu	0.45980	-1.96246	-0.20155
O	1.87908	-3.06222	-0.93174
O	-0.69238	-3.56738	0.37749
C	1.87441	-4.31991	-0.90955
C	-0.29176	-4.74487	0.21575
C	0.90414	-5.18941	-0.38009
C	3.11854	-4.94173	-1.58212
C	-1.28484	-5.81002	0.73412
H	1.08462	-6.25939	-0.43912
F	4.23748	-4.46384	-1.02682
F	3.15140	-6.28039	-1.48460
F	3.13530	-4.62802	-2.88517
F	-1.62792	-5.54289	2.00124
F	-0.79169	-7.05669	0.69610
F	-2.40285	-5.79152	-0.00710

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.06751504721

Zero-point correction (ZPE) = -5468.784368 .28314610839

Internal Energy (U) = -5468.948900 .11861500021

Enthalpy (H) = -5468.746075 .321439374984603

Gibbs Free Energy (G) = -5468.864692 .20282234891

Frequencies -- 6.22 8.86 11.43 18.30 23.07 26.59

Mono Cu(I) DiMeDHF-Z-Cis Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.21502976776

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0008808	0.0010000	yes	0.0001911	0.0005000	yes
Grad	0.0001828	0.0010000	yes	0.0000379	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.46389	2.04343	-0.36092
C	0.40884	2.08728	1.09844
C	-0.61702	1.93518	1.97637
C	-0.61236	2.48511	-1.33455
O	-1.26340	1.23028	-1.43410
C	-1.03221	-4.06803	-1.01210
C	-0.18366	-2.80364	-0.74355
C	1.13154	-2.97096	-0.25916
C	1.96025	-1.87923	0.01089
O	1.70663	-0.64740	-0.11864
Cu	0.03008	0.10026	-0.74437
C	3.38594	-2.14438	0.53623
F	3.55505	-1.55214	1.72524
F	4.28816	-1.63763	-0.31274
F	3.64778	-3.44995	0.68569
O	-0.77631	-1.73096	-0.99233
F	-2.13152	-4.05132	-0.25049
F	-0.36452	-5.20149	-0.74602
F	-1.40942	-4.10339	-2.29371
H	1.48577	2.03149	-0.76018
H	1.39891	2.22365	1.54985
H	-0.34711	2.05814	3.03293
H	-0.12148	2.73511	-2.29814
H	1.51068	-3.97508	-0.09124
C	-1.52994	3.64107	-0.97215
H	-0.97727	4.59488	-1.00437
H	-2.34170	3.69167	-1.71570
H	-1.98210	3.53561	0.02235

C	-2.03568	1.53551	1.72763
H	-2.28284	0.65502	2.34818
H	-2.72775	2.33272	2.05589
H	-2.23724	1.29918	0.67474

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.21502976776

Zero-point correction (ZPE) = -2888.999946 .21508287249

Internal Energy (U) = -2889.137971 .07705796030

Enthalpy (H) = -2888.976961 .238068576401132

Gibbs Free Energy (G) = -2889.054020 .16100935485

Frequencies -- 22.16 28.60 29.91 32.64 57.74 77.39

Dual Cu(I) DiMeDHF-Z-Cis Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

```
============================================================
Method: B3-LYP      |  Basis: def2-SVP            |  Atoms:  47
Charge: 0     |  Spin: 1                          | Basis Functions:   584
------------------------------------------------------------------------------
Energy =    -5469.05486514104
------------------------------------------------------------------------------
Item      Max Val.     ||  Criteria   Pass? |   RMS Val.  ||  Criteria   Pass?
Energy   0.0000007  ||  0.0000010   yes
Step      0.0003733  ||  0.0010000   yes   |  0.0000743  ||  0.0005000   yes
Grad      0.0000555  ||  0.0010000   yes   |  0.0000106  ||  0.0005000   yes
============================================================
Atomic Coordinates (Angstroms)
Type   X        Y        Z
------------------------------------------------------------------------------
C         1.60537        2.47308       -0.87280
C         1.86123        2.71167        0.53377
C         1.06887        2.86989        1.63166
C         0.42814        2.84531       -1.77503
O        -0.19615        1.56555       -1.88534
C         0.52767       -3.67886       -2.01525
C         1.20295       -2.39559       -1.48063
C         2.40499       -2.52090       -0.75267
C         3.05722       -1.41547       -0.20562
O         2.72406       -0.19389       -0.24692
Cu        1.11656        0.47998       -1.06249
C         4.37951       -1.63830        0.55654
F         4.28446       -1.15212        1.79837
F         5.37601       -0.99476       -0.06688
F         4.71464       -2.93186        0.64092
O         0.58448       -1.34415       -1.75654
F        -0.68553       -3.81101       -1.46665
F         1.23121       -4.78514       -1.73488
F         0.38327       -3.60562       -3.34191
C        -5.14580       -1.44741        0.01348
C        -3.71227       -0.87138        0.04839
C        -2.83317       -1.36326        1.03000
C        -1.49280       -0.95552        1.17674
C        -0.67932       -1.56467        2.34096
O        -0.85311       -0.12342        0.49375
O        -3.51664       -0.00589       -0.84475
Cu       -1.84578        0.81667       -1.25581
F        -0.40050       -0.60675        3.24723
```

F	0.48938	-2.04575	1.89014
F	-1.31013	-2.55489	2.98222
F	-6.04322	-0.46820	0.18772
F	-5.36245	-2.37212	0.96159
F	-5.38020	-2.01774	-1.17456
H	2.53814	2.35786	-1.43931
H	2.93547	2.72167	0.75026
H	1.61926	3.09225	2.55482
H	0.85297	3.09858	-2.76498
H	2.83074	-3.50908	-0.60334
H	-3.21391	-2.11418	1.71745
C	-0.51756	3.96850	-1.39500
H	0.02054	4.93021	-1.36506
H	-1.29980	4.04399	-2.16745
H	-1.00807	3.81151	-0.42708
C	-0.39808	2.71129	1.82167
H	-0.57217	1.98552	2.63451
H	-0.84988	3.66409	2.15392
H	-0.92062	2.34032	0.93484

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05486514104

Zero-point correction (ZPE) = -5468.771338 .28352698828

Internal Energy (U) = -5468.939251 .11561362690

Enthalpy (H) = -5468.733261 .321603153336245

Gibbs Free Energy (G) = -5468.848877 .20598746077

Frequencies -- 8.63 11.79 20.83 21.04 26.11 29.99

Dual Cu(I) DiMeDHF-Z-Cis Suprafacial Copper Migration (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.03999170906

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000006	0.0000010	yes			
Step	0.0003612	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0004239	0.0010000	yes	0.0000716	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.73781	-2.24373	0.65146
C	-1.24065	-1.49808	1.73874
C	0.08093	-1.29772	2.15559
C	-0.90717	-2.74781	-0.52865
O	-0.33558	-1.51289	-0.98025
C	-1.98163	3.46968	-2.45619
C	-2.43256	2.25428	-1.61178
C	-3.66543	2.33567	-0.92753
C	-4.13903	1.30431	-0.10972
O	-3.60140	0.18756	0.14030
Cu	-1.88066	-0.40274	-0.57014
C	-5.49068	1.48993	0.61089
F	-5.32655	1.35330	1.93310
F	-6.35828	0.55533	0.20156
F	-6.04102	2.69023	0.38607
O	-1.61570	1.30587	-1.61477
F	-0.91123	4.03982	-1.88791
F	-2.93697	4.40528	-2.56633
F	-1.64451	3.07881	-3.68738
H	-2.81952	-2.41449	0.61978
H	-1.98709	-0.84052	2.20612
H	0.24193	-0.38340	2.73919
H	-1.64576	-3.07812	-1.28433
H	-4.26426	3.23622	-1.03267
C	1.14326	-2.33070	2.40815
H	1.15316	-2.51151	3.50095
H	0.96012	-3.29394	1.92341
H	2.15383	-1.96801	2.16211

C	0.11396	-3.87510	-0.43200
H	-0.28900	-4.73854	0.12230
H	0.36817	-4.20907	-1.44953
H	1.04908	-3.54935	0.04112
C	3.61290	2.07074	2.03289
C	3.15153	1.11484	0.91336
C	3.99439	0.90471	-0.18071
C	3.67006	0.01394	-1.23073
C	4.67667	-0.13444	-2.39744
O	2.64356	-0.68666	-1.35323
O	2.01762	0.60520	1.15284
Cu	1.10849	-0.66228	-0.00327
F	4.15413	0.37645	-3.51798
F	4.94608	-1.42632	-2.61272
F	5.83884	0.49467	-2.16119
F	2.71395	3.04477	2.20993
F	4.79793	2.64124	1.77904
F	3.72185	1.39438	3.18729
H	4.94008	1.43819	-0.21976

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.03999170906

Zero-point correction (ZPE) = -5468.757340 .28265096454

Internal Energy (U) = -5468.924640 .11535130483

Enthalpy (H) = -5468.719938 .320052972193960

Gibbs Free Energy (G) = -5468.835291 .20470008675

Frequencies -- i77.48 7.31 8.24 10.56 16.23 22.48

Dual Cu(I) DiMeDHF-Z-Cis Antarafacial Copper Migration (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.02771963083

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000008	0.0000010	yes			
Step	0.0003604	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0003848	0.0010000	yes	0.0000706	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.86609	-2.25604	-0.11491
C	-0.12708	-1.92601	1.06143
H	-0.00662	-2.78926	1.73793
C	0.48554	-0.75410	1.50939
H	1.20122	-0.92939	2.32369
C	-0.28364	-2.02943	-1.50450
H	-1.07301	-2.28050	-2.24273
O	-0.09304	-0.61714	-1.50333
C	-3.91187	3.30541	-1.17364
C	-3.65967	1.82720	-0.79476
C	-4.72492	1.08656	-0.23906
C	-4.58027	-0.24227	0.16754
O	-3.55360	-0.98165	0.11811
Cu	-1.84519	-0.43192	-0.59013
C	-5.79850	-0.96358	0.78184
F	-5.52550	-1.32070	2.04310
F	-6.07603	-2.07129	0.08504
F	-6.89683	-0.19860	0.79689
O	-2.49100	1.43647	-1.01677
F	-3.14601	4.09864	-0.41616
F	-5.19008	3.66966	-0.99344
F	-3.59867	3.51402	-2.45444
C	5.61594	-1.51833	0.07479
C	4.40955	-0.55398	0.03450
C	4.64045	0.80821	0.29156
C	3.60548	1.76153	0.28581
C	3.94959	3.22149	0.65375
O	2.39003	1.58756	0.03273

O	3.32055	-1.12282	-0.22496
Cu	1.50427	-0.20388	-0.40239
F	3.24039	3.58920	1.73320
F	3.62966	4.04376	-0.35116
F	5.24812	3.40305	0.93730
F	5.42312	-2.45753	1.01202
F	6.77418	-0.89978	0.34836
F	5.75093	-2.13597	-1.10607
H	-1.59327	-3.07224	-0.01011
H	-5.69122	1.56848	-0.11743
H	5.65143	1.13422	0.52067
C	-0.09577	0.64586	1.57662
H	0.69099	1.39623	1.73188
H	-0.67228	0.96899	0.69740
H	-0.77229	0.68260	2.45200
C	0.95402	-2.84386	-1.85834
H	0.71376	-3.91952	-1.88820
H	1.29761	-2.54415	-2.86160
H	1.77561	-2.68518	-1.14340

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.02771963083

Zero-point correction (ZPE) = -5468.746211 .28150832488

Internal Energy (U) = -5468.914047 .11367176221

Enthalpy (H) = -5468.708729 .318990317307726

Gibbs Free Energy (G) = -5468.822398 .20532092097

Frequencies -- i100.28 9.23 15.86 17.13 25.47 28.34

Mono Cu(I) DiMeDHF-Z-Cis Metalaoxinane (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22503182874

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0008714	0.0010000	yes	0.0002089	0.0005000	yes
Grad	0.0000734	0.0010000	yes	0.0000139	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.34794	3.08394	-0.94369
C	-0.27253	2.27142	-1.83629
C	0.20068	0.96286	-2.26728
C	1.52239	2.63264	-0.12207
C	0.61204	-1.76305	3.50618
C	0.26561	-1.54877	2.01407
C	-0.64231	-2.43912	1.39702
C	-0.98599	-2.30130	0.05228
C	-1.97010	-3.30609	-0.57864
C	1.29782	2.89410	1.38062
C	-0.71178	0.12691	-3.12334
O	1.93802	1.35539	-0.41049
O	-0.58795	-1.43405	-0.77877
O	0.84607	-0.57501	1.49131
Cu	0.61269	0.04077	-0.44927
F	-1.36247	-3.98419	-1.56065
F	-3.01368	-2.65559	-1.11071
F	-2.44408	-4.19292	0.30566
F	-0.03295	-2.81106	4.04144
F	0.28237	-0.67467	4.21155
F	1.92476	-1.97191	3.64698
H	-0.03768	4.09354	-0.76621
H	-1.23069	2.60411	-2.25657
H	1.25905	0.92278	-2.54470
H	2.35108	3.31141	-0.45363
H	-1.07816	-3.24772	1.97749
H	2.20252	2.59999	1.93287
H	1.08254	3.95558	1.58748

H	0.46096	2.28460	1.75708
H	-0.77468	0.60038	-4.12270
H	-0.33083	-0.89305	-3.26242
H	-1.73064	0.05808	-2.71462

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22503182874

Zero-point correction (ZPE) = -2889.010786 .21424493674

Internal Energy (U) = -2889.148030 .07700118063

Enthalpy (H) = -2888.988014 .237017347911524

Gibbs Free Energy (G) = -2889.065012 .16001906715

Frequencies -- 13.78 23.84 27.57 33.52 61.28 76.29

Dual Cu(I) DiMeDHF-Z-Cis Metalaoxinane (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07611703167

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000006	0.0000010	yes			
Step	0.0007590	0.0010000	yes	0.0001492	0.0005000	yes
Grad	0.0000826	0.0010000	yes	0.0000201	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.19722	3.73214	-0.62909
C	-1.74286	2.88716	-1.54717
C	-1.14242	1.66997	-2.06241
C	0.05701	3.44769	0.14393
O	0.54278	2.17203	-0.12790
C	5.36536	-1.46057	0.51559
C	3.95623	-0.96014	0.12353
C	3.11961	-1.84527	-0.58528
C	1.80510	-1.55054	-0.99238
O	1.17182	-0.48016	-0.83774
Cu	2.14458	1.21785	0.25842
C	1.00125	-2.66031	-1.70821
F	0.48566	-2.19016	-2.85597
F	-0.02553	-3.05234	-0.93246
F	1.72659	-3.74559	-2.00257
O	3.74014	0.21592	0.51308
F	6.29843	-0.64048	0.01572
F	5.62773	-2.69907	0.06871
F	5.49473	-1.47219	1.84826
C	-0.73535	-1.04303	3.67789
C	-1.12396	-0.80264	2.20180
C	-2.06795	-1.66001	1.60294
C	-2.49775	-1.47581	0.28594
C	-3.56351	-2.43080	-0.29104
O	-2.14333	-0.59464	-0.54749
O	-0.54350	0.17762	1.68135
Cu	-0.76080	0.72996	-0.25733
F	-3.08345	-3.06405	-1.36526

F	-4.64079	-1.72716	-0.66888
F	-3.96471	-3.35349	0.59266
F	-1.34614	-2.11216	4.20720
F	-1.06844	0.02696	4.41167
F	0.58433	-1.22629	3.78163
H	-1.71911	4.66500	-0.39105
H	-2.74978	3.12246	-1.91504
H	-0.06584	1.70508	-2.25311
H	0.80604	4.17408	-0.25472
H	3.51572	-2.82964	-0.82057
H	-2.48539	-2.47817	2.18338
C	-0.10751	3.72116	1.64603
H	0.85871	3.55675	2.14725
H	-0.43175	4.75619	1.84065
H	-0.83924	3.02628	2.08612
C	-1.92123	0.79811	-2.99821
H	-1.91518	1.27828	-3.99712
H	-1.45313	-0.18971	-3.10758
H	-2.96597	0.66371	-2.68517

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07611703167

Zero-point correction (ZPE) = -5468.793123 .28299375644

Internal Energy (U) = -5468.961956 .11416006737

Enthalpy (H) = -5468.755355 .320761408784783

Gibbs Free Energy (G) = -5468.869516 .20660067739

Frequencies -- 8.71 16.06 17.58 25.21 27.23 27.42

Mono Cu(I) DiMeDHF-Z-Cis Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22295336064

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0007866	0.0010000	yes	0.0000929	0.0005000	yes
Grad	0.0000316	0.0010000	yes	0.0000068	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.21735	2.98629	0.62596
C	-0.80815	2.62002	-0.18255
C	-0.71547	1.69877	-1.31154
C	1.55874	2.30871	0.58839
C	1.62882	-3.16723	2.08521
C	0.78407	-2.38359	1.05345
C	-0.36057	-3.01277	0.51211
C	-1.19250	-2.35170	-0.38993
C	-2.44588	-3.07552	-0.91959
C	-1.99508	1.25652	-1.96700
C	2.69367	3.34841	0.39886
O	1.66604	1.36669	-0.40612
O	-1.07606	-1.18268	-0.86236
O	1.20084	-1.23200	0.81476
Cu	0.29759	0.10369	-0.44868
F	-2.38927	-3.18185	-2.25282
F	-3.54308	-2.37265	-0.60646
F	-2.58628	-4.30683	-0.41164
F	1.24238	-4.44744	2.19921
F	1.51161	-2.59507	3.29117
F	2.91745	-3.15465	1.73862
H	0.05875	3.75469	1.39074
H	-1.80826	3.01620	0.03765
H	0.11363	1.88956	-1.99943
H	-0.60475	-4.02776	0.81283
H	-2.41701	2.12162	-2.51543
H	-1.83142	0.44991	-2.69307
H	-2.74741	0.91630	-1.24037

H	1.70771	1.87605	1.61087
H	2.58802	3.84768	-0.57621
H	2.67456	4.10474	1.19944
H	3.65994	2.82592	0.42392

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22295336064

Zero-point correction (ZPE) = -2889.008327 .21462581662

Internal Energy (U) = -2889.145914 .07703865521

Enthalpy (H) = -2888.985539 .237413462994565

Gibbs Free Energy (G) = -2889.062580 .16037328544

Frequencies -- 15.01 21.59 28.37 35.35 52.73 80.92

Dual Cu(I) DiMeDHF-Z-Cis Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07083784262

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008422	0.0010000	yes	0.0000932	0.0005000	yes
Grad	0.0000878	0.0010000	yes	0.0000150	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.36950	3.69401	0.85493
C	-2.43255	3.33311	0.08621
C	-2.42846	2.37882	-1.01127
C	-0.04004	3.00389	0.84768
O	-0.01034	1.93223	-0.05025
C	2.12705	-3.46118	-1.18766
C	2.41672	-1.99036	-0.81778
C	3.75036	-1.60926	-0.58810
C	4.12427	-0.30863	-0.19897
O	3.39397	0.69206	0.00623
Cu	1.41266	0.63269	-0.16101
C	5.62479	-0.02684	0.03724
F	5.83945	0.28296	1.32384
F	6.02149	1.01262	-0.70842
F	6.41023	-1.07175	-0.26706
O	1.38081	-1.28263	-0.76313
F	1.24013	-3.98211	-0.32367
F	3.21923	-4.23753	-1.16989
F	1.59231	-3.53640	-2.41462
C	-0.08923	-2.47992	2.39784
C	-0.96388	-1.69200	1.39672
C	-1.99221	-2.37761	0.71564
C	-2.87652	-1.72048	-0.13828
C	-4.02221	-2.52307	-0.78722
O	-2.90208	-0.49549	-0.47244
O	-0.69467	-0.47059	1.32599
Cu	-1.54017	0.78084	-0.03083
F	-3.98947	-2.37881	-2.11690

F	-5.20138	-2.06216	-0.34853
F	-3.95985	-3.82990	-0.50789
F	-0.23986	-3.80343	2.27886
F	-0.43713	-2.13594	3.64803
F	1.20234	-2.18572	2.23376
H	-1.49727	4.48707	1.59924
H	-3.40640	3.77567	0.33379
H	-1.57489	2.44360	-1.69456
H	4.52884	-2.35945	-0.69804
H	-2.10548	-3.44740	0.86880
C	-3.73355	2.00790	-1.65170
H	-4.05349	2.84299	-2.30593
H	-3.64319	1.11136	-2.27900
H	-4.52904	1.83334	-0.91205
H	0.13071	2.65886	1.89382
C	1.11396	3.97034	0.50310
H	0.98439	4.37135	-0.51341
H	1.15516	4.80583	1.21871
H	2.06401	3.41711	0.54820

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07083784262

Zero-point correction (ZPE) = -5468.787767 .28306993241

Internal Energy (U) = -5468.956447 .11439059282

Enthalpy (H) = -5468.749996 .320841393561167

Gibbs Free Energy (G) = -5468.864385 .20645213424

Frequencies -- 6.02 12.20 21.46 26.41 29.49 32.87

Mono Cu(I) DiMeDHF-Z-Cis Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20831476650

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0006465	0.0010000	yes	0.0001068	0.0005000	yes
Grad	0.0007521	0.0010000	yes	0.0001250	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.72451	-0.85796	-1.58598
C	-2.57015	0.46786	-1.52579
C	-1.90448	1.09640	-0.35901
C	-2.15355	-1.63823	-0.42834
C	3.75286	-2.05025	0.51652
C	2.74948	-0.87614	0.41840
C	3.27390	0.43483	0.33469
C	2.46158	1.56427	0.19369
C	3.13845	2.94234	0.04462
C	-2.72993	1.69102	0.74793
C	-3.19253	-2.54664	0.24314
O	-1.69148	-0.71251	0.52607
O	1.20022	1.62770	0.15195
O	1.55182	-1.22793	0.40873
Cu	-0.02504	0.11675	0.28760
F	2.65563	3.79807	0.95379
F	2.88485	3.44769	-1.17210
F	4.46954	2.88993	0.19575
F	5.02206	-1.64183	0.67503
F	3.70022	-2.79129	-0.59972
F	3.44351	-2.83752	1.55187
H	-3.20037	-1.36848	-2.42799
H	-2.88202	1.12987	-2.34284
H	-1.09149	1.78273	-0.66078
H	4.35181	0.56935	0.36214
H	-2.09829	1.98695	1.59911
H	-3.21464	2.61056	0.36840
H	-3.50626	0.99543	1.09155

H	-1.32673	-2.28036	-0.80302
H	-4.03918	-1.95159	0.61911
H	-3.57250	-3.29277	-0.47351
H	-2.73274	-3.07824	1.08898

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20831476650

Zero-point correction (ZPE) = -2888.994755 .21355935294

Internal Energy (U) = -2889.130366 .07794826551

Enthalpy (H) = -2888.972085 .236228926544318

Gibbs Free Energy (G) = -2889.050036 .15827844606

Frequencies -- i326.97 15.14 22.71 24.59 29.19 37.71

Dual Cu(I) DiMeDHF-Z-Cis Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

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Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04987663737

Item	Max Val.	Criteria Pass?	RMS Val.	Criteria Pass?
Energy	0.0000010	0.0000010	yes	
Step	0.0005613	0.0010000	yes	0.0000861 / 0.0005000	yes
Grad	0.0002956	0.0010000	yes	0.0000508 / 0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.64698	-0.97745	-1.66946
C	-0.47879	0.39375	-1.56562
C	0.44490	0.95678	-0.53296
C	0.14146	-1.77899	-0.65356
O	0.57406	-0.86918	0.32876
C	-4.98974	2.86724	0.66116
C	-4.46267	1.48038	0.23563
C	-5.30552	0.36654	0.38803
C	-4.91639	-0.93652	0.03223
O	-3.81723	-1.32106	-0.44550
Cu	-2.31841	-0.10067	-0.82792
C	-5.92867	-2.08471	0.23474
F	-5.43927	-2.97643	1.10507
F	-6.14668	-2.71211	-0.92705
F	-7.11033	-1.65803	0.70141
O	-3.29173	1.51443	-0.22452
F	-4.17486	3.40135	1.57993
F	-6.22394	2.81916	1.18037
F	-5.01811	3.68796	-0.39635
C	6.03102	-2.20955	0.50538
C	5.02940	-1.03796	0.37119
C	5.55350	0.27097	0.26222
C	4.74250	1.39651	0.09010
C	5.41634	2.77232	-0.08852
O	3.48039	1.45673	0.03948
O	3.83110	-1.39167	0.35637
Cu	2.26585	-0.06110	0.17287
F	4.94622	3.63928	0.81595

F	5.14157	3.25805	-1.30829
F	6.74885	2.72115	0.04210
F	7.30097	-1.79732	0.63943
F	5.96760	-2.98961	-0.58280
F	5.72622	-2.95649	1.57106
H	-1.03922	-1.45716	-2.57279
H	-0.70973	1.05657	-2.41060
H	1.28462	1.47801	-1.02899
H	-6.30054	0.51847	0.79756
H	6.63122	0.40630	0.29338
C	-0.08108	1.73240	0.64024
H	0.73669	2.17110	1.23013
H	-0.72141	2.55488	0.27209
H	-0.70521	1.09650	1.28405
H	0.99907	-2.23998	-1.19130
C	-0.64564	-2.90309	0.02435
H	-1.51083	-2.50002	0.57190
H	-1.01534	-3.61620	-0.72959
H	0.00477	-3.44152	0.72862

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04987663737

Zero-point correction (ZPE) = -5468.767568 .28230817264

Internal Energy (U) = -5468.934540 .11533654211

Enthalpy (H) = -5468.730425 .319451181971648

Gibbs Free Energy (G) = -5468.845763 .20411353173

Frequencies -- i311.42 7.48 10.03 13.07 18.95 22.27

Mono Cu(I) DiMeDHF-Z-Cis Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20994683908

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0008740	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0003448	0.0010000	yes	0.0000407	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.65886	3.01474	1.66687
C	-0.64843	2.75742	1.56246
C	-1.18618	2.07336	0.36434
C	1.51467	2.50103	0.53690
C	2.15281	-3.37741	-1.16956
C	0.96189	-2.44038	-0.85986
C	-0.31587	-3.02268	-0.69297
C	-1.45411	-2.26526	-0.39884
C	-2.80022	-2.99667	-0.21881
C	2.57286	1.49515	1.00056
C	-1.79594	2.87994	-0.74915
O	0.65815	2.00318	-0.45960
O	-1.55015	-1.01464	-0.24831
O	1.27163	-1.23286	-0.79060
Cu	-0.08824	0.27652	-0.35884
F	-3.69775	-2.53052	-1.09737
F	-3.28109	-2.78127	1.01413
F	-2.70393	-4.32218	-0.39431
F	1.80808	-4.67455	-1.19125
F	3.10839	-3.22388	-0.24428
F	2.67844	-3.07443	-2.36356
H	1.10597	3.51516	2.53024
H	-1.35623	2.99489	2.36584
H	-1.82381	1.20947	0.62821
H	2.03089	3.37101	0.07651
H	-0.41710	-4.10053	-0.78716
H	3.12993	1.10736	0.13494
H	3.28561	1.96398	1.69941

H	2.09910	0.64094	1.51130
H	-2.04636	2.24297	-1.61089
H	-2.74299	3.32049	-0.38414
H	-1.12887	3.68968	-1.07222

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20994683908

Zero-point correction (ZPE) = -2888.996387 .21355935294

Internal Energy (U) = -2889.132671 .07727485864

Enthalpy (H) = -2888.973794 .236152750566810

Gibbs Free Energy (G) = -2889.051070 .15887642748

Frequencies -- i327.03 16.65 25.08 28.54 29.75 45.01

Dual Cu(I) DiMeDHF-Z-Cis Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

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Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05025436947

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0006532	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0007945	0.0010000	yes	0.0001082	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.87987	0.89515	1.78431
C	-0.48393	0.66914	1.68342
C	-1.00749	-0.30298	0.67644
C	1.70781	0.11434	0.78135
O	0.81276	-0.33849	-0.20369
C	-2.71838	5.15202	-1.04573
C	-1.39134	4.59551	-0.48627
C	-0.22158	5.35231	-0.66529
C	1.03996	4.92979	-0.20888
O	1.33561	3.86642	0.39439
Cu	0.00087	2.48504	0.84809
C	2.24992	5.86265	-0.43677
F	3.22497	5.20827	-1.07596
F	2.72982	6.27784	0.74308
F	1.93854	6.94832	-1.15868
O	-1.52185	3.48106	0.08570
F	-3.22459	4.29738	-1.94433
F	-2.57221	6.34201	-1.64424
F	-3.61184	5.29454	-0.05950
C	2.25446	-5.69750	-1.01625
C	1.06951	-4.76106	-0.68480
C	-0.20973	-5.33765	-0.51275
C	-1.34140	-4.58046	-0.19395
C	-2.69106	-5.30729	-0.01993
O	-1.42823	-3.33196	-0.01314
O	1.38688	-3.55522	-0.60172
Cu	0.04751	-2.06153	-0.12218
F	-3.58291	-4.83398	-0.89973

F	-3.17303	-5.09325	1.21225
F	-2.59770	-6.63174	-0.19969
F	1.90100	-6.99051	-1.06827
F	3.20819	-5.56956	-0.08477
F	2.78298	-5.36783	-2.20078
H	1.34334	1.32961	2.67639
H	-1.15580	0.89552	2.52201
H	-1.46505	-1.16629	1.19488
H	2.39913	0.80682	0.26088
H	-0.29358	6.30513	-1.18248
H	-0.31829	-6.41297	-0.62651
C	2.52874	-0.99433	1.44549
H	3.03404	-1.59763	0.67686
H	3.28962	-0.57247	2.12219
H	1.87904	-1.66287	2.03606
C	-1.84013	0.16384	-0.48379
H	-2.25892	-0.68364	-1.04539
H	-2.68082	0.77178	-0.10197
H	-1.25471	0.80670	-1.15636

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05025436947

Zero-point correction (ZPE) = -5468.767793 .28246052459

Internal Energy (U) = -5468.936179 .11407489786

Enthalpy (H) = -5468.730810 .319443564373898

Gibbs Free Energy (G) = -5468.844883 .20537043536

Frequencies -- i309.36 7.82 10.78 14.78 24.41 25.07

Mono Cu(I) DiMeDHF-Z-Cis Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27811550316

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0007912	0.0010000	yes	0.0001103	0.0005000	yes
Grad	0.0001598	0.0010000	yes	0.0000337	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.53833	-1.91288	0.64778
C	0.46289	-2.50728	0.01259
C	-0.63717	-2.71532	1.04603
C	1.16736	-1.71493	2.11251
C	-2.39612	1.52627	-2.80908
C	-1.11929	1.30312	-1.96961
C	-0.31472	2.41603	-1.66936
C	0.84721	2.32161	-0.88401
C	1.65270	3.60885	-0.60439
C	-2.06849	-2.43561	0.62152
C	1.57847	-0.41258	2.77760
O	-0.25330	-1.84298	2.10708
O	1.34720	1.29840	-0.35049
O	-0.95111	0.10390	-1.62972
Cu	0.52574	-0.50241	-0.45501
F	1.74772	3.81102	0.71601
F	1.09788	4.70150	-1.14909
F	2.89248	3.48978	-1.09666
F	-3.47531	1.18977	-2.08962
F	-2.37199	0.75780	-3.90402
F	-2.54587	2.79946	-3.20354
H	2.57344	-1.90701	0.29376
H	0.49677	-3.05476	-0.93389
H	-0.56426	-3.77331	1.39205
H	1.61360	-2.56542	2.67985
H	-0.60861	3.39000	-2.05122
H	-2.38545	-3.15703	-0.14828
H	-2.74176	-2.53582	1.48632

H	-2.16933	-1.42211	0.20530
H	1.16691	-0.36698	3.79727
H	2.67604	-0.34802	2.84462
H	1.21805	0.45692	2.20771

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27811550316

Zero-point correction (ZPE) = -2889.061356 .21675874399

Internal Energy (U) = -2889.202280 .07583492623

Enthalpy (H) = -2889.039018 .239096952097488

Gibbs Free Energy (G) = -2889.114855 .16326035499

Frequencies -- 20.80 27.38 32.52 38.29 44.28 84.55

Dual Cu(I) DiMeDHF-Z-Cis Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11126364820

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008913	0.0010000	yes	0.0001333	0.0005000	yes
Grad	0.0004689	0.0010000	yes	0.0000810	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.31555	-2.43323	1.09487
C	-1.59054	-2.38782	0.58788
C	-2.53463	-1.93711	1.69032
C	-0.36228	-2.00234	2.55130
O	-1.66115	-1.43548	2.69848
C	5.55039	1.64935	-0.95988
C	4.11072	1.11588	-0.76879
C	3.80849	-0.16040	-1.29472
C	2.55882	-0.78646	-1.20336
O	1.50620	-0.32328	-0.68406
Cu	1.49893	1.70434	0.18273
C	2.43543	-2.22380	-1.75223
F	1.25272	-2.39849	-2.35534
F	2.49762	-3.10238	-0.72766
F	3.39919	-2.54321	-2.61822
O	3.37272	1.91573	-0.14503
F	5.52110	2.81690	-1.61101
F	6.32940	0.80897	-1.65779
F	6.12502	1.84756	0.23202
C	-3.63708	0.83885	-2.74926
C	-2.47523	0.91887	-1.73008
C	-2.30119	2.13520	-1.01946
C	-1.28429	2.33198	-0.09172
C	-1.14928	3.71038	0.58196
O	-0.42454	1.47311	0.29727
O	-1.82102	-0.13505	-1.63083
Cu	-0.49452	-0.78436	-0.23872
F	-1.32943	3.59878	1.90242

F	-2.02027	4.60977	0.11521
F	0.09228	4.19677	0.38031
F	-4.53703	-0.06317	-2.32576
F	-3.18562	0.44626	-3.94297
F	-4.27395	2.00801	-2.90921
H	0.52965	-2.97702	0.66700
H	-1.94015	-2.88009	-0.32407
H	-3.05556	-2.85071	2.06097
H	-0.28273	-2.92646	3.16971
H	4.60660	-0.69551	-1.80364
H	-2.97455	2.96066	-1.23501
C	-3.57904	-0.88777	1.34475
H	-4.22300	-1.22925	0.51916
H	-4.21236	-0.67926	2.22021
H	-3.08772	0.04899	1.04380
C	0.69178	-1.01140	3.01884
H	0.51658	-0.73954	4.07083
H	1.69934	-1.44937	2.93643
H	0.64978	-0.09341	2.41235

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11126364820

Zero-point correction (ZPE) = -5468.827165 .28409830811

Internal Energy (U) = -5468.994959 .11630406768

Enthalpy (H) = -5468.789302 .321961180430532

Gibbs Free Energy (G) = -5468.905607 .20565609527

Frequencies -- 6.38 10.84 18.29 20.48 24.74 26.04

Mono Cu(I) DiMeDHF-Z-Cis Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27588137608

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0008614	0.0010000	yes	0.0001316	0.0005000	yes
Grad	0.0000535	0.0010000	yes	0.0000150	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.29176	-1.71592	0.77557
C	0.34902	-2.24546	-0.08673
C	-0.93422	-2.48974	0.69765
C	0.66799	-1.59705	2.15821
C	-1.79697	1.72374	-3.44786
C	-0.82548	1.53420	-2.26121
C	-0.19853	2.67483	-1.72623
C	0.73929	2.60791	-0.68206
C	1.37799	3.92230	-0.18299
C	-1.18724	-3.97626	0.96461
C	0.91856	-0.31367	2.93383
O	-0.72946	-1.75282	1.90587
O	1.16175	1.58985	-0.07484
O	-0.69129	0.33461	-1.91201
Cu	0.49784	-0.23660	-0.43077
F	1.21234	4.04093	1.13978
F	0.85235	5.01140	-0.76286
F	2.69359	3.91684	-0.43782
F	-2.96604	1.12636	-3.19272
F	-1.27808	1.16686	-4.55150
F	-2.04403	3.01397	-3.71810
H	2.37406	-1.70959	0.61608
H	0.55389	-2.73051	-1.04576
H	-1.81928	-2.05970	0.19745
H	1.04219	-2.45325	2.76453
H	-0.44608	3.64806	-2.14156
H	-2.05688	-4.08984	1.62956
H	-1.39831	-4.51057	0.02390

H	-0.31700	-4.45258	1.44409
H	0.34002	-0.32440	3.86986
H	1.98674	-0.22387	3.18861
H	0.62950	0.56998	2.34541

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27588137608

Zero-point correction (ZPE) = -2889.059084 .21679683198

Internal Energy (U) = -2889.199452 .07642884157

Enthalpy (H) = -2889.036696 .239184554471622

Gibbs Free Energy (G) = -2889.113127 .16275378474

Frequencies -- 20.24 26.77 27.73 34.04 38.60 81.36

Dual Cu(I) DiMeDHF-Z-Cis Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11045236287

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0001462	0.0010000	yes	0.0000221	0.0005000	yes
Grad	0.0000997	0.0010000	yes	0.0000190	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.35521	-1.86882	1.23379
C	-1.26585	-2.22836	0.27158
C	-2.66723	-1.97906	0.80496
C	-1.11508	-1.37724	2.45488
O	-2.44154	-1.17614	1.96720
C	5.91579	1.20087	-0.34673
C	4.40454	0.88791	-0.45186
C	4.02724	-0.34722	-1.02340
C	2.70273	-0.78838	-1.15704
O	1.65156	-0.16377	-0.85428
Cu	1.77301	1.80938	0.09405
C	2.46153	-2.21994	-1.68060
F	1.45070	-2.23807	-2.55807
F	2.10881	-3.01744	-0.64803
F	3.53299	-2.76297	-2.26357
O	3.68424	1.80802	0.00785
F	6.21306	2.27650	-1.08507
F	6.68868	0.18756	-0.76726
F	6.24012	1.46403	0.92373
C	-3.59718	1.30293	-2.72615
C	-2.37613	1.31198	-1.77589
C	-2.08098	2.51588	-1.07957
C	-1.00550	2.64260	-0.21214
C	-0.74782	3.99505	0.47279
O	-0.17227	1.73023	0.12017
O	-1.78198	0.22086	-1.71277
Cu	-0.43802	-0.40198	-0.32697
F	-0.86821	3.86727	1.80033

F	-1.58069	4.95667	0.06727
F	0.51094	4.40197	0.21618
F	-4.51612	0.44492	-2.25798
F	-3.23272	0.89976	-3.94588
F	-4.17832	2.50540	-2.84236
H	0.69208	-2.17669	1.26224
H	-1.06208	-2.85736	-0.59978
H	-3.27955	-1.38653	0.10365
H	-1.10458	-2.20570	3.20023
H	4.82034	-1.01068	-1.35884
H	-2.71601	3.38171	-1.24937
C	-3.40832	-3.27717	1.13848
H	-4.36674	-3.04156	1.62575
H	-3.61851	-3.85228	0.22199
H	-2.81866	-3.91354	1.81770
C	-0.61456	-0.11711	3.14334
H	-1.28195	0.14321	3.97900
H	0.39655	-0.28000	3.55048
H	-0.58307	0.73329	2.44598

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11045236287

Zero-point correction (ZPE) = -5468.826049 .28440301202

Internal Energy (U) = -5468.994207 .11624501682

Enthalpy (H) = -5468.788277 .322174473167554

Gibbs Free Energy (G) = -5468.904522 .20593032879

Frequencies -- 7.07 11.35 14.32 16.14 27.12 27.80

4. Cu(I)-catalyzed rearrangement of Z-Trans dimethylvinyloxiranes

4.a. Additional Figures

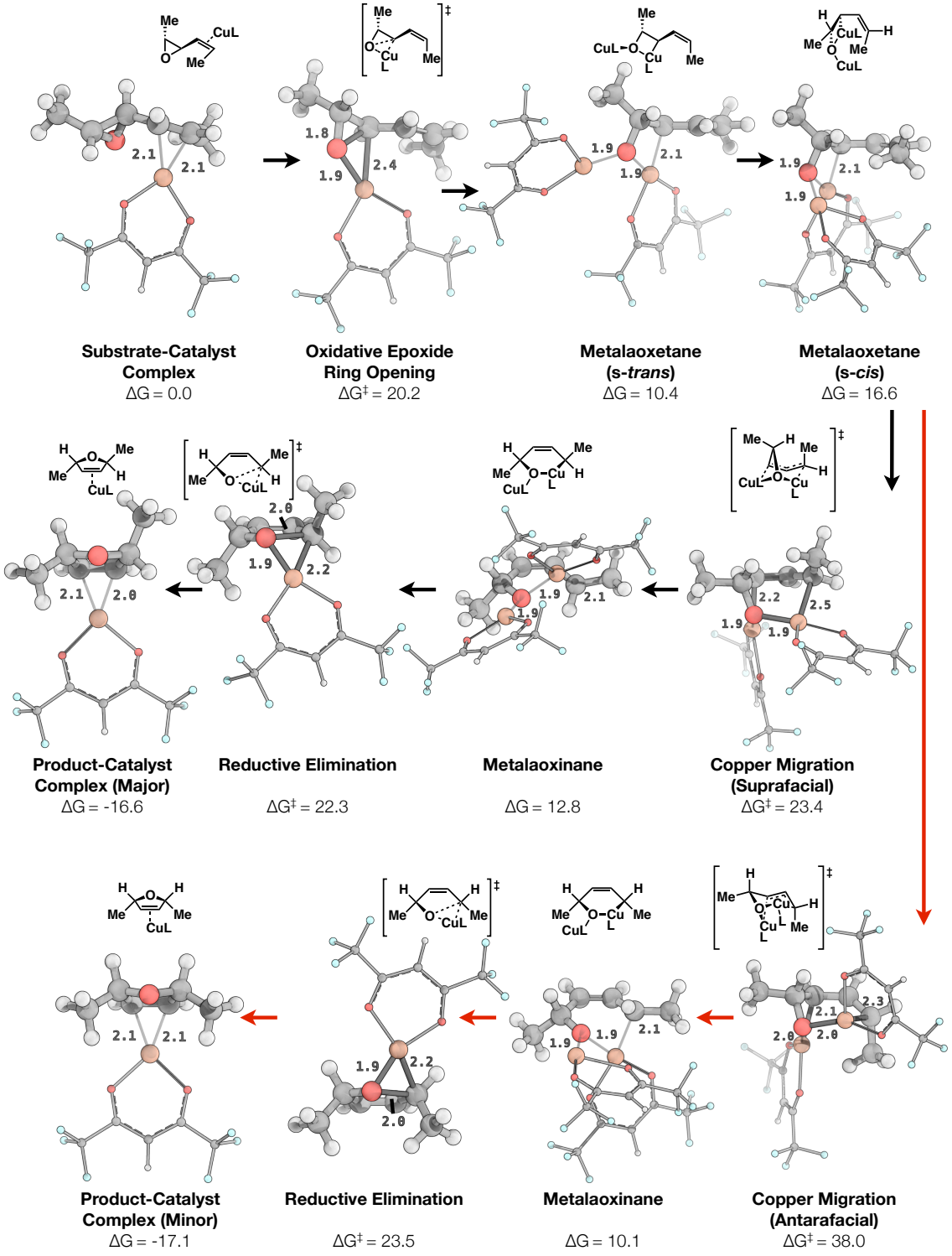


Figure 10. Structures of stationary points for both major and minor pathways for Z-Trans VO. All structures, energies, and free energy corrections

computed at the B3LYP/def2-SVP level of theory, as implemented in Turbomole. Figures rendered using Pymol.

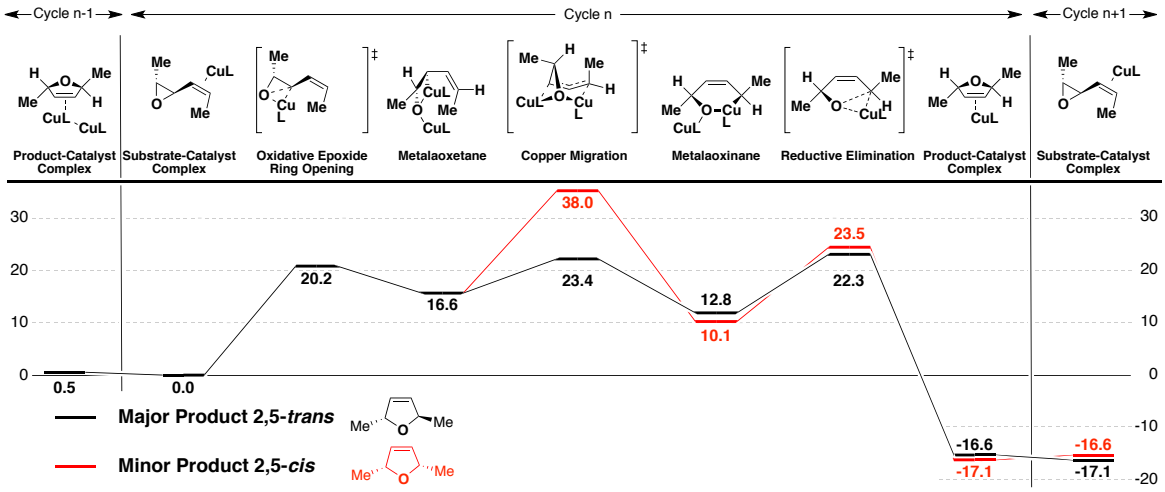


Figure 11. Reaction coordinate of Cu(I)-catalyzed ring expansion of Z-Trans VO.

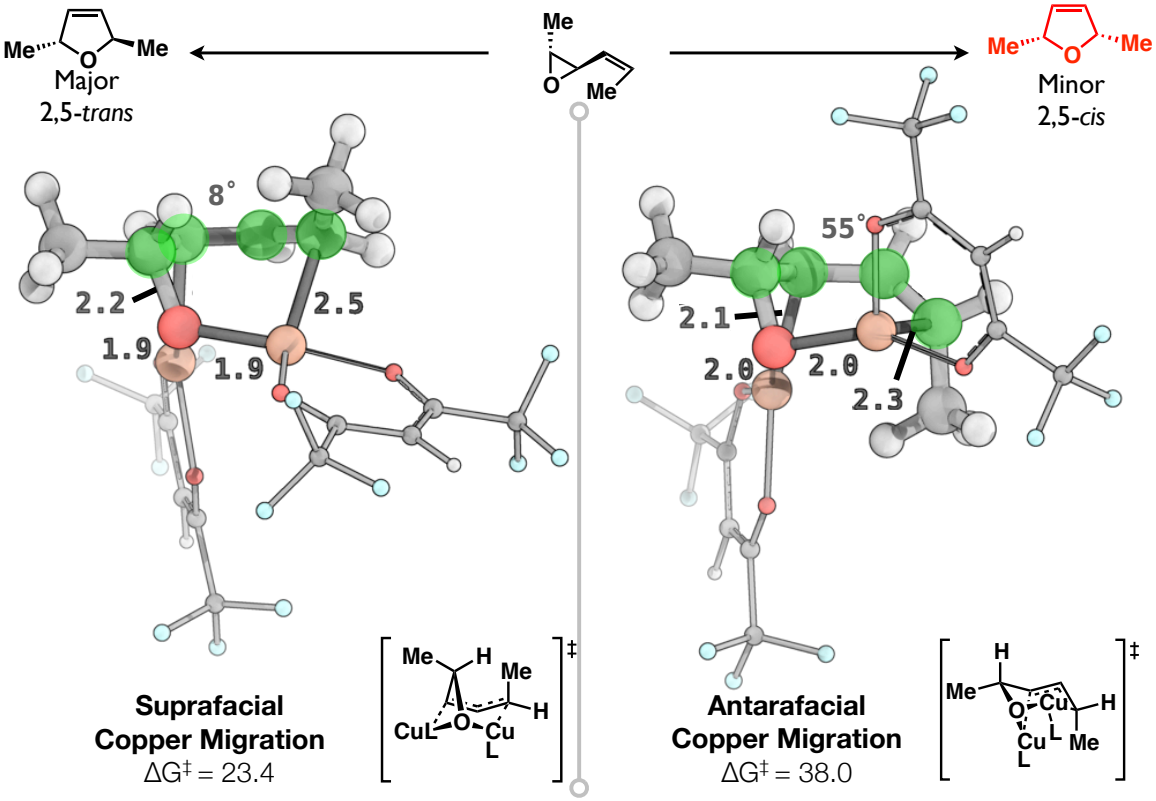


Figure 12. Stereoselective copper migration of Z-Trans VO showing π-allyl distortion (green highlight with dihedral), and TS bond distances.

4.b. Geometries, Energies, and Thermal Corrections
Mono Cu(I) DiMeDHF-Z-Trans Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP		Atoms: 32		
Charge: 0	Spin: 1		Basis Functions: 366		

Energy = -2889.24679824241

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0004077	0.0010000	yes	0.0000699	0.0005000	yes
Grad	0.0000550	0.0010000	yes	0.0000132	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.88457	3.22043	-0.25576
C	-1.72986	1.68747	-0.35821
C	-2.86608	0.88647	-0.15402
H	-3.80905	1.37237	0.08174
C	-2.83591	-0.51820	-0.24439
O	-1.85568	-1.26210	-0.49550
C	-4.15158	-1.29723	-0.02249
F	-4.48092	-1.96418	-1.13698
F	-5.18289	-0.50244	0.29962
F	-3.99714	-2.18941	0.96277
O	-0.55792	1.32457	-0.63822
F	-1.67157	3.78275	-1.45390
F	-0.98288	3.71805	0.60012
F	-3.10091	3.59806	0.16276
Cu	-0.01778	-0.57953	-0.78121
C	2.74062	-0.42309	0.09345
H	3.74285	-0.86548	0.22278
C	1.98568	-0.93065	-1.09921
H	2.22460	-0.45354	-2.05866
C	1.28857	-2.13281	-1.11387
H	0.97067	-2.50801	-2.09607
C	2.51888	0.90817	0.68782
H	1.73040	1.53051	0.24214
O	2.00979	-0.28223	1.31281
C	1.19243	-3.12183	0.02057
H	0.17803	-3.54607	0.08472
H	1.88363	-3.96497	-0.16232

H	1.44470	-2.67346	0.99114
C	3.59787	1.64846	1.43212
H	4.10457	2.36588	0.76553
H	3.16360	2.21784	2.26976
H	4.34787	0.95418	1.84094

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.24679824241

Zero-point correction (ZPE) = -2889.031753 .21504478450

Internal Energy (U) = -2889.168647 .07815040114

Enthalpy (H) = -2889.008504 .238293295534780

Gibbs Free Energy (G) = -2889.086653 .16014475751

Frequencies -- 21.40 29.94 31.84 34.21 43.88 64.63

Dual Cu(I) DiMeDHF-Z-Trans Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 64
Charge: 0 | Spin: 1 | Basis Functions: 732

Energy = -5778.54307443494

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000100	yes			
Step	0.0008982	0.0010000	yes	0.0001086	0.0005000	yes
Grad	0.0001156	0.0010000	yes	0.0000200	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.70781	-0.64236	2.23182
C	0.71276	-0.32723	1.93256
C	1.79968	-1.30004	2.18913
C	-1.62409	0.23955	2.77856
O	1.32562	-1.06498	0.85395
C	-5.77292	-2.07347	-0.23397
C	-4.77208	-0.91406	-0.01662
C	-5.22377	0.39853	-0.27649
C	-4.41657	1.53536	-0.11465
C	-5.02840	2.91520	-0.44119
O	-3.22333	1.60762	0.27377
O	-3.64721	-1.29007	0.37471
Cu	-2.02210	0.04014	0.72793
F	-4.29936	3.52853	-1.38719
F	-5.02000	3.69308	0.65065
F	-6.29264	2.84616	-0.88365
F	-5.97886	-2.72710	0.91785
F	-5.27397	-2.95179	-1.12000
F	-6.96682	-1.66958	-0.69336
H	-0.95279	-1.71127	2.23718
H	0.99546	0.73218	1.94135
H	1.49413	-2.28526	2.57031
H	-2.54763	-0.20197	3.17223
H	-6.24531	0.53557	-0.62063
C	4.77566	2.65145	0.14419
C	4.30468	1.28648	-0.40112
C	5.24241	0.24267	-0.45914
C	4.88872	-1.08797	-0.76351

O	3.76839	-1.54675	-1.08128
Cu	2.10695	-0.38775	-1.27023
C	5.98273	-2.17031	-0.62574
F	5.99985	-2.96714	-1.69689
F	5.71790	-2.93225	0.45319
F	7.21314	-1.66114	-0.46887
O	3.07869	1.25779	-0.67597
F	4.24588	2.83762	1.36976
F	4.35966	3.65100	-0.63767
F	6.10735	2.74418	0.26102
C	0.61950	-1.28097	-2.41235
C	0.63750	0.06982	-2.68348
C	-0.55799	0.73810	-2.03830
O	-1.03885	-0.28605	-1.13444
C	-0.59682	-1.60032	-1.56327
H	6.27555	0.45823	-0.19912
H	1.15396	-2.05451	-2.97046
H	1.19804	0.55275	-3.48877
H	-1.32781	0.90736	-2.81966
H	-0.33276	-2.15275	-0.64873
C	-1.39333	1.67914	3.15594
C	3.20716	-0.89014	2.52491
C	-1.68887	-2.34291	-2.32932
C	-0.31374	2.04468	-1.30440
H	-0.51551	2.12173	2.66406
H	-1.24835	1.76587	4.24816
H	-2.26978	2.29138	2.89361
H	3.42883	0.12728	2.17250
H	3.92947	-1.58621	2.07091
H	3.35179	-0.92026	3.61730
H	-1.97991	-1.79931	-3.24248
H	-2.57608	-2.47223	-1.69327
H	-1.32581	-3.34034	-2.62603
H	0.45655	1.92272	-0.52815
H	-1.24747	2.41614	-0.85852
H	0.05079	2.80019	-2.01860

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5778.54307443494

Zero-point correction (ZPE) = -5778.109633 .43344131201

Internal Energy (U) = -5778.409545 .13352874813

Enthalpy (H) = -5778.063143 .479931113787445

Gibbs Free Energy (G) = -5778.196671 .34640264011

Frequencies -- 10.38 12.53 16.27 22.55 26.59 31.83

Mono Cu(I) DiMeDHF-Z-Trans Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.21073169224

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0006273	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0003357	0.0010000	yes	0.0000896	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.20231	-0.97493	0.07392
C	2.46358	0.11754	-0.84457
C	2.50716	1.42892	-0.50981
C	2.45879	-2.37947	-0.26197
C	2.90143	-3.36173	0.79849
C	2.21444	2.05722	0.81303
O	1.06400	-2.26955	-0.42114
H	2.01809	-0.76109	1.12979
H	2.70049	-0.16998	-1.87404
H	2.77861	2.12662	-1.31083
H	2.98188	-2.53005	-1.22366
H	2.65402	-4.38726	0.48204
H	3.99085	-3.30280	0.95638
H	2.38785	-3.16655	1.75270
H	1.30252	2.67162	0.72902
H	2.05265	1.33175	1.62251
H	3.03490	2.73187	1.11206
C	-4.48686	-1.19534	0.03775
C	-3.09275	-0.53778	-0.10140
C	-3.03639	0.87500	-0.16382
C	-1.83466	1.57811	-0.30476
C	-1.89409	3.11597	-0.41419
O	-0.65963	1.12576	-0.37393
O	-2.14897	-1.35266	-0.15003
Cu	-0.16745	-0.77876	-0.33126
F	-1.49440	3.50984	-1.63205
F	-1.06476	3.67852	0.48509
F	-3.11783	3.61795	-0.20304

F -4.76570 -1.92186 -1.05332
F -5.47611 -0.29971 0.19409
F -4.50858 -2.01340 1.09686
H -3.96539 1.43623 -0.10992
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.21073169224
Zero-point correction (ZPE) = -2888.997896 .21283568115
Internal Energy (U) = -2889.130479 .08025238449
Enthalpy (H) = -2888.974281 .236449836879090
Gibbs Free Energy (G) = -2889.054532 .15619884187

Frequencies -- i268.26 15.94 19.06 33.03 36.50 41.08

Dual Cu(I) DiMeDHF-Z-Trans Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05254760836

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0008661	0.0010000	yes	0.0001306	0.0005000	yes
Grad	0.0006111	0.0010000	yes	0.0000788	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	5.04682	-2.53426	-0.11669
C	4.42016	-1.12797	-0.22493
C	5.25483	-0.00889	-0.08064
C	4.78024	1.31473	-0.14864
C	5.79736	2.46522	0.02154
C	-0.16462	-1.00964	0.15043
H	-0.28183	-0.73148	1.20162
C	0.09179	0.03517	-0.84566
C	0.21634	1.40211	-0.59309
C	0.09842	-2.42494	-0.12539
O	3.60154	1.71426	-0.32952
O	3.17909	-1.15376	-0.44119
O	-1.30711	-2.31497	-0.24063
Cu	2.08057	0.48690	-0.56952
F	5.78504	3.24907	-1.06184
F	7.05129	2.02569	0.19960
F	5.46739	3.21134	1.08221
F	4.88822	-3.19738	-1.26804
F	4.43053	-3.23177	0.85162
F	6.35380	-2.50460	0.16914
H	6.31497	-0.17056	0.09516
H	0.06392	-0.30149	-1.88897
H	0.23880	2.05221	-1.47603
H	0.58379	-2.61678	-1.09715
C	-6.82415	-1.22017	-0.11825
C	-5.42183	-0.56534	-0.08929
C	-5.35647	0.84925	-0.06809
H	-6.28553	1.41249	-0.04173

C	-4.14899	1.55201	-0.10319
O	-2.97020	1.09753	-0.13365
Cu	-2.49822	-0.80161	-0.13406
C	-4.19698	3.09337	-0.13876
F	-3.73612	3.54103	-1.31607
F	-3.40882	3.60403	0.82457
F	-5.42704	3.59004	0.03663
O	-4.47756	-1.38059	-0.10930
F	-7.00855	-1.84434	-1.28972
F	-7.81822	-0.32974	0.03154
F	-6.93737	-2.12653	0.85809
C	0.59447	-3.34748	0.96118
H	0.34285	-4.38969	0.70952
H	1.68899	-3.26563	1.04883
H	0.12844	-3.10689	1.92956
C	-0.00523	2.10542	0.71851
H	-1.03707	2.49329	0.74541
H	0.13006	1.45240	1.59344
H	0.68219	2.95891	0.82146

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05254760836

Zero-point correction (ZPE) = -5468.770429 .28211773270

Internal Energy (U) = -5468.936781 .11576579641

Enthalpy (H) = -5468.732574 .319972987417577

Gibbs Free Energy (G) = -5468.848338 .20420875170

Frequencies -- i271.03 8.21 12.06 16.82 22.71 29.07

Mono Cu(I) DiMeDHF-Z-Trans Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22556391245

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000004	II	0.0000010	yes					
Step	0.0006643	II	0.0010000	yes	I	0.0001500	II	0.0005000	yes
Grad	0.0000495	II	0.0010000	yes	I	0.0000146	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.83505	-0.86099	-0.57243
C	2.03325	0.26507	-1.45684
C	2.35704	1.53516	-1.09622
C	1.81692	-2.27478	-1.10381
C	-4.51238	-0.93366	0.02307
C	-3.05364	-0.43118	0.13110
C	-2.82435	0.83507	0.71698
C	-1.53243	1.33107	0.89677
C	-1.35326	2.69602	1.59124
C	2.61328	-3.28992	-0.30122
C	2.53964	2.09062	0.27631
O	0.42465	-2.48348	-1.00665
O	-0.43167	0.79823	0.57307
O	-2.20176	-1.23620	-0.29713
Cu	-0.19836	-0.91234	-0.30873
F	-0.61665	3.51491	0.82253
F	-0.70781	2.53671	2.75446
F	-2.51545	3.30932	1.84382
F	-4.74353	-1.44113	-1.18847
F	-5.40854	0.04130	0.24310
F	-4.72281	-1.89578	0.93128
H	2.06946	-0.74303	0.49267
H	1.94592	0.04748	-2.52751
H	2.52937	2.24355	-1.91626
H	2.14486	-2.29960	-2.16389
H	-3.67218	1.43149	1.04312
H	2.40099	-4.30410	-0.67555
H	3.69828	-3.10736	-0.38359

H	2.32190	-3.25452	0.76125
H	1.86151	2.94748	0.42479
H	2.33519	1.36627	1.07500
H	3.56749	2.47831	0.39774

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22556391245

Zero-point correction (ZPE) = -2889.010938 .21462581662

Internal Energy (U) = -2889.147843 .07772001124

Enthalpy (H) = -2888.987742 .237821004474232

Gibbs Free Energy (G) = -2889.065461 .16010286072

Frequencies -- 18.07 25.64 34.28 37.02 66.26 77.08

Dual Cu(I) DiMeDHF-Z-Trans Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.06928530782

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000010	II	0.0000100	yes					
Step	0.0001747	II	0.0010000	yes	I	0.0000340	II	0.0005000	yes
Grad	0.0003224	II	0.0010000	yes	I	0.0000726	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.28127	1.35227	-0.45301
H	2.51644	1.43998	0.61540
C	2.56031	2.46920	-1.31422
C	2.89063	3.73605	-0.93025
C	2.18182	-0.05990	-0.99624
O	0.77021	-0.26462	-0.85839
H	2.51295	2.26652	-2.39058
H	3.10773	4.44692	-1.73697
H	2.43642	-0.08032	-2.07244
C	-4.07766	1.20897	0.21239
C	-2.63400	1.75915	0.27957
C	-2.42885	3.04627	0.82465
H	-3.28963	3.62015	1.15789
C	-1.15346	3.59880	0.96271
O	-0.03576	3.11115	0.62098
Cu	0.21901	1.38089	-0.18647
C	-1.01582	4.97808	1.63924
F	-0.26651	5.79361	0.88203
F	-0.40572	4.84149	2.82410
F	-2.19432	5.57510	1.84535
O	-1.76056	0.97196	-0.14828
F	-4.30717	0.66349	-0.98308
F	-4.99470	2.16653	0.41707
F	-4.24529	0.26963	1.14817
C	2.99000	-1.10940	-0.25756
H	2.75324	-2.10909	-0.65588
H	4.07123	-0.93126	-0.38122
H	2.75220	-1.09573	0.81915

C	3.00885	4.28035	0.45194
H	2.29782	5.11392	0.58467
H	2.80129	3.54209	1.23716
H	4.01774	4.70164	0.61217
Cu	-0.21257	-1.82377	-0.38928
O	0.56194	-3.47569	-1.30704
O	-1.56143	-2.82151	0.59555
C	0.09189	-4.61978	-1.09717
C	-1.70059	-4.06917	0.52035
C	-0.97583	-4.99013	-0.25645
C	0.82364	-5.73338	-1.87973
C	-2.82133	-4.60797	1.43668
H	-1.24592	-6.04102	-0.19585
F	0.76961	-5.48622	-3.19486
F	0.30697	-6.95383	-1.67144
F	2.11556	-5.76979	-1.52048
F	-3.98474	-4.01345	1.14824
F	-2.99853	-5.93372	1.32334
F	-2.52840	-4.34446	2.71807

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.06928530782

Zero-point correction (ZPE) = -5468.786367 .28291758046

Internal Energy (U) = -5468.949232 .12005266144

Enthalpy (H) = -5468.748063 .321222273448706

Gibbs Free Energy (G) = -5468.868115 .20116933020

Frequencies -- 1.86 7.31 9.84 18.12 21.50 26.73

Mono Cu(I) DiMeDHF-Z-Trans Metalaoxetane (s-*cis*)

Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: | Basis Functions: 366

Energy = -2889.22149921010

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000005	0.0000010	yes			
Step	0.0007658	0.0010000	yes	0.0001504	0.0005000	yes
Grad	0.0000910	0.0010000	yes	0.0000219	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.32513	2.02909	-0.12092
C	0.35616	2.00398	1.33208
C	-0.67247	2.02686	2.22128
C	-0.82601	2.53086	-0.96026
O	-1.38619	1.26294	-1.24562
C	-1.17706	-4.04720	-1.08637
C	-0.32960	-2.80180	-0.73676
C	0.95963	-2.99814	-0.19538
C	1.77263	-1.92395	0.17486
O	1.52956	-0.68638	0.08647
Cu	-0.11374	0.10003	-0.58411
C	3.15192	-2.21863	0.79933
F	3.18002	-1.77864	2.06536
F	4.11467	-1.58586	0.11999
F	3.44553	-3.52569	0.81172
O	-0.90354	-1.71599	-0.97034
F	-2.29263	-4.05779	-0.34802
F	-0.52248	-5.19681	-0.85937
F	-1.52676	-4.02071	-2.37567
H	1.30785	2.02058	-0.61008
H	1.36418	1.92976	1.75438
H	-0.38213	2.05849	3.27871
H	-1.52717	3.15148	-0.37060
H	1.32568	-4.01113	-0.05304
C	-0.42360	3.28564	-2.21689
H	-1.31019	3.44729	-2.85021
H	0.01303	4.26857	-1.97093
H	0.30930	2.70517	-2.80088

C	-2.14372	1.94900	1.96035
H	-2.61443	1.26260	2.68464
H	-2.62343	2.93261	2.12161
H	-2.38013	1.60378	0.94466

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22149921010

Zero-point correction (ZPE) = -2889.006568 .21493052053

Internal Energy (U) = -2889.143644 .07785514686

Enthalpy (H) = -2888.983491 .238007635619126

Gibbs Free Energy (G) = -2889.061346 .16015237511

Frequencies -- 18.57 25.10 27.31 30.47 58.54 72.15

Dual Cu(I) DiMeDHF-Z-Trans Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: * | Basis Functions: 584

Energy = -5469.06414246118

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0008655	0.0010000	yes	0.0001467	0.0005000	yes
Grad	0.0000620	0.0010000	yes	0.0000112	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.46775	2.44485	-0.68140
C	1.70630	2.53951	0.73670
C	0.86370	2.79292	1.78001
C	0.24793	2.88117	-1.47138
O	-0.23226	1.59885	-1.89498
C	0.34998	-3.66585	-2.00636
C	1.04689	-2.40215	-1.45304
C	2.21406	-2.56365	-0.67859
C	2.89191	-1.47772	-0.12022
O	2.61155	-0.24573	-0.18985
Cu	1.03023	0.46990	-1.03204
C	4.17602	-1.74262	0.69217
F	4.05897	-1.22573	1.91965
F	5.22053	-1.15550	0.09202
F	4.45040	-3.04733	0.81465
O	0.47302	-1.33135	-1.75622
F	-0.87207	-3.77653	-1.47174
F	1.02636	-4.78937	-1.72709
F	0.22167	-3.57905	-3.33328
C	-5.05386	-1.58096	0.13419
C	-3.64315	-0.94875	0.13132
C	-2.76657	-1.29576	1.17715
C	-1.45586	-0.80060	1.31565
C	-0.62662	-1.27514	2.53028
O	-0.84809	0.00933	0.57755
O	-3.46628	-0.16886	-0.83995
Cu	-1.84056	0.71697	-1.29009
F	-0.28967	-0.21593	3.29101

F	0.51325	-1.85166	2.11539
F	-1.26590	-2.15050	3.31518
F	-5.98127	-0.62720	0.30108
F	-5.22186	-2.48656	1.11027
F	-5.29001	-2.18900	-1.03293
H	2.38281	2.38797	-1.28688
H	2.74785	2.34633	1.01160
H	1.35630	2.85147	2.75869
H	-0.49244	3.38423	-0.83021
H	2.59716	-3.56546	-0.50598
H	-3.12676	-1.99886	1.92369
C	0.55938	3.76084	-2.66819
H	-0.35632	3.92248	-3.25909
H	0.94535	4.74275	-2.34697
H	1.30600	3.27915	-3.31991
C	-0.61532	2.97105	1.83004
H	-1.01701	2.36770	2.66071
H	-0.86657	4.02335	2.06126
H	-1.13692	2.66699	0.91612

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.06414246118

Zero-point correction (ZPE) = -5468.780805 .28333654834

Internal Energy (U) = -5468.948516 .11562611842

Enthalpy (H) = -5468.742695 .321446992582354

Gibbs Free Energy (G) = -5468.858318 .20582368242

Frequencies -- 7.46 8.93 22.57 28.19 29.71 31.58

Dual Cu(I) DiMeDHF-Z-Trans Suprafacial Copper Migration (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.05136659506

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000010	yes			
Step	0.0003997	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0009828	0.0010000	yes	0.0002124	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.16585	-2.54853	0.75867
C	-0.83724	-1.73637	1.86728
C	0.43056	-1.31261	2.27356
C	-0.12599	-2.92934	-0.27680
O	0.15673	-1.61925	-0.80068
C	-2.26254	3.00921	-2.32224
C	-2.54602	1.69910	-1.55243
C	-3.82695	1.52098	-0.98713
C	-4.16972	0.38437	-0.24798
O	-3.45410	-0.62015	0.02967
Cu	-1.59868	-0.84662	-0.52218
C	-5.59471	0.28134	0.33397
F	-5.53748	0.18124	1.66852
F	-6.20366	-0.81322	-0.13872
F	-6.35612	1.34074	0.03137
O	-1.57085	0.91464	-1.51228
F	-1.23829	3.65574	-1.75529
F	-3.31787	3.83717	-2.33615
F	-1.93759	2.73500	-3.58975
H	-2.18707	-2.93631	0.67241
H	-1.68605	-1.23798	2.35191
H	0.42630	-0.45204	2.95292
H	0.78717	-3.37663	0.15024
H	-4.57138	2.30065	-1.12265
C	1.72293	-2.08240	2.33285
H	1.72721	-2.65437	3.28174
H	1.88146	-2.81274	1.52887
H	2.58653	-1.40240	2.38080

C	-0.64378	-3.85858	-1.36572
H	0.10315	-3.94205	-2.16874
H	-0.84119	-4.86462	-0.96078
H	-1.57811	-3.47142	-1.80582
C	2.97623	2.96701	2.13172
C	2.82659	1.86198	1.06493
C	3.78011	1.78742	0.04464
C	3.74157	0.79936	-0.96452
C	4.85447	0.80464	-2.03939
O	2.90048	-0.11265	-1.11586
O	1.82268	1.12021	1.27070
Cu	1.32634	-0.38312	0.14152
F	4.32249	1.01768	-3.24750
F	5.47596	-0.38106	-2.05949
F	5.78152	1.75010	-1.82393
F	1.89984	3.76099	2.12988
F	4.05711	3.73527	1.93972
F	3.07907	2.41184	3.34867
H	4.58475	2.51779	0.02947

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05136659506

Zero-point correction (ZPE) = -5468.768944 .28242243661

Internal Energy (U) = -5468.935425 .11594067779

Enthalpy (H) = -5468.731515 .319851105853565

Gibbs Free Energy (G) = -5468.847454 .20391166539

Frequencies -- i63.99 5.45 7.86 9.48 21.97 23.71

Dual Cu(I) DiMeDHF-Z-Trans Antarafacial Copper Migration (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.02889019094

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000010	yes			
Step	0.0006561	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0008945	0.0010000	yes	0.0001201	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.56773	-1.95018	0.29739
C	0.07507	-1.39567	1.45387
H	0.23459	-2.15332	2.23984
C	0.56568	-0.13231	1.77256
H	1.24211	-0.14573	2.63789
C	0.09516	-1.85422	-1.06834
H	1.14335	-2.20557	-1.02738
O	0.04045	-0.43319	-1.26656
C	-4.10639	3.19518	-1.07898
C	-3.74178	1.73633	-0.71844
C	-4.76293	0.88637	-0.24299
C	-4.51626	-0.43218	0.14840
O	-3.41693	-1.05980	0.17595
Cu	-1.72850	-0.34292	-0.42180
C	-5.70726	-1.30067	0.60718
F	-5.46869	-1.81453	1.81833
F	-5.87987	-2.31450	-0.25055
F	-6.85304	-0.61059	0.66749
O	-2.53198	1.45883	-0.88434
F	-3.42722	4.03425	-0.28749
F	-5.41401	3.45033	-0.92774
F	-3.77779	3.45374	-2.34684
C	5.43661	-1.92353	-0.56800
C	4.41760	-0.78452	-0.32716
C	4.91512	0.46258	0.11291
C	4.08807	1.55214	0.41526
C	4.75046	2.86304	0.89228
O	2.83123	1.63303	0.35078

O	3.23053	-1.11194	-0.53460
Cu	1.60084	0.20573	-0.21869
F	4.21752	3.25203	2.05920
F	4.53857	3.83613	-0.00319
F	6.07526	2.74773	1.06609
F	5.23019	-2.90926	0.31955
F	6.71223	-1.52625	-0.44614
F	5.28194	-2.43500	-1.79462
H	-1.23209	-2.80545	0.48046
H	-5.77760	1.26958	-0.17840
H	5.98845	0.57941	0.23574
C	-0.05802	1.23763	1.59633
H	0.71655	2.01825	1.62336
H	-0.65394	1.38367	0.68502
H	-0.72531	1.41242	2.46256
C	-0.63600	-2.61144	-2.16972
H	-1.70304	-2.33550	-2.21707
H	-0.17447	-2.38214	-3.14126
H	-0.56673	-3.69800	-1.99810

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.02889019094

Zero-point correction (ZPE) = -5468.747458 .28143214890

Internal Energy (U) = -5468.913653 .11523660989

Enthalpy (H) = -5468.709865 .319024596497604

Gibbs Free Energy (G) = -5468.825104 .20378597502

Frequencies -- i117.47 8.62 14.34 15.34 18.40 20.14

Mono Cu(I) DiMeDHF-Z-Trans Metalaoxinane (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22295336064

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0007866	0.0010000	yes	0.0000929	0.0005000	yes
Grad	0.0000316	0.0010000	yes	0.0000068	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.21735	2.98629	0.62596
C	-0.80815	2.62002	-0.18255
C	-0.71547	1.69877	-1.31154
C	1.55874	2.30871	0.58839
C	1.62882	-3.16723	2.08521
C	0.78407	-2.38359	1.05345
C	-0.36057	-3.01277	0.51211
C	-1.19250	-2.35170	-0.38993
C	-2.44588	-3.07552	-0.91959
C	-1.99508	1.25652	-1.96700
C	2.69367	3.34841	0.39886
O	1.66604	1.36669	-0.40612
O	-1.07606	-1.18268	-0.86236
O	1.20084	-1.23200	0.81476
Cu	0.29759	0.10369	-0.44868
F	-2.38927	-3.18185	-2.25282
F	-3.54308	-2.37265	-0.60646
F	-2.58628	-4.30683	-0.41164
F	1.24238	-4.44744	2.19921
F	1.51161	-2.59507	3.29117
F	2.91745	-3.15465	1.73862
H	0.05875	3.75469	1.39074
H	-1.80826	3.01620	0.03765
H	0.11363	1.88956	-1.99943
H	-0.60475	-4.02776	0.81283
H	-2.41701	2.12162	-2.51543
H	-1.83142	0.44991	-2.69307
H	-2.74741	0.91630	-1.24037

H 1.70771 1.87605 1.61087
H 2.58802 3.84768 -0.57621
H 2.67456 4.10474 1.19944
H 3.65994 2.82592 0.42392
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22295336064
Zero-point correction (ZPE) = -2889.008327 .21462581662
Internal Energy (U) = -2889.145914 .07703865521
Enthalpy (H) = -2888.985539 .237413462994565
Gibbs Free Energy (G) = -2889.062580 .16037328544

Frequencies -- 15.01 21.59 28.37 35.35 52.73 80.92

Dual Cu(I) DiMeDHF-Z-Trans Metalaoxinane (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07083784262

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008422	0.0010000	yes	0.0000932	0.0005000	yes
Grad	0.0000878	0.0010000	yes	0.0000150	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.36950	3.69401	0.85493
C	-2.43255	3.33311	0.08621
C	-2.42846	2.37882	-1.01127
C	-0.04004	3.00389	0.84768
O	-0.01034	1.93223	-0.05025
C	2.12705	-3.46118	-1.18766
C	2.41672	-1.99036	-0.81778
C	3.75036	-1.60926	-0.58810
C	4.12427	-0.30863	-0.19897
O	3.39397	0.69206	0.00623
Cu	1.41266	0.63269	-0.16101
C	5.62479	-0.02684	0.03724
F	5.83945	0.28296	1.32384
F	6.02149	1.01262	-0.70842
F	6.41023	-1.07175	-0.26706
O	1.38081	-1.28263	-0.76313
F	1.24013	-3.98211	-0.32367
F	3.21923	-4.23753	-1.16989
F	1.59231	-3.53640	-2.41462
C	-0.08923	-2.47992	2.39784
C	-0.96388	-1.69200	1.39672
C	-1.99221	-2.37761	0.71564
C	-2.87652	-1.72048	-0.13828
C	-4.02221	-2.52307	-0.78722
O	-2.90208	-0.49549	-0.47244
O	-0.69467	-0.47059	1.32599
Cu	-1.54017	0.78084	-0.03083
F	-3.98947	-2.37881	-2.11690

F	-5.20138	-2.06216	-0.34853
F	-3.95985	-3.82990	-0.50789
F	-0.23986	-3.80343	2.27886
F	-0.43713	-2.13594	3.64803
F	1.20234	-2.18572	2.23376
H	-1.49727	4.48707	1.59924
H	-3.40640	3.77567	0.33379
H	-1.57489	2.44360	-1.69456
H	4.52884	-2.35945	-0.69804
H	-2.10548	-3.44740	0.86880
C	-3.73355	2.00790	-1.65170
H	-4.05349	2.84299	-2.30593
H	-3.64319	1.11136	-2.27900
H	-4.52904	1.83334	-0.91205
H	0.13071	2.65886	1.89382
C	1.11396	3.97034	0.50310
H	0.98439	4.37135	-0.51341
H	1.15516	4.80583	1.21871
H	2.06401	3.41711	0.54820

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07083784262

Zero-point correction (ZPE) = -5468.787767 .28306993241

Internal Energy (U) = -5468.956447 .11439059282

Enthalpy (H) = -5468.749996 .320841393561167

Gibbs Free Energy (G) = -5468.864385 .20645213424

Frequencies -- 6.02 12.20 21.46 26.41 29.49 32.87

Mono Cu(I) DiMeDHF-Z-Trans Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.22503182874

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0008714	0.0010000	yes	0.0002089	0.0005000	yes
Grad	0.0000734	0.0010000	yes	0.0000139	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.34794	3.08394	-0.94369
C	-0.27253	2.27142	-1.83629
C	0.20068	0.96286	-2.26728
C	1.52239	2.63264	-0.12207
C	0.61204	-1.76305	3.50618
C	0.26561	-1.54877	2.01407
C	-0.64231	-2.43912	1.39702
C	-0.98599	-2.30130	0.05228
C	-1.97010	-3.30609	-0.57864
C	1.29782	2.89410	1.38062
C	-0.71178	0.12691	-3.12334
O	1.93802	1.35539	-0.41049
O	-0.58795	-1.43405	-0.77877
O	0.84607	-0.57501	1.49131
Cu	0.61269	0.04077	-0.44927
F	-1.36247	-3.98419	-1.56065
F	-3.01368	-2.65559	-1.11071
F	-2.44408	-4.19292	0.30566
F	-0.03295	-2.81106	4.04144
F	0.28237	-0.67467	4.21155
F	1.92476	-1.97191	3.64698
H	-0.03768	4.09354	-0.76621
H	-1.23069	2.60411	-2.25657
H	1.25905	0.92278	-2.54470
H	2.35108	3.31141	-0.45363
H	-1.07816	-3.24772	1.97749
H	2.20252	2.59999	1.93287
H	1.08254	3.95558	1.58748

H	0.46096	2.28460	1.75708
H	-0.77468	0.60038	-4.12270
H	-0.33083	-0.89305	-3.26242
H	-1.73064	0.05808	-2.71462

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.22503182874

Zero-point correction (ZPE) = -2889.010786 .21424493674

Internal Energy (U) = -2889.148030 .07700118063

Enthalpy (H) = -2888.988014 .237017347911524

Gibbs Free Energy (G) = -2889.065012 .16001906715

Frequencies -- 13.78 23.84 27.57 33.52 61.28 76.29

Dual Cu(I) DiMeDHF-Z-Trans Metalaoxinane (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.07611703167

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000006	0.0000010	yes			
Step	0.0007590	0.0010000	yes	0.0001492	0.0005000	yes
Grad	0.0000826	0.0010000	yes	0.0000201	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.19722	3.73214	-0.62909
C	-1.74286	2.88716	-1.54717
C	-1.14242	1.66997	-2.06241
C	0.05701	3.44769	0.14393
O	0.54278	2.17203	-0.12790
C	5.36536	-1.46057	0.51559
C	3.95623	-0.96014	0.12353
C	3.11961	-1.84527	-0.58528
C	1.80510	-1.55054	-0.99238
O	1.17182	-0.48016	-0.83774
Cu	2.14458	1.21785	0.25842
C	1.00125	-2.66031	-1.70821
F	0.48566	-2.19016	-2.85597
F	-0.02553	-3.05234	-0.93246
F	1.72659	-3.74559	-2.00257
O	3.74014	0.21592	0.51308
F	6.29843	-0.64048	0.01572
F	5.62773	-2.69907	0.06871
F	5.49473	-1.47219	1.84826
C	-0.73535	-1.04303	3.67789
C	-1.12396	-0.80264	2.20180
C	-2.06795	-1.66001	1.60294
C	-2.49775	-1.47581	0.28594
C	-3.56351	-2.43080	-0.29104
O	-2.14333	-0.59464	-0.54749
O	-0.54350	0.17762	1.68135
Cu	-0.76080	0.72996	-0.25733
F	-3.08345	-3.06405	-1.36526

F	-4.64079	-1.72716	-0.66888
F	-3.96471	-3.35349	0.59266
F	-1.34614	-2.11216	4.20720
F	-1.06844	0.02696	4.41167
F	0.58433	-1.22629	3.78163
H	-1.71911	4.66500	-0.39105
H	-2.74978	3.12246	-1.91504
H	-0.06584	1.70508	-2.25311
H	0.80604	4.17408	-0.25472
H	3.51572	-2.82964	-0.82057
H	-2.48539	-2.47817	2.18338
C	-0.10751	3.72116	1.64603
H	0.85871	3.55675	2.14725
H	-0.43175	4.75619	1.84065
H	-0.83924	3.02628	2.08612
C	-1.92123	0.79811	-2.99821
H	-1.91518	1.27828	-3.99712
H	-1.45313	-0.18971	-3.10758
H	-2.96597	0.66371	-2.68517

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.07611703167

Zero-point correction (ZPE) = -5468.793123 .28299375644

Internal Energy (U) = -5468.961956 .11416006737

Enthalpy (H) = -5468.755355 .320761408784783

Gibbs Free Energy (G) = -5468.869516 .20660067739

Frequencies -- 8.71 16.06 17.58 25.21 27.23 27.42

Mono Cu(I) DiMeDHF-Z-Trans Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp		Basis: def2-SVP		Atoms: 32	
Charge: 0	Spin: 1			Basis Functions: 366	

Energy = -2889.20994683908

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0008740	0.0010000	yes	0.0001054	0.0005000	yes
Grad	0.0003448	0.0010000	yes	0.0000407	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.65886	3.01474	1.66687
C	-0.64843	2.75742	1.56246
C	-1.18618	2.07336	0.36434
C	1.51467	2.50103	0.53690
C	2.15281	-3.37741	-1.16956
C	0.96189	-2.44038	-0.85986
C	-0.31587	-3.02268	-0.69297
C	-1.45411	-2.26526	-0.39884
C	-2.80022	-2.99667	-0.21881
C	2.57286	1.49515	1.00056
C	-1.79594	2.87994	-0.74915
O	0.65815	2.00318	-0.45960
O	-1.55015	-1.01464	-0.24831
O	1.27163	-1.23286	-0.79060
Cu	-0.08824	0.27652	-0.35884
F	-3.69775	-2.53052	-1.09737
F	-3.28109	-2.78127	1.01413
F	-2.70393	-4.32218	-0.39431
F	1.80808	-4.67455	-1.19125
F	3.10839	-3.22388	-0.24428
F	2.67844	-3.07443	-2.36356
H	1.10597	3.51516	2.53024
H	-1.35623	2.99489	2.36584
H	-1.82381	1.20947	0.62821
H	2.03089	3.37101	0.07651
H	-0.41710	-4.10053	-0.78716
H	3.12993	1.10736	0.13494
H	3.28561	1.96398	1.69941

H	2.09910	0.64094	1.51130
H	-2.04636	2.24297	-1.61089
H	-2.74299	3.32049	-0.38414
H	-1.12887	3.68968	-1.07222

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20994683908

Zero-point correction (ZPE) = -2888.996387 .21355935294

Internal Energy (U) = -2889.132671 .07727485864

Enthalpy (H) = -2888.973794 .236152750566810

Gibbs Free Energy (G) = -2889.051070 .15887642748

Frequencies -- i327.03 16.65 25.08 28.54 29.75 45.01

Dual Cu(I) DiMeDHF-Z-Trans Reductive Elimination TS (Major)
Using: TURBOMOLE V6.3

Method: B3-LYP	Basis: def2-SVP	Atoms: 47
Charge: 0	Spin: 1	Basis Functions: 584

Energy = -5469.05025436947

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0006532	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0007945	0.0010000	yes	0.0001082	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.87987	0.89515	1.78431
C	-0.48393	0.66914	1.68342
C	-1.00749	-0.30298	0.67644
C	1.70781	0.11434	0.78135
O	0.81276	-0.33849	-0.20369
C	-2.71838	5.15202	-1.04573
C	-1.39134	4.59551	-0.48627
C	-0.22158	5.35231	-0.66529
C	1.03996	4.92979	-0.20888
O	1.33561	3.86642	0.39439
Cu	0.00087	2.48504	0.84809
C	2.24992	5.86265	-0.43677
F	3.22497	5.20827	-1.07596
F	2.72982	6.27784	0.74308
F	1.93854	6.94832	-1.15868
O	-1.52185	3.48106	0.08570
F	-3.22459	4.29738	-1.94433
F	-2.57221	6.34201	-1.64424
F	-3.61184	5.29454	-0.05950
C	2.25446	-5.69750	-1.01625
C	1.06951	-4.76106	-0.68480
C	-0.20973	-5.33765	-0.51275
C	-1.34140	-4.58046	-0.19395
C	-2.69106	-5.30729	-0.01993
O	-1.42823	-3.33196	-0.01314
O	1.38688	-3.55522	-0.60172
Cu	0.04751	-2.06153	-0.12218
F	-3.58291	-4.83398	-0.89973

F	-3.17303	-5.09325	1.21225
F	-2.59770	-6.63174	-0.19969
F	1.90100	-6.99051	-1.06827
F	3.20819	-5.56956	-0.08477
F	2.78298	-5.36783	-2.20078
H	1.34334	1.32961	2.67639
H	-1.15580	0.89552	2.52201
H	-1.46505	-1.16629	1.19488
H	2.39913	0.80682	0.26088
H	-0.29358	6.30513	-1.18248
H	-0.31829	-6.41297	-0.62651
C	2.52874	-0.99433	1.44549
H	3.03404	-1.59763	0.67686
H	3.28962	-0.57247	2.12219
H	1.87904	-1.66287	2.03606
C	-1.84013	0.16384	-0.48379
H	-2.25892	-0.68364	-1.04539
H	-2.68082	0.77178	-0.10197
H	-1.25471	0.80670	-1.15636

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.05025436947

Zero-point correction (ZPE) = -5468.767793 .28246052459

Internal Energy (U) = -5468.936179 .11407489786

Enthalpy (H) = -5468.730810 .319443564373898

Gibbs Free Energy (G) = -5468.844883 .20537043536

Frequencies -- i309.36 7.82 10.78 14.78 24.41 25.07

Mono Cu(I) DiMeDHF-Z-Trans Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.20831476650

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0006465	0.0010000	yes	0.0001068	0.0005000	yes
Grad	0.0007521	0.0010000	yes	0.0001250	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.72451	-0.85796	-1.58598
C	-2.57015	0.46786	-1.52579
C	-1.90448	1.09640	-0.35901
C	-2.15355	-1.63823	-0.42834
C	3.75286	-2.05025	0.51652
C	2.74948	-0.87614	0.41840
C	3.27390	0.43483	0.33469
C	2.46158	1.56427	0.19369
C	3.13845	2.94234	0.04462
C	-2.72993	1.69102	0.74793
C	-3.19253	-2.54664	0.24314
O	-1.69148	-0.71251	0.52607
O	1.20022	1.62770	0.15195
O	1.55182	-1.22793	0.40873
Cu	-0.02504	0.11675	0.28760
F	2.65563	3.79807	0.95379
F	2.88485	3.44769	-1.17210
F	4.46954	2.88993	0.19575
F	5.02206	-1.64183	0.67503
F	3.70022	-2.79129	-0.59972
F	3.44351	-2.83752	1.55187
H	-3.20037	-1.36848	-2.42799
H	-2.88202	1.12987	-2.34284
H	-1.09149	1.78273	-0.66078
H	4.35181	0.56935	0.36214
H	-2.09829	1.98695	1.59911
H	-3.21464	2.61056	0.36840
H	-3.50626	0.99543	1.09155

H -1.32673 -2.28036 -0.80302
H -4.03918 -1.95159 0.61911
H -3.57250 -3.29277 -0.47351
H -2.73274 -3.07824 1.08898
==========

Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.20831476650
Zero-point correction (ZPE) = -2888.994755 .21355935294
Internal Energy (U) = -2889.130366 .07794826551
Enthalpy (H) = -2888.972085 .236228926544318
Gibbs Free Energy (G) = -2889.050036 .15827844606

Frequencies -- i326.97 15.14 22.71 24.59 29.19 37.71

Dual Cu(I) DiMeDHF-Z-Trans Reductive Elimination TS (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.04987663737

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0005613	0.0010000	yes	0.0000861	0.0005000	yes
Grad	0.0002956	0.0010000	yes	0.0000508	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.64698	-0.97745	-1.66946
C	-0.47879	0.39375	-1.56562
C	0.44490	0.95678	-0.53296
C	0.14146	-1.77899	-0.65356
O	0.57406	-0.86918	0.32876
C	-4.98974	2.86724	0.66116
C	-4.46267	1.48038	0.23563
C	-5.30552	0.36654	0.38803
C	-4.91639	-0.93652	0.03223
O	-3.81723	-1.32106	-0.44550
Cu	-2.31841	-0.10067	-0.82792
C	-5.92867	-2.08471	0.23474
F	-5.43927	-2.97643	1.10507
F	-6.14668	-2.71211	-0.92705
F	-7.11033	-1.65803	0.70141
O	-3.29173	1.51443	-0.22452
F	-4.17486	3.40135	1.57993
F	-6.22394	2.81916	1.18037
F	-5.01811	3.68796	-0.39635
C	6.03102	-2.20955	0.50538
C	5.02940	-1.03796	0.37119
C	5.55350	0.27097	0.26222
C	4.74250	1.39651	0.09010
C	5.41634	2.77232	-0.08852
O	3.48039	1.45673	0.03948
O	3.83110	-1.39167	0.35637
Cu	2.26585	-0.06110	0.17287
F	4.94622	3.63928	0.81595

F	5.14157	3.25805	-1.30829
F	6.74885	2.72115	0.04210
F	7.30097	-1.79732	0.63943
F	5.96760	-2.98961	-0.58280
F	5.72622	-2.95649	1.57106
H	-1.03922	-1.45716	-2.57279
H	-0.70973	1.05657	-2.41060
H	1.28462	1.47801	-1.02899
H	-6.30054	0.51847	0.79756
H	6.63122	0.40630	0.29338
C	-0.08108	1.73240	0.64024
H	0.73669	2.17110	1.23013
H	-0.72141	2.55488	0.27209
H	-0.70521	1.09650	1.28405
H	0.99907	-2.23998	-1.19130
C	-0.64564	-2.90309	0.02435
H	-1.51083	-2.50002	0.57190
H	-1.01534	-3.61620	-0.72959
H	0.00477	-3.44152	0.72862

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.04987663737

Zero-point correction (ZPE) = -5468.767568 .28230817264

Internal Energy (U) = -5468.934540 .11533654211

Enthalpy (H) = -5468.730425 .319451181971648

Gibbs Free Energy (G) = -5468.845763 .20411353173

Frequencies -- i311.42 7.48 10.03 13.07 18.95 22.27

Mono Cu(I) DiMeDHF-Z-Trans Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27588137608

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0008614	0.0010000	yes	0.0001316	0.0005000	yes
Grad	0.0000535	0.0010000	yes	0.0000150	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.29176	-1.71592	0.77557
C	0.34902	-2.24546	-0.08673
C	-0.93422	-2.48974	0.69765
C	0.66799	-1.59705	2.15821
C	-1.79697	1.72374	-3.44786
C	-0.82548	1.53420	-2.26121
C	-0.19853	2.67483	-1.72623
C	0.73929	2.60791	-0.68206
C	1.37799	3.92230	-0.18299
C	-1.18724	-3.97626	0.96461
C	0.91856	-0.31367	2.93383
O	-0.72946	-1.75282	1.90587
O	1.16175	1.58985	-0.07484
O	-0.69129	0.33461	-1.91201
Cu	0.49784	-0.23660	-0.43077
F	1.21234	4.04093	1.13978
F	0.85235	5.01140	-0.76286
F	2.69359	3.91684	-0.43782
F	-2.96604	1.12636	-3.19272
F	-1.27808	1.16686	-4.55150
F	-2.04403	3.01397	-3.71810
H	2.37406	-1.70959	0.61608
H	0.55389	-2.73051	-1.04576
H	-1.81928	-2.05970	0.19745
H	1.04219	-2.45325	2.76453
H	-0.44608	3.64806	-2.14156
H	-2.05688	-4.08984	1.62956
H	-1.39831	-4.51057	0.02390

H -0.31700 -4.45258 1.44409
H 0.34002 -0.32440 3.86986
H 1.98674 -0.22387 3.18861
H 0.62950 0.56998 2.34541
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27588137608
Zero-point correction (ZPE) = -2889.059084 .21679683198
Internal Energy (U) = -2889.199452 .07642884157
Enthalpy (H) = -2889.036696 .239184554471622
Gibbs Free Energy (G) = -2889.113127 .16275378474

Frequencies -- 20.24 26.77 27.73 34.04 38.60 81.36

Dual Cu(I) DiMeDHF-Z-Trans Product-Catalyst Complex (Major)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11045236287

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0001462	0.0010000	yes	0.0000221	0.0005000	yes
Grad	0.0000997	0.0010000	yes	0.0000190	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.35521	-1.86882	1.23379
C	-1.26585	-2.22836	0.27158
C	-2.66723	-1.97906	0.80496
C	-1.11508	-1.37724	2.45488
O	-2.44154	-1.17614	1.96720
C	5.91579	1.20087	-0.34673
C	4.40454	0.88791	-0.45186
C	4.02724	-0.34722	-1.02340
C	2.70273	-0.78838	-1.15704
O	1.65156	-0.16377	-0.85428
Cu	1.77301	1.80938	0.09405
C	2.46153	-2.21994	-1.68060
F	1.45070	-2.23807	-2.55807
F	2.10881	-3.01744	-0.64803
F	3.53299	-2.76297	-2.26357
O	3.68424	1.80802	0.00785
F	6.21306	2.27650	-1.08507
F	6.68868	0.18756	-0.76726
F	6.24012	1.46403	0.92373
C	-3.59718	1.30293	-2.72615
C	-2.37613	1.31198	-1.77589
C	-2.08098	2.51588	-1.07957
C	-1.00550	2.64260	-0.21214
C	-0.74782	3.99505	0.47279
O	-0.17227	1.73023	0.12017
O	-1.78198	0.22086	-1.71277
Cu	-0.43802	-0.40198	-0.32697
F	-0.86821	3.86727	1.80033

F	-1.58069	4.95667	0.06727
F	0.51094	4.40197	0.21618
F	-4.51612	0.44492	-2.25798
F	-3.23272	0.89976	-3.94588
F	-4.17832	2.50540	-2.84236
H	0.69208	-2.17669	1.26224
H	-1.06208	-2.85736	-0.59978
H	-3.27955	-1.38653	0.10365
H	-1.10458	-2.20570	3.20023
H	4.82034	-1.01068	-1.35884
H	-2.71601	3.38171	-1.24937
C	-3.40832	-3.27717	1.13848
H	-4.36674	-3.04156	1.62575
H	-3.61851	-3.85228	0.22199
H	-2.81866	-3.91354	1.81770
C	-0.61456	-0.11711	3.14334
H	-1.28195	0.14321	3.97900
H	0.39655	-0.28000	3.55048
H	-0.58307	0.73329	2.44598

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11045236287

Zero-point correction (ZPE) = -5468.826049 .28440301202

Internal Energy (U) = -5468.994207 .11624501682

Enthalpy (H) = -5468.788277 .322174473167554

Gibbs Free Energy (G) = -5468.904522 .20593032879

Frequencies -- 7.07 11.35 14.32 16.14 27.12 27.80

Mono Cu(I) DiMeDHF-Z-Trans Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.27811550316

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0007912	0.0010000	yes	0.0001103	0.0005000	yes
Grad	0.0001598	0.0010000	yes	0.0000337	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.53833	-1.91288	0.64778
C	0.46289	-2.50728	0.01259
C	-0.63717	-2.71532	1.04603
C	1.16736	-1.71493	2.11251
C	-2.39612	1.52627	-2.80908
C	-1.11929	1.30312	-1.96961
C	-0.31472	2.41603	-1.66936
C	0.84721	2.32161	-0.88401
C	1.65270	3.60885	-0.60439
C	-2.06849	-2.43561	0.62152
C	1.57847	-0.41258	2.77760
O	-0.25330	-1.84298	2.10708
O	1.34720	1.29840	-0.35049
O	-0.95111	0.10390	-1.62972
Cu	0.52574	-0.50241	-0.45501
F	1.74772	3.81102	0.71601
F	1.09788	4.70150	-1.14909
F	2.89248	3.48978	-1.09666
F	-3.47531	1.18977	-2.08962
F	-2.37199	0.75780	-3.90402
F	-2.54587	2.79946	-3.20354
H	2.57344	-1.90701	0.29376
H	0.49677	-3.05476	-0.93389
H	-0.56426	-3.77331	1.39205
H	1.61360	-2.56542	2.67985
H	-0.60861	3.39000	-2.05122
H	-2.38545	-3.15703	-0.14828
H	-2.74176	-2.53582	1.48632

H	-2.16933	-1.42211	0.20530
H	1.16691	-0.36698	3.79727
H	2.67604	-0.34802	2.84462
H	1.21805	0.45692	2.20771

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27811550316

Zero-point correction (ZPE) = -2889.061356 .21675874399

Internal Energy (U) = -2889.202280 .07583492623

Enthalpy (H) = -2889.039018 .239096952097488

Gibbs Free Energy (G) = -2889.114855 .16326035499

Frequencies -- 20.80 27.38 32.52 38.29 44.28 84.55

Dual Cu(I) DiMeDHF-Z-Trans Product-Catalyst Complex (Minor)
Using: TURBOMOLE V6.3

==========

Method: B3-LYP | Basis: def2-SVP | Atoms: 47
Charge: 0 | Spin: 1 | Basis Functions: 584

Energy = -5469.11126364820

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000010	0.0000010	yes			
Step	0.0008913	0.0010000	yes	0.0001333	0.0005000	yes
Grad	0.0004689	0.0010000	yes	0.0000810	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.31555	-2.43323	1.09487
C	-1.59054	-2.38782	0.58788
C	-2.53463	-1.93711	1.69032
C	-0.36228	-2.00234	2.55130
O	-1.66115	-1.43548	2.69848
C	5.55039	1.64935	-0.95988
C	4.11072	1.11588	-0.76879
C	3.80849	-0.16040	-1.29472
C	2.55882	-0.78646	-1.20336
O	1.50620	-0.32328	-0.68406
Cu	1.49893	1.70434	0.18273
C	2.43543	-2.22380	-1.75223
F	1.25272	-2.39849	-2.35534
F	2.49762	-3.10238	-0.72766
F	3.39919	-2.54321	-2.61822
O	3.37272	1.91573	-0.14503
F	5.52110	2.81690	-1.61101
F	6.32940	0.80897	-1.65779
F	6.12502	1.84756	0.23202
C	-3.63708	0.83885	-2.74926
C	-2.47523	0.91887	-1.73008
C	-2.30119	2.13520	-1.01946
C	-1.28429	2.33198	-0.09172
C	-1.14928	3.71038	0.58196
O	-0.42454	1.47311	0.29727
O	-1.82102	-0.13505	-1.63083
Cu	-0.49452	-0.78436	-0.23872
F	-1.32943	3.59878	1.90242

F	-2.02027	4.60977	0.11521
F	0.09228	4.19677	0.38031
F	-4.53703	-0.06317	-2.32576
F	-3.18562	0.44626	-3.94297
F	-4.27395	2.00801	-2.90921
H	0.52965	-2.97702	0.66700
H	-1.94015	-2.88009	-0.32407
H	-3.05556	-2.85071	2.06097
H	-0.28273	-2.92646	3.16971
H	4.60660	-0.69551	-1.80364
H	-2.97455	2.96066	-1.23501
C	-3.57904	-0.88777	1.34475
H	-4.22300	-1.22925	0.51916
H	-4.21236	-0.67926	2.22021
H	-3.08772	0.04899	1.04380
C	0.69178	-1.01140	3.01884
H	0.51658	-0.73954	4.07083
H	1.69934	-1.44937	2.93643
H	0.64978	-0.09341	2.41235

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5469.11126364820

Zero-point correction (ZPE) = -5468.827165 .28409830811

Internal Energy (U) = -5468.994959 .11630406768

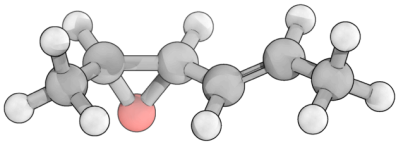
Enthalpy (H) = -5468.789302 .321961180430532

Gibbs Free Energy (G) = -5468.905607 .20565609527

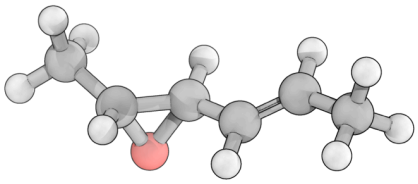
Frequencies -- 6.38 10.84 18.29 20.48 24.74 26.04

5. Substrates and catalyst

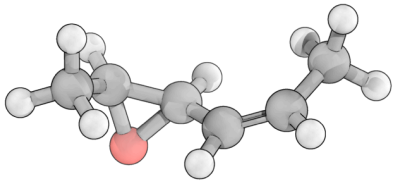
5.a. Additional Figures



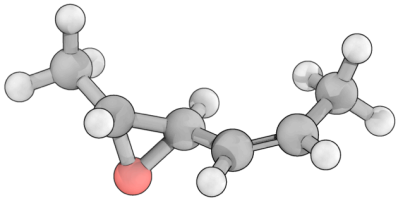
E-*Cis*



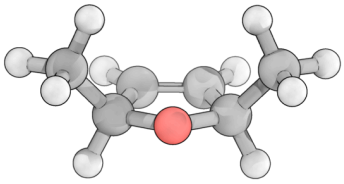
E-*Trans*



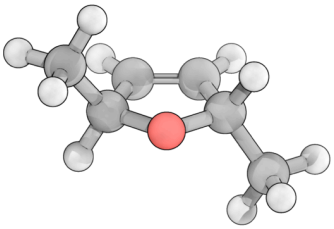
Z-*Cis*



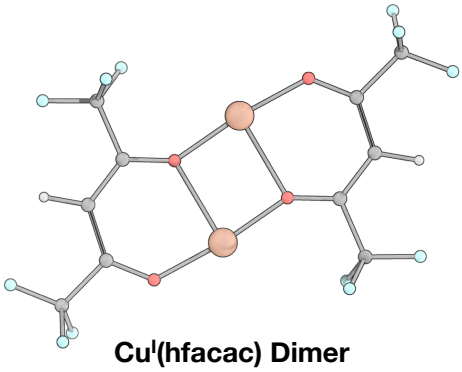
Z-*Trans*



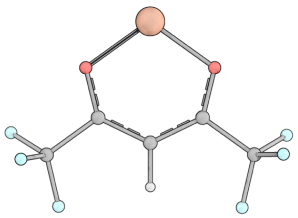
***cis*-2,5-dimethyldihydrofuran**



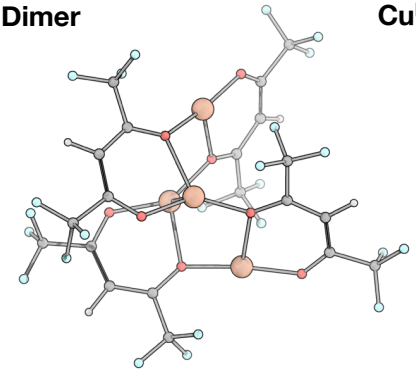
***trans*-2,5-dimethyldihydrofuran**



Cu^{I}(hfacac) Dimer



Cu^{I}(hfacac)



Cu^{I}(hfacac) Tetramer

Figure 13. Geometries of substrates, products and catalyst isomers studied.

5.b. Geometries, Energies, and Thermal Corrections

E-Cis

Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 17
Charge: OPT | Spin: 21 | Basis Functions: 148

Energy = -309.40217864897

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000002	II	0.0000010	yes					
Step	0.0008395	II	0.0010000	yes	I	0.0001705	II	0.0005000	yes
Grad	0.0003617	II	0.0010000	yes	I	0.0000919	II	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.00193	0.37656	0.49476
H	-0.94426	0.72913	0.06935
C	1.11553	0.15648	-0.45514
H	2.07575	-0.09081	0.02315
C	0.94078	-0.29769	-1.85670
H	1.79266	-0.84822	-2.28944
C	0.10566	0.17369	1.81593
H	1.07275	-0.16114	2.21651
O	1.23208	1.06151	-1.56353
C	-0.38443	-0.61126	-2.50454
H	-0.35521	-0.34135	-3.57320
H	-0.60128	-1.69044	-2.43709
H	-1.21292	-0.05766	-2.04096
C	-0.99392	0.36447	2.81686
H	-1.92598	0.70790	2.34162
H	-1.21071	-0.57519	3.35622
H	-0.70843	1.10402	3.58620

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -309.40217864897
Zero-point correction (ZPE) = -309.2565301 .14564846899
Internal Energy (U) = -309.3606079 .04157066703
Enthalpy (H) = -309.2474542 .154724439409789
Gibbs Free Energy (G) = -309.2890230 .11315560578

Frequencies -- 77.93 142.82 159.28 185.58 210.08 287.11

E-Trans
Using: TURBOMOLE V6.3
==========
Method: b3-lyp | Basis: def2-SVP | Atoms: 17
Charge: OPT | Spin: 25 | Basis Functions: 148

Energy = -309.40410371966

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0001606	0.0010000	yes	0.0000247	0.0005000	yes
Grad	0.0000418	0.0010000	yes	0.0000116	0.0005000	yes

==========
Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.44539	0.49274	0.57089
H	-1.39492	0.90095	0.20208
C	0.57635	0.21480	-0.46251
H	1.54714	-0.13567	-0.08078
C	0.22399	-0.16147	-1.84915
H	-0.84990	-0.21965	-2.08993
C	-0.26647	0.27640	1.88123
H	0.70296	-0.11913	2.21504
O	0.67387	1.15239	-1.54707
C	1.11895	-1.01217	-2.71428
H	0.81587	-2.07141	-2.66817
H	1.05756	-0.68872	-3.76673
H	2.16897	-0.93003	-2.39431
C	-1.28340	0.52746	2.95365
H	-2.22256	0.92836	2.54171
H	-1.51974	-0.39996	3.50572
H	-0.90328	1.24512	3.70260

==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -309.40410371966
Zero-point correction (ZPE) = -309.2585314 .14557229301
Internal Energy (U) = -309.3626432 .04146051447
Enthalpy (H) = -309.2494402 .154663498627783
Gibbs Free Energy (G) = -309.2909024 .11320131137

Frequencies -- 84.27 145.57 152.80 202.79 214.50 289.68

Z-Cis
Using: TURBOMOLE V6.3
==========
Method: b3-lyp | Basis: def2-SVP | Atoms: 17
Charge: OPT | Spin: 22 | Basis Functions: 148

Energy = -309.39973647481

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000005	0.0000010	yes			
Step	0.0008204	0.0010000	yes	0.0001606	0.0005000	yes
Grad	0.0002055	0.0010000	yes	0.0000443	0.0005000	yes

==========
Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.56927	0.65098	0.39044
H	-1.49155	0.90158	-0.14313
C	0.61087	0.42075	-0.47598
H	1.58626	0.44589	0.02918
C	0.55978	-0.34228	-1.74968
H	1.50544	-0.81754	-2.05941
C	-0.60084	0.59388	1.73221
H	-1.56542	0.79567	2.21476
O	0.60979	1.07631	-1.75307
C	-0.67299	-1.01041	-2.30463
H	-0.66553	-0.96186	-3.40617
H	-0.69520	-2.07456	-2.01626
H	-1.59749	-0.53419	-1.95013
C	0.52789	0.27896	2.67097
H	1.49507	0.15570	2.16285
H	0.63939	1.07385	3.42916
H	0.32378	-0.65271	3.22891

==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -309.39973647481
Zero-point correction (ZPE) = -309.2538594 .14587699692
Internal Energy (U) = -309.3577649 .04197153149
Enthalpy (H) = -309.2447987 .154937732146811
Gibbs Free Energy (G) = -309.2867713 .11296516584

Frequencies -- 40.26 134.84 159.71 180.95 222.60 296.21

Z-Trans

Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 17

Charge: OPT | Spin: 20 | Basis Functions: 148

Energy = -309.40170082407

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0006859	0.0010000	yes	0.0001455	0.0005000	yes
Grad	0.0000305	0.0010000	yes	0.0000117	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.06783	0.57513	0.51990
H	-2.06351	0.70401	0.07995
C	0.00843	0.35103	-0.47154
H	1.03837	0.35074	-0.09043
C	-0.23014	-0.38889	-1.73174
H	-1.25049	-0.77103	-1.89606
C	-0.93966	0.63570	1.85518
H	-1.85598	0.80518	2.43446
O	-0.14120	1.02807	-1.73152
C	0.85858	-1.14608	-2.44886
H	0.84276	-2.21266	-2.16954
H	0.71714	-1.08085	-3.54062
H	1.84985	-0.73174	-2.20941
C	0.31303	0.49771	2.67149
H	1.22069	0.38362	2.06147
H	0.45110	1.37747	3.32441
H	0.24885	-0.37742	3.34284

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -309.40170082407

Zero-point correction (ZPE) = -309.2558619 .14583890893

Internal Energy (U) = -309.3599689 .04173192129

Enthalpy (H) = -309.2468240 .154876791364805

Gibbs Free Energy (G) = -309.2885566 .11314417939

Frequencies -- 55.64 141.34 160.25 185.54 216.65 292.86

***cis*-2,5-dimethyldihydrofuran**
Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  17
Charge: OPT| Spin: 16                    | Basis Functions:   148
----------------------------------------------------------------------------------------------------
Energy =     -309.43234263791
----------------------------------------------------------------------------------------------------
Item      Max Val.    || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000000  || 0.0000010   yes
Step      0.0005412  || 0.0010000   yes  |  0.0000900 || 0.0005000   yes
Grad      0.0001827  || 0.0010000   yes  |  0.0000393 || 0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
----------------------------------------------------------------------------------------------------
C       -0.38398      -1.06240       1.00179
H       -0.31210      -1.70014       1.88573
C       -0.31417      -1.45201      -0.27206
H       -0.17318      -2.47188      -0.63720
C       -0.47964      -0.25971      -1.18380
H       -1.43839      -0.34190      -1.74304
C       -0.60473       0.42978       1.07119
H       -1.61767       0.64289       1.48046
O       -0.55289       0.85385      -0.29191
C        0.64719      -0.05211      -2.19365
H        0.67387      -0.87594      -2.92623
H        0.49344       0.89061      -2.74134
H        1.62072      -0.00198      -1.68097
C        0.41839       1.20139       1.90181
H        1.44012       0.99147       1.54808
H        0.23551       2.28368       1.81439
H        0.34751       0.92440       2.96674
==========================================================
Thermodynamic Analysis
Tempurature = 298.15 Kelvin     Pressure = 101325 Pa
----------------------------------------------------------------------------------------------------
SCF Energy =     -309.43234263791
Zero-point correction (ZPE) = -309.2847897    .14755286843
Internal Energy (U) = -309.3931351    .03920749720
Enthalpy (H) = -309.2766774    .155665212732011
Gibbs Free Energy (G) = -309.3158848    .11645783441
----------------------------------------------------------------------------------------------------
Frequencies -- 74.16 209.47 234.96 248.10 304.87 379.68
```

***trans*-2,5-dimethyldihydrofuran**
Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp        |  Basis: def2-SVP          |  Atoms:  17
Charge: OPT|  Spin: 13                    |  Basis Functions:   148
----------------------------------------------------------------------------------------------------
Energy =     -309.43222697477
----------------------------------------------------------------------------------------------------
Item      Max Val.     ||  Criteria     Pass? |   RMS Val.  ||  Criteria     Pass?
Energy    0.0000002  ||  0.0000010   yes
Step      0.0004938   ||  0.0010000   yes   |  0.0001157  ||  0.0005000   yes
Grad      0.0000721   ||  0.0010000   yes   |  0.0000197  ||  0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type   X         Y         Z
----------------------------------------------------------------------------------------------------
C        -0.02507      -0.96565       1.03980
H        -0.07596      -1.58349       1.93918
C         0.21785      -1.38449      -0.20314
H         0.41103      -2.41184      -0.52032
C         0.18614      -0.21478      -1.15680
H         1.18147      -0.07465      -1.63084
C        -0.21937       0.53139       1.05048
H        -1.24361       0.78824       1.39583
O        -0.08893       0.91154      -0.32103
C        -0.86101      -0.32447      -2.26557
H        -0.88489       0.60559      -2.85449
H        -0.62549      -1.15901      -2.94682
H        -1.86213      -0.49080      -1.83700
C         0.78382       1.29593       1.91527
H         1.81609       1.04951       1.61972
H         0.63672       2.38049       1.79410
H         0.65334       1.04649       2.98163
==========================================================
Thermodynamic Analysis
Tempurature = 298.15 Kelvin     Pressure = 101325 Pa
----------------------------------------------------------------------------------------------------
SCF Energy =     -309.43222697477
Zero-point correction (ZPE) = -309.2846741    .14755286843
Internal Energy (U) = -309.3929581    .03926881924
Enthalpy (H) = -309.2765236    .155703300720765
Gibbs Free Energy (G) = -309.3157919    .11643498162
----------------------------------------------------------------------------------------------------
Frequencies -- 70.29 197.24 239.98 250.39 305.66 362.50
```

Cu(I) hfacac Dimer
Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  30
Charge: 0     | Spin: 1                         | Basis Functions:   436
----------------------------------------------------------------------------------------------
Energy =    -5159.65428184342
----------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000000  || 0.0000100   yes
Step      0.0006210   || 0.0010000   yes  |  0.0001108  || 0.0005000   yes
Grad      0.0000850   || 0.0010000   yes  |  0.0000263  || 0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
----------------------------------------------------------------------------------------------
C        4.24255      -1.33854       2.60765
C        2.95702      -1.15874       1.76378
C        2.43658      -2.30482       1.11458
C        1.31978      -2.30577       0.27751
C        0.87002      -3.62627      -0.37573
O        0.61184      -1.29955      -0.02456
O        2.54502       0.02444       1.75129
Cu       1.04192       0.77924       0.85773
F        0.93579      -3.51493      -1.71032
F       -0.40636      -3.88003      -0.05040
F        1.61094      -4.67391      -0.00712
F        4.07598      -0.80973       3.82173
F        5.26026      -0.70708       2.00920
F        4.58806      -2.62553       2.75908
H        2.94842      -3.24991       1.27730
C       -4.26346       1.31854      -2.57042
C       -2.95219       1.15737      -1.76397
C       -2.45598       2.29612      -1.08467
C       -1.29040       2.32150      -0.31667
C       -0.88406       3.63226       0.38320
O       -0.49572       1.35282      -0.13038
O       -2.49038      -0.00619      -1.82024
Cu      -0.95818      -0.74377      -0.96737
F        0.29168       4.05921      -0.09768
F       -0.73132       3.41309       1.69836
F       -1.78015       4.60938       0.22429
F       -5.18543       0.46631      -2.11116
F       -4.03937       1.04201      -3.85924
```

F -4.77165 2.55729 -2.49531
H -3.03122 3.21520 -1.16046
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5159.65428184342
Zero-point correction (ZPE) = -5159.518650 .13563132795
Internal Energy (U) = -5159.557757 .09652430210
Enthalpy (H) = -5159.489528 .164753006848698
Gibbs Free Energy (G) = -5159.586054 .06822701425

Frequencies -- 8.84 15.56 21.65 25.31 26.79 28.54

Cu(I) hfacac
Using: TURBOMOLE V6.3
==========
Method: b3-lyp | Basis: def2-SVP | Atoms: 15
Charge: 0 | Spin: 1 | Basis Functions: 218

Energy = -2579.78724649463

Item	Max Val.	II	Criteria	Pass?	I	RMS Val.	II	Criteria	Pass?
Energy	0.0000003	II	0.0000010	yes					
Step	0.0006682	II	0.0010000	yes	I	0.0001495	II	0.0005000	yes
Grad	0.0000528	II	0.0010000	yes	I	0.0000202	II	0.0005000	yes

==========
Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.75500	-2.19219	-1.08833
C	0.11335	-1.32073	-0.15082
C	-0.17313	0.05983	-0.08632
C	0.50619	1.04004	0.66902
C	0.03655	2.50635	0.52581
O	1.48778	0.92057	1.45615
O	1.00211	-1.99225	0.44667
Cu	2.10986	-0.90352	1.59650
F	0.98396	3.22185	-0.09614
F	-0.16802	3.04606	1.73109
F	-1.09802	2.62782	-0.17854
F	-1.34389	-3.17026	-0.39080
F	0.01764	-2.75563	-2.02555
F	-1.71691	-1.49761	-1.71263
H	-1.00247	0.40969	-0.69612

==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2579.78724649463
Zero-point correction (ZPE) = -2579.719906 .06733956411
Internal Energy (U) = -2579.730472 .05677399126
Enthalpy (H) = -2579.706020 .081226047511336
Gibbs Free Energy (G) = -2579.762794 .02445248878

Frequencies -- 21.39 26.36 83.69 88.76 112.65 155.51

Cu(I) hfacac Tetramer
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 60
Charge: 0	Spin: 1	Basis Functions: 872

Energy = -10319.34132707470

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0000769	0.0001000	yes	0.0000149	0.0000500	yes
Grad	0.0000149	0.0010000	yes	0.0000032	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	5.18501	-1.62243	-2.70103
C	3.78799	-1.44690	-2.05910
C	2.66838	-1.34762	-2.92376
C	1.35731	-1.18219	-2.48736
C	0.24585	-1.04458	-3.54483
O	0.95675	-1.09717	-1.28159
O	3.81693	-1.40954	-0.81169
Cu	2.37683	-1.17397	0.44559
F	-0.19600	0.22934	-3.57149
F	-0.80196	-1.82127	-3.21897
F	0.63918	-1.37002	-4.77375
F	5.75644	-2.74176	-2.24789
F	5.96540	-0.58712	-2.37351
F	5.13379	-1.69470	-4.03945
H	2.84604	-1.40617	-3.99457
C	0.73515	4.77492	-3.64658
C	0.44519	3.80827	-2.47235
C	1.44208	3.67727	-1.47174
C	1.36631	2.79264	-0.40007
C	2.55936	2.71545	0.57060
O	0.41324	1.99191	-0.13342
O	-0.64897	3.21528	-2.56741
Cu	-1.38396	1.82192	-1.46151
F	3.44823	3.69046	0.39973
F	3.19821	1.53750	0.40465
F	2.12603	2.75645	1.84128
F	-0.34168	5.50662	-3.92971
F	1.05950	4.06251	-4.73474

F	1.75133	5.61016	-3.38394
H	2.32879	4.30122	-1.55477
C	-2.36689	-0.52250	4.64891
C	-1.17374	-0.51654	3.66383
C	-0.19090	-1.52620	3.80174
C	0.90503	-1.65533	2.95812
C	1.88782	-2.81559	3.19716
O	1.21811	-0.89091	1.98203
O	-1.22015	0.40858	2.82642
Cu	0.02318	0.79092	1.35056
F	3.07170	-2.33851	3.60096
F	2.08930	-3.48401	2.04532
F	1.45280	-3.68586	4.10851
F	-3.51961	-0.54247	3.96429
F	-2.34702	0.58737	5.39399
F	-2.35444	-1.57675	5.47233
H	-0.32265	-2.26473	4.58782
C	-3.87404	-3.06235	1.82529
C	-3.21369	-1.95375	0.97151
C	-3.97902	-0.80403	0.65634
C	-3.49990	0.25487	-0.10368
C	-4.41551	1.46621	-0.35253
O	-2.35265	0.34158	-0.66177
O	-2.03539	-2.21018	0.64827
Cu	-0.80563	-1.13509	-0.44893
F	-4.74827	1.52957	-1.64863
F	-3.75646	2.59981	-0.04616
F	-5.53584	1.43135	0.36793
F	-3.13858	-3.29339	2.92190
F	-3.93256	-4.19651	1.11913
F	-5.11545	-2.74948	2.21408
H	-4.98633	-0.73256	1.05863

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -10319.34132707470

Zero-point correction (ZPE) = -10319.06995 .27137691987

Internal Energy (U) = -10319.17251 .16880822782

Enthalpy (H) = -10319.01056 .330763314631565

Gibbs Free Energy (G) = -10319.17936 .16195774577

Frequencies -- 9.59 11.54 14.57 16.54 18.30 19.92

6. Cu(I)-catalyzed rearrangement of unsubstituted vinyloxiranes

6.a. Additional Figures

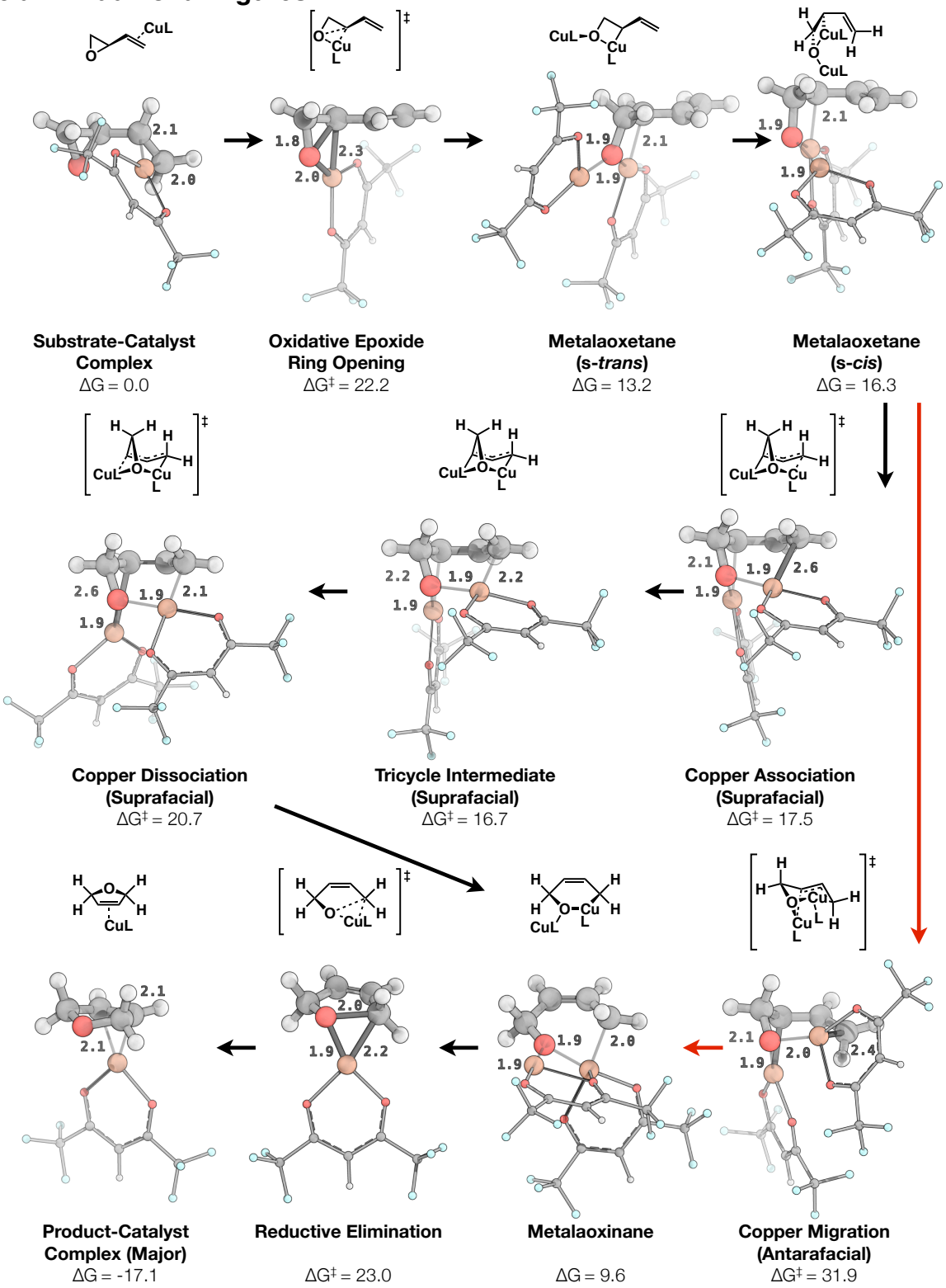


Figure 14. Structures of stationary points for both major and minor pathways for simple VO. All structures, energies, and free energy corrections computed

at the B3LYP/def2-SVP level of theory, as implemented in Turbomole. Figures rendered using Pymol.

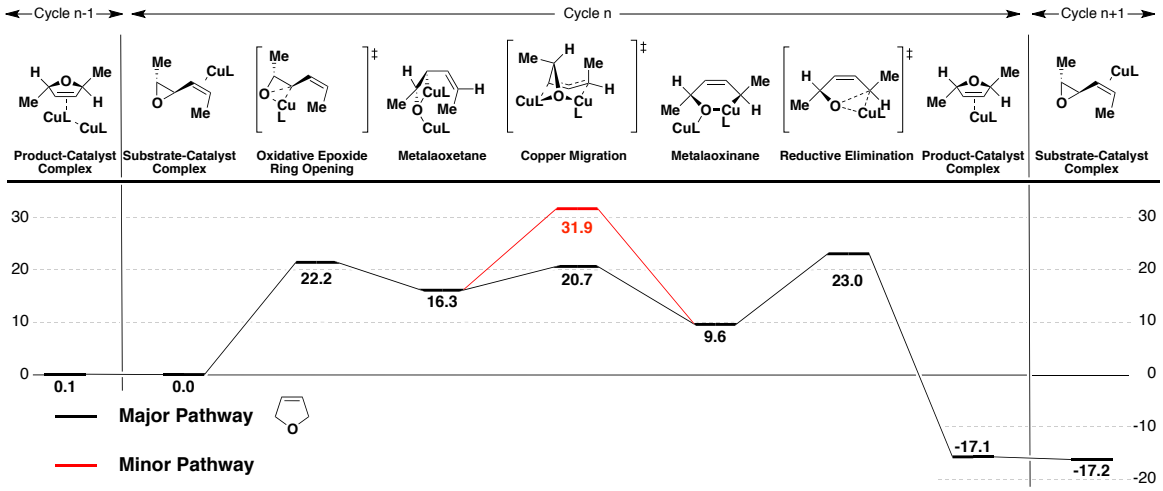


Figure 15. Reaction coordinate of Cu(I)-catalyzed ring expansion of simple VO.

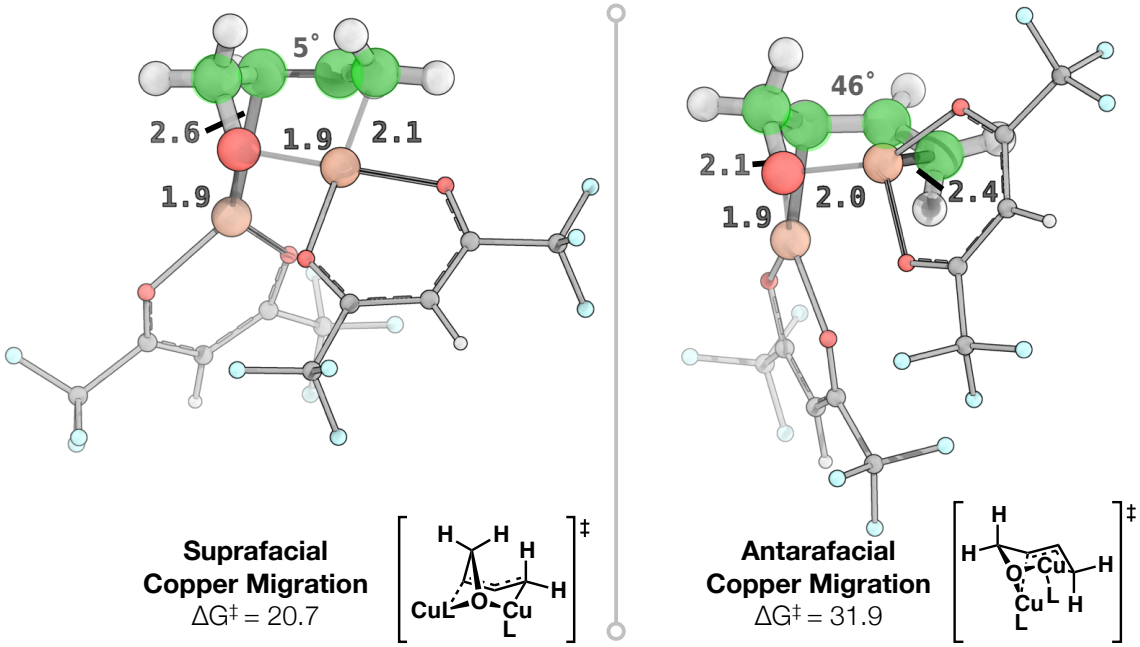


Figure 16. Copper migration of simple VO showing π-allyl distortion (green highlight with dihedral), and TS bond distances.

6.b. Geometries, Energies, and Thermal Corrections
Mono Copper Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 26
Charge: 0	Spin:	Basis Functions: 318

Energy = -2810.72049716515

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0009184	0.0010000	yes	0.0001299	0.0005000	yes
Grad	0.0000462	0.0010000	yes	0.0000144	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.26895	3.00084	-0.11695
C	-1.13365	1.46408	-0.17256
C	-2.28506	0.68346	0.01173
H	-3.23248	1.18607	0.18711
C	-2.26244	-0.72478	-0.01879
O	-1.27694	-1.48410	-0.18703
C	-3.59310	-1.48296	0.19122
F	-3.79777	-2.34032	-0.81477
F	-4.65332	-0.66336	0.25574
F	-3.54619	-2.18358	1.33149
O	0.04313	1.07701	-0.40199
F	-1.04372	3.52586	-1.32964
F	-0.36437	3.51051	0.72868
F	-2.48201	3.40366	0.28537
Cu	0.56999	-0.82710	-0.46185
C	3.35572	-0.50466	0.31848
H	4.40720	-0.83403	0.36857
C	2.58864	-1.11390	-0.81704
H	2.81111	-0.71883	-1.81728
C	1.92309	-2.32246	-0.69589
H	1.90850	-2.86211	0.25736
H	1.60299	-2.88046	-1.58162
C	3.02723	0.79304	0.93055
H	2.17215	1.37241	0.56258
H	3.83002	1.36854	1.40932
O	2.70023	-0.44285	1.57720

Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.72049716515
Zero-point correction (ZPE) = -2810.561060 .15943632092
Internal Energy (U) = -2810.648947 .07154919679
Enthalpy (H) = -2810.540958 .179538764082972
Gibbs Free Energy (G) = -2810.612506 .10799087451

Frequencies -- 19.26 28.29 31.90 41.85 57.08 66.43

Mono Copper Oxidative Epoxide Ring Opening TS

Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 26
Charge: 0 | Spin: 1 | Basis Functions: 318

Energy = -2810.68215675954

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0005893	0.0010000	yes	0.0001179	0.0005000	yes
Grad	0.0002549	0.0010000	yes	0.0000586	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.45304	-1.45097	-0.00066
C	2.72762	-0.85591	-1.30203
C	2.71429	0.47161	-1.51957
C	2.63297	-2.88360	0.25666
O	1.27117	-2.79764	-0.07073
C	-4.04516	-0.33617	-0.17540
C	-2.53520	-0.12037	0.08130
C	-2.10964	1.17100	0.46506
C	-0.76746	1.49177	0.70990
O	0.24048	0.73735	0.65625
Cu	0.16122	-1.19564	0.12014
C	-0.41873	2.94353	1.09919
F	0.49217	3.43919	0.24447
F	0.11397	2.98122	2.32867
F	-1.47843	3.76331	1.08632
O	-1.84413	-1.14745	-0.10087
F	-4.25559	-0.61328	-1.46990
F	-4.78808	0.73786	0.13736
F	-4.49386	-1.36790	0.54816
H	2.32201	-0.78499	0.85870
H	2.99096	-1.54954	-2.10812
H	2.41013	1.17621	-0.73954
H	2.98805	0.88232	-2.49488
H	3.22899	-3.45557	-0.47248
H	2.84586	-3.18986	1.29419
H	-2.85667	1.95352	0.56779

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.68215675954
Zero-point correction (ZPE) = -2810.524777 .15737956953
Internal Energy (U) = -2810.609367 .07278926477
Enthalpy (H) = -2810.504293 .177862892577800
Gibbs Free Energy (G) = -2810.577083 .10507333457

Frequencies -- i289.80 19.79 25.76 33.83 38.30 45.65

Mono Coper Metalaoxetane (s-*trans*)

Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 26
Charge: 0	Spin:	Basis Functions: 318

Energy = -2810.69649641630

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000007	0.0000010	yes			
Step	0.0004016	0.0010000	yes	0.0000698	0.0005000	yes
Grad	0.0001137	0.0010000	yes	0.0000270	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	3.75620	-1.33691	0.18854
C	2.36498	-0.69607	-0.02427
C	2.28083	0.71263	-0.09462
H	3.18680	1.30418	0.00402
C	1.06060	1.36262	-0.28600
O	-0.08985	0.85071	-0.40631
C	1.03919	2.90144	-0.37849
F	0.62490	3.28127	-1.59415
F	2.24094	3.44985	-0.16180
F	0.18553	3.40398	0.52362
O	1.43282	-1.52301	-0.12071
F	4.72249	-0.42052	0.35330
F	4.07849	-2.08881	-0.86915
F	3.74130	-2.11808	1.27213
Cu	-0.51431	-1.03852	-0.33802
C	-2.53453	-0.82687	-0.39923
H	-2.53786	-0.16766	-1.27628
C	-2.81921	-0.22971	0.89243
H	-3.01792	-0.92799	1.71453
C	-2.87892	1.10021	1.12180
H	-3.14924	1.49055	2.10642
H	-2.65242	1.82700	0.33703
C	-2.70575	-2.30785	-0.61672
H	-3.11753	-2.55254	-1.61509
H	-3.34725	-2.78634	0.14951
O	-1.35028	-2.66358	-0.48249

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.69649641630
Zero-point correction (ZPE) = -2810.537440 .15905544103
Internal Energy (U) = -2810.625492 .07100411197
Enthalpy (H) = -2810.517235 .179260721765069
Gibbs Free Energy (G) = -2810.588238 .10825749043

Frequencies -- 22.66 31.23 36.78 40.62 74.32 95.11

Mono Copper Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 26
Charge: 0	Spin: 1	Basis Functions: 318

Energy = -2810.69509471073

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000010	yes			
Step	0.0004137	0.0010000	yes	0.0000714	0.0005000	yes
Grad	0.0000956	0.0010000	yes	0.0000254	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.35789	-3.92584	0.42018
C	0.04057	-2.43721	0.29023
C	1.09865	-1.95072	1.09008
H	1.59461	-2.62595	1.78216
C	1.52888	-0.62492	1.00941
O	1.07815	0.30489	0.27865
C	2.70947	-0.16948	1.89149
F	3.74449	0.18821	1.12084
F	3.12959	-1.12706	2.72810
F	2.35230	0.89237	2.62454
O	-0.63537	-1.80371	-0.54873
F	0.31324	-4.55331	1.39780
F	-0.10598	-4.56496	-0.72790
F	-1.66318	-4.03121	0.68309
Cu	-0.40488	0.15118	-0.95805
C	-0.48529	2.09998	-1.50987
H	0.56049	2.12246	-1.84020
C	-0.77320	2.75501	-0.24144
H	0.09165	2.91140	0.41213
C	-1.99086	3.15711	0.18205
H	-2.10805	3.65627	1.14727
H	-2.89912	2.99402	-0.40453
C	-1.52518	1.80105	-2.55551
H	-1.15802	1.98596	-3.58378
H	-2.46976	2.36269	-2.42643
O	-1.66530	0.43176	-2.26159

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.69509471073
Zero-point correction (ZPE) = -2810.535886 .15920779299
Internal Energy (U) = -2810.623569 .07152534933
Enthalpy (H) = -2810.515666 .179428308915586
Gibbs Free Energy (G) = -2810.587191 .10790327213

Frequencies -- 20.97 23.80 35.26 39.78 75.91 81.72

Mono Copper Metalaoxipane

Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 26
Charge: 0 | Spin: 1 | Basis Functions: 318

Energy = -2810.70263303777

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0009158	0.0010000	yes	0.0001607	0.0005000	yes
Grad	0.0003144	0.0010000	yes	0.0000627	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-3.33957	-1.53051	0.10161
C	-2.14155	-0.57563	-0.10913
C	-2.37766	0.81669	-0.09318
H	-3.39135	1.18336	0.04166
C	-1.33696	1.73508	-0.23917
O	-0.10063	1.51032	-0.39596
C	-1.66571	3.24216	-0.21219
F	-1.00661	3.83874	0.78841
F	-2.97343	3.48071	-0.04456
F	-1.28493	3.81412	-1.36048
O	-1.04831	-1.15936	-0.26753
F	-4.50564	-0.87682	0.21411
F	-3.15761	-2.24230	1.22088
F	-3.43974	-2.37980	-0.92447
Cu	0.73152	-0.22717	-0.51186
C	3.29713	-1.46361	0.83202
H	3.89493	-1.92172	1.62741
C	3.27545	-0.11791	0.67130
H	3.76325	0.50515	1.43179
C	2.57273	0.57433	-0.39861
H	2.36466	1.63879	-0.23625
H	2.85711	0.32992	-1.42767
C	2.41750	-2.35981	0.01628
H	1.80058	-2.96951	0.72212
H	3.09115	-3.10507	-0.47439
O	1.70371	-1.74014	-0.97217

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.70263303777
Zero-point correction (ZPE) = -2810.543882 .15875073712
Internal Energy (U) = -2810.632359 .07027392542
Enthalpy (H) = -2810.524198 .178434212409109
Gibbs Free Energy (G) = -2810.594470 .10816227046

Frequencies -- 20.21 24.49 28.00 40.53 74.12 90.77

Mono Copper Reductive Elimination TS

Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 26
Charge: 0 | Spin: 1 | Basis Functions: 318

Energy = -2810.68224653823

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0007615	0.0010000	yes	0.0001179	0.0005000	yes
Grad	0.0003671	0.0010000	yes	0.0000528	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.70224	0.03818	3.40131
H	1.45226	-0.14894	4.44890
C	1.73284	1.25597	2.84764
H	1.45798	2.16099	3.40086
C	2.06661	1.38005	1.41463
H	1.41220	2.07240	0.85351
H	3.11663	1.52462	1.13864
C	1.97826	-1.08749	2.44664
H	2.84616	-1.68074	2.80176
H	1.11346	-1.78077	2.38683
O	2.33973	-0.54436	1.20352
C	-2.06269	-2.69278	-1.45867
C	-1.25059	-1.39450	-1.23949
C	-1.64924	-0.23440	-1.94309
C	-0.98697	0.99178	-1.81887
C	-1.51864	2.19869	-2.62011
O	0.02629	1.27508	-1.11895
O	-0.30010	-1.52064	-0.43937
Cu	0.97584	0.04102	0.04257
F	-0.57232	2.65444	-3.45119
F	-1.85077	3.19508	-1.78750
F	-2.60022	1.90062	-3.35438
F	-2.57945	-3.11346	-0.29650
F	-3.07511	-2.53802	-2.32613
F	-1.26367	-3.65790	-1.93018
H	-2.51073	-0.29492	-2.60239

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.68224653823
Zero-point correction (ZPE) = -2810.524219 .15802706534
Internal Energy (U) = -2810.610946 .07130050184
Enthalpy (H) = -2810.504577 .177668643835155
Gibbs Free Energy (G) = -2810.575878 .10636832619

Frequencies -- i410.26 16.20 23.49 28.10 33.43 53.98

Mono Copper Product-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 26
Charge: 0 | Spin: | Basis Functions: 318

Energy = -2810.75005270414

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0004992	0.0010000	yes	0.0001060	0.0005000	yes
Grad	0.0000704	0.0010000	yes	0.0000227	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.68011	-2.52823	0.05374
C	-1.84569	-1.23497	-0.08282
C	-2.50695	0.00030	0.03760
H	-3.57616	0.00053	0.23075
C	-1.84511	1.23530	-0.08249
O	-0.62532	1.44998	-0.30039
C	-2.67879	2.52892	0.05515
F	-2.18211	3.29540	1.03377
F	-3.96858	2.28965	0.33422
F	-2.62986	3.22971	-1.08534
O	-0.62594	-1.45016	-0.30040
F	-3.97049	-2.28839	0.32957
F	-2.18611	-3.29442	1.03395
F	-2.62865	-3.22957	-1.08630
Cu	0.69935	-0.00040	-0.50843
C	2.60700	0.69206	-0.80271
H	2.58008	1.33539	-1.68667
C	2.60683	-0.69361	-0.80193
H	2.57979	-1.33794	-1.68515
C	3.14248	-1.15360	0.54160
H	2.57133	-1.97004	1.01122
H	4.19453	-1.49812	0.42461
C	3.14282	1.15350	0.54024
H	4.19498	1.49757	0.42282
H	2.57192	1.97068	1.00889
O	3.05878	0.00045	1.36450

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2810.75005270414
Zero-point correction (ZPE) = -2810.588673 .16137880835
Internal Energy (U) = -2810.679459 .07059302716
Enthalpy (H) = -2810.569203 .180848990896107
Gibbs Free Energy (G) = -2810.639795 .11025710984

Frequencies -- 22.92 25.90 28.52 30.37 52.41 81.39

Dual Copper Substrate-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 52
Charge: 0 | Spin: 1 | Basis Functions: 636

Energy = -5621.49043892705

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0000736	0.0001000	yes	0.0000126	0.0000500	yes
Grad	0.0000334	0.0010000	yes	0.0000063	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.52967	-0.16310	2.66801
C	0.79692	-0.13860	1.99763
C	1.81138	-1.18992	2.21048
C	-1.14777	0.99900	3.08558
O	1.04854	-1.15475	1.00500
C	-5.15787	-2.20807	-0.19657
C	-4.39269	-0.91833	0.17995
C	-4.84686	0.29515	-0.37734
C	-4.19669	1.52673	-0.18858
C	-4.70871	2.74044	-0.99492
O	-3.18961	1.79168	0.51345
O	-3.40264	-1.12123	0.91785
Cu	-2.02997	0.38254	1.32299
F	-3.84890	2.98797	-2.00542
F	-4.76740	3.83439	-0.23359
F	-5.91941	2.54639	-1.53712
F	-5.46020	-2.91734	0.89461
F	-4.37728	-2.97442	-0.98269
F	-6.29752	-1.97532	-0.86497
H	-0.87394	-1.13669	3.03700
H	1.16996	0.85157	1.70637
H	2.87311	-0.93528	2.10767
H	-0.68688	1.97745	2.91294
H	-5.73135	0.27301	-1.00867
C	4.41695	2.44752	0.70827
C	3.97619	1.13992	0.01616
C	4.93213	0.12908	-0.16861
C	4.61407	-1.14567	-0.68683

O	3.49831	-1.58428	-1.04631
Cu	1.81880	-0.44821	-1.11160
C	5.75701	-2.18108	-0.80243
F	5.75581	-2.74367	-2.01449
F	5.58180	-3.15097	0.10810
F	6.96996	-1.64462	-0.59851
O	2.75369	1.12758	-0.28253
F	3.76849	2.56762	1.88229
F	4.10370	3.50826	-0.04195
F	5.73111	2.49411	0.96431
C	0.18915	-1.12456	-2.22715
C	0.34386	0.23545	-2.40290
C	-0.71108	0.95693	-1.59880
O	-1.20888	-0.05653	-0.71808
C	-0.97281	-1.35457	-1.28512
H	5.96186	0.33063	0.11502
H	0.58024	-1.90543	-2.88467
H	0.89339	0.71703	-3.21618
H	-1.52030	1.34272	-2.25171
H	-0.77309	-2.05599	-0.46397
H	-1.97755	0.97085	3.79789
H	1.58749	-2.03572	2.87213
H	-1.86691	-1.70842	-1.83644
H	-0.33794	1.79877	-0.99555

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5621.49043892705

Zero-point correction (ZPE) = -5621.168481 .32195776893

Internal Energy (U) = -5621.368871 .12156754301

Enthalpy (H) = -5621.127868 .362570594039969

Gibbs Free Energy (G) = -5621.249437 .24100174884

Frequencies -- 8.89 13.52 18.07 20.39 24.24 27.16

Dual Copper Oxidative Epoxide Ring Opening TS
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 41
Charge: 0	Spin:	Basis Functions: 536

Energy = -5390.52386577256

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000004	0.0000010	yes			
Step	0.0005264	0.0010000	yes	0.0000925	0.0005000	yes
Grad	0.0008660	0.0010000	yes	0.0001482	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	5.14676	-2.20171	0.90661
C	4.33745	-1.02318	0.32221
C	4.95510	0.23455	0.23861
C	4.31621	1.36777	-0.29752
C	5.10723	2.69352	-0.36544
C	-0.24642	-1.58217	-0.03584
C	0.12115	-0.94083	-1.29899
C	0.05797	0.43029	-1.52760
C	-0.08673	-3.02389	0.16206
O	3.14863	1.46176	-0.75722
O	3.17260	-1.34724	-0.03587
O	-1.43282	-2.91382	-0.23418
Cu	1.91395	-0.05737	-0.81992
F	5.22738	3.08419	-1.63972
F	6.33890	2.58534	0.15215
F	4.45876	3.64985	0.30623
F	5.31718	-3.14297	-0.03026
F	4.48470	-2.75176	1.93152
F	6.35643	-1.83159	1.34593
C	-6.75354	-0.45671	-0.21824
C	-5.23732	-0.24275	0.00391
C	-4.80121	1.04918	0.37692
C	-3.45632	1.36649	0.59992
O	-2.44964	0.60803	0.52772
Cu	-2.54181	-1.32482	0.01714
C	-3.09704	2.81475	0.99090
F	-2.17153	3.29919	0.14508
F	-2.57731	2.84625	2.22564

F	-4.14811	3.64352	0.96514
O	-4.55097	-1.27181	-0.18348
F	-6.98390	-0.82492	-1.48498
F	-7.47791	0.64698	0.02584
F	-7.20324	-1.42655	0.58628
H	-0.41446	-0.95080	0.84335
H	5.97555	0.33627	0.59838
H	0.32062	-1.62359	-2.13382
H	-0.39217	1.10411	-0.79013
H	0.19321	0.82307	-2.53968
H	0.54706	-3.56174	-0.55972
H	0.06966	-3.37938	1.19285
H	-5.54401	1.83450	0.48821

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.52386577256

Zero-point correction (ZPE) = -5390.297432 .22643309314

Internal Energy (U) = -5390.413424 .11044099903

Enthalpy (H) = -5390.262654 .261210838368018

Gibbs Free Energy (G) = -5390.373094 .15077130348

Frequencies -- i294.60 8.65 10.70 11.99 17.39 22.28

Dual Copper Metalaoxetane (s-*trans*)
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 41
Charge: 0	Spin: 1	Basis Functions: 536

Energy = -5390.53887786453

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0000522	0.0001000	yes	0.0000091	0.0000500	yes
Grad	0.0000169	0.0010000	yes	0.0000051	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.18394	1.43405	1.02533
H	-2.73666	1.86198	0.17875
C	-2.09730	2.22500	2.22832
C	-2.42409	3.53795	2.30609
C	-2.00499	-0.06678	1.05079
O	-0.71021	-0.17456	0.46317
H	-1.74751	1.70817	3.13071
H	-2.75149	4.09792	1.42598
H	-2.00868	-0.48211	2.07385
C	3.63846	2.03478	-1.47582
C	2.22385	2.42637	-0.99007
C	1.85869	3.78949	-1.00719
H	2.57477	4.52346	-1.36623
C	0.60294	4.22486	-0.57608
O	-0.35350	3.53773	-0.11176
Cu	-0.32221	1.62729	0.15112
C	0.26535	5.72734	-0.66729
F	-0.19023	6.17142	0.50920
F	-0.69296	5.91841	-1.58321
F	1.32250	6.47172	-1.01133
O	1.52554	1.45571	-0.61668
F	4.28897	1.39366	-0.50082
F	4.36900	3.10143	-1.83111
F	3.55068	1.22217	-2.53241
Cu	0.08248	-1.80017	-0.10417
O	-1.24971	-3.15839	0.65640
O	1.22113	-3.10847	-0.94914
C	-1.09175	-4.38385	0.44218

C	0.98507	-4.34522	-0.91612
C	-0.07286	-5.02594	-0.28960
C	-2.18178	-5.26543	1.09482
C	2.03314	-5.17951	-1.68507
H	-0.10502	-6.10881	-0.37277
F	-3.39497	-4.88047	0.67668
F	-2.04622	-6.56990	0.81362
F	-2.14277	-5.12848	2.42789
F	2.07765	-4.79306	-2.96606
F	1.77127	-6.49561	-1.66373
F	3.24792	-4.99638	-1.15298
H	-2.76488	-0.60742	0.46123
H	-2.36567	4.07964	3.25350

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.53887786453

Zero-point correction (ZPE) = -5390.311606 .22727102889

Internal Energy (U) = -5390.426390 .11248733831

Enthalpy (H) = -5390.276204 .262673417136169

Gibbs Free Energy (G) = -5390.388693 .15018474845

Frequencies -- 7.05 8.65 10.37 18.90 22.20 27.67

Dual Copper Metalaoxetane (s-*cis*)
Using: TURBOMOLE V6.3

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============================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  41
Charge: 0     | Spin: 1                         | Basis Functions:   536
------------------------------------------------------------------------------------------------
Energy =    -5390.53680866891
------------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000002  || 0.0000010   yes
Step      0.0004666   || 0.0010000   yes  |  0.0000723  || 0.0005000   yes
Grad      0.0001624   || 0.0010000   yes  |  0.0000349  || 0.0005000   yes
============================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
------------------------------------------------------------------------------------------------
C       -1.47663      -2.94894      -0.80295
C       -0.99447      -2.92621       0.51947
C        0.37528      -2.91261       0.80421
C       -0.44710      -2.86916      -1.90331
O        0.05949      -1.54111      -1.70178
C       -1.49335       3.47413      -0.41800
C       -2.04571       2.03143      -0.47642
C       -3.38086       1.80545      -0.07925
C       -3.95613       0.53000      -0.06987
O       -3.43153      -0.57512      -0.38906
Cu       -1.60119      -0.78492      -1.00951
C       -5.41848       0.38070       0.39925
F       -5.46472      -0.37919       1.50168
F       -6.14596      -0.21935      -0.54984
F       -5.99619       1.55542       0.68276
O       -1.21291       1.19039      -0.88617
F       -0.40894       3.51166       0.36425
F       -2.38483       4.34957       0.06888
F       -1.14192       3.87993      -1.64225
C        4.39040       1.39773      -1.78053
C        3.51865       0.61461      -0.77115
C        3.80508       0.74796       0.60545
C        3.06891       0.08431       1.58901
C        3.45623       0.29276       3.06792
O        2.08068      -0.69540       1.45156
O        2.62490      -0.07711      -1.30549
Cu        1.31454      -1.18903      -0.25709
F        3.67291      -0.89039       3.65614
```

F	2.45946	0.90389	3.71949
F	4.56161	1.03516	3.21346
F	4.92786	0.55404	-2.66842
F	5.39129	2.06395	-1.18563
F	3.64106	2.28374	-2.44332
H	-2.53648	-3.12567	-1.01010
H	-1.70925	-2.78931	1.33813
H	0.71941	-2.80011	1.83451
H	1.07751	-3.41398	0.12370
H	0.35458	-3.62977	-1.83816
H	-0.89984	-2.95842	-2.90540
H	-3.98208	2.65156	0.24292
H	4.62871	1.38738	0.91090

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Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.53680866891

Zero-point correction (ZPE) = -5390.308928 .22788043671

Internal Energy (U) = -5390.427347 .10946098194

Enthalpy (H) = -5390.274352 .262456315600272

Gibbs Free Energy (G) = -5390.383816 .15299183322

Frequencies -- 5.42 8.96 9.15 18.60 27.63 28.45

Dual Copper Suprafacial Copper Migration TS
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 41
Charge: 0 | Spin: 1 | Basis Functions: 536

Energy = -5390.53598068066

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0004395	0.0010000	yes	0.0000925	0.0005000	yes
Grad	0.0005770	0.0010000	yes	0.0000947	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.55756	-2.89126	-1.10674
C	-1.15082	-2.98137	0.25980
C	0.16505	-3.00985	0.65054
C	-0.49239	-2.76914	-2.16380
O	-0.08619	-1.41090	-1.93241
C	-1.36761	3.39914	-0.14619
C	-1.97550	1.98427	-0.28075
C	-3.26664	1.75297	0.23907
C	-3.88269	0.49872	0.18736
O	-3.44158	-0.58027	-0.30610
Cu	-1.69139	-0.77969	-1.10063
C	-5.27974	0.33504	0.82165
F	-5.21353	-0.53145	1.84166
F	-6.14186	-0.14775	-0.07913
F	-5.77159	1.48825	1.29029
O	-1.22815	1.16484	-0.86350
F	-0.16265	3.32387	0.42588
F	-2.13020	4.21553	0.59463
F	-1.22605	3.94982	-1.35656
C	4.63039	1.41392	-1.78155
C	3.62351	0.66506	-0.87718
C	3.79115	0.75034	0.52254
C	2.92728	0.12598	1.42912
C	3.20999	0.27550	2.93924
O	1.90144	-0.57362	1.19391
O	2.74081	0.04866	-1.51452
Cu	1.24307	-0.94337	-0.59570
F	3.34361	-0.93443	3.50053

F	2.18850	0.89830	3.54012
F	4.32521	0.97227	3.19655
F	5.20211	0.55742	-2.63645
F	5.60789	2.01593	-1.08699
F	3.99471	2.35215	-2.49185
H	-2.60215	-3.07881	-1.37572
H	-1.93128	-2.91787	1.02578
H	0.44786	-2.95219	1.70336
H	0.97395	-3.22869	-0.05271
H	0.34957	-3.47721	-2.05804
H	-0.89864	-2.88030	-3.18296
H	-3.79469	2.57514	0.71478
H	4.62679	1.32502	0.91267

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.53598068066

Zero-point correction (ZPE) = -5390.308366 .22761382079

Internal Energy (U) = -5390.428410 .10757021895

Enthalpy (H) = -5390.274373 .261606953451059

Gibbs Free Energy (G) = -5390.381941 .15403925291

Frequencies -- i48.95 6.11 9.58 11.19 19.26 27.82

Dual Copper Antarafacial Copper Migration TS
Using: TURBOMOLE V6.3

Method: b3-lyp		Basis: def2-SVP			Atoms: 41		
Charge: 0	Spin: 1				Basis Functions: 536		

Energy = -5390.51179066632

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0004754	0.0010000	yes	0.0000925	0.0005000	yes
Grad	0.0009655	0.0010000	yes	0.0001668	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.33446	-2.86969	-0.64029
C	-0.75354	-2.76797	0.66653
H	-1.06760	-3.55952	1.36401
C	0.15033	-1.85228	1.15208
H	0.16576	-0.80294	0.83041
C	-0.46552	-2.74926	-1.87165
H	-1.04815	-2.98407	-2.78121
O	-0.08627	-1.38055	-1.88613
C	-1.82266	3.30572	0.23114
C	-2.31674	1.87806	-0.10039
C	-3.64822	1.52750	0.21643
C	-4.15088	0.24115	0.00405
O	-3.56364	-0.77369	-0.47775
Cu	-1.71497	-0.80702	-0.98787
C	-5.61587	-0.05673	0.38850
F	-5.66350	-1.09283	1.23407
F	-6.31870	-0.37776	-0.70377
F	-6.21634	0.98557	0.97602
O	-1.44021	1.14540	-0.61101
F	-0.90184	3.23887	1.20009
F	-2.81576	4.10160	0.65785
F	-1.27156	3.86818	-0.84263
C	5.33998	-1.35281	0.89487
C	4.08007	-0.67407	0.31703
C	4.06256	0.71987	0.21703
C	2.95619	1.43899	-0.29885
C	3.06933	2.98011	-0.39493
O	1.87209	0.98256	-0.70990

O	3.18465	-1.51013	0.00089
Cu	1.44300	-1.06733	-0.71507
F	2.04232	3.55915	0.23640
F	3.03816	3.35914	-1.67876
F	4.20414	3.45525	0.14406
F	5.02407	-2.02973	2.00916
F	6.30923	-0.48105	1.20699
F	5.84173	-2.22522	0.01226
H	-2.25843	-3.45362	-0.72057
H	-4.30159	2.27940	0.65067
H	4.93890	1.27361	0.54313
H	0.40665	-3.43389	-1.84143
H	0.64729	-2.03796	2.10855

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.51179066632

Zero-point correction (ZPE) = -5390.285586 .22620456520

Internal Energy (U) = -5390.404096 .10769399863

Enthalpy (H) = -5390.251246 .260544298564825

Gibbs Free Energy (G) = -5390.358939 .15285090766

Frequencies -- i88.04 9.81 14.31 17.35 22.62 26.74

Dual Copper Tricyclic Intermediate
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 41
Charge: 0 | Spin: | Basis Functions: 536

Energy = -5390.53696449256

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0009602	0.0010000	yes	0.0001933	0.0005000	yes
Grad	0.0005793	0.0010000	yes	0.0000784	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.34341	-2.25371	-1.91956
C	-0.80773	-2.83271	-0.75164
C	0.56653	-2.87415	-0.51400
C	-0.37175	-1.58929	-2.86324
O	0.05685	-0.47736	-2.05908
C	-2.25647	3.56142	0.75992
C	-2.51004	2.09645	0.33311
C	-3.70933	1.47593	0.74533
C	-4.03570	0.16590	0.38072
O	-3.37069	-0.64325	-0.32787
Cu	-1.63154	-0.26152	-1.11061
C	-5.36761	-0.43534	0.87517
F	-5.12762	-1.53573	1.59989
F	-6.12666	-0.78407	-0.17102
F	-6.07337	0.41335	1.63291
O	-1.59554	1.61039	-0.37078
F	-1.06494	3.67004	1.35365
F	-3.18673	4.01927	1.61105
F	-2.26215	4.35111	-0.32016
C	4.59242	2.04847	-1.12680
C	3.68244	0.97571	-0.48400
C	4.01037	0.50037	0.80481
C	3.26433	-0.48987	1.44974
C	3.72440	-0.97087	2.84255
O	2.22693	-1.09221	1.04568
O	2.72693	0.62633	-1.21096
Cu	1.39698	-0.79132	-0.68135
F	4.00659	-2.28027	2.79983

F	2.75114	-0.78610	3.74119
F	4.81631	-0.32819	3.27764
F	5.10750	1.57746	-2.26883
F	5.61232	2.40526	-0.33151
F	3.88379	3.14519	-1.40776
H	-2.39887	-2.39054	-2.17443
H	-1.49739	-3.14125	0.04140
H	0.95050	-3.23923	0.44088
H	1.26607	-2.93651	-1.35948
H	0.47960	-2.22460	-3.17312
H	-0.86180	-1.23058	-3.78421
H	-4.40370	2.03586	1.36602
H	4.88103	0.91014	1.30892

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.53696449256

Zero-point correction (ZPE) = -5390.309122 .22784234872

Internal Energy (U) = -5390.428367 .10859679537

Enthalpy (H) = -5390.274553 .262410610013767

Gibbs Free Energy (G) = -5390.383149 .15381453378

Frequencies -- 7.79 10.32 11.13 18.97 30.96 32.22

Dual Copper Metalaoxetane Ring Opening TS
Using: TURBOMOLE V6.3

Method: b3-lyp	Basis: def2-SVP	Atoms: 41
Charge: 0	Spin: 1	Basis Functions: 536

Energy = -5390.53149515096

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000500	0.0000010	no			
Step	0.0089140	0.0010000	no	0.0016630	0.0005000	no
Grad	0.0018041	0.0010000	no	0.0003831	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.79207	-1.96242	2.67995
C	-0.09639	-2.70285	1.94178
C	-1.48404	-2.35374	1.90128
C	0.25521	-0.71727	3.33984
O	-0.20884	0.12582	2.27621
C	4.34131	2.76096	-0.23842
C	3.46692	1.48717	-0.17184
C	3.69678	0.47819	-1.13193
C	2.96667	-0.71700	-1.16844
O	2.01960	-1.08394	-0.42061
Cu	1.29099	0.00095	1.03914
C	3.37068	-1.78543	-2.20706
F	2.28984	-2.31266	-2.78951
F	4.03393	-2.77855	-1.59203
F	4.16564	-1.29939	-3.17092
O	2.62253	1.50036	0.75247
F	3.58506	3.81587	-0.56728
F	5.32795	2.66575	-1.14410
F	4.90013	3.00294	0.95220
C	-2.57433	3.30215	-0.86195
C	-2.60482	1.80699	-0.45868
C	-3.50533	0.98258	-1.16726
C	-3.63359	-0.37816	-0.89276
C	-4.66332	-1.16555	-1.73779
O	-3.02577	-1.06986	-0.02218
O	-1.83362	1.46920	0.46459
Cu	-1.65536	-0.41690	1.16169
F	-4.66925	-2.45672	-1.42212

F	-4.38593	-1.04982	-3.04449
F	-5.89639	-0.67501	-1.53727
F	-3.78750	3.84973	-0.68161
F	-2.26127	3.42447	-2.16167
F	-1.69173	3.98516	-0.14699
H	1.84749	-2.24006	2.75291
H	0.27126	-3.48994	1.27515
H	-2.14600	-2.90715	1.23009
H	-1.95740	-2.03097	2.84055
H	-0.56724	-0.93257	4.04974
H	1.03742	-0.18303	3.90495
H	4.48132	0.63049	-1.86820
H	-4.11466	1.42023	-1.95745

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.53149515096

Zero-point correction (ZPE) = -5390.303652 .22784234872

Internal Energy (U) = -5390.424533 .10696154090

Enthalpy (H) = -5390.269857 .261637423842062

Gibbs Free Energy (G) = -5390.376819 .15467532232

Frequencies -- i19.58 8.24 8.91 17.80 21.45 24.37

Dual Copper Metalaoxipane

Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  41
Charge: 0     | Spin: 1                         | Basis Functions:   536
----------------------------------------------------------------------------------------------
Energy =    -5390.54943929733
----------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000003  || 0.0000010   yes
Step      0.0009369   || 0.0010000   yes  |  0.0001596  || 0.0005000   yes
Grad      0.0000390   || 0.0010000   yes  |  0.0000087  || 0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
----------------------------------------------------------------------------------------------
C        4.58275      -2.45597      -1.59633
C        3.42269      -1.66252      -0.95204
C        2.98533      -0.49356      -1.60492
H        3.49404      -0.21296      -2.52390
C        1.93245       0.32832      -1.16044
O        1.23539       0.19884      -0.12575
C        1.55335       1.55147      -2.02674
F        0.30274       1.40112      -2.50290
F        2.36594       1.73945      -3.07400
F        1.57346       2.66526      -1.28366
O        3.00349      -2.19803       0.10657
F        5.10879      -1.84312      -2.66803
F        4.15134      -3.66225      -1.98745
F        5.56538      -2.63539      -0.70567
Cu       1.59473      -1.54136       1.20036
C       -0.79840       0.09770       4.30639
H       -1.28458      -0.09013       5.26970
C       -0.82540       1.34499       3.76770
H       -1.44584       2.10085       4.26508
C       -0.17603       1.74238       2.53470
H       -0.49454       2.69251       2.09341
H        0.88694       1.51728       2.40363
C       -0.23594      -1.09033       3.59643
H        0.60727      -1.47869       4.21178
H       -1.00014      -1.90014       3.60841
O        0.24220      -0.80840       2.32757
C       -2.70522      -2.21758      -1.63925
C       -2.26897      -0.91956      -0.92283
```

C	-2.70605	0.31368	-1.44454
C	-2.39272	1.52895	-0.83266
C	-2.97204	2.82937	-1.42825
O	-1.70033	1.74176	0.20512
O	-1.55779	-1.11347	0.08999
Cu	-0.75858	0.37314	1.17896
F	-2.00718	3.73194	-1.60990
F	-3.87290	3.34514	-0.57889
F	-3.58213	2.62744	-2.60303
F	-3.46860	-2.95355	-0.82214
F	-3.40815	-1.97593	-2.75459
F	-1.63247	-2.93995	-1.97329
H	-3.31428	0.32128	-2.34456

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.54943929733

Zero-point correction (ZPE) = -5390.321825 .22761382079

Internal Energy (U) = -5390.442192 .10724657484

Enthalpy (H) = -5390.287181 .262258258058751

Gibbs Free Energy (G) = -5390.394424 .15501430542

Frequencies -- 9.13 15.26 23.87 27.32 27.54 34.43

Dual Copper Reductive Elimination TS

Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 41
Charge: 0 | Spin: 1 | Basis Functions: 536

Energy = -5390.52110000154

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000009	0.0000010	yes			
Step	0.0004500	0.0001000	no	0.0000925	0.0000500	no
Grad	0.0002223	0.0010000	yes	0.0000455	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	5.94378	-1.72094	0.63474
C	4.88847	-0.60562	0.44926
C	5.34379	0.72452	0.29910
H	6.41352	0.91488	0.31215
C	4.47378	1.80386	0.11769
O	3.20929	1.79925	0.07985
C	5.07233	3.20962	-0.09262
F	4.73948	3.66495	-1.30929
F	6.40891	3.22576	0.00108
F	4.58487	4.06252	0.81528
O	3.70908	-1.01927	0.45164
F	7.20379	-1.26487	0.56883
F	5.79415	-2.65328	-0.31383
F	5.78142	-2.30847	1.82610
Cu	2.08818	0.22373	0.21314
C	-0.66093	-0.86801	-1.79982
H	-0.96406	-1.33188	-2.74386
C	-0.63925	0.50692	-1.60130
H	-0.90115	1.20311	-2.40755
C	0.17621	1.04183	-0.47545
H	0.91239	1.79595	-0.81062
H	-0.33945	1.37278	0.43162
C	0.17932	-1.62061	-0.79704
H	1.08538	-2.03443	-1.28668
H	-0.37618	-2.47510	-0.36637
O	0.46475	-0.74138	0.26099
C	-5.29560	1.98731	1.22868
C	-4.61081	0.77697	0.55715

C	-5.24638	-0.47522	0.62371
C	-4.69194	-1.64408	0.07374
C	-5.46778	-2.97009	0.22790
O	-3.60283	-1.77754	-0.54384
O	-3.51417	1.06837	0.01180
Cu	-2.38514	-0.27523	-0.88007
F	-4.75530	-3.82916	0.96780
F	-5.67180	-3.52400	-0.97253
F	-6.66092	-2.80856	0.81643
F	-5.49735	2.95608	0.32846
F	-6.47931	1.67892	1.77665
F	-4.50764	2.47443	2.19592
H	-6.20486	-0.54402	1.13118

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.52110000154

Zero-point correction (ZPE) = -5390.293943 .22715676492

Internal Energy (U) = -5390.412352 .10874782929

Enthalpy (H) = -5390.260007 .261092765602881

Gibbs Free Energy (G) = -5390.368755 .15234433741

Frequencies -- i372.53 9.03 9.80 10.24 20.19 23.85

Dual Copper Product-Catalyst Complex
Using: TURBOMOLE V6.3

Method: b3-lyp | Basis: def2-SVP | Atoms: 41
Charge: 0 | Spin: | Basis Functions: 536

Energy = -5390.58592706604

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0006907	0.0010000	yes	0.0001683	0.0005000	yes
Grad	0.0000968	0.0010000	yes	0.0000300	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.15453	-1.65673	2.28581
C	-0.99257	-0.99557	2.65754
C	-0.59597	0.39116	3.13046
C	1.33013	-0.73764	2.54610
O	0.73713	0.55437	2.64615
C	4.85151	1.09823	-1.12663
C	3.39017	0.63560	-0.91342
C	3.05714	-0.68103	-1.30946
C	1.79367	-1.26447	-1.15747
O	0.74074	-0.71260	-0.73388
Cu	0.80836	1.44024	0.08110
C	1.62901	-2.75514	-1.51823
F	0.65824	-2.91489	-2.42234
F	1.27358	-3.44373	-0.41280
F	2.74486	-3.31156	-2.00088
O	2.67407	1.51024	-0.37369
F	4.87610	2.22107	-1.85030
F	5.60235	0.18330	-1.75931
F	5.42584	1.34940	0.05739
C	-4.68143	-0.82203	-1.47885
C	-3.38649	-0.22673	-0.87349
C	-3.17805	1.17029	-1.00182
C	-2.05759	1.82644	-0.49885
C	-1.88290	3.33027	-0.78089
O	-1.13345	1.32200	0.21332
O	-2.64928	-1.07774	-0.33905
Cu	-0.85239	-0.95828	0.55431
F	-1.91632	4.02294	0.36553

F	-2.81923	3.82693	-1.59472
F	-0.68276	3.54536	-1.35077
F	-5.35778	-1.48594	-0.53348
F	-4.37897	-1.68154	-2.45814
F	-5.49849	0.11242	-1.98811
H	0.25852	-2.73320	2.12817
H	-1.96432	-1.44968	2.86670
H	-1.21277	1.21024	2.73328
H	-0.62328	0.43477	4.24070
H	1.82906	-1.02373	3.49746
H	2.09741	-0.71523	1.75824
H	3.84797	-1.29068	-1.73872
H	-3.91636	1.75287	-1.54692

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -5390.58592706604

Zero-point correction (ZPE) = -5390.356713 .22921351632

Internal Energy (U) = -5390.477893 .10803354105

Enthalpy (H) = -5390.322034 .263892232776295

Gibbs Free Energy (G) = -5390.430071 .15585604998

Frequencies -- 11.52 15.60 19.66 23.58 27.33 32.03

7. Geometries, Energies, and Thermal Corrections for allyl anion Me-allyl

Using: TURBOMOLE V6.3

==========

Method: b3-lyp | Basis: def2-SVP | Atoms: 11
Charge: -1 | Spin: 1 | Basis Functions: 91

Energy = -156.34735315904

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0000927	0.0001000	yes	0.0000317	0.0000500	yes
Grad	0.0000085	0.0010000	yes	0.0000030	0.0005000	yes

==========

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.04764	-1.68827	0.42202
H	-0.07832	-2.59757	1.03439
H	-0.03979	-1.82392	-0.66664
C	-0.02069	-0.42306	1.01337
H	-0.03230	-0.43130	2.12081
C	0.01834	0.85239	0.44656
H	0.03417	1.73583	1.09653
C	0.03755	1.05517	-1.03675
H	0.06501	2.12782	-1.31415
H	0.91251	0.57614	-1.54985
H	-0.84883	0.61677	-1.56629

==========

Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -156.34735315904
Zero-point correction (ZPE) = -156.2569322 .09042088530
Internal Energy (U) = -156.3129174 .03443573379
Enthalpy (H) = -156.2502406 .097112547620599
Gibbs Free Energy (G) = -156.2846755 .06267759429

Frequencies -- 129.74 226.86 230.75 344.82 424.02 585.80

Me-allyl-9
Using: TURBOMOLE V6.3
==========
Method: b3-lyp | Basis: def2-SVP | Atoms: 11
Charge: -1 | Spin: 1 | Basis Functions: 91

Energy = -156.34703263472

Item Max Val. || Criteria Pass? | RMS Val. || Criteria Pass?
Energy 0.0000000 || 0.0000010 yes
Step 0.0000742 || 0.0001000 yes | 0.0000174 || 0.0000500 yes
Grad 0.0000110 || 0.0010000 yes | 0.0000039 || 0.0005000 yes
==========
Atomic Coordinates (Angstroms)
Type X Y Z

C -0.01191 -1.57056 -0.56463
H -0.05924 -2.66119 -0.45935
H 0.03143 -1.17254 -1.58593
C -0.00345 -0.73935 0.55701
H -0.04314 -1.27362 1.52631
C 0.09074 0.65101 0.66943
H -0.01475 1.11423 1.65924
C 0.00830 1.54135 -0.53335
H 0.03745 2.61599 -0.26330
H 0.83973 1.38434 -1.26621
H -0.91832 1.39450 -1.15131
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -156.34703263472
Zero-point correction (ZPE) = -156.2564974 .09053514926
Internal Energy (U) = -156.3127888 .03424381851
Enthalpy (H) = -156.2498743 .097158253207103
Gibbs Free Energy (G) = -156.2841188 .06291373982

Frequencies -- 136.00 224.41 265.55 352.91 439.15 585.16

Me-allyl-39
Using: TURBOMOLE V6.3
==========
Method: b3-lyp | Basis: def2-SVP | Atoms: 11
Charge: -1 | Spin: 1 | Basis Functions: 91

Energy = -156.34028054646

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000000	0.0000010	yes			
Step	0.0000865	0.0001000	yes	0.0000229	0.0000500	yes
Grad	0.0000165	0.0010000	yes	0.0000051	0.0005000	yes

==========
Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.03354	-1.63747	-0.52935
H	-0.24641	-2.68906	-0.38816
H	0.22658	-1.31665	-1.56207
C	-0.03899	-0.73203	0.52475
H	-0.22207	-1.21525	1.50625
C	0.29048	0.63776	0.62416
H	0.06549	1.08193	1.61015
C	-0.00504	1.58850	-0.51354
H	0.09598	2.64638	-0.19725
H	0.67564	1.48131	-1.39195
H	-1.03319	1.48489	-0.95528

==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -156.34028054646
Zero-point correction (ZPE) = -156.2495168 .09076367720
Internal Energy (U) = -156.3060662 .03421429308
Enthalpy (H) = -156.2430194 .097261090776739
Gibbs Free Energy (G) = -156.2772334 .06304704778

Frequencies -- 107.07 209.79 278.71 423.47 525.87 637.55

8. Figures, Geometries, Energies, and Thermal Corrections for catalyst complexation

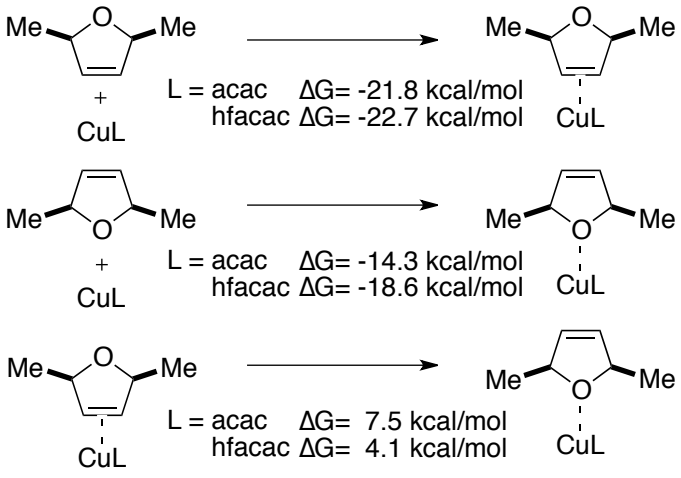


Figure 17. Complexation energies for Cu(I) with product. With more electronegative ligands, Cu coordinates with the Oxygen-lp more strongly. But the complexation with the π-system is still preferred, presumably due to back bonding.

Cu(I) hfacac

Using: TURBOMOLE V6.3

```
==========================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  15
Charge: 0     | Spin: 1                         | Basis Functions:   218
----------------------------------------------------------------------------------------------
Energy =    -2579.78724649463
----------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000003  || 0.0000010   yes
Step      0.0006682  || 0.0010000   yes  |  0.0001495  || 0.0005000   yes
Grad      0.0000528  || 0.0010000   yes  |  0.0000202  || 0.0005000   yes
==========================================================
Atomic Coordinates (Angstroms)
Type  X       Y       Z
----------------------------------------------------------------------------------------------
C       -0.75500      -2.19219      -1.08833
C        0.11335      -1.32073      -0.15082
C       -0.17313       0.05983      -0.08632
C        0.50619       1.04004       0.66902
C        0.03655       2.50635       0.52581
O        1.48778       0.92057       1.45615
O        1.00211      -1.99225       0.44667
Cu       2.10986      -0.90352       1.59650
F        0.98396       3.22185      -0.09614
```

F	-0.16802	3.04606	1.73109
F	-1.09802	2.62782	-0.17854
F	-1.34389	-3.17026	-0.39080
F	0.01764	-2.75563	-2.02555
F	-1.71691	-1.49761	-1.71263
H	-1.00247	0.40969	-0.69612

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2579.78724649463

Zero-point correction (ZPE) = -2579.719906 .06733956411

Internal Energy (U) = -2579.730472 .05677399126

Enthalpy (H) = -2579.706020 .081226047511336

Gibbs Free Energy (G) = -2579.762794 .02445248878

Frequencies -- 21.39 26.36 83.69 88.76 112.65 155.51

Cu(I) acac

Using: TURBOMOLE V6.4

```
============================================================
Method: b3-lyp        |  Basis: def2-SVP            |  Atoms:  15
Charge: 0     |  Spin: 1                            |  Basis Functions:   164
------------------------------------------------------------------------------------------------
Energy =    -1984.99121625433
------------------------------------------------------------------------------------------------
Item      Max Val.     ||  Criteria     Pass? |   RMS Val.  ||  Criteria     Pass?
Energy    0.0000000  ||  0.0000010   yes
Step       0.0007137   ||  0.0010000   yes   |  0.0001278  ||  0.0005000   yes
Grad       0.0000473   ||  0.0010000   yes   |  0.0000141  ||  0.0005000   yes
============================================================
Atomic Coordinates (Angstroms)
Type   X         Y         Z
------------------------------------------------------------------------------------------------
C         -0.79082       -2.16695       -1.08553
C          0.10497       -1.34033       -0.18257
C         -0.14034        0.05779       -0.09913
C          0.51530        1.07755        0.64412
C          0.00392        2.49878        0.50487
O          1.50993        0.95210        1.43637
O          1.00822       -2.01339        0.42058
Cu         2.07361       -0.87351        1.52724
H          0.81702        3.13705        0.12103
H         -0.25699        2.88660        1.50310
H         -0.86716        2.58568       -0.15831
H         -1.27130       -2.95886       -0.48791
H         -0.16909       -2.67562       -1.84051
H         -1.56436       -1.57473       -1.59226
H         -0.97290        0.40782       -0.71108
============================================================
Thermodynamic Analysis
Tempurature = 298.15 Kelvin     Pressure = 101325 Pa
------------------------------------------------------------------------------------------------
SCF Energy =    -1984.99121625433
Zero-point correction (ZPE) = -1984.879428    .11178824699
Internal Energy (U) = -1984.945778    .04543736250
Enthalpy (H) = -1984.869258    .121957342684785
Gibbs Free Energy (G) = -1984.914697    .07651876940
------------------------------------------------------------------------------------------------
Frequencies -- 79.91 92.44 118.92 157.51 171.29 182.10
```

Cis-DiMeDHF-π-Cu(I) hfacac

Using: TURBOMOLE V6.4

```
==============================================================
Method: b3-lyp       | Basis: def2-SVP          | Atoms:  32
Charge: 0     | Spin: 1                         | Basis Functions:   366
--------------------------------------------------------------------------------------------
Energy =    -2889.27811593941
--------------------------------------------------------------------------------------------
Item      Max Val.     || Criteria     Pass? |  RMS Val.  || Criteria     Pass?
Energy    0.0000003  || 0.0000010   yes
Step      0.0001599   || 0.0010000   yes  |  0.0000287  || 0.0005000   yes
Grad      0.0001728   || 0.0010000   yes  |  0.0000325  || 0.0005000   yes
==============================================================
Atomic Coordinates (Angstroms)
Type  X        Y        Z
--------------------------------------------------------------------------------------------
C        1.53823      -1.91295       0.64766
C        0.46260      -2.50707       0.01253
C       -0.63725      -2.71524       1.04618
C        1.16767      -1.71537       2.11251
C       -2.39575       1.52601      -2.80997
C       -1.11931       1.30314      -1.96981
C       -0.31489       2.41614      -1.66953
C        0.84678       2.32187      -0.88378
C        1.65215       3.60921      -0.60414
C       -2.06862      -2.43507       0.62214
C        1.57912      -0.41324       2.77784
O       -0.25298      -1.84330       2.10742
O        1.34671       1.29871      -0.35007
O       -0.95115       0.10401      -1.62969
Cu       0.52557      -0.50225      -0.45471
F        1.74736       3.81125       0.71626
F        1.09705       4.70183      -1.14864
F        2.89186       3.49037      -1.09666
F       -3.47536       1.18992      -2.09094
F       -2.37108       0.75703      -3.90454
F       -2.54518       2.79902      -3.20513
H        2.57326      -1.90716       0.29338
H        0.49620      -3.05430      -0.93410
H       -0.56447      -3.77336       1.39183
H        1.61399      -2.56606       2.67950
H       -0.60873       3.39004      -2.05156
H       -2.38595      -3.15613      -0.14783
H       -2.74169      -2.53540       1.48709
```

H -2.16932 -1.42141 0.20630
H 1.16789 -0.36788 3.79765
H 2.67671 -0.34881 2.84452
H 1.21858 0.45645 2.20829
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.27811593941
Zero-point correction (ZPE) = -2889.061357 .21675874399
Internal Energy (U) = -2889.202281 .07583492623
Enthalpy (H) = -2889.039018 .239096952097488
Gibbs Free Energy (G) = -2889.114851 .16326416379

Frequencies -- 20.80 27.39 32.52 38.33 44.27 84.54

Cis-DiMeDHF-π-Cu(I) acac
Using: TURBOMOLE V6.4

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 312

Energy = -2294.48023726234

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000002	0.0000010	yes			
Step	0.0009628	0.0010000	yes	0.0001540	0.0005000	yes
Grad	0.0000379	0.0010000	yes	0.0000089	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.52210	-1.87300	0.61801
C	0.43133	-2.45616	-0.00971
C	-0.63737	-2.70866	1.04569
C	1.19072	-1.73099	2.09777
C	-2.36366	1.53849	-2.86153
C	-1.14955	1.30252	-1.98460
C	-0.31733	2.39844	-1.66407
C	0.84084	2.35135	-0.85616
C	1.61396	3.63229	-0.61088
C	-2.07873	-2.40713	0.67192
C	1.59831	-0.44063	2.78853
O	-0.22750	-1.88207	2.13362
O	1.31849	1.31540	-0.29533
O	-0.98249	0.10132	-1.60371
Cu	0.48998	-0.45665	-0.43466
H	1.66249	3.82283	0.47394
H	1.17513	4.50554	-1.11259
H	2.65297	3.49884	-0.95472
H	-3.26944	1.22813	-2.31490
H	-2.29670	0.89387	-3.75335
H	-2.47211	2.58502	-3.17739
H	2.55049	-1.86497	0.24516
H	0.44825	-2.98890	-0.96491
H	-0.56019	-3.78024	1.34720
H	1.66650	-2.58943	2.62861
H	-0.59696	3.36969	-2.07387
H	-2.42091	-3.09767	-0.11552
H	-2.72965	-2.53415	1.55057

H	-2.17740	-1.37880	0.29365
H	1.21294	-0.42784	3.81961
H	2.69639	-0.35992	2.82812
H	1.20906	0.43349	2.24552

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2294.48023726234

Zero-point correction (ZPE) = -2294.219029 .26120742687

Internal Energy (U) = -2294.415366 .06487077210

Enthalpy (H) = -2294.200500 .279736836097929

Gibbs Free Energy (G) = -2294.265371 .21486577095

Frequencies -- 28.42 45.48 57.40 81.66 98.24 101.78

Cis-DiMeDHF-O-lp-Cu(I) hfacac

Using: TURBOMOLE V6.4

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 366

Energy = -2889.26786306754

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000001	0.0000010	yes			
Step	0.0009971	0.0010000	yes	0.0001633	0.0005000	yes
Grad	0.0001667	0.0010000	yes	0.0000538	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.54113	-3.86848	1.31846
C	1.58503	-3.23604	1.85631
C	1.75313	-1.86344	1.26186
C	-0.13760	-3.00888	0.28593
C	1.76964	-0.70170	2.24534
C	-1.62361	-2.75228	0.49331
O	0.59999	-1.75878	0.37834
H	0.20000	-4.87752	1.55823
H	2.25886	-3.62968	2.61991
H	2.66261	-1.81904	0.63000
H	0.02297	-3.41841	-0.73172
H	2.66467	-0.76545	2.88507
H	1.80237	0.25836	1.70700
H	0.87625	-0.72346	2.88876
H	-2.19322	-3.68572	0.35819
H	-1.81639	-2.36443	1.50555
H	-1.98840	-2.01931	-0.24431
C	-2.77897	2.23729	-2.67785
C	-1.53207	1.89494	-1.83376
C	-0.65301	2.94068	-1.49743
C	0.51200	2.76286	-0.72513
C	1.38232	4.00466	-0.42796
O	0.96658	1.70501	-0.22721
O	-1.46024	0.67582	-1.53577
Cu	-0.00095	-0.06910	-0.43949
F	1.52422	4.16186	0.89599
F	0.87074	5.14325	-0.92078
F	2.60507	3.84718	-0.95565

F -3.89338 1.94870 -1.98943
F -2.79098 1.50843 -3.80188
F -2.84130 3.53111 -3.02980
H -0.88742 3.94156 -1.85009
==========
Thermodynamic Analysis
Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2889.26786306754
Zero-point correction (ZPE) = -2889.051447 .21641595209
Internal Energy (U) = -2889.188001 .07986174037
Enthalpy (H) = -2889.028442 .239420700001897
Gibbs Free Energy (G) = -2889.108304 .15955820248

Frequencies -- 6.86 21.41 25.53 30.41 37.74 57.33

Cis-DiMeDHF-O-lp-Cu(I) acac

Using: TURBOMOLE V6.4

Method: b3-lyp | Basis: def2-SVP | Atoms: 32
Charge: 0 | Spin: 1 | Basis Functions: 312

Energy = -2294.46470099847

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Energy	0.0000003	0.0000010	yes			
Step	0.0007997	0.0010000	yes	0.0001426	0.0005000	yes
Grad	0.0000433	0.0010000	yes	0.0000116	0.0005000	yes

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	0.54961	-3.85188	1.33084
C	1.60255	-3.20896	1.83823
C	1.74995	-1.84287	1.22213
C	-0.15196	-3.00462	0.30245
C	1.78627	-0.66728	2.18887
C	-1.63516	-2.75039	0.53402
O	0.57866	-1.75282	0.36640
H	0.21705	-4.85904	1.59033
H	2.29441	-3.59050	2.59199
H	2.64598	-1.80332	0.57017
H	-0.01135	-3.42665	-0.71360
H	2.70056	-0.71536	2.80277
H	1.78880	0.28274	1.63183
H	0.91211	-0.68893	2.85861
H	-2.20777	-3.68329	0.40638
H	-1.81109	-2.36265	1.54949
H	-2.00495	-2.01233	-0.19609
C	-2.75307	2.28825	-2.71817
C	-1.56089	1.89516	-1.86141
C	-0.64875	2.90641	-1.47647
C	0.51757	2.75184	-0.68618
C	1.35278	3.98690	-0.38797
O	0.94807	1.66945	-0.18897
O	-1.49594	0.66200	-1.56779
Cu	-0.05439	-0.06375	-0.46543
H	1.41374	4.12651	0.70430
H	0.95586	4.90363	-0.84610
H	2.38341	3.82056	-0.74306

H	-3.68118	1.98064	-2.20857
H	-2.71500	1.72947	-3.66813
H	-2.79781	3.36463	-2.93489
H	-0.86809	3.91648	-1.82597

==========

Thermodynamic Analysis

Tempurature = 298.15 Kelvin Pressure = 101325 Pa

SCF Energy = -2294.46470099847

Zero-point correction (ZPE) = -2294.203950 .26075037100

Internal Energy (U) = -2294.396028 .06867273875

Enthalpy (H) = -2294.184682 .280018687214708

Gibbs Free Energy (G) = -2294.253354 .21134644079

Frequencies -- 11.84 27.50 35.41 62.51 85.22 95.02

9. Transformation Between Mono- to Dual-Catalyst Explanation Figure

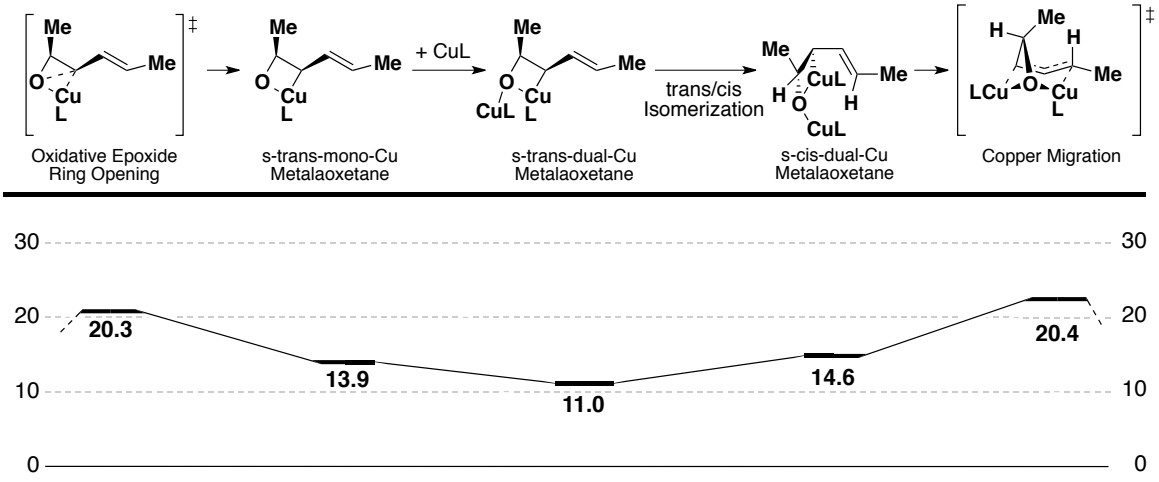


Figure 18. Transformation between mono- and dual-catalyst species and relative computed energies.

10. How Relative Energies of Figure 1 were Computed

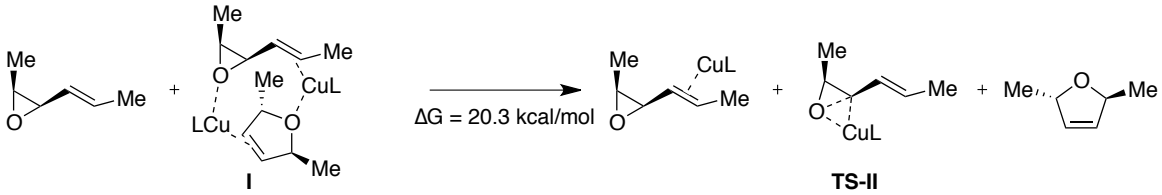


Figure 19. Explanation of relative computed energies between steps.

11. PDB files for Copper Migration TSs from Figure 3

Suprafacial Migration TS:

```
COMPND    0  1 F Last
AUTHOR    GENERATED BY OPEN BABEL 2.3.90
HETATM    1  C   LIG     1      -1.634  -2.978   0.006  1.00  0.00           C
HETATM    2  C   LIG     1      -1.097  -2.461   1.174  1.00  0.00           C
HETATM    3  C   LIG     1       0.262  -2.142   1.406  1.00  0.00           C
HETATM    4  C   LIG     1      -0.838  -3.094  -1.280  1.00  0.00           C
HETATM    5  O   LIG     1      -0.445  -1.738  -1.511  1.00  0.00           O
HETATM    6  C   LIG     1      -0.574   2.820   1.265  1.00  0.00           C
HETATM    7  C   LIG     1      -1.503   1.829   0.528  1.00  0.00           C
HETATM    8  C   LIG     1      -2.884   2.116   0.490  1.00  0.00           C
HETATM    9  C   LIG     1      -3.842   1.250  -0.062  1.00  0.00           C
HETATM   10  O   LIG     1      -3.685   0.117  -0.593  1.00  0.00           O
HETATM   11 CU   LIG     1      -1.996  -0.732  -0.947  1.00  0.00          Cu
HETATM   12  C   LIG     1      -5.323   1.689  -0.030  1.00  0.00           C
HETATM   13  F   LIG     1      -6.058   0.775   0.616  1.00  0.00           F
HETATM   14  F   LIG     1      -5.796   1.795  -1.278  1.00  0.00           F
HETATM   15  F   LIG     1      -5.506   2.869   0.580  1.00  0.00           F
HETATM   16  O   LIG     1      -0.916   0.827   0.062  1.00  0.00           O
HETATM   17  F   LIG     1      -0.174   2.273   2.428  1.00  0.00           F
HETATM   18  F   LIG     1      -1.163   3.989   1.546  1.00  0.00           F
HETATM   19  F   LIG     1       0.520   3.072   0.536  1.00  0.00           F
HETATM   20  C   LIG     1       2.457   2.219  -3.150  1.00  0.00           C
HETATM   21  C   LIG     1       2.343   1.286  -1.922  1.00  0.00           C
HETATM   22  C   LIG     1       3.232   1.492  -0.842  1.00  0.00           C
HETATM   23  C   LIG     1       3.220   0.679   0.290  1.00  0.00           C
HETATM   24  C   LIG     1       4.316   0.892   1.354  1.00  0.00           C
HETATM   25  O   LIG     1       2.442  -0.281   0.570  1.00  0.00           O
HETATM   26  O   LIG     1       1.460   0.412  -2.030  1.00  0.00           O
HETATM   27 CU   LIG     1       0.938  -0.840  -0.503  1.00  0.00          Cu
HETATM   28  F   LIG     1       5.244  -0.071   1.240  1.00  0.00           F
HETATM   29  F   LIG     1       3.801   0.821   2.587  1.00  0.00           F
HETATM   30  F   LIG     1       4.932   2.074   1.229  1.00  0.00           F
HETATM   31  F   LIG     1       2.782   1.506  -4.235  1.00  0.00           F
HETATM   32  F   LIG     1       3.387   3.172  -2.990  1.00  0.00           F
HETATM   33  F   LIG     1       1.285   2.820  -3.379  1.00  0.00           F
HETATM   34  H   LIG     1      -2.695  -3.246  -0.008  1.00  0.00           H
HETATM   35  H   LIG     1      -1.805  -2.167   1.958  1.00  0.00           H
HETATM   36  H   LIG     1       1.036  -2.739   0.917  1.00  0.00           H
HETATM   37  H   LIG     1      -3.228   3.053   0.920  1.00  0.00           H
HETATM   38  H   LIG     1       3.959   2.297  -0.904  1.00  0.00           H
HETATM   39  C   LIG     1       0.660  -1.418   2.651  1.00  0.00           C
HETATM   40  H   LIG     1       0.643  -2.130   3.501  1.00  0.00           H
```

```
HETATM   41  H   LIG     1       1.674  -1.008   2.579  1.00  0.00          H
HETATM   42  H   LIG     1      -0.040  -0.602   2.888  1.00  0.00          H
HETATM   43  H   LIG     1      -1.547  -3.378  -2.082  1.00  0.00          H
HETATM   44  C   LIG     1       0.318  -4.086  -1.362  1.00  0.00          C
HETATM   45  H   LIG     1       1.113  -3.903  -0.625  1.00  0.00          H
HETATM   46  H   LIG     1      -0.045  -5.117  -1.223  1.00  0.00          H
HETATM   47  H   LIG     1       0.770  -4.015  -2.364  1.00  0.00          H
CONECT    1    4   11   34    2
CONECT    1
CONECT    2    1    3   35
CONECT    3   27   36    2   39
CONECT    3
CONECT    4   43    5   44    1
CONECT    4
CONECT    5    4   27
CONECT    6    7   19   18   17
CONECT    6
CONECT    7   16    8    6
CONECT    8    9    7   37
CONECT    9   10   12    8
CONECT   10   11    9
CONECT   11   10    1   16
CONECT   12   14    9   15   13
CONECT   12
CONECT   13   12
CONECT   14   12
CONECT   15   12
CONECT   16   11    7
CONECT   17    6
CONECT   18    6
CONECT   19    6
CONECT   20   31   33   32   21
CONECT   20
CONECT   21   20   26   22
CONECT   22   21   38   23
CONECT   23   22   25   24
CONECT   24   23   30   28   29
CONECT   24
CONECT   25   27   23
CONECT   26   21   27
CONECT   27   26    5   25    3
CONECT   27
CONECT   28   24
CONECT   29   24
```

```
CONECT   30   24
CONECT   31   20
CONECT   32   20
CONECT   33   20
CONECT   34    1
CONECT   35    2
CONECT   36    3
CONECT   37    8
CONECT   38   22
CONECT   39    3   41   42   40
CONECT   39
CONECT   40   39
CONECT   41   39
CONECT   42   39
CONECT   43    4
CONECT   44   47    4   46   45
CONECT   44
CONECT   45   44
CONECT   46   44
CONECT   47   44
MASTER        0    0    0    0    0    0    0    0   47    0   47    0
END
```

Antarafacial Migration TS:

```
COMPND    0  1 0 Last
AUTHOR    GENERATED BY OPEN BABEL 2.3.90
HETATM    1  C   LIG     1      -1.311  -2.497  -0.811  1.00  0.00          C
HETATM    2  C   LIG     1      -0.851  -2.394   0.529  1.00  0.00          C
HETATM    3  H   LIG     1      -1.219  -3.193   1.191  1.00  0.00          H
HETATM    4  C   LIG     1      -0.017  -1.465   1.139  1.00  0.00          C
HETATM    5  H   LIG     1      -0.034  -0.417   0.808  1.00  0.00          H
HETATM    6  C   LIG     1      -0.441  -2.191  -2.015  1.00  0.00          C
HETATM    7  H   LIG     1      -1.072  -2.304  -2.919  1.00  0.00          H
HETATM    8  O   LIG     1      -0.128  -0.813  -1.880  1.00  0.00          O
HETATM    9  C   LIG     1      -2.331   3.315   1.102  1.00  0.00          C
HETATM   10  C   LIG     1      -2.688   2.003   0.367  1.00  0.00          C
HETATM   11  C   LIG     1      -4.038   1.596   0.335  1.00  0.00          C
HETATM   12  C   LIG     1      -4.455   0.391  -0.242  1.00  0.00          C
HETATM   13  O   LIG     1      -3.761  -0.505  -0.802  1.00  0.00          O
HETATM   14 CU   LIG     1      -1.840  -0.409  -1.003  1.00  0.00         Cu
HETATM   15  C   LIG     1      -5.960   0.045  -0.216  1.00  0.00          C
HETATM   16  F   LIG     1      -6.151  -1.120   0.416  1.00  0.00          F
HETATM   17  F   LIG     1      -6.424  -0.079  -1.465  1.00  0.00          F
HETATM   18  F   LIG     1      -6.694   0.978   0.406  1.00  0.00          F
```

```
HETATM   19  O   LIG     1      -1.696   1.407  -0.114  1.00  0.00          O
HETATM   20  F   LIG     1      -1.648   3.022   2.220  1.00  0.00          F
HETATM   21  F   LIG     1      -3.415   4.020   1.456  1.00  0.00          F
HETATM   22  F   LIG     1      -1.565   4.088   0.334  1.00  0.00          F
HETATM   23  C   LIG     1       4.974  -0.494   1.543  1.00  0.00          C
HETATM   24  C   LIG     1       3.908   0.044   0.568  1.00  0.00          C
HETATM   25  C   LIG     1       4.107   1.297  -0.010  1.00  0.00          C
HETATM   26  C   LIG     1       3.159   1.898  -0.876  1.00  0.00          C
HETATM   27  C   LIG     1       3.471   3.316  -1.415  1.00  0.00          C
HETATM   28  O   LIG     1       2.070   1.432  -1.259  1.00  0.00          O
HETATM   29  O   LIG     1       2.939  -0.758   0.421  1.00  0.00          O
HETATM   30 CU   LIG     1       1.361  -0.450  -0.676  1.00  0.00         Cu
HETATM   31  F   LIG     1       2.552   4.184  -0.976  1.00  0.00          F
HETATM   32  F   LIG     1       3.444   3.318  -2.752  1.00  0.00          F
HETATM   33  F   LIG     1       4.677   3.765  -1.028  1.00  0.00          F
HETATM   34  F   LIG     1       4.410  -0.761   2.735  1.00  0.00          F
HETATM   35  F   LIG     1       5.978   0.366   1.753  1.00  0.00          F
HETATM   36  F   LIG     1       5.499  -1.634   1.076  1.00  0.00          F
HETATM   37  H   LIG     1      -2.170  -3.159  -0.973  1.00  0.00          H
HETATM   38  H   LIG     1      -4.787   2.245   0.782  1.00  0.00          H
HETATM   39  H   LIG     1       5.012   1.846   0.235  1.00  0.00          H
HETATM   40  C   LIG     1       0.630  -1.695   2.463  1.00  0.00          C
HETATM   41  H   LIG     1       0.478  -2.720   2.831  1.00  0.00          H
HETATM   42  H   LIG     1       1.715  -1.511   2.370  1.00  0.00          H
HETATM   43  H   LIG     1       0.256  -0.977   3.215  1.00  0.00          H
HETATM   44  C   LIG     1       0.781  -3.090  -2.178  1.00  0.00          C
HETATM   45  H   LIG     1       1.425  -3.050  -1.284  1.00  0.00          H
HETATM   46  H   LIG     1       0.484  -4.137  -2.350  1.00  0.00          H
HETATM   47  H   LIG     1       1.362  -2.750  -3.050  1.00  0.00          H
CONECT    1    6   14   37    2
CONECT    1
CONECT    2    1    4    3
CONECT    3    2
CONECT    4   30    2    5   40
CONECT    4
CONECT    5    4
CONECT    6    7   44    8    1
CONECT    6
CONECT    7    6
CONECT    8    6   30
CONECT    9   22   10   21   20
CONECT    9
CONECT   10   19   11    9
CONECT   11   12   10   38
```

```
CONECT  12  13  15  11
CONECT  13  14  12
CONECT  14   1  13  19
CONECT  15  17  12  18  16
CONECT  15
CONECT  16  15
CONECT  17  15
CONECT  18  15
CONECT  19  14  10
CONECT  20   9
CONECT  21   9
CONECT  22   9
CONECT  23  24  36  35  34
CONECT  23
CONECT  24  25  29  23
CONECT  25  26  39  24
CONECT  26  27  28  25
CONECT  27  32  33  31  26
CONECT  27
CONECT  28  26  30
CONECT  29  30  24
CONECT  30   8  28  29   4
CONECT  30
CONECT  31  27
CONECT  32  27
CONECT  33  27
CONECT  34  23
CONECT  35  23
CONECT  36  23
CONECT  37   1
CONECT  38  11
CONECT  39  25
CONECT  40   4  42  41  43
CONECT  40
CONECT  41  40
CONECT  42  40
CONECT  43  40
CONECT  44  47  46   6  45
CONECT  44
CONECT  45  44
CONECT  46  44
CONECT  47  44
MASTER      0   0   0   0   0   0   0   0  47   0  47   0
END
```

Appendix II.

Computational Data for Chapter 3

Catalytic Efficiency is a Function of How Rhodium(I) (5 + 2) Catalysts Accommodate a Conserved Substrate Transition State Geometry: Induced Fit Model for Explaining Transition Metal Catalysis

1. RhCOCl

1.a. Additional Figures

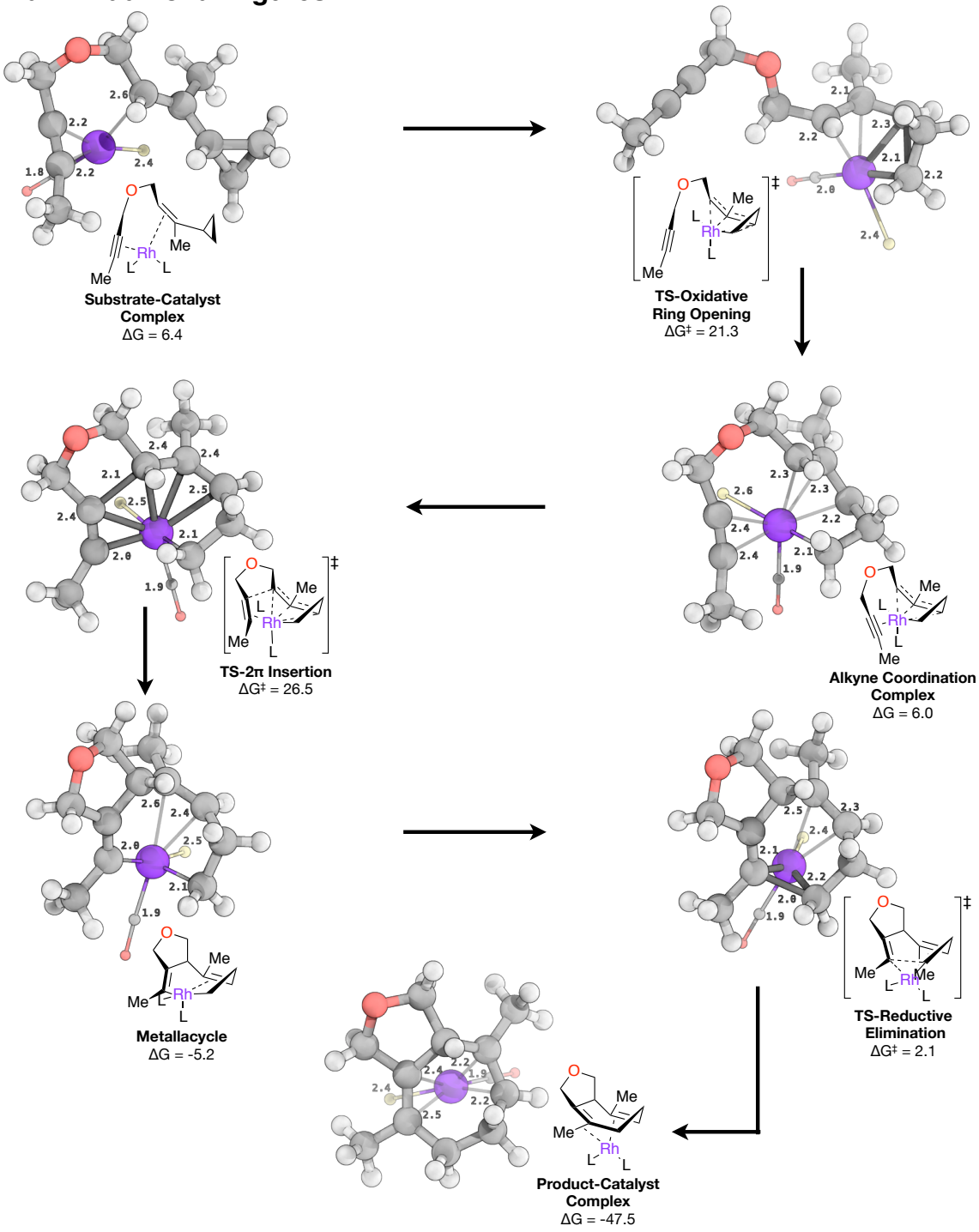


Figure S1. Computed geometries for RhCOCl.

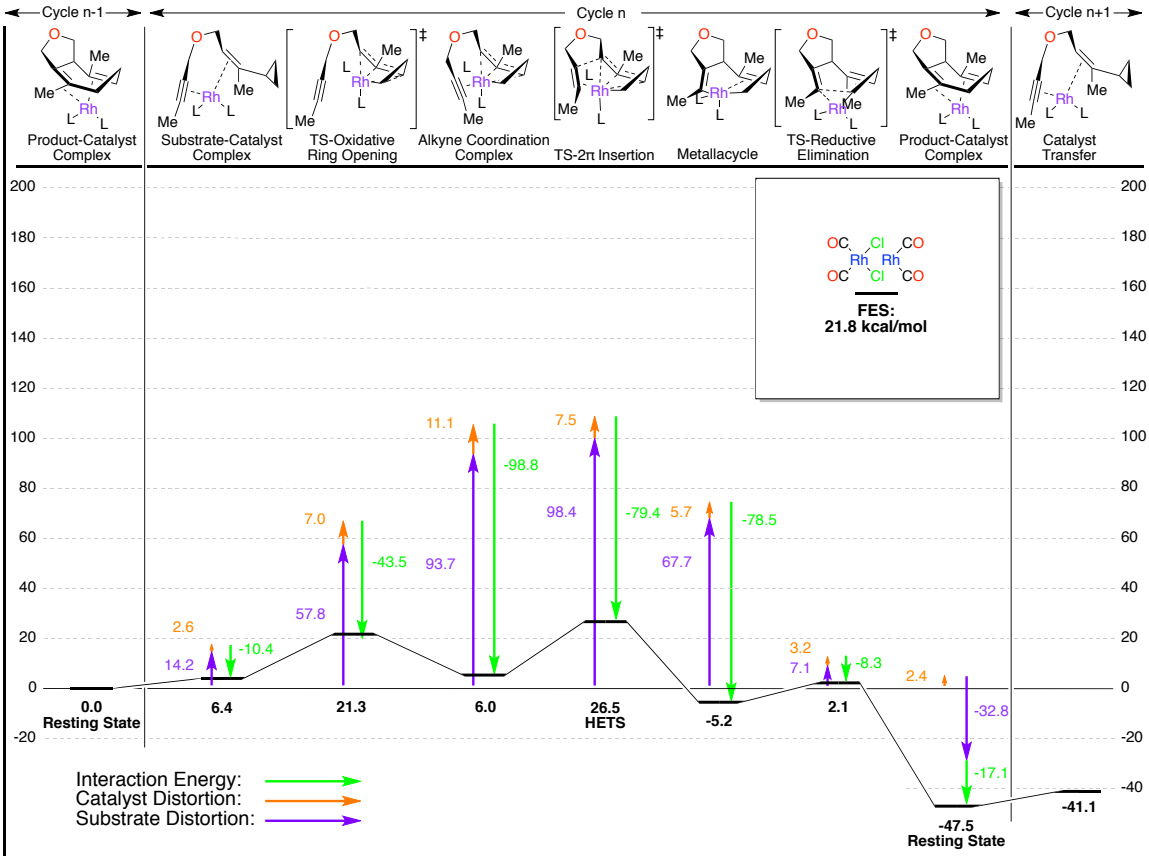


Figure S2. Reaction coordinate diagram for RhCOCl. Interaction, catalyst and substrate distortion shown with colored arrows.

Substrate-Catalyst Complex RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(maxcycle=250,nofreeze) freq=noraman b3lyp geom=connectivity gen pseudo=read scf=(direct,tight,maxcycle=300,xqc) gfinput gfprint iop(1/8=20)

#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)] #Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -1187.01306971 Predicted Change= -1.499199D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003 II	0.00045	[YES]	0.00000 II	0.00030	[YES]

Displ 0.00355 ll 0.00180 [NO] 0.00355 ll 0.00180 [YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.807424	1.590133	-0.019938
Rh	-0.641912	-0.511335	-0.080754
C	1.926540	0.811925	-0.107824
C	2.574178	0.337044	1.143586
C	-1.973663	1.138630	0.335331
C	-1.903756	0.497542	1.405736
H	0.491233	1.903844	0.972564
C	0.193617	2.424220	-1.134267
H	0.872366	3.241973	-1.408448
H	0.003342	1.834005	-2.043132
C	-2.144250	2.254746	-0.626654
H	-2.405251	1.856706	-1.618913
H	-2.956633	2.911618	-0.295872
C	-1.981324	-1.739513	-0.339891
O	-2.834282	-2.492123	-0.518761
Cl	0.754029	-2.098108	-1.221851
H	2.094887	0.709601	2.046246
C	3.203501	-1.041605	1.271865
C	4.088274	0.163059	1.243034
H	4.682578	0.341344	0.352026
H	3.047459	-1.555356	2.216364
H	3.161272	-1.689523	0.403216
H	4.557785	0.497498	2.164082
O	-0.994908	3.083445	-0.707499
C	-2.173032	0.074193	2.789982
H	-2.831278	0.795950	3.288982
H	-2.656312	-0.909150	2.813607
H	-1.244206	-0.003946	3.365561
C	2.623260	0.567870	-1.421012
H	1.957037	0.709794	-2.273482
H	3.456461	1.278479	-1.517445
H	3.025714	-0.444965	-1.489573

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1187.01306971 Predicted Change= -1.499199D-07
Zero-point correction (ZPE)= -1186.7584 0.25464
Internal Energy (U)= -1186.7388 0.27421

Enthalpy (H)=		-1186.7379	0.27515
Gibbs Free Energy (G)=	-1186.8075	0.20548	

Frequencies --	33.9518	52.0300	62.6374

SCF Energy (M06) = -1186.544315

SCF Energy (M06/def2-tzvp) = -1187.909664

Oxidative-Addition TS RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
#Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -1186.98663596 Predicted Change= -3.808433D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00380 II	0.00180	[NO]	0.00380 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.365884	-0.454310	-0.638512
Rh	1.560462	-0.344896	-0.222272
C	-4.682297	0.023094	0.238351
C	-3.838942	0.599142	1.295028
C	-1.697900	0.067013	0.395792
C	-0.465472	0.735365	-0.146970
C	0.495236	1.348216	0.657813
C	1.644114	1.990607	0.002505
C	1.600384	2.787171	-1.258806
C	2.172925	1.448000	-1.618160
H	3.250341	1.397217	-1.723007
H	1.606955	0.859331	-2.338073
H	2.271361	3.642005	-1.304235
H	0.608332	3.002865	-1.649928
H	-0.519953	1.012425	-1.199147
H	-3.677623	-0.149753	2.088925
H	-4.342117	1.458496	1.752695
H	-1.455381	-0.609057	1.226706
H	-2.167067	-0.538274	-0.389538
H	2.495966	2.192896	0.644507
O	-2.589756	1.099222	0.831643

C	-6.201028	-1.030318	-1.689350
H	-6.059822	-0.504803	-2.641664
H	-5.965865	-2.088772	-1.853739
H	-7.264375	-0.961866	-1.429016
C	0.417385	1.410325	2.162174
H	1.415342	1.436845	2.610476
H	-0.122083	2.318477	2.461854
H	-0.121445	0.553091	2.569795
C	3.299043	-1.102607	-0.148267
O	4.355915	-1.541076	-0.032810
Cl	0.672469	-2.405656	0.545610

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1186.98663596 Predicted Change= -3.808433D-09
Zero-point correction (ZPE)= -1186.7338 0.25279
Internal Energy (U)= -1186.7140 0.27255
Enthalpy (H)= -1186.7131 0.27349
Gibbs Free Energy (G)= -1186.7860 0.20061

Frequencies -- -193.8067 18.8719 21.2927
SCF Energy (M06) = -1186.514763
SCF Energy (M06/def2-tzvp) = -1187.884564

Alkyne Coordination Complex RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(loose,modredundant,maxcycle=250) b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Modredundant Input: B 3 6 3.0000 F
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1187.01835077 Predicted Change= -4.027491D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00011 ll	0.00045	[YES]	0.00001 ll	0.00030	[YES]
Displ	0.00637 ll	0.00180	[NO]	0.00637 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.115996	2.034345	-0.475157
Rh	-0.439552	-0.213036	-0.001073
C	0.102614	2.094985	-0.310097
C	1.491218	2.526663	-0.043280
C	2.759085	0.553832	-0.419083
C	1.670560	-0.389535	-0.859012
C	1.372599	-1.610795	-0.205718
C	0.172338	-2.272052	-0.583599
C	-0.467034	-2.130483	-1.966860
C	-1.045274	-0.713909	-1.954356
H	-2.132144	-0.688529	-2.050271
H	-0.593818	-0.015610	-2.663262
H	-1.247930	-2.888744	-2.082707
H	0.269561	-2.300042	-2.763564
H	1.407041	-0.277728	-1.907711
H	1.686399	2.386664	1.029259
H	1.565398	3.593599	-0.281491
H	3.707423	0.298513	-0.909738

H	2.908337	0.513129	0.667180
H	-0.128396	-3.117966	0.030142
O	2.486528	1.891847	-0.828406
C	-2.526175	2.340942	-0.745839
H	-2.911743	1.736606	-1.573837
H	-3.148909	2.148541	0.134585
H	-2.631742	3.397575	-1.018170
C	2.162194	-2.101954	0.983628
H	3.151836	-2.432805	0.641691
H	2.290151	-1.322918	1.738636
H	1.665059	-2.949161	1.463077
C	-2.156543	-0.594432	0.762692
O	-3.157394	-0.838711	1.268068
Cl	0.280747	0.273810	2.410426

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1187.01835077 Predicted Change= -4.027491D-07
Zero-point correction (ZPE)= -1186.7635 0.25477
Internal Energy (U)= -1186.7446 0.27370
Enthalpy (H)= -1186.7436 0.27465
Gibbs Free Energy (G)= -1186.8100 0.20834

Frequencies -- 59.3022 70.5780 76.6907
SCF Energy (M06) = -1186.54779
SCF Energy (M06/def2-tzvp) = -1187.912115

2π-Insertion TS RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp gen pseudo=read scf=(direct,tight,maxcycle=300,xqc) gfinput gfprint opt=(maxcycle=250,modredundant) iop(1/8=20) geom=connectivity

Modredundant Input: B 4 7 F

#b3lyp GenChk ChkBas scf=(direct,tight,maxcycle=300,xqc) opt=(calcfc,ts,noeigentest,maxcycle=250,nofreeze) freq=noraman iop(1/8=20) gfinput gfprint Geom=AllCheck Guess=Read SCRF=Check

#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)] #Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -1186.99268497 Predicted Change= -8.573902D-10

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00033 II	0.00180	[YES]	0.00033 II	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.139240	1.793994	-0.599653
Rh	-0.710721	-0.091092	-0.035516
Cl	-0.556260	0.491741	2.427793
C	1.081572	1.410759	-0.509539
C	2.458516	1.947115	-0.261832
C	2.991866	-0.221253	0.121860
C	1.624526	-0.595041	-0.434958
C	0.940780	-1.746376	0.204926
C	-0.048450	-2.432966	-0.474414
C	-0.456337	-2.183544	-1.921012
C	-0.866649	-0.709214	-2.045634
C	-2.549024	0.106466	0.123117
O	-3.685344	0.245366	0.233867
H	-1.878896	-0.588156	-2.434787
H	-0.182781	-0.097888	-2.641228
H	-1.295939	-2.843416	-2.160315
H	0.361107	-2.461906	-2.603541

H	1.654808	-0.662214	-1.521354
H	2.517879	2.296262	0.782087
H	2.657187	2.791453	-0.929880
H	3.717065	-1.003831	-0.126885
H	2.956488	-0.102551	1.213718
H	-0.495062	-3.282404	0.038555
O	3.439980	0.962288	-0.504263
C	-0.971276	3.000059	-0.834746
H	-1.532483	3.246155	0.073650
H	-0.350281	3.861274	-1.109587
H	-1.695696	2.827307	-1.638574
C	1.361673	-2.194781	1.587057
H	0.736468	-3.026703	1.922394
H	2.404032	-2.539586	1.576387
H	1.260130	-1.386799	2.317262

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1186.99268497 Predicted Change= -8.573902D-10
Zero-point correction (ZPE)= -1186.7374 0.25527
Internal Energy (U)= -1186.7197 0.27289
Enthalpy (H)= -1186.7188 0.27384
Gibbs Free Energy (G)= -1186.7823 0.21037

Frequencies -- -225.6127 63.9476 71.6126
SCF Energy (M06) = -1186.517152
SCF Energy (M06/def2-tzvp) = -1187.879585

Metallacycle RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(maxcycle=250,nofreeze) freq=noraman b3lyp geom=connectivity gen pseudo=read scf=(direct,tight,maxcycle=300,xqc) gfinput gfprint iop(1/8=20)

#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)] #Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -1187.04655064 Predicted Change= -1.442490D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00746 II	0.00180	[NO]	0.00746 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.657333	1.359567	-0.057338
Rh	0.961932	0.108749	-0.070975
Cl	2.714392	-1.452492	-0.862153
C	-1.874508	0.800343	0.025831
C	-3.231928	1.432816	-0.272726
C	-3.446601	-0.856486	-0.510084
C	-2.161412	-0.661272	0.317241
C	-0.972352	-1.573196	0.073560
C	-0.007740	-1.737507	1.031737
C	0.094880	-0.957926	2.338163
C	1.000035	0.229398	2.011519
C	2.221385	1.472013	-0.311077
O	3.028414	2.278191	-0.422946
H	2.051561	0.065819	2.254527
H	0.649223	1.193434	2.377925
H	0.527396	-1.592489	3.121309
H	-0.885689	-0.616907	2.681155
H	-2.468932	-0.753869	1.369724
H	-3.230074	1.953829	-1.242626
H	-3.563912	2.145444	0.493237

H	-4.075962	-1.684386	-0.171181
H	-3.224923	-0.992510	-1.579672
H	0.771903	-2.472268	0.847289
O	-4.168026	0.350664	-0.287858
C	-0.484558	2.842037	-0.295834
H	0.085949	3.308368	0.518619
H	0.062808	3.048735	-1.224308
H	-1.445971	3.367212	-0.356591
C	-0.938191	-2.406408	-1.186297
H	0.015236	-2.929943	-1.286879
H	-1.751613	-3.144965	-1.174028
H	-1.081771	-1.787944	-2.079743

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1187.04655064 Predicted Change= -1.442490D-07
Zero-point correction (ZPE)= -1186.7889 0.25762
Internal Energy (U)= -1186.7711 0.27544
Enthalpy (H)= -1186.7701 0.27638
Gibbs Free Energy (G)= -1186.8353 0.21118

Frequencies -- 31.9510 42.0925 78.2664
SCF Energy (M06) = -1186.568483
SCF Energy (M06/def2-tzvp) = -1187.927433

Reductive Elimination TS RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp gen pseudo=read scf=(direct,tight,maxcycle=300,xqc) gfinput gfprint opt=(maxcycle=250,modredundant) iop(1/8=20) geom=connectivity

Modredundant Input: B 1 11 F

#b3lyp GenChk ChkBas scf=(direct,tight,maxcycle=300,xqc) opt=(calcfc,ts,noeigentest,maxcycle=250,nofreeze) freq=noraman iop(1/8=20) gfinput gfprint Geom=AllCheck Guess=Read SCRF=Check

#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)] #Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -1187.02343046 Predicted Change= -1.153524D-10

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00015 II	0.00180	[YES]	0.00015 II	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-0.565840	1.403128	0.142482
Rh	1.020141	0.034897	0.055340
Cl	2.375158	-1.661800	-0.947907
C	-1.760516	0.806500	-0.047101
C	-2.949312	1.393776	-0.791352
C	-3.103015	-0.903060	-0.903097
C	-2.126616	-0.634724	0.260120
C	-0.930954	-1.557329	0.453091
C	-0.111137	-1.378824	1.537218
C	-0.291169	-0.245955	2.539989
C	0.273300	1.038129	1.920784
C	2.306685	1.232157	-0.583891
O	3.126444	1.940743	-0.966219
H	1.327073	1.208819	2.166244
H	-0.268456	1.937265	2.213609
H	0.245836	-0.480448	3.465687
H	-1.348582	-0.120135	2.800579

H	-2.738330	-0.664313	1.178567
H	-2.645454	1.834760	-1.754215
H	-3.482558	2.169401	-0.223516
H	-3.810275	-1.715493	-0.716281
H	-2.562721	-1.105286	-1.840483
H	0.648679	-2.130095	1.739335
O	-3.851275	0.305462	-0.996235
C	-0.351488	2.854481	-0.233174
H	-0.174727	2.949932	-1.312217
H	-1.222452	3.474325	0.016579
H	0.515165	3.286028	0.275935
C	-0.818254	-2.781291	-0.419942
H	0.082306	-3.352825	-0.190605
H	-1.698709	-3.421133	-0.264039
H	-0.782282	-2.522166	-1.482188

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1187.02343046 Predicted Change= -1.153524D-10
Zero-point correction (ZPE)= -1186.7668 0.25653
Internal Energy (U)= -1186.7497 0.27372
Enthalpy (H)= -1186.7487 0.27466
Gibbs Free Energy (G)= -1186.8118 0.21156

Frequencies -- -379.7070 45.8650 51.2967
SCF Energy (M06) = -1186.55735
SCF Energy (M06/def2-tzvp) = -1187.916615

Product-Catalyst Complex RhCOCl

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(maxcycle=250,nofreeze) freq=noraman b3lyp geom=connectivity gen pseudo=read scf=(direct,tight,maxcycle=300,xqc) gfinput gfprint iop(1/8=20)

#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClO2Rh C1[X(C12H16ClO2Rh)] #Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -1187.10407546 Predicted Change= -3.807245D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00194 II	0.00180	[NO]	0.00194 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.249600	-1.064014	1.047561
Rh	-0.828481	-0.160302	-0.012927
C	1.592817	-0.241396	0.007880
C	2.281454	-0.722522	-1.268901
C	2.046706	1.522657	-1.526007
C	1.557778	1.298325	-0.074846
C	0.137046	1.768142	0.233270
C	-0.397198	1.399413	1.483923
C	0.464041	0.852563	2.613198
C	0.857029	-0.621202	2.446133
H	0.020124	-1.252066	2.768887
H	1.691523	-0.868772	3.122189
H	-0.072415	0.961919	3.561040
H	1.367909	1.472660	2.700669
H	2.286384	1.750279	0.617302
H	1.559334	-1.147577	-1.982447
H	3.060159	-1.465660	-1.074148
H	2.610185	2.449567	-1.658044
H	1.200014	1.515394	-2.228636
H	-1.306903	1.909371	1.795590

C	-2.583948	0.370629	-0.323700
O	-3.671563	0.695181	-0.509875
Cl	-1.259514	-2.215739	-1.134395
O	2.916963	0.436820	-1.796488
C	-0.446395	2.927525	-0.544607
H	0.158202	3.831343	-0.376254
H	-0.474768	2.747370	-1.622791
H	-1.466093	3.145493	-0.212021
C	1.483416	-2.556238	0.931748
H	1.401301	-2.916591	-0.094166
H	2.485416	-2.799268	1.315875
H	0.755700	-3.111603	1.530382

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1187.10407546 Predicted Change= -3.807245D-08
Zero-point correction (ZPE)= -1186.8441 0.25988
Internal Energy (U)= -1186.8270 0.27707
Enthalpy (H)= -1186.8260 0.27801
Gibbs Free Energy (G)= -1186.8891 0.21492

Frequencies -- 48.6950 59.0418 78.6943
SCF Energy (M06) = -1186.639709
SCF Energy (M06/def2-tzvp) = -1187.997234

2. RhCOD

2.a. Additional Figures

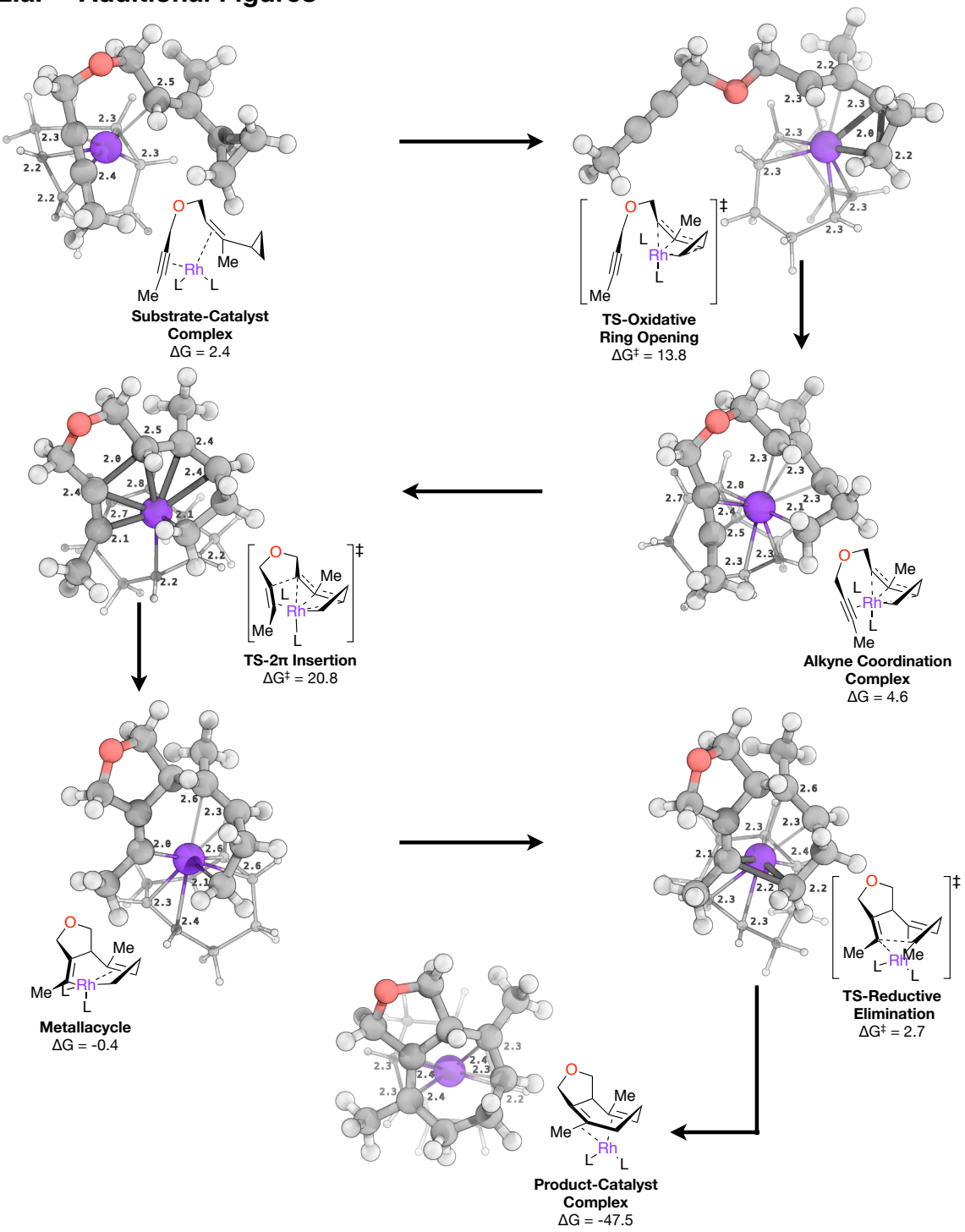


Figure S3. Computed geometries for RhCOD.

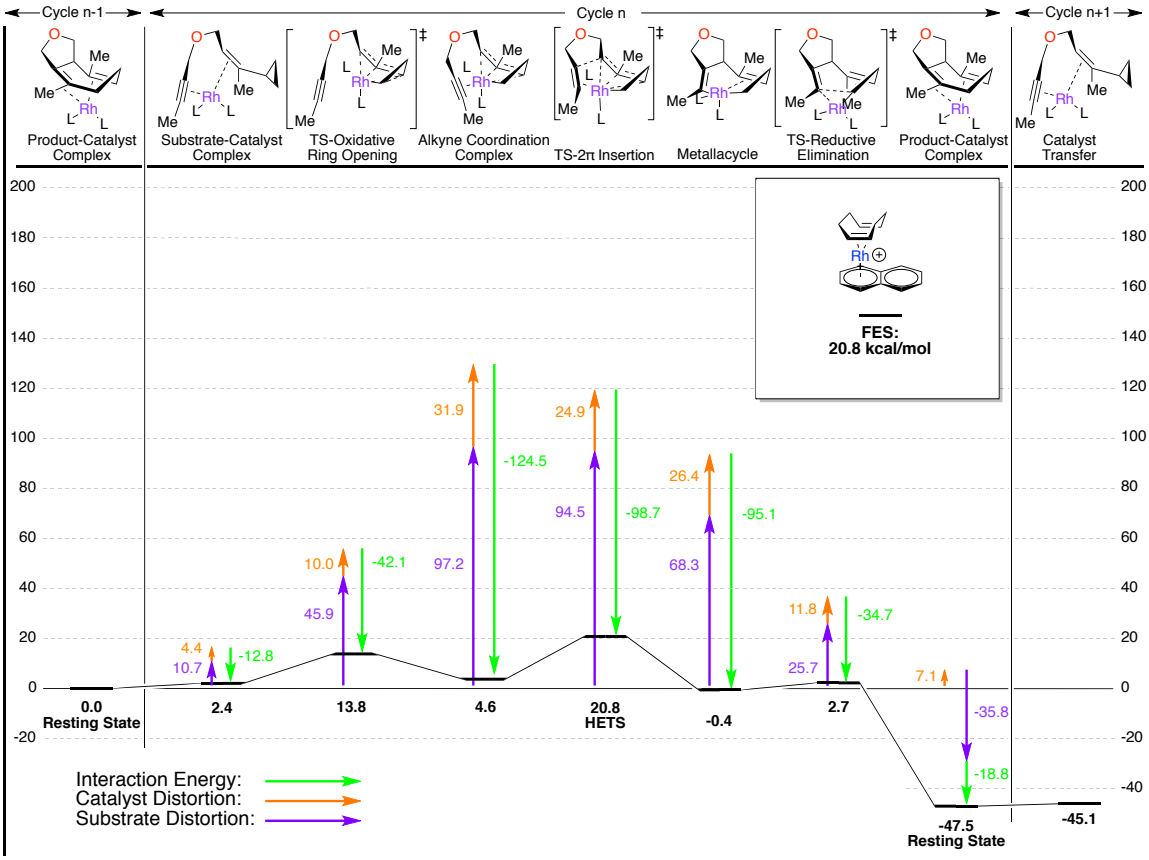


Figure S4. Reaction coordinate diagram for RhCOD. Interaction, catalyst and substrate distortion shown with colored arrows.

Substrate-Catalyst Complex RhCOD

Using Gaussian 03: IA64L-G03RevD.01 13-Oct-2005

==========

freq=noraman b3lyp gen pseudo gfprint gfinput scf=(direct,xqc,maxcycle=300) geom=check guess=read

---

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]
#Atoms= 49
Charge = 1 Multiplicity = 1

SCF Energy= -925.282766214 Predicted Change= -3.221468D-07

==========

Optimization incomplete.

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00006 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00538 II	0.00180	[NO]	0.00538 II	0.00180	[NO]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
Rh	-0.440257	0.169179	0.083972
C	2.131303	-0.951294	-0.731676
C	2.594473	-1.850916	0.361082
C	4.024100	-1.697701	0.894077
C	2.854589	-1.416272	1.785846
C	0.150309	2.347689	0.483751
C	0.055185	1.958283	1.648072
H	4.600929	-2.605010	1.045968
H	4.597167	-0.850809	0.527503
H	2.615057	-2.132934	2.566163
H	2.664889	-0.383255	2.062324
H	2.284861	-2.886773	0.236029
C	-2.408881	0.131772	1.060541
H	-2.301024	0.713163	1.971875
C	-2.947864	-1.280089	1.263593
C	-2.482239	0.872563	-0.133195
H	-2.434816	1.955607	-0.027329
C	-3.046869	0.404800	-1.455628
C	-0.939489	-2.020414	-0.140514
H	0.029906	-2.507818	-0.076335
C	-1.268177	-1.405935	-1.341072
C	-2.674314	-1.052642	-1.797447
H	-0.516175	-1.419991	-2.125141
H	-3.287507	-1.379763	2.299226
C	-1.894260	-2.371936	0.979922
H	-3.836400	-1.425192	0.642067
H	-4.139593	0.535096	-1.458669
H	-2.663742	1.069735	-2.238189
H	-3.392915	-1.750411	-1.359441
H	-2.736241	-1.193592	-2.881350
H	-1.297520	-2.539988	1.882941
H	-2.384955	-3.332068	0.759514
C	1.985770	0.399846	-0.571901
H	2.289198	0.830462	0.378459
C	1.945388	1.424768	-1.700069
H	2.902850	1.424254	-2.234180
C	0.528493	3.094841	-0.746875
H	-0.225775	2.946542	-1.534195
O	1.817049	2.749542	-1.205977
H	1.156573	1.212026	-2.437738
H	0.566339	4.162960	-0.508689
C	0.056518	1.741346	3.098103

H	0.435586	2.643883	3.592698
H	-0.945254	1.539775	3.489912
H	0.705630	0.903534	3.373887
C	2.062874	-1.615620	-2.085038
H	3.083557	-1.887135	-2.387549
H	1.496607	-2.553973	-2.053590
H	1.646461	-0.976263	-2.866541

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.282766214 Predicted Change= -3.221468D-07
Zero-point correction (ZPE)= -924.8534 0.42932
Internal Energy (U)= -924.8299 0.45285
Enthalpy (H)= -924.8289 0.45380
Gibbs Free Energy (G)= -924.9057 0.37701

Frequencies -- 34.9833 44.7152 51.7861
SCF Energy (M06) = -924.6561001
SCF Energy (M06/def2-tzvp) = -926.0497593

Oxidative-Addition TS RhCOD

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=(gdiis,modredundant,maxcycle=250) b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Modredundant Input: B 3 5 F
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]
#Atoms= 49
Charge = 1 Multiplicity = 1

SCF Energy= -925.270265099 Predicted Change= -5.640279D-10

==========

Optimization completed on the basis of negligible forces. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00218 II	0.00180	[NO]	0.00218 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	1.010903	-0.035936	-0.343069
C	1.143881	-2.130767	0.463043
C	2.240183	-2.012147	-0.472950
C	2.209792	-2.398884	-1.917632
C	1.948436	-0.933963	-2.133248
C	-4.609321	-0.433721	0.118337
C	-5.399660	0.353400	-0.348558
H	3.155842	-2.778597	-2.303115
H	1.388312	-3.061666	-2.190265
H	2.822456	-0.348716	-2.403310
H	1.033809	-0.678605	-2.679890
H	3.224168	-1.828603	-0.048839
C	-0.469933	1.440538	0.688812
H	-1.410273	0.925746	0.498609
C	-0.317294	2.830754	0.090631
C	0.347454	0.907992	1.666513
H	-0.041945	0.052500	2.212579
C	1.583991	1.529687	2.276816

C	1.745020	1.936642	-1.174987
H	2.124056	1.691404	-2.165052
C	2.575841	1.652000	-0.100587
C	2.486624	2.290592	1.277631
H	3.514210	1.150207	-0.329505
H	-1.314160	3.211827	-0.152904
C	0.543470	2.860483	-1.191575
H	0.090816	3.511762	0.842889
H	1.294560	2.201127	3.099290
H	2.166038	0.725259	2.740296
H	2.146939	3.324692	1.169262
H	3.495855	2.348155	1.698066
H	-0.080543	2.575355	-2.046700
H	0.877978	3.888166	-1.399417
C	-0.156768	-1.971837	-0.032458
H	-0.335469	-2.095246	-1.100520
C	-1.425439	-2.077869	0.767640
H	-1.778625	-3.124761	0.722940
C	-3.698878	-1.404199	0.707592
H	-3.676800	-1.295672	1.804420
O	-2.374905	-1.212035	0.180392
H	-1.278832	-1.840037	1.832732
H	-4.029926	-2.432022	0.489129
C	-6.361274	1.294838	-0.915257
H	-6.061796	1.604693	-1.923309
H	-7.354691	0.837525	-0.991021
H	-6.453324	2.195666	-0.297555
C	1.487182	-2.397317	1.909165
H	1.610070	-3.478603	2.054022
H	2.431065	-1.919857	2.189400
H	0.708986	-2.065640	2.599166

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.270265099 Predicted Change= -5.640279D-10
Zero-point correction (ZPE)= -924.8426 0.42760
Internal Energy (U)= -924.8193 0.45091
Enthalpy (H)= -924.8184 0.45185
Gibbs Free Energy (G)= -924.8958 0.37439

Frequencies -- -213.5920 21.2559 36.5263
SCF Energy (M06) = -924.6352954
SCF Energy (M06/def2-tzvp) = -926.0314525

Alkyne Coordination Complex RhCOD

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

opt=maxcycle=250 freq=noraman b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]

#Atoms= 49

Charge = 1 Multiplicity = 1

SCF Energy= -925.284643782 Predicted Change= -9.616118D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00316 ll	0.00180	[NO]	0.00316 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.326215	-1.959885	0.003125
C	0.490086	-2.138868	1.130751
C	0.822112	-1.582104	2.514865
C	0.614627	-0.078251	2.359107
C	1.278113	1.905915	-0.279424
C	0.517359	2.349845	0.582703
H	0.141764	-2.013914	3.254328
H	1.841373	-1.854186	2.815789
H	-0.208614	0.317948	2.957478
H	1.506191	0.537810	2.489208
H	-0.245168	-2.937096	1.070816
C	2.171371	-0.823303	0.006223
H	2.593927	-0.494353	0.951563
C	3.011406	-0.392495	-1.169659
H	3.953586	-0.954344	-1.177039
C	2.336575	1.866748	-1.320760
H	1.889020	1.661729	-2.306520
O	3.391810	0.969058	-1.060295
H	2.507334	-0.571173	-2.131173
H	2.793303	2.860963	-1.362043
C	-0.126258	3.227865	1.567851
H	0.459439	4.149974	1.658613

H	-1.143055	3.501891	1.269427
H	-0.170020	2.761691	2.557789
C	1.214065	-2.893124	-1.178641
H	2.010328	-3.644773	-1.096763
H	0.260377	-3.427355	-1.188119
H	1.349417	-2.392851	-2.140607
Rh	0.031527	-0.062679	0.364812
C	-1.406982	-0.777820	-1.934689
C	-1.093263	0.536200	-2.008176
C	-2.137216	-0.648795	0.989391
C	-2.107424	0.730362	0.841868
C	-2.726950	-1.336590	-1.452128
H	-0.708415	-1.487724	-2.367680
H	-0.177642	0.801927	-2.532727
C	-1.961373	1.701192	-1.590287
H	-1.980746	-1.026447	1.998091
C	-2.773254	-1.659043	0.058287
H	-1.924065	1.292313	1.752877
C	-2.776394	1.512330	-0.285573
H	-3.531151	-0.643688	-1.712960
H	-2.940528	-2.259822	-2.001803
H	-1.314444	2.575993	-1.481012
H	-2.654705	1.946152	-2.408064
H	-3.822764	-1.783907	0.366730
H	-2.306022	-2.633524	0.234235
H	-3.032251	2.507005	0.094954
H	-3.736545	1.036783	-0.508566

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.284643782 Predicted Change= -9.616118D-08
Zero-point correction (ZPE)= -924.8539 0.43066
Internal Energy (U)= -924.8314 0.45321
Enthalpy (H)= -924.8304 0.45416
Gibbs Free Energy (G)= -924.9025 0.38208

Frequencies -- 61.0702 75.5528 86.6094
SCF Energy (M06) = -924.6576917
SCF Energy (M06/def2-tzvp) = -926.0514691

2π-Insertion TS RhCOD

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant) geom=connectivity

Modredundant Input: B 5 12 F

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]

#Atoms= 49

Charge = 1 Multiplicity = 1

SCF Energy= -925.262229380 Predicted Change= -9.095485D-10

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00046 II	0.00180	[YES]	0.00046 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.316985	-1.791183	-0.291983
C	0.612451	-2.367463	0.751860
C	0.739400	-1.975789	2.220321
C	0.426027	-0.480115	2.320574
C	1.682740	1.363075	0.009106
C	0.641350	1.813756	0.608597
H	0.022644	-2.565452	2.798825
H	1.736364	-2.233443	2.605646
H	-0.383649	-0.244869	3.014067
H	1.287140	0.150835	2.551581
H	0.023665	-3.252244	0.517894
C	2.182172	-0.619359	-0.043250
H	2.560678	-0.571398	0.975651
C	3.309948	-0.353772	-1.039076
H	4.079671	-1.124387	-0.925652
C	2.888307	1.848781	-0.746926
H	2.596614	2.081428	-1.785338
O	3.907778	0.879995	-0.725194

H	2.949224	-0.366697	-2.077873
H	3.273608	2.760297	-0.279555
C	0.177254	3.041967	1.304886
H	0.950065	3.818301	1.263574
H	-0.742142	3.446143	0.873060
H	-0.022489	2.825552	2.361439
C	1.291717	-2.428524	-1.665506
H	2.230965	-2.969293	-1.840286
H	0.477929	-3.153783	-1.746853
H	1.188050	-1.700088	-2.474260
Rh	-0.184488	-0.099506	0.366610
C	-1.608909	-0.503616	-1.959543
C	-1.214055	0.790434	-1.917986
C	-2.230289	-0.621562	0.978229
C	-2.122582	0.781288	0.959023
C	-2.947058	-1.029001	-1.492488
H	-0.960840	-1.215998	-2.462676
H	-0.280290	1.048604	-2.414999
C	-2.012415	1.958396	-1.382869
H	-2.124629	-1.093774	1.953388
C	-2.952274	-1.503048	-0.021725
H	-1.926501	1.243092	1.923874
C	-2.787847	1.702396	-0.066055
H	-3.716860	-0.268807	-1.647553
H	-3.233157	-1.877278	-2.123732
H	-1.320541	2.792899	-1.235786
H	-2.719960	2.298869	-2.152770
H	-3.993434	-1.615573	0.319204
H	-2.518220	-2.507721	0.036689
H	-2.969266	2.670246	0.412822
H	-3.782423	1.302390	-0.287404

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.262229380 Predicted Change= -9.095485D-10
Zero-point correction (ZPE)= -924.8320 0.43019
Internal Energy (U)= -924.8106 0.45162
Enthalpy (H)= -924.8096 0.45257
Gibbs Free Energy (G)= -924.8795 0.38272

Frequencies -- -237.9369 63.3908 68.4420
SCF Energy (M06) = -924.6324734
SCF Energy (M06/def2-tzvp) = -926.0245505

Metallacycle RhCOD

Using Gaussian 03: IA64L-G03RevD.01 13-Oct-2005

==========

opt=maxcycle=250 freq=noraman b3lyp gen pseudo gfprint gfinput
scf=(direct,xqc,maxcycle=300) geom=check guess=read
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]
#Atoms= 49
Charge = 1 Multiplicity = 1

SCF Energy= -925.303843887 Predicted Change= -4.934228D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.04333 ll	0.00180	[NO]	0.04333 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.412375	0.010127	-0.109396
C	-1.560846	-1.599026	0.162488
C	-0.669824	-1.901777	-0.842857
C	-0.679945	-1.333900	-2.261504
C	0.277916	-0.149929	-2.196415
C	-2.390803	0.765528	-0.137896
C	-1.161208	1.288602	-0.282515
H	-0.343851	-2.096697	-2.973572
H	-1.682777	-1.015958	-2.557286
H	1.289975	-0.366769	-2.536535
H	-0.092722	0.777351	-2.630058
H	0.046381	-2.695584	-0.644977
C	2.318542	-1.254638	1.194816
H	1.678893	-1.966300	1.715630
C	2.976492	-0.194317	2.053956
C	2.587616	-1.492900	-0.113584
H	2.177712	-2.399673	-0.552800
C	3.528269	-0.723016	-1.008919
C	1.690990	1.676537	0.784619
H	0.966546	2.475598	0.897993
C	2.208510	1.480354	-0.483454
C	3.539302	0.812643	-0.813153

H	1.800742	2.112062	-1.268031
H	3.057409	-0.576156	3.077148
C	2.198913	1.138113	2.103141
H	4.001731	-0.025511	1.715717
H	4.551092	-1.104896	-0.878329
H	3.270802	-0.951760	-2.048143
H	4.256751	1.084134	-0.033502
H	3.919622	1.266055	-1.734054
H	1.334110	1.029851	2.771922
H	2.822649	1.915171	2.572040
C	-2.748715	-0.702965	-0.105132
H	-3.175830	-0.969357	-1.083725
C	-3.945277	-0.667893	0.870114
H	-4.624279	-1.518821	0.776368
C	-3.694485	1.508524	0.141277
H	-4.069873	2.071945	-0.722452
O	-4.648680	0.494584	0.454477
H	-3.580601	2.210837	0.981152
H	-3.616771	-0.582911	1.917901
C	-1.001592	2.784224	-0.467389
H	-1.880965	3.210574	-0.963898
H	-0.888947	3.315129	0.488306
H	-0.138571	3.043826	-1.088685
C	-1.477505	-2.299701	1.495208
H	-1.483989	-1.588883	2.329738
H	-2.355405	-2.945643	1.628822
H	-0.585357	-2.926757	1.573490

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.303843887 Predicted Change= -4.934228D-06
Zero-point correction (ZPE)= -924.8713 0.43252
Internal Energy (U)= -924.8496 0.45416
Enthalpy (H)= -924.8487 0.45510
Gibbs Free Energy (G)= -924.9199 0.38393

Frequencies -- 31.1516 61.4716 82.9671
SCF Energy (M06) = -924.667433
SCF Energy (M06/def2-tzvp) = -926.0553635

Reductive Elimination TS RhCOD

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant) geom=connectivity

Modredundant Input: B 4 6 F

Modredundant Input: B 4 29 2.2000 F

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]

#Atoms= 49

Charge = 1 Multiplicity = 1

SCF Energy= -925.291041139 Predicted Change= -2.287980D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00192 II	0.00180	[NO]	0.00192 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.506327	-1.563004	0.475778
C	0.705253	-1.405530	1.585638
C	0.907979	-0.307722	2.624447
C	0.239235	0.953283	2.096241
C	2.248079	0.794854	-0.115313
C	1.059924	1.392559	0.110276
H	0.448964	-0.607917	3.573174
H	1.973195	-0.142331	2.816394
H	-0.797765	1.078071	2.412553
H	0.781121	1.877461	2.279475
H	0.021607	-2.214407	1.834608
C	2.668287	-0.616949	0.241028
H	3.277898	-0.574045	1.158479
C	3.666178	-0.895545	-0.906340
H	4.399752	-1.672322	-0.679644
C	3.413041	1.388284	-0.898479
H	3.896475	2.226452	-0.379820

O	4.362360	0.336009	-1.027663
H	3.085499	1.749184	-1.886763
H	3.146658	-1.152073	-1.843187
C	0.893708	2.868232	-0.181085
H	1.698636	3.453725	0.280354
H	0.940475	3.059600	-1.261655
H	-0.048784	3.281393	0.182895
C	1.442190	-2.815606	-0.361164
H	1.344756	-2.601757	-1.430889
H	2.379133	-3.375341	-0.237994
H	0.625241	-3.473873	-0.054486
Rh	-0.491509	0.013029	0.194137
C	-1.812572	1.304953	-1.162338
C	-2.199862	1.508143	0.156188
C	-1.782590	-1.610977	-0.855962
C	-2.460950	-1.400851	0.324926
C	-2.550184	0.456968	-2.188314
H	-1.100237	2.014057	-1.572746
H	-1.787878	2.382412	0.654539
C	-3.391793	0.910399	0.871661
H	-1.099085	-2.455234	-0.883226
C	-2.106915	-1.022828	-2.214631
H	-2.211175	-2.048504	1.162745
C	-3.705306	-0.552269	0.495282
H	-3.627015	0.532963	-2.012017
H	-2.377062	0.888518	-3.179071
H	-3.200588	0.968861	1.949645
H	-4.272476	1.545993	0.692885
H	-2.877948	-1.634195	-2.706542
H	-1.211373	-1.114622	-2.839087
H	-4.323762	-0.990854	1.285052
H	-4.305437	-0.593953	-0.417578

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.291041139 Predicted Change= -2.287980D-08
Zero-point correction (ZPE)= -924.8595 0.43150
Internal Energy (U)= -924.8385 0.45252
Enthalpy (H)= -924.8375 0.45346
Gibbs Free Energy (G)= -924.9071 0.38386

Frequencies -- -326.1231 42.6173 54.6085
SCF Energy (M06) = -924.6623814

SCF Energy (M06/def2-tzvp) = -926.0507014

Product-Catalyst Complex RhCOD

Using Gaussian 03: IA64L-G03RevD.01 13-Oct-2005

==========

freq=noraman b3lyp gen pseudo gfprint gfinput
scf=(direct,xqc,maxcycle=300) geom=check guess=read

Pointgroup= C1 Stoichiometry= C19H28ORh(1+) C1[X(C19H28ORh)]
#Atoms= 49
Charge = 1 Multiplicity = 1

SCF Energy= -925.368591573 Predicted Change= -1.347109D-05

==========

Optimization incomplete.

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00013 ll	0.00045	[YES]	0.00002 ll	0.00030	[YES]
Displ	0.05113 ll	0.00180	[NO]	0.05113 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.380093	0.043756	0.202338
C	1.349080	-1.152390	1.260289
C	0.868716	-0.229795	2.170243
C	1.540387	1.108915	2.427373
C	1.330824	2.174520	1.339441
C	1.869197	0.499752	-0.548486
C	1.370126	1.704418	-0.106307
H	1.179656	1.511956	3.377833
H	2.615745	0.927960	2.562594
H	0.371380	2.679525	1.506125
H	2.092603	2.962118	1.449190
H	0.216427	-0.601689	2.957880
C	-1.932852	1.227234	-1.023766
H	-1.465336	2.206257	-1.091922
C	-3.290414	1.198069	-0.339760
C	-1.400328	0.227273	-1.820194
H	-0.583353	0.511723	-2.480435
C	-2.007277	-1.125845	-2.116129
C	-2.255117	-0.484109	1.299845
H	-1.940181	-0.630316	2.331464
C	-1.998560	-1.526485	0.413496
C	-2.715830	-1.774371	-0.906441
H	-1.461093	-2.381510	0.814464

H	-3.685810	2.218621	-0.314204
C	-3.230659	0.655944	1.105560
H	-3.749555	-1.425664	-0.833904
H	-2.704937	-1.041106	-2.962923
H	-1.200663	-1.783932	-2.457557
H	-3.994568	0.617870	-0.941473
H	-2.773385	-2.854825	-1.072757
H	-2.937278	1.465723	1.782965
H	-4.233132	0.340905	1.432445
C	2.412190	-0.678561	0.278639
H	3.319057	-0.372727	0.824024
C	2.833223	-1.659933	-0.839328
H	3.672953	-2.302170	-0.567761
C	2.293170	0.221408	-1.995114
H	2.781900	1.081127	-2.462442
O	3.248119	-0.820233	-1.902370
H	1.446447	-0.081204	-2.632110
H	1.987937	-2.290611	-1.156201
C	1.140913	2.827049	-1.099929
H	0.396836	3.540865	-0.733029
H	2.077007	3.387832	-1.232041
H	0.827792	2.478931	-2.087678
C	1.102411	-2.631135	1.435625
H	2.027644	-3.100287	1.799884
H	0.327834	-2.822666	2.183615
H	0.832087	-3.141630	0.507364

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -925.368591573 Predicted Change= -1.347109D-05
Zero-point correction (ZPE)= -924.9345 0.43409
Internal Energy (U)= -924.9132 0.45538
Enthalpy (H)= -924.9122 0.45633
Gibbs Free Energy (G)= -924.9829 0.38564

Frequencies -- 30.6187 47.1145 64.0949
SCF Energy (M06) = -924.7442374
SCF Energy (M06/def2-tzvp) = -926.1306984

3. RhNHC-IPr

3.a. Additional Figures

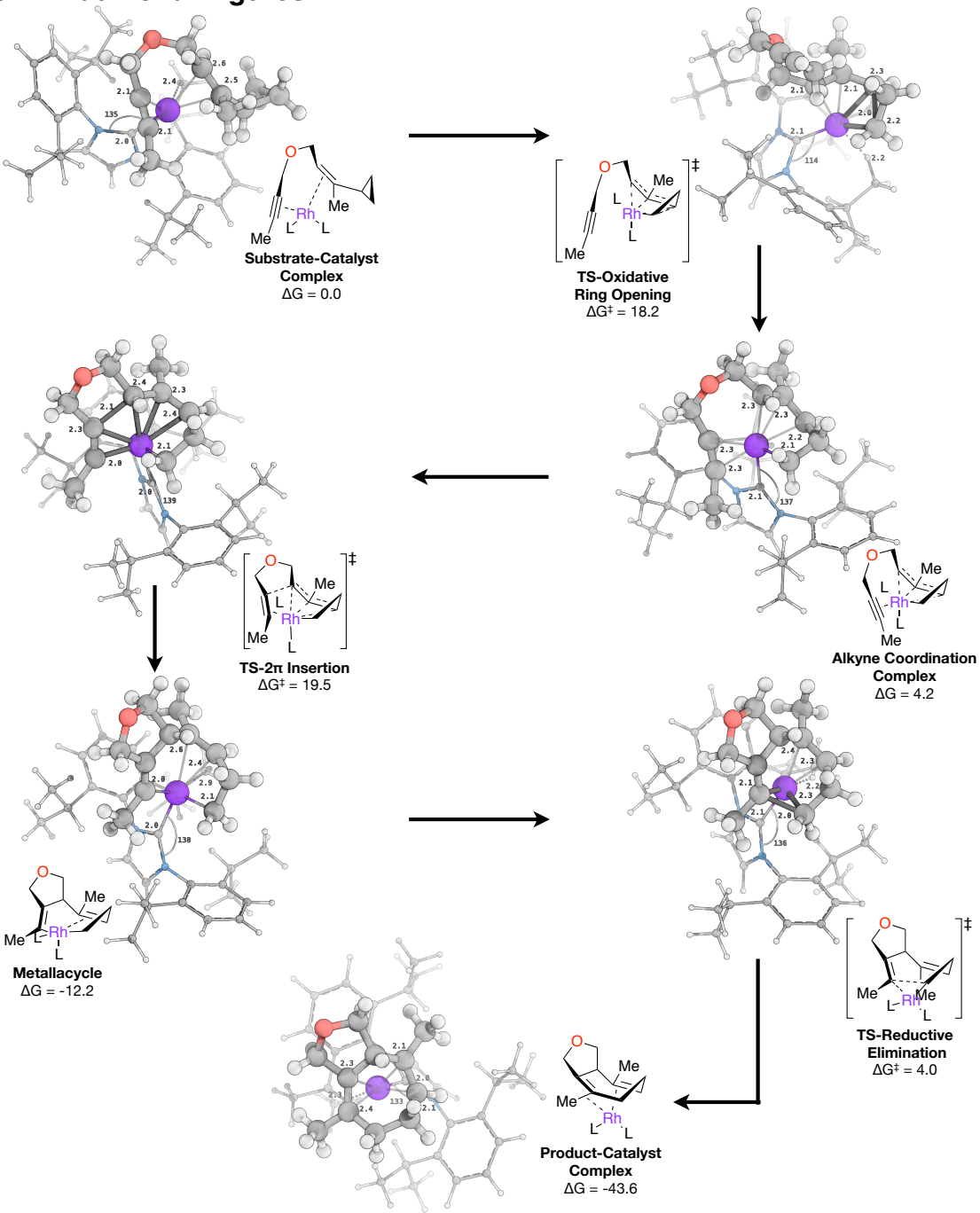


Figure S5. Computed geometries for RhNHC-IPr.

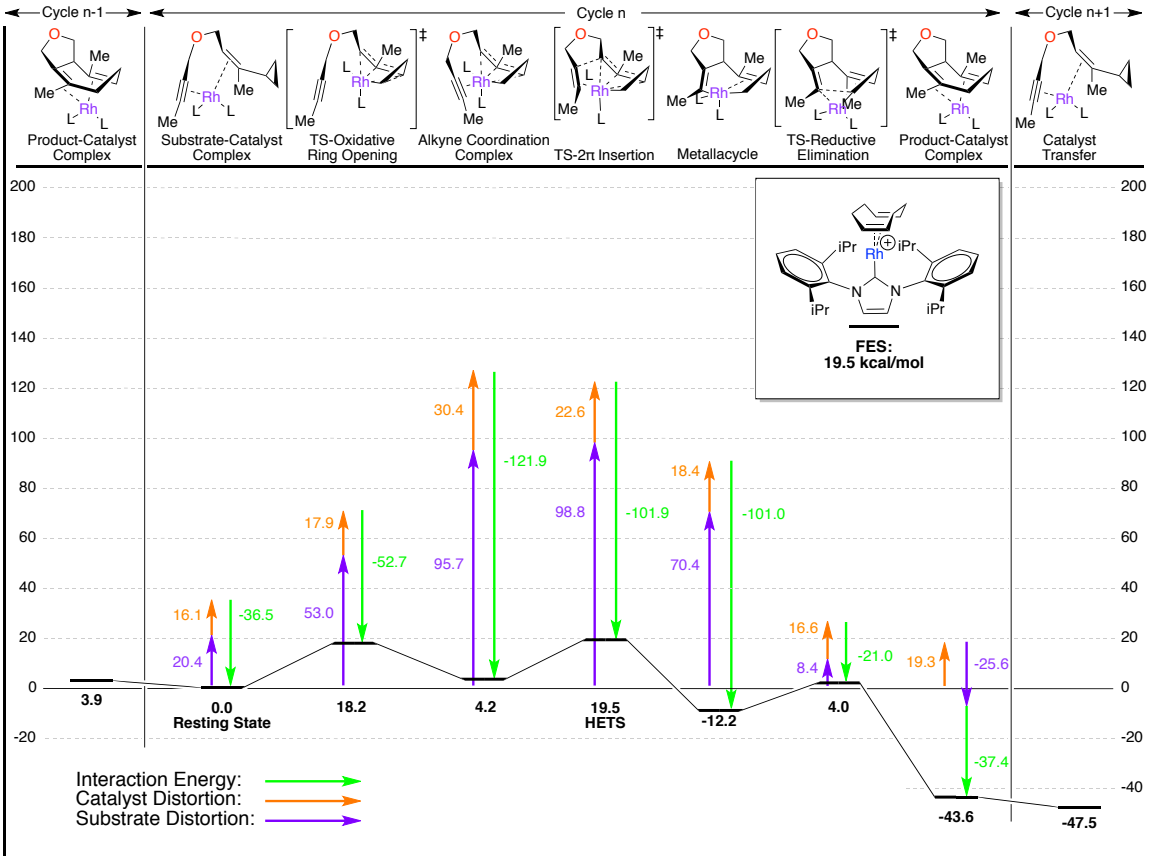


Figure S6. Reaction coordinate diagram for NHC-IPr. Interaction, catalyst and substrate distortion shown with colored arrows.

Substrate-Catalyst Complex RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]

#Atoms= 94

Charge = 1 Multiplicity = 1

SCF Energy= -1773.31167298 Predicted Change= -1.087739D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.01779 II	0.00180	[NO]	0.01779 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.428446	-0.899424	-0.417532
C	-1.919469	-2.620840	-1.378708
C	-3.231069	-2.168201	-0.813212
C	-4.382882	-3.168478	-0.735737
C	-3.788685	-2.605768	0.522526
C	1.240774	-1.469534	-1.512336
C	0.629449	-0.635489	-2.237270
H	-5.365514	-2.834648	-1.055292
H	-4.159200	-4.204881	-0.973796
H	-4.361825	-1.871174	1.079303
H	-3.206694	-3.278404	1.145308
H	-3.535129	-1.177467	-1.151658
C	-0.938825	-3.186920	-0.594319
H	-1.136245	-3.286681	0.474035
C	0.228530	-4.033648	-1.063097
H	0.062674	-5.062632	-0.723979
C	2.134436	-2.611561	-1.194905
H	2.542939	-3.007736	-2.140079
O	1.468670	-3.641059	-0.478275
H	0.311353	-4.058551	-2.156755
H	2.968982	-2.294348	-0.565106
C	0.381221	0.232485	-3.401436
H	1.132504	0.045019	-4.178047
H	-0.608451	0.049240	-3.831126
H	0.433016	1.291469	-3.126348
C	-1.901043	-2.641707	-2.891620
H	-2.504906	-3.485479	-3.250714
H	-2.362397	-1.732982	-3.293145
H	-0.899798	-2.736957	-3.313513
C	0.313950	0.840190	0.297804
N	1.565055	1.287877	0.622677
N	-0.522786	1.855926	0.671619
C	1.493571	2.554391	1.200057
C	2.830035	0.577296	0.540848
C	0.187643	2.912317	1.228833
C	-1.968746	1.771344	0.638163
H	2.378407	3.065923	1.542649
C	3.156203	-0.338050	1.564246
C	3.729164	0.914526	-0.494159
H	-0.302344	3.799565	1.597644
C	-2.666735	2.307866	-0.465428

C	-2.621841	1.199126	1.753051
C	2.233531	-0.653507	2.737960
C	4.420126	-0.942274	1.508231
C	4.978482	0.281506	-0.493398
C	3.411803	1.953506	-1.566720
C	-1.959812	3.035506	-1.604716
C	-4.063838	2.210818	-0.447341
C	-4.020080	1.124368	1.710484
C	-1.859946	0.682021	2.971589
C	1.997874	-2.167770	2.902314
H	1.260057	-0.194953	2.541828
C	2.779816	-0.034096	4.041554
H	4.704536	-1.649942	2.280604
C	5.322465	-0.639010	0.493350
H	5.696380	0.518804	-1.271877
C	4.116669	3.293986	-1.266389
H	2.331324	2.134972	-1.553210
C	3.781092	1.471034	-2.982677
H	-0.903945	2.743884	-1.584927
C	-2.024296	4.563750	-1.390703
C	-2.515193	2.666360	-2.992251
H	-4.637744	2.616074	-1.274366
C	-4.733507	1.618740	0.621533
H	-4.557704	0.692088	2.548551
H	-0.842832	1.084251	2.931380
C	-1.745115	-0.853650	2.947727
C	-2.473538	1.161606	4.301116
H	2.915609	-2.691390	3.192328
H	1.630953	-2.622814	1.976077
H	1.261775	-2.347640	3.694475
H	2.900165	1.051455	3.952995
H	3.756078	-0.457570	4.302523
H	2.096314	-0.233535	4.874851
H	6.299458	-1.113573	0.475688
H	5.205408	3.169759	-1.264494
H	3.828137	3.701134	-0.291699
H	3.864316	4.038420	-2.029997
H	3.356120	0.485078	-3.195003
H	4.865594	1.404658	-3.120555
H	3.405208	2.178733	-3.730009
H	-1.575844	4.859996	-0.436326
H	-3.062087	4.915450	-1.394265
H	-1.488414	5.085019	-2.191812
H	-3.534217	3.040251	-3.139167

H	-2.529907	1.582245	-3.147580
H	-1.894079	3.115984	-3.774752
H	-5.818361	1.561096	0.614036
H	-1.242151	-1.204169	2.031663
H	-2.730306	-1.329395	2.988940
H	-1.156582	-1.213030	3.799012
H	-3.463450	0.728201	4.480025
H	-2.573981	2.251661	4.324380
H	-1.831669	0.861993	5.136569

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1773.31167298 Predicted Change= -1.087739D-07
Zero-point correction (ZPE)= -1772.4906 0.82103
Internal Energy (U)= -1772.4443 0.86731
Enthalpy (H)= -1772.4434 0.86825
Gibbs Free Energy (G)= -1772.5704 0.74124

Frequencies -- 12.8667 24.6478 30.3515
SCF Energy (M06) = -1772.045947
SCF Energy (M06/def2-tzvp) = -1773.748655

Oxidative-Addition TS RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,readfc,ts,noeigentest,gdiis) freq geom=check guess=read
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]
#Atoms= 94
Charge = 1 Multiplicity = 1

SCF Energy= -1773.28176816 Predicted Change= -3.953775D-09

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00786 ll	0.00180	[NO]	0.00786 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.129874	-3.876549	-0.782163
Rh	0.530586	0.447678	-1.202848
C	3.033821	-4.155026	-0.348294
C	1.738184	-4.556961	0.214836
C	0.524763	-2.475112	0.046235
C	1.045884	-1.607554	-1.072845
C	0.269351	-1.360403	-2.255859
C	0.904146	-0.520952	-3.248200
C	2.367053	-0.427062	-3.554601
C	2.263967	0.716673	-2.585485
H	2.138935	1.697786	-3.037693
H	2.930374	0.690961	-1.720350
H	2.601151	-0.179443	-4.589720
H	2.959522	-1.274962	-3.211528
H	2.130131	-1.636931	-1.168585
H	1.765880	-4.458472	1.311822
H	1.544609	-5.610117	-0.014155
H	-0.527184	-2.261334	0.234235
H	1.082496	-2.275054	0.970296
H	0.241787	-0.048344	-3.970846
O	0.603406	-3.858163	-0.299565

C	5.460413	-3.578992	-1.309022
H	5.460299	-3.552969	-2.405217
H	5.835465	-2.614483	-0.946507
H	6.177084	-4.348845	-0.999387
C	-1.075813	-1.969238	-2.551511
H	-1.655756	-1.340934	-3.234174
H	-0.925570	-2.944535	-3.033369
H	-1.666231	-2.135316	-1.648723
C	-0.601261	0.673746	0.559775
N	-1.842977	0.413156	1.072560
N	-0.030351	1.509059	1.479197
C	-2.034481	1.098958	2.272233
C	-2.885863	-0.396091	0.468160
C	-0.894866	1.784927	2.531341
C	1.284079	2.081267	1.283142
H	-2.962602	1.037969	2.816581
C	-3.629018	0.147723	-0.601529
C	-3.167363	-1.669420	1.018377
H	-0.622438	2.436133	3.347015
C	2.399141	1.468485	1.896090
C	1.392237	3.241524	0.482950
C	-3.447726	1.576574	-1.108421
C	-4.633648	-0.651344	-1.162854
C	-4.185201	-2.418542	0.413513
C	-2.479216	-2.216907	2.270286
C	2.263182	0.272184	2.832836
C	3.655280	2.036091	1.650957
C	2.677270	3.753937	0.260753
C	0.171626	3.931386	-0.123978
C	-3.242816	1.643088	-2.632928
H	-2.549965	1.995252	-0.645389
C	-4.640396	2.455875	-0.675666
H	-5.223949	-0.262106	-1.986464
C	-4.903369	-1.924461	-0.671691
H	-4.425512	-3.401096	0.805671
C	-3.372778	-2.001298	3.512974
H	-1.551810	-1.653718	2.425531
C	-2.104247	-3.709413	2.166820
H	1.270393	-0.164131	2.678424
C	2.347575	0.728501	4.305510
C	3.298378	-0.832791	2.552087
H	4.536746	1.598349	2.108452
C	3.796618	3.156612	0.834318
H	2.801920	4.640733	-0.352479

H	-0.718449	3.569597	0.400846
C	0.007027	3.567566	-1.611529
C	0.204852	5.461775	0.054300
H	-4.116809	1.276024	-3.181490
H	-2.375795	1.048342	-2.941281
H	-3.075197	2.679707	-2.946870
H	-4.766294	2.452520	0.412582
H	-5.577533	2.102519	-1.120163
H	-4.487806	3.492654	-0.996957
H	-5.687786	-2.526058	-1.121892
H	-4.309275	-2.562410	3.418459
H	-3.634709	-0.948818	3.661402
H	-2.860259	-2.351523	4.415975
H	-1.504371	-3.936319	1.280516
H	-2.992971	-4.349267	2.143651
H	-1.526592	-4.001527	3.051145
H	1.581858	1.474742	4.543936
H	3.324861	1.174230	4.523157
H	2.209155	-0.125017	4.978433
H	4.319527	-0.504596	2.774740
H	3.271637	-1.164227	1.508348
H	3.095784	-1.700845	3.189227
H	4.783024	3.576551	0.658933
H	-0.169354	2.481909	-1.758659
H	0.891802	3.844347	-2.195048
H	-0.862992	4.071880	-2.046633
H	1.005204	5.929071	-0.529363
H	0.348940	5.736568	1.104069
H	-0.741654	5.897160	-0.283630

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1773.28176816 Predicted Change= -3.953775D-09
Zero-point correction (ZPE)= -1772.4629 0.81882
Internal Energy (U)= -1772.4164 0.86532
Enthalpy (H)= -1772.4154 0.86627
Gibbs Free Energy (G)= -1772.5456 0.73607

Frequencies -- -219.7296 11.4576 16.0260
SCF Energy (M06) = -1772.011779
SCF Energy (M06/def2-tzvp) = -1773.717276

Alkyne Coordination Complex RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

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opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

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Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]
#Atoms= 94

Charge = 1 Multiplicity = 1

SCF Energy= -1773.31389410 Predicted Change= -2.601199D-07

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00829 II	0.00180	[NO]	0.00829 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.129204	1.140698	-2.264655
Rh	0.524481	-0.733964	-1.079874
C	2.044628	0.317162	-2.419364
C	3.328433	-0.286270	-2.858812
C	2.792523	-2.592849	-2.791417
C	1.349000	-2.479655	-2.372063
C	0.823592	-3.013730	-1.173326
C	-0.511375	-2.676841	-0.826981
C	-1.547920	-2.284686	-1.886807
C	-1.119075	-0.889160	-2.319155
H	-1.818508	-0.100738	-2.055316
H	-0.772032	-0.781628	-3.349054
H	-2.544207	-2.269343	-1.438693
H	-1.561710	-3.004965	-2.715556
H	0.680593	-2.340388	-3.217122
H	3.989721	-0.429613	-1.988566
H	3.815004	0.422571	-3.537303
H	2.933506	-3.468845	-3.435269
H	3.468438	-2.698465	-1.930004
H	-0.875594	-3.025883	0.133420
O	3.197068	-1.485793	-3.589882
C	0.330221	2.351465	-2.508553

H	0.056857	2.860412	-1.581260
H	0.897266	3.050712	-3.133297
H	-0.593926	2.099382	-3.037150
C	1.692666	-3.757435	-0.186083
H	1.167502	-3.917921	0.757255
H	1.952504	-4.740709	-0.597877
H	2.633484	-3.239387	0.025915
C	-0.376096	0.438699	0.437573
N	0.432451	1.075571	1.352871
N	-1.645611	0.824065	0.800212
C	-0.314101	1.856944	2.229155
C	1.869301	0.900661	1.508722
C	-1.609948	1.702076	1.883836
C	-2.933652	0.349879	0.312533
H	0.149775	2.438904	3.008394
C	2.339719	-0.226659	2.231232
C	2.741262	1.909546	1.040232
H	-2.512472	2.117859	2.301064
C	-3.656705	1.145478	-0.602905
C	-3.477877	-0.826447	0.882312
C	1.406013	-1.182814	2.978712
C	3.727539	-0.379278	2.349455
C	4.118313	1.701731	1.198683
C	2.252476	3.244086	0.482499
C	-3.157175	2.496127	-1.109036
C	-4.919588	0.689178	-1.004870
C	-4.743532	-1.231707	0.438420
C	-2.794313	-1.598334	2.010504
C	2.023340	-2.563858	3.264626
H	0.509998	-1.335856	2.366397
C	0.963681	-0.564941	4.326641
H	4.126831	-1.233173	2.884583
C	4.609554	0.560803	1.822582
H	4.813858	2.454210	0.842136
C	2.304934	4.331329	1.580314
H	1.205578	3.126195	0.187125
C	3.042002	3.721861	-0.750657
H	-2.086160	2.561690	-0.895211
C	-3.852699	3.650265	-0.354078
C	-3.344148	2.676885	-2.627978
H	-5.497184	1.275137	-1.712336
C	-5.453742	-0.492247	-0.503198
H	-5.189138	-2.131917	0.847851
H	-1.715820	-1.426101	1.934346

C	-3.028770	-3.119967	1.949174
C	-3.259040	-1.067778	3.386112
H	2.781833	-2.509477	4.053399
H	2.489971	-3.008768	2.382597
H	1.245170	-3.247681	3.620683
H	0.416161	0.371893	4.201044
H	1.836257	-0.367550	4.959620
H	0.310477	-1.262435	4.863461
H	5.681120	0.419553	1.932172
H	3.335277	4.497459	1.913965
H	1.713513	4.061113	2.461143
H	1.918747	5.281133	1.193598
H	3.095470	2.949616	-1.523077
H	4.065729	4.010963	-0.490088
H	2.561897	4.608048	-1.180326
H	-3.682338	3.594122	0.726159
H	-4.935370	3.629849	-0.521468
H	-3.475907	4.617804	-0.704686
H	-4.400981	2.766897	-2.900176
H	-2.928268	1.838440	-3.197626
H	-2.849814	3.596718	-2.959634
H	-6.434504	-0.826994	-0.828617
H	-2.831692	-3.534267	0.955012
H	-4.056684	-3.384917	2.218940
H	-2.373039	-3.625021	2.666984
H	-4.339505	-1.205238	3.507336
H	-3.038247	-0.004022	3.513042
H	-2.757350	-1.613377	4.193590

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1773.31389410 Predicted Change= -2.601199D-07
Zero-point correction (ZPE)= -1772.4918 0.82204
Internal Energy (U)= -1772.4464 0.86747
Enthalpy (H)= -1772.4454 0.86841
Gibbs Free Energy (G)= -1772.5679 0.74598

Frequencies -- 20.3922 25.8838 33.9922
SCF Energy (M06) = -1772.043934
SCF Energy (M06/def2-tzvp) = -1773.750339

2π-Insertion TS RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

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b3lyp geom=check gen pseudo=read gfprint gfinput guess=read
scf=(direct,tight,maxcycle=300,xqc) guess=read
opt=(gdiis,maxcycle=250,readfc,ts,noeigentest,nofreeze) freq
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

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Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]
#Atoms= 94
Charge = 1 Multiplicity = 1

SCF Energy= -1773.29653225 Predicted Change= -2.049915D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00265 ll	0.00180	[NO]	0.00265 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.007771	-2.408540	0.530665
Rh	-0.625866	-0.815213	-0.684332
C	-1.922029	-2.697831	-0.338142
C	-3.142501	-3.569510	-0.470273
C	-3.441628	-2.466203	-2.430458
C	-2.022899	-1.934367	-2.274323
C	-1.761513	-0.533106	-2.669238
C	-0.480258	-0.137289	-3.019299
C	0.694733	-1.103317	-3.126968
C	0.891640	-1.733304	-1.746453
H	1.848013	-1.501587	-1.289334
H	0.696133	-2.807549	-1.692351
H	1.588009	-0.549260	-3.424577
H	0.512927	-1.852993	-3.910686
H	-1.313601	-2.648833	-2.687778
H	-3.969011	-3.117997	0.105551
H	-2.934796	-4.561537	-0.057297
H	-3.663344	-2.614639	-3.492319
H	-4.187109	-1.776016	-2.008618
H	-0.338001	0.884766	-3.360590
O	-3.519220	-3.732466	-1.816327

C	-2.919352	0.441244	-2.726904
H	-3.631417	0.144959	-3.507297
H	-3.469247	0.492805	-1.780727
H	-2.569725	1.447723	-2.963017
C	-0.477175	-3.017148	1.782645
H	0.478788	-3.509051	1.578388
H	-0.299454	-2.270763	2.560812
H	-1.165309	-3.773751	2.178409
C	0.515868	0.384444	0.512028
N	-0.150355	1.294343	1.299773
N	1.831259	0.523689	0.881720
C	0.724207	1.959836	2.151847
C	-1.542067	1.677152	1.139542
C	1.959667	1.479507	1.890943
C	3.024021	-0.034638	0.262944
H	0.382396	2.710083	2.846451
C	-1.837936	2.749516	0.263112
C	-2.533193	1.045826	1.923756
H	2.921542	1.723932	2.311094
C	3.623157	-1.180043	0.828300
C	3.601558	0.666982	-0.821942
C	-0.753209	3.594393	-0.404370
C	-3.183826	3.105219	0.113163
C	-3.862690	1.443499	1.726322
C	-2.187440	0.062562	3.037230
C	3.085026	-1.861998	2.082613
C	4.796840	-1.656645	0.228916
C	4.772240	0.138406	-1.379947
C	3.056967	2.000218	-1.332836
C	-1.025863	3.913571	-1.884538
H	0.188149	3.039239	-0.363108
C	-0.553444	4.906668	0.387207
H	-3.448581	3.923125	-0.549364
C	-4.188406	2.448291	0.819771
H	-4.650688	0.977758	2.308731
C	-2.095918	0.805595	4.389018
H	-1.197178	-0.349563	2.821823
C	-3.172989	-1.113578	3.147393
H	2.032156	-1.583368	2.192967
C	3.833974	-1.361744	3.337676
C	3.158192	-3.398807	2.008878
H	5.282190	-2.538339	0.633643
C	5.359574	-1.015757	-0.869803
H	5.240674	0.646246	-2.216591

H	2.007850	2.077097	-1.031023
C	3.098920	2.144157	-2.865152
C	3.821739	3.174576	-0.681605
H	-1.926995	4.521480	-2.018664
H	-1.139559	3.004005	-2.481798
H	-0.188444	4.485039	-2.299927
H	-0.304598	4.716148	1.436307
H	-1.462911	5.517650	0.367680
H	0.259171	5.496504	-0.051486
H	-5.225454	2.744241	0.688555
H	-3.060059	1.253452	4.654795
H	-1.351218	1.608148	4.363674
H	-1.814880	0.109977	5.187818
H	-3.295684	-1.627201	2.188630
H	-4.161682	-0.788921	3.488843
H	-2.805683	-1.839439	3.880967
H	3.740006	-0.278506	3.466327
H	4.901964	-1.598872	3.274228
H	3.434663	-1.842840	4.237827
H	4.190763	-3.760568	2.056066
H	2.713124	-3.786492	1.085725
H	2.628925	-3.840110	2.860569
H	6.268687	-1.405667	-1.318561
H	2.603947	1.309056	-3.370699
H	4.123929	2.204915	-3.245686
H	2.592213	3.068747	-3.163168
H	4.883258	3.142715	-0.951704
H	3.753994	3.152326	0.410427
H	3.415271	4.132764	-1.025180

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1773.29653225 Predicted Change= -2.049915D-08
Zero-point correction (ZPE)= -1772.4746 0.82184
Internal Energy (U)= -1772.4300 0.86647
Enthalpy (H)= -1772.4291 0.86741
Gibbs Free Energy (G)= -1772.5501 0.74638

Frequencies -- -205.4828 29.4456 33.7696
SCF Energy (M06) = -1772.020053
SCF Energy (M06/def2-tzvp) = -1773.724226

Metallacycle RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

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opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]

#Atoms= 94

Charge = 1 Multiplicity = 1

SCF Energy= -1773.34912438 Predicted Change= -2.109130D-07

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00923 ll	0.00180	[NO]	0.00923 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.207346	-1.861837	0.368127
Rh	-0.498249	-0.466687	-0.886023
C	-2.231213	-2.595852	-0.089255
C	-3.130989	-3.543258	0.706073
C	-4.270006	-2.907947	-1.204147
C	-2.787116	-2.606232	-1.499595
C	-2.407892	-1.390012	-2.319416
C	-1.200079	-1.327046	-2.961931
C	-0.055188	-2.332058	-2.859366
C	0.846085	-1.742596	-1.775389
H	1.643141	-1.103692	-2.163386
H	1.256307	-2.455781	-1.059165
H	0.456565	-2.429628	-3.825036
H	-0.418323	-3.322938	-2.574978
H	-2.397528	-3.505810	-1.998014
H	-3.519540	-3.055033	1.613198
H	-2.630771	-4.471991	1.006737
H	-4.812626	-3.347456	-2.044859
H	-4.807232	-2.011088	-0.858985
H	-1.031150	-0.480948	-3.630443
O	-4.196995	-3.889055	-0.176953
C	-0.589856	-2.092061	1.719028

H	0.382980	-2.581273	1.607333
H	-0.427551	-1.172370	2.283650
H	-1.215792	-2.755863	2.328479
C	-3.446779	-0.312200	-2.522991
H	-4.321178	-0.720752	-3.046074
H	-3.804146	0.093142	-1.569083
H	-3.054364	0.515581	-3.119629
C	0.666024	0.532740	0.455867
N	1.984487	0.568935	0.821285
N	0.094722	1.586182	1.123121
C	2.216228	1.624860	1.699764
C	3.085292	-0.224168	0.291516
C	1.035312	2.261728	1.888887
C	-1.270025	2.038126	0.911948
H	3.199936	1.821592	2.094288
C	3.568966	-1.317883	1.039810
C	3.692795	0.201208	-0.912319
H	0.777333	3.125582	2.480783
C	-1.543373	2.812678	-0.240781
C	-2.257114	1.750111	1.880948
C	3.034626	-1.683503	2.421962
C	4.645605	-2.037827	0.503718
C	4.765314	-0.558014	-1.395475
C	3.291954	1.484361	-1.638319
C	-0.456762	3.323178	-1.185313
C	-2.871715	3.203456	-0.455912
C	-3.563737	2.178135	1.614366
C	-1.943441	1.082866	3.216139
C	2.869401	-3.201931	2.624371
H	2.048892	-1.222840	2.538485
C	3.950368	-1.105501	3.523827
H	5.039492	-2.888657	1.049505
C	5.229609	-1.673963	-0.705041
H	5.253700	-0.262388	-2.318208
C	4.257150	2.631395	-1.265122
H	2.293779	1.774160	-1.295549
C	3.218024	1.331677	-3.169129
H	0.502360	2.904694	-0.867253
C	-0.331783	4.858464	-1.084350
C	-0.683639	2.890402	-2.645109
H	-3.116167	3.795350	-1.332773
C	-3.875380	2.877847	0.451396
H	-4.347377	1.970689	2.335747
H	-0.942124	0.645507	3.152259

C	-2.927080	-0.049420	3.565685
C	-1.910083	2.134777	4.346785
H	3.836843	-3.711533	2.686921
H	2.303361	-3.667460	1.810262
H	2.341983	-3.398587	3.564066
H	4.040498	-0.016294	3.453036
H	4.959447	-1.526714	3.453439
H	3.552213	-1.346548	4.515870
H	6.063352	-2.247671	-1.099437
H	5.278947	2.401976	-1.587336
H	4.280070	2.806844	-0.184366
H	3.951081	3.563865	-1.753068
H	2.557150	0.511341	-3.470017
H	4.202125	1.146138	-3.612225
H	2.834936	2.255961	-3.615705
H	-0.139213	5.177142	-0.054426
H	-1.245979	5.358347	-1.422646
H	0.494521	5.213228	-1.710333
H	-1.621590	3.288333	-3.047993
H	-0.721127	1.797275	-2.738585
H	0.129992	3.254674	-3.281940
H	-4.897326	3.197497	0.268501
H	-3.013798	-0.772916	2.748871
H	-3.929178	0.335913	3.782159
H	-2.584788	-0.579188	4.461227
H	-2.887846	2.614457	4.467015
H	-1.176746	2.924525	4.148778
H	-1.647776	1.660954	5.299196

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1773.34912438 Predicted Change= -2.109130D-07
Zero-point correction (ZPE)= -1772.5256 0.82349
Internal Energy (U)= -1772.4806 0.86843
Enthalpy (H)= -1772.4797 0.86937
Gibbs Free Energy (G)= -1772.6033 0.74581

Frequencies -- 14.6753 25.0346 29.1482
SCF Energy (M06) = -1772.069882
SCF Energy (M06/def2-tzvp) = -1773.768725

Reductive Elimination TS RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

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b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,readfc,ts,noeigentest) freq
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

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Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]
#Atoms= 94
Charge = 1 Multiplicity = 1

SCF Energy= -1773.31019756 Predicted Change= -4.276102D-09

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00151 II	0.00180	[YES]	0.00151 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.571588	-2.180603	0.286174
Rh	-0.488849	-0.510819	-0.920629
C	-1.741831	-2.838680	0.107162
C	-2.534517	-3.601957	1.152707
C	-3.991088	-2.895961	-0.497400
C	-2.590731	-2.836367	-1.142216
C	-2.237068	-1.705644	-2.096425
C	-1.028552	-1.743669	-2.759660
C	0.035049	-2.802498	-2.495609
C	0.743957	-2.402669	-1.203085
H	1.587353	-1.723691	-1.350337
H	1.109658	-3.239078	-0.609159
H	0.751868	-2.835192	-3.323743
H	-0.409223	-3.800714	-2.414063
H	-2.464673	-3.799414	-1.665291
H	-2.621969	-3.036818	2.093305
H	-2.095251	-4.580162	1.395027
H	-4.769448	-3.291422	-1.154327
H	-4.304267	-1.910158	-0.119664
H	-0.876232	-1.069838	-3.601914
O	-3.818517	-3.822631	0.570844

C	0.174345	-2.272952	1.594063
H	-0.323084	-1.683198	2.373271
H	0.231935	-3.310629	1.949273
H	1.191835	-1.899028	1.494879
C	-3.334776	-0.757352	-2.517701
H	-2.985218	-0.053185	-3.277386
H	-4.172445	-1.323338	-2.947573
H	-3.733157	-0.183451	-1.673196
C	0.568690	0.710859	0.350286
N	-0.071379	1.768603	0.937120
N	1.894306	0.917106	0.639941
C	0.828220	2.622853	1.562578
C	-1.490636	2.035912	0.818876
C	2.058694	2.091716	1.371679
C	3.031641	0.125854	0.201515
H	0.507763	3.519199	2.069529
C	-1.941434	2.720207	-0.331614
C	-2.351353	1.657523	1.869431
H	3.033612	2.436307	1.674684
C	3.712872	-0.677950	1.146085
C	3.470193	0.257149	-1.135905
C	-0.980623	3.206827	-1.414773
C	-3.317472	2.954580	-0.444239
C	-3.715182	1.934215	1.709185
C	-1.842392	1.029590	3.163259
C	3.379945	-0.694284	2.639319
C	4.803260	-1.427193	0.683634
C	4.564797	-0.520452	-1.536058
C	2.883402	1.275560	-2.111593
C	-0.921899	2.221390	-2.594633
H	0.023293	3.254856	-0.980105
C	-1.313356	4.624386	-1.919020
H	-3.704552	3.471278	-1.316537
C	-4.196525	2.559897	0.561721
H	-4.410579	1.661789	2.496571
C	-1.757457	2.088032	4.284134
H	-0.827871	0.658066	2.982125
C	-2.695943	-0.167540	3.618597
H	2.365423	-0.302327	2.771232
C	4.346193	0.229287	3.416100
C	3.420969	-2.103284	3.264240
H	5.345188	-2.060692	1.377914
C	5.215962	-1.366199	-0.643466
H	4.926134	-0.445994	-2.556696

H	1.924622	1.620497	-1.714747
C	2.612402	0.692288	-3.510432
C	3.810394	2.507270	-2.208192
H	-1.907517	2.079193	-3.049059
H	-0.549847	1.224770	-2.279715
H	-0.229970	2.570171	-3.369333
H	-1.390310	5.332968	-1.088313
H	-2.254800	4.655850	-2.477699
H	-0.523919	4.975108	-2.592361
H	-5.259211	2.761408	0.461050
H	-2.746700	2.504080	4.505902
H	-1.101004	2.920931	4.009421
H	-1.366577	1.639263	5.204126
H	-2.814297	-0.901809	2.815236
H	-3.696531	0.140270	3.940708
H	-2.221779	-0.663036	4.473076
H	4.327112	1.259817	3.047852
H	5.377464	-0.130791	3.330322
H	4.082585	0.246550	4.479496
H	4.444094	-2.488680	3.327451
H	2.826089	-2.827919	2.700869
H	3.030446	-2.064685	4.286845
H	6.063380	-1.958671	-0.976228
H	1.960021	-0.186556	-3.461454
H	3.535889	0.398355	-4.020370
H	2.124247	1.443754	-4.141200
H	4.793552	2.230317	-2.604851
H	3.965383	2.972115	-1.228419
H	3.377983	3.260640	-2.876666

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1773.31019756 Predicted Change= -4.276102D-09
Zero-point correction (ZPE)= -1772.4878 0.82233
Internal Energy (U)= -1772.4435 0.86661
Enthalpy (H)= -1772.4426 0.86755
Gibbs Free Energy (G)= -1772.5634 0.74672

Frequencies -- -424.7894 26.3770 27.5935
SCF Energy (M06) = -1772.045125
SCF Energy (M06/def2-tzvp) = -1773.743704

Product-Catalyst Complex RhNHC-IPr

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

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opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C38H52N2ORh(1+) C1[X(C38H52N2ORh)]

#Atoms= 94

Charge = 1 Multiplicity = 1

SCF Energy= -1773.38853685 Predicted Change= -8.281237D-09

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00102 ll	0.00180	[YES]	0.00102 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.543716	-3.440435	-0.389300
Rh	-0.318953	-1.069375	-0.146760
C	-1.501292	-2.797085	-1.141053
C	-3.009558	-2.827568	-0.881404
C	-2.772465	-1.698832	-2.836649
C	-1.319928	-2.125190	-2.514660
C	-0.312735	-1.003269	-2.284334
C	0.974151	-1.397431	-1.805369
C	1.470201	-2.832397	-1.909020
C	0.857207	-3.785578	-0.868703
H	1.509654	-3.811914	0.011371
H	0.842723	-4.816178	-1.255679
H	2.558204	-2.843843	-1.798170
H	1.262662	-3.195553	-2.925704
H	-0.971171	-2.834962	-3.280557
H	-3.328209	-2.030707	-0.186598
H	-3.359487	-3.787967	-0.493791
H	-3.016821	-1.740937	-3.899838
H	-2.978755	-0.685139	-2.461776
H	1.753738	-0.642298	-1.846530
O	-3.592254	-2.639427	-2.159889
C	-0.490959	0.318463	-2.988191

H	-0.375800	0.170420	-4.072843
H	-1.477002	0.758329	-2.825851
H	0.265187	1.039641	-2.668854
C	-0.932579	-4.171793	0.880196
H	-1.904625	-3.869252	1.274522
H	-0.970575	-5.253528	0.687068
H	-0.184784	-4.019661	1.666645
C	0.327169	0.795048	0.384455
N	1.569014	1.329900	0.592971
N	-0.537267	1.734357	0.881086
C	1.474321	2.569019	1.219929
C	2.847116	0.701095	0.317988
C	0.156745	2.822512	1.401713
C	-1.983101	1.622369	0.909812
H	2.351201	3.138804	1.482256
C	3.362137	-0.212953	1.259585
C	3.555470	1.080876	-0.843498
H	-0.350305	3.661385	1.850083
C	-2.743360	2.520598	0.131238
C	-2.581518	0.651153	1.751877
C	2.675900	-0.519175	2.588225
C	4.598615	-0.806062	0.971523
C	4.790156	0.460564	-1.072749
C	3.060423	2.164606	-1.800362
C	-2.128257	3.594534	-0.765645
C	-4.140572	2.428363	0.217385
C	-3.979554	0.603255	1.783559
C	-1.763249	-0.283891	2.651637
C	2.395642	-2.022080	2.768775
H	1.709673	-0.006221	2.603557
C	3.501847	0.033034	3.768923
H	5.024345	-1.517174	1.673082
C	5.301785	-0.482692	-0.184873
H	5.364299	0.724701	-1.955016
C	3.792651	3.498182	-1.534378
H	1.994757	2.330471	-1.604857
C	3.201874	1.774578	-3.284408
H	-1.054593	3.398804	-0.853362
C	-2.305242	4.999007	-0.148907
C	-2.711122	3.575887	-2.192846
H	-4.754202	3.110088	-0.362730
C	-4.753546	1.482877	1.028186
H	-4.478371	-0.121424	2.415827
H	-0.911049	-0.686897	2.061782

C	-2.546185	-1.500653	3.170159
C	-1.151346	0.477194	3.847894
H	3.319748	-2.609850	2.792082
H	1.774848	-2.405074	1.950614
H	1.869858	-2.200232	3.714013
H	3.669543	1.111086	3.670536
H	4.482285	-0.451684	3.833144
H	2.978911	-0.144068	4.715530
H	6.261264	-0.950737	-0.385613
H	4.868593	3.394648	-1.714190
H	3.660704	3.838683	-0.501834
H	3.413338	4.281904	-2.199680
H	2.725333	0.813374	-3.504749
H	4.251268	1.703804	-3.589230
H	2.734164	2.537803	-3.915958
H	-1.870068	5.070658	0.853750
H	-3.366670	5.257365	-0.063587
H	-1.826054	5.755531	-0.780028
H	-3.765340	3.871771	-2.207925
H	-2.637213	2.584481	-2.650387
H	-2.166113	4.284211	-2.826335
H	-5.837061	1.428509	1.078323
H	-3.054050	-2.043992	2.367004
H	-3.300063	-1.205679	3.907941
H	-1.861062	-2.192780	3.670156
H	-1.952372	0.894657	4.468652
H	-0.503362	1.300007	3.536015
H	-0.561194	-0.202658	4.472370

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1773.38853685 Predicted Change= -8.281237D-09
Zero-point correction (ZPE)= -1772.5631 0.82538
Internal Energy (U)= -1772.5187 0.86975
Enthalpy (H)= -1772.5178 0.87070
Gibbs Free Energy (G)= -1772.6398 0.74869

Frequencies -- 15.7615 23.4679 33.7136
SCF Energy (M06) = -1772.122855
SCF Energy (M06/def2-tzvp) = -1773.819378

4. $RhTPPh_3$

4.a. Additional Figures

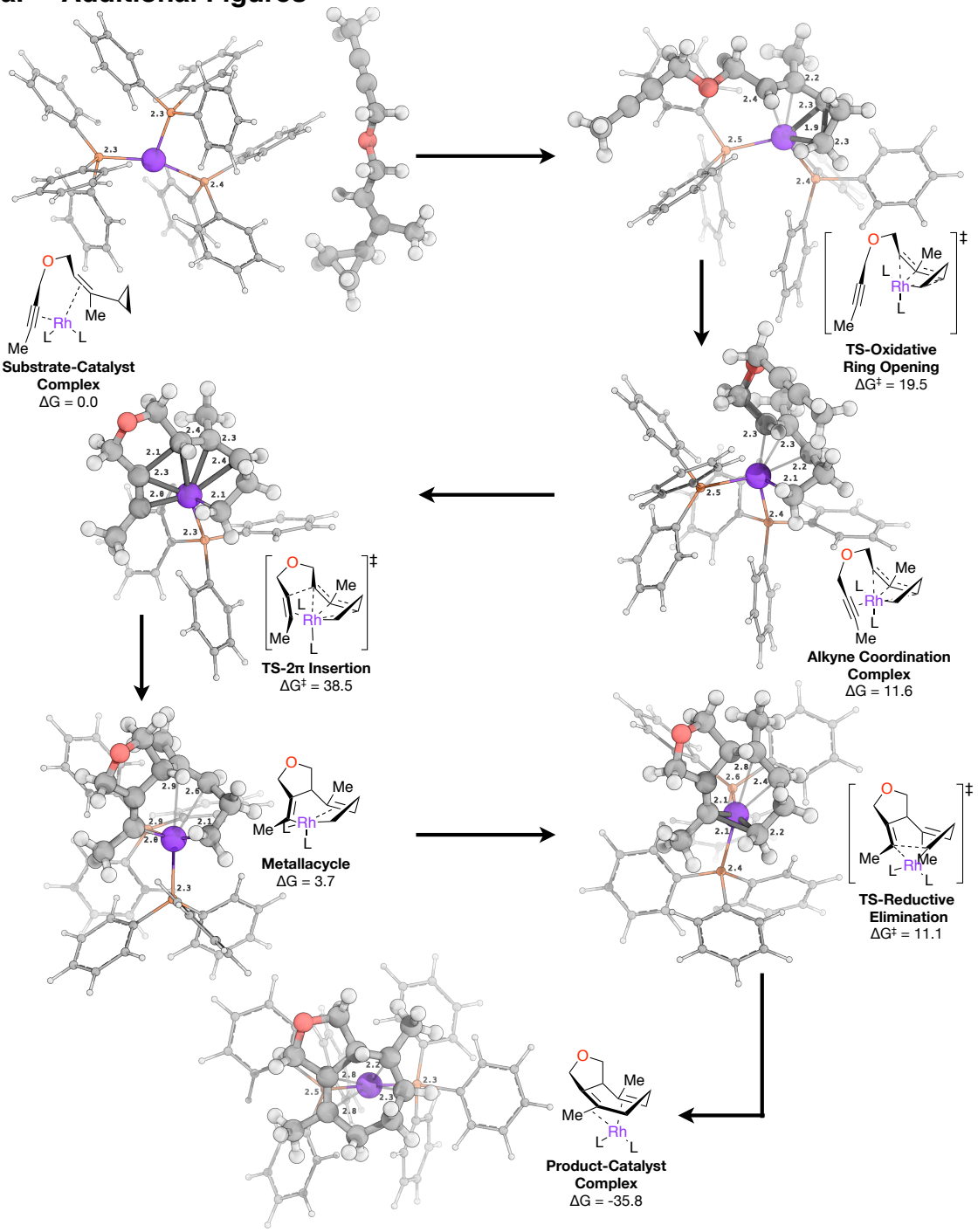


Figure S7. Computed geometries for Wilkinson's catalyst.

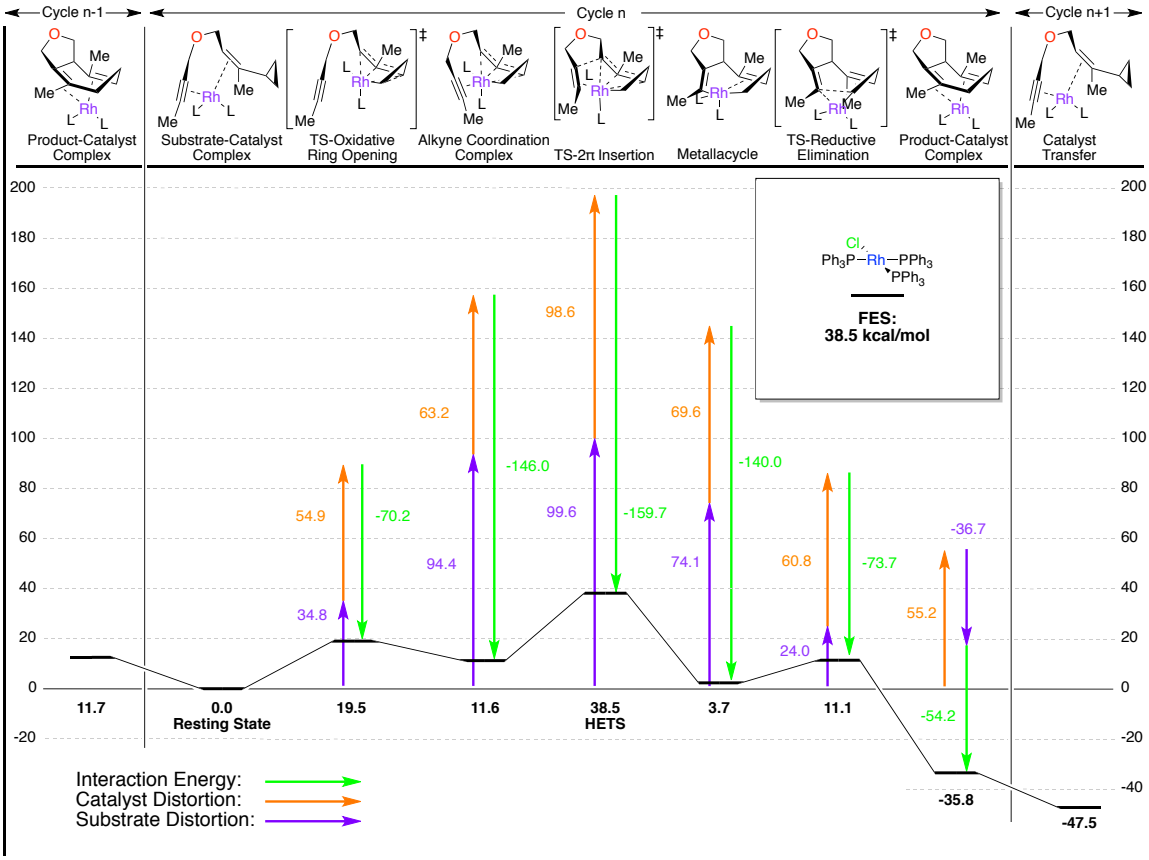


Figure S8. Reaction coordinate diagram for Wilkinson's catalyst. Interaction, catalyst and substrate distortion shown with colored arrows.

$Rh(PPh_3)_3$ (Tris)

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C54H45P3Rh(1+) C1[X(C54H45P3Rh)] #Atoms= 103

Charge = 1 Multiplicity = 1

SCF Energy= -3218.26561799 Predicted Change= -1.415008D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00238 II	0.00180	[NO]	0.00238 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.066340	0.440675	0.052843
P	2.286551	1.076997	0.043226
P	0.257368	-1.807448	0.045907
C	3.209126	1.211288	1.626065
C	2.734779	0.534845	2.759299
C	4.334897	2.045110	1.746655
C	3.386781	0.669254	3.987385
C	4.985132	2.175022	2.973106
C	4.514158	1.484558	4.093851
C	1.816095	2.819231	-0.332824
C	2.210150	3.533107	-1.476602
C	0.913212	3.419681	0.569120
C	1.712981	4.815024	-1.707170
C	0.407867	4.698980	0.324299
C	0.806263	5.396924	-0.815154
C	3.477478	0.557281	-1.250824
C	3.022969	0.502165	-2.581476
C	4.793137	0.166109	-0.966534
C	3.877906	0.102471	-3.607004
C	5.643154	-0.245955	-1.995623
C	5.192712	-0.270951	-3.315392
C	-0.349876	-2.668169	1.561265
C	-0.987320	-1.942176	2.577011
C	-0.145456	-4.049068	1.739610
C	-1.434456	-2.581291	3.736529
C	-0.598628	-4.686354	2.894430
C	-1.246084	-3.954635	3.894117
C	-0.668233	-2.512455	-1.387414
C	-1.507156	-3.630912	-1.290742
C	-0.493855	-1.901935	-2.642373
C	-2.142352	-4.136598	-2.427651
C	-1.120077	-2.415772	-3.777195
C	-1.946426	-3.537339	-3.671622
C	1.947568	-2.548465	-0.128288
C	2.425851	-3.043833	-1.350268
C	3.703294	-3.602062	-1.436510
C	4.054285	-3.179040	0.913067
C	4.519539	-3.673150	-0.308004
P	-2.344835	0.675463	0.020421
C	-2.998125	1.288721	1.635166

C	-2.089902	1.698880	2.624127
C	-4.375073	1.386021	1.900458
C	-2.541728	2.205253	3.844325
C	-4.825955	1.893818	3.119792
C	-3.911690	2.305956	4.092481
C	-2.586756	2.080977	-1.155604
C	-1.842043	2.072867	-2.348499
C	-3.472472	3.143003	-0.916283
C	-1.993513	3.094013	-3.288092
C	-3.616681	4.165762	-1.855002
C	-2.881901	4.142462	-3.042427
C	-3.614899	-0.564602	-0.488492
C	-4.207866	-0.533494	-1.758752
C	-3.992568	-1.574623	0.413945
C	-5.164449	-1.486756	-2.115242
C	-4.953134	-2.519682	0.056010
C	-5.542619	-2.478250	-1.209870
H	1.845550	-0.083749	2.678938
H	4.698839	2.598404	0.885432
H	3.011558	0.140016	4.858836
H	5.854826	2.820476	3.056341
H	5.021338	1.590216	5.048617
H	2.913573	3.096375	-2.177486
H	-0.284528	5.149131	1.029627
H	0.642331	2.905012	1.487957
H	0.422207	6.394955	-1.004732
H	2.039036	5.365817	-2.585100
H	1.998132	0.780523	-2.813801
H	5.157876	0.175150	0.054444
H	3.517960	0.078230	-4.631826
H	6.660633	-0.545366	-1.761045
H	5.859323	-0.584746	-4.113583
H	-1.924088	-2.002489	4.514738
H	-1.123818	-0.872321	2.462032
H	0.378773	-4.625661	0.983499
H	-1.591784	-4.453286	4.795167
H	-0.437736	-5.753602	3.017491
H	0.140508	-1.023356	-2.726012
H	-1.678737	-4.107669	-0.332562
H	-0.966707	-1.939317	-4.741644
H	-2.793532	-5.001073	-2.335654
H	-2.438819	-3.936903	-4.553584
H	1.801635	-3.014744	-2.235938
H	4.053837	-3.988252	-2.389359

H	4.678329	-3.237514	1.800511
H	5.509160	-4.116017	-0.376152
H	-5.096469	1.058023	1.158479
H	-1.022274	1.600033	2.440503
H	-5.893047	1.963686	3.310998
H	-1.825280	2.514522	4.600386
H	-4.266560	2.697530	5.041548
H	-1.147037	1.259197	-2.538975
H	-4.050348	3.176528	0.001127
H	-1.416985	3.071133	-4.208713
H	-4.307295	4.981006	-1.658054
H	-2.999987	4.939095	-3.771534
H	-3.551331	-1.618437	1.405063
H	-3.938093	0.240269	-2.469655
H	-5.244291	-3.285445	0.769764
H	-5.621143	-1.443696	-3.100072
H	-6.295284	-3.211450	-1.485751
C	2.780304	-2.620334	1.002319
H	2.428097	-2.261083	1.963505

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3218.26561799 Predicted Change= -1.415008D-08
Zero-point correction (ZPE)= -3217.4360 0.82953
Internal Energy (U)= -3217.3834 0.88217
Enthalpy (H)= -3217.3824 0.88311
Gibbs Free Energy (G)= -3217.5302 0.73539

Frequencies -- 13.6178 15.4121 17.8334
SCF Energy (M06) = -3720.038519
SCF Energy (M06/def2-tzvp) = -3218.471068

$Rh(PPh_3)_3$ (Tris)-Substrate-Complex

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C65H61OP3Rh(1+) C1[X(C65H61OP3Rh)] #Atoms= 131
Charge = 1 Multiplicity = 1

SCF Energy= -3722.14632596 Predicted Change= -4.302477D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00511 ll	0.00180	[NO]	0.00511 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.441799	0.341149	-0.684550
C	6.704454	0.537945	-2.115834
C	7.754126	-0.395439	-1.593037
C	8.982330	0.153431	-0.883852
C	7.977868	-0.680983	-0.130350
C	0.904485	1.380754	-1.851179
C	-0.191441	1.208213	-2.520294
C	5.638788	0.884631	-1.374897
C	4.559406	1.858565	-1.730860
C	2.218881	2.066747	-1.950722
O	3.288680	1.197785	-1.646535
C	-0.883413	1.478408	-3.805121
C	6.996071	1.037454	-3.512277
H	9.951912	-0.275405	-1.121609
H	9.001300	1.220041	-0.675427
H	8.252599	-1.694501	0.148405
H	7.354125	-0.176582	0.601423
H	7.967773	-1.223918	-2.269626
H	5.521928	0.441667	-0.388802
H	4.560691	2.701986	-1.018638
H	2.334973	2.464319	-2.976419

H	4.687915	2.279859	-2.737566
H	2.222787	2.933252	-1.267157
H	-0.143751	1.692460	-4.588180
H	-1.501273	0.635325	-4.128861
H	-1.542731	2.350100	-3.718843
H	7.167678	0.189915	-4.188988
H	6.196089	1.647259	-3.938344
H	7.918837	1.631857	-3.522765
P	-1.597533	2.084704	0.234693
P	-2.212183	-1.522525	-0.837881
C	-2.944164	2.866430	-0.756244
C	-3.532052	2.209425	-1.841011
C	-3.410375	4.146791	-0.398475
C	-4.566020	2.814092	-2.562057
C	-4.442796	4.745523	-1.117125
C	-5.021300	4.081767	-2.203529
C	-0.552689	3.580925	0.574311
C	-0.019921	4.281284	-0.523172
C	-0.361265	4.102935	1.862613
C	0.690897	5.464975	-0.335606
C	0.358773	5.287271	2.047805
C	0.886978	5.970417	0.953024
C	-2.385882	1.697556	1.850417
C	-1.589315	1.252055	2.919674
C	-3.768316	1.844114	2.046162
C	-2.158559	0.987010	4.164721
C	-4.335104	1.572321	3.292962
C	-3.533493	1.151382	4.354816
C	-1.150576	-2.971872	-1.295076
C	-0.102931	-2.772742	-2.212337
C	-1.343293	-4.258919	-0.768225
C	0.704571	-3.835731	-2.617404
C	-0.525334	-5.318116	-1.165956
C	0.494668	-5.112468	-2.095434
C	-3.379217	-2.201728	0.427057
C	-4.349875	-3.163294	0.080188
C	-3.298720	-1.778260	1.758660
C	-5.208309	-3.685061	1.045422
C	-4.163039	-2.301558	2.725715
C	-5.117557	-3.253290	2.372664
C	-3.358112	-1.399299	-2.305372
C	-2.967327	-1.787059	-3.596681
C	-3.844784	-1.662325	-4.677193
C	-5.532308	-0.767153	-3.206849

C	-5.129844	-1.153235	-4.487373
P	1.291650	-0.776738	1.187523
C	2.631387	0.371346	1.751947
C	3.833570	-0.117027	2.293982
C	2.444697	1.755382	1.668573
C	4.815069	0.764181	2.747953
C	3.426123	2.639751	2.126171
C	4.613333	2.145730	2.666321
C	0.698985	-1.498015	2.793387
C	1.112481	-1.008314	4.043281
C	-0.218174	-2.562909	2.765162
C	0.629851	-1.573777	5.227018
C	-0.689288	-3.135026	3.947466
C	-0.268274	-2.641023	5.184005
C	2.318349	-2.154455	0.471234
C	3.068445	-1.867841	-0.682702
C	2.441022	-3.422420	1.058361
C	3.930815	-2.822724	-1.221314
C	3.294242	-4.380879	0.504055
C	4.044642	-4.084414	-0.633404
H	-3.183077	1.226853	-2.127302
H	-2.969344	4.677423	0.439057
H	-5.009050	2.286156	-3.401160
H	-4.792712	5.733246	-0.831053
H	-5.821702	4.554256	-2.765807
H	-0.173514	3.907852	-1.530565
H	0.492544	5.677642	3.052642
H	-0.781575	3.604194	2.727618
H	1.438666	6.894657	1.098698
H	1.086724	5.996364	-1.196473
H	-0.522789	1.110364	2.784764
H	-4.404869	2.175381	1.233893
H	-1.526883	0.641498	4.977121
H	-5.405594	1.693456	3.431239
H	-3.976978	0.948999	5.325692
H	1.506615	-3.660270	-3.327572
H	0.085154	-1.783005	-2.621779
H	-2.135686	-4.444268	-0.052164
H	1.126657	-5.939341	-2.405640
H	-0.692133	-6.307579	-0.749200
H	-2.559837	-1.042738	2.049971
H	-4.437118	-3.502999	-0.946906
H	-4.083543	-1.957345	3.752301
H	-5.949426	-4.427020	0.761626

H	-5.791117	-3.657445	3.123319
H	-1.986889	-2.217701	-3.765912
H	-3.524144	-1.980945	-5.665209
H	-6.534956	-0.382142	-3.041643
H	-5.815065	-1.068500	-5.325957
H	1.532882	2.147056	1.233574
H	4.004411	-1.187090	2.360693
H	3.258062	3.710763	2.055652
H	5.737029	0.371940	3.168802
H	5.379660	2.829671	3.020543
H	1.824230	-0.192213	4.100721
H	-0.554327	-2.965933	1.814389
H	0.971664	-1.185944	6.183076
H	-1.388936	-3.964618	3.899520
H	-0.633310	-3.087430	6.104747
H	1.890765	-3.669750	1.958596
H	3.015584	-0.886939	-1.142947
H	3.379398	-5.355735	0.976802
H	4.522347	-2.569241	-2.096948
H	4.718311	-4.826876	-1.052833
C	-4.654393	-0.883559	-2.128233
H	-4.991556	-0.585300	-1.140158

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3722.14632596 Predicted Change= -4.302477D-08
Zero-point correction (ZPE)= -3721.0707 1.07562
Internal Energy (U)= -3721.0031 1.14318
Enthalpy (H)= -3721.0021 1.14413
Gibbs Free Energy (G)= -3721.1819 0.96434

Frequencies -- 9.6914 13.3363 19.0278=
SCF Energy (M06) = -3720.052968

Triphenylphosphine

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

#b3lyp/gen opt freq

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C18H15P C1[X(C18H15P)] #Atoms= 34

Charge = 0 Multiplicity = 1

SCF Energy= -1036.28170050 Predicted Change= -2.351745D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00014 ll	0.00045	[YES]	0.00003 ll	0.00030	[YES]
Displ	0.05710 ll	0.00180	[NO]	0.05710 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
P	-0.000749	-0.000526	-1.207752
C	1.153888	-1.206357	-0.402573
C	1.314475	-2.451047	-1.035482
C	1.891507	-0.947631	0.763277
C	2.170248	-3.418014	-0.507559
H	0.767305	-2.660599	-1.951868
C	2.757054	-1.911527	1.286047
H	1.792918	0.011307	1.263065
C	2.896176	-3.149124	0.655153
H	2.278367	-4.376177	-1.009294
H	3.322703	-1.693771	2.188575
H	3.571048	-3.897165	1.062886
C	0.467226	1.602931	-0.404574
C	-0.136575	2.122412	0.751089
C	1.479165	2.353445	-1.027890
C	0.268016	3.353497	1.273009
H	-0.927694	1.565362	1.243850
C	1.891363	3.577320	-0.500496
H	1.943639	1.976206	-1.936211
C	1.284063	4.081981	0.651776
H	-0.211929	3.742353	2.167649
H	2.678368	4.141300	-0.994496
H	1.596683	5.039921	1.059070

C	-1.623528	-0.396481	-0.404167
C	-2.780740	0.094199	-1.033285
C	-1.769722	-1.170927	0.757129
C	-4.046412	-0.162662	-0.505789
H	-2.687542	0.678356	-1.946064
C	-3.037620	-1.438288	1.279105
H	-0.890601	-1.569583	1.254208
C	-4.177925	-0.932655	0.652217
H	-4.929435	0.228630	-1.004452
H	-3.132998	-2.042136	2.178100
H	-5.163547	-1.142560	1.059343

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1036.28170050 Predicted Change= -2.351745D-06
Zero-point correction (ZPE)= -1036.0072 0.27440
Internal Energy (U)= -1035.9913 0.29030
Enthalpy (H)= -1035.9904 0.29125
Gibbs Free Energy (G)= -1036.0536 0.22806

Frequencies -- 22.4218 26.1225 39.9091
SCF Energy (M06) = -1035.690649
SCF Energy (M06/def2-tzvp) = -1035.978894

Substrate

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

b3lyp/6-31+G* 5D gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(gdiis,maxcycle=250) freq=noraman geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31+G(d) Freq

---

Pointgroup= C1 Stoichiometry= C11H16O C1[X(C11H16O)] #Atoms= 28

Charge = 0 Multiplicity = 1

SCF Energy= -503.909332222 Predicted Change= -1.355676D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.01064 ll	0.00180	[NO]	0.01064 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.205750	-0.371089	0.345458
C	3.329212	0.591144	0.595869
C	4.545544	0.619446	-0.317538
C	3.607306	1.802672	-0.256352
C	-3.617219	-0.183469	-0.185615
C	-4.612708	0.391851	0.194214
H	5.531549	0.705667	0.132984
H	4.511839	0.002916	-1.213072
H	3.945911	2.706616	0.243659
H	2.977024	1.986828	-1.121502
H	3.567307	0.703367	1.655169
C	1.112175	-0.010671	-0.348427
H	1.036033	1.015205	-0.704366
C	-0.066184	-0.860752	-0.716155
H	-0.122558	-0.971169	-1.815038
C	-2.432242	-0.895732	-0.659086
H	-2.424433	-1.923209	-0.255436
O	-1.252051	-0.208331	-0.257370
H	-0.006624	-1.872589	-0.290010
H	-2.459220	-0.982025	-1.759429
C	-5.806613	1.101328	0.651252
H	-6.402305	0.483353	1.334218

H	-5.531865	2.018870	1.186003
H	-6.448262	1.386134	-0.191577
C	2.444689	-1.737551	0.947860
H	3.310199	-2.222416	0.475888
H	2.684723	-1.643087	2.015832
H	1.588829	-2.410874	0.856757

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -503.909332222 Predicted Change= -1.355676D-06
Zero-point correction (ZPE)= -503.6673 0.24202
Internal Energy (U)= -503.6527 0.25663
Enthalpy (H)= -503.6517 0.25757
Gibbs Free Energy (G)= -503.7119 0.19739

Frequencies -- 17.8485 32.7582 42.0991
SCF Energy (M06) = -503.505363
SCF Energy (M06/def2-tzvp) = -503.7101042

Substrate-Catalyst Complex $RhPPh_3$ (Mono)

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

opt=maxcycle=250 freq=noraman b3lyp/gen geom=connectivity gfinput gfprint pseudo=read scf=(direct,tight,maxcycle=300,xqc)
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)] #Atoms= 63
Charge = 1 Multiplicity = 1

SCF Energy= -1649.53216441 Predicted Change= -1.029713D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00613 ll	0.00180	[NO]	0.00613 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.003731	-0.459715	-0.105567
Rh	-0.562771	-1.414376	0.342250
C	5.349772	-0.412762	-0.151213
C	6.040337	0.750820	0.475951
C	0.173065	-2.169032	-1.385860
C	-0.972864	-2.703327	-1.195995
H	3.479034	0.368262	0.371853
C	3.106149	-1.531266	-0.632726
H	3.657023	-2.401746	-1.010410
H	2.434560	-1.890864	0.167293
C	1.377067	-1.904598	-2.236157
H	1.858395	-2.870909	-2.461679
H	1.039560	-1.474667	-3.186381
H	5.357118	1.431785	0.979267
C	7.416376	0.647067	1.116414
C	7.250735	1.429430	-0.151432
H	7.662023	1.015863	-1.067544
H	7.573215	1.184235	2.047430
H	7.938358	-0.303561	1.062823
H	7.285317	2.514203	-0.105176
O	2.299242	-0.988619	-1.696831

C	-2.143167	-3.528586	-1.559326
H	-1.873662	-4.223473	-2.364034
H	-2.512927	-4.111730	-0.710448
H	-2.961689	-2.893098	-1.918292
C	6.210979	-1.483115	-0.778191
H	5.635423	-2.197453	-1.369585
H	6.964116	-1.044115	-1.442198
H	6.755064	-2.048781	-0.011376
P	-1.630630	0.505993	0.062796
C	-3.192685	0.589958	-0.853189
C	-3.454581	1.639085	-1.749327
C	-4.139720	-0.439433	-0.689348
C	-4.657728	1.665468	-2.455945
H	-2.727633	2.430493	-1.896392
C	-5.341369	-0.399887	-1.393235
H	-3.935455	-1.265220	-0.014005
C	-5.601074	0.652328	-2.277066
H	-4.855728	2.479799	-3.146263
H	-6.073123	-1.190511	-1.256128
H	-6.536388	0.678269	-2.828222
C	-0.629262	1.987197	-0.256038
C	0.603485	1.876330	-0.919518
C	-1.081177	3.242979	0.192739
C	1.369641	3.023181	-1.141959
H	0.980741	0.909811	-1.242603
C	-0.307370	4.378396	-0.036869
H	-2.026962	3.334415	0.720069
C	0.916310	4.268825	-0.705973
H	2.323707	2.934240	-1.652705
H	-0.656019	5.346665	0.309725
H	1.516904	5.156758	-0.880708
C	-1.906758	0.324365	1.855037
C	-3.149081	0.235000	2.507402
C	-0.721556	-0.026076	2.554043
C	-3.198380	-0.161245	3.840805
H	-4.062462	0.486206	1.977802
C	-0.791621	-0.448106	3.889829
H	0.258895	0.155113	2.102392
C	-2.026961	-0.512570	4.528415
H	-4.155317	-0.200198	4.352999
H	0.119327	-0.700103	4.424073
H	-2.084986	-0.827979	5.565686

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1649.53216441 Predicted Change= -1.029713D-08

Zero-point correction (ZPE)= -1649.0110 0.52113

Internal Energy (U)= -1648.9778 0.55428

Enthalpy (H)= -1648.9769 0.55522

Gibbs Free Energy (G)= -1649.0822 0.44991

Frequencies -- 9.0904 13.7030 18.5281

SCF Energy (M06) = -1648.568622

SCF Energy (M06/def2-tzvp) = -1650.134581

Ox.-Add. TS $RhPPh_3$ (Mono)

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)] #Atoms= 63
Charge = 1 Multiplicity = 1

SCF Energy= -1649.52183423 Predicted Change= -6.233666D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00144 II	0.00180	[YES]	0.00144 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.829118	-1.387199	-0.291643
P	0.525510	0.942336	-0.061881
C	1.921371	0.820341	-1.249317
C	3.240318	1.259306	-1.025525
C	1.647121	0.015280	-2.383986
C	4.247249	0.925402	-1.926017
H	3.467736	1.873471	-0.160147
C	2.676410	-0.325457	-3.276945
H	0.615818	-0.232627	-2.641344
C	3.971244	0.127429	-3.046851
H	5.256557	1.291505	-1.760810
H	2.449531	-0.918925	-4.157958
H	4.767337	-0.123497	-3.741420
C	-0.818406	1.833708	-0.914500
C	-0.579152	3.038467	-1.600942
C	-2.112693	1.292094	-0.882767
C	-1.630405	3.694564	-2.238566
H	0.421911	3.459565	-1.638551
C	-3.161195	1.960534	-1.519276
H	-2.300559	0.350688	-0.373187

C	-2.921716	3.157711	-2.194812
H	-1.443316	4.622681	-2.770834
H	-4.159708	1.535621	-1.481104
H	-3.737596	3.674101	-2.692598
C	1.044791	1.946888	1.374347
C	0.373763	3.129159	1.724069
C	2.107187	1.496643	2.180014
C	0.770303	3.853803	2.849676
H	-0.454572	3.485745	1.121621
C	2.505848	2.230905	3.295944
H	2.624715	0.574837	1.930118
C	1.836404	3.410524	3.633453
H	0.244518	4.767496	3.110753
H	3.334325	1.880401	3.904748
H	2.143399	3.978548	4.506680
C	0.794157	-2.540110	1.493361
C	1.712370	-3.290224	0.664033
C	1.388591	-4.425485	-0.253907
C	1.317977	-3.321054	-1.272718
C	-4.988558	-0.886532	0.651704
C	-5.924156	-0.738249	-0.100410
H	2.190388	-5.153370	-0.376675
H	0.440908	-4.923441	-0.048451
H	2.216680	-3.160765	-1.862332
H	0.376016	-3.233320	-1.822844
H	2.770969	-3.119327	0.846782
C	-0.542718	-2.411439	1.017179
H	-0.943753	-3.179389	0.355506
C	-1.636731	-1.736472	1.801212
H	-1.294128	-0.807056	2.280679
C	-3.903483	-1.076468	1.606162
H	-3.707868	-0.143567	2.160341
O	-2.715126	-1.490333	0.919589
H	-1.961724	-2.419021	2.609367
H	-4.180259	-1.841760	2.349599
C	-7.062184	-0.580936	-1.002805
H	-7.464214	0.438317	-0.966734
H	-6.773277	-0.792090	-2.039178
H	-7.872286	-1.270077	-0.737395
C	1.276138	-1.994027	2.814527
H	1.031711	-2.704821	3.615653
H	2.361794	-1.858283	2.816237
H	0.807951	-1.037905	3.060880

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-1649.52183423	Predicted Change= -6.233666D-10
Zero-point correction (ZPE)=	-1649.0024	0.51943
Internal Energy (U)=	-1648.9696	0.55215
Enthalpy (H)=	-1648.9687	0.55309
Gibbs Free Energy (G)=	-1649.0704	0.45140

Frequencies -- -214.8780 13.6117 24.5064
SCF Energy (M06) = -1648.557021
SCF Energy (M06/def2-tzvp) = -1650.121832

Alkyne Coord. Complex $RhPPh_3$ (Mono)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)]
#Atoms= 63

Charge = 1 Multiplicity = 1

SCF Energy= -1649.54758210 Predicted Change= -8.612871D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.01659 ll	0.00180	[NO]	0.01659 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.532579	2.039793	-0.231417
Rh	0.216199	-1.320426	-0.943594
C	4.470409	1.232055	0.669390
C	4.441108	0.282951	1.790294
C	2.382612	-0.855578	1.258363
C	2.151546	-0.978892	-0.237483
C	2.293137	-2.277184	-0.906664
C	1.953332	-2.317228	-2.247975
C	1.841071	-1.075371	-3.142672
C	0.661349	-0.255221	-2.631508
H	-0.237428	-0.333931	-3.254928
H	0.871172	0.792039	-2.405517
H	1.690836	-1.393787	-4.178664
H	2.780245	-0.508780	-3.109135
H	2.550503	-0.119917	-0.776916
H	3.983245	0.760706	2.670601
H	5.461723	-0.001811	2.065444
H	1.889761	-1.658375	1.815365
H	1.976982	0.095286	1.625268
H	1.878809	-3.292308	-2.725334
O	3.779543	-0.955737	1.520504
C	4.652795	3.017724	-1.311527

H	3.671781	3.320799	-1.697033
H	5.163446	3.921299	-0.958025
H	5.234906	2.616617	-2.149378
C	2.575529	-3.540424	-0.129524
H	2.496056	-4.425719	-0.765770
H	3.589157	-3.490983	0.284112
H	1.894617	-3.665806	0.720082
P	-1.272111	0.182136	0.073261
C	-1.264971	-0.207378	1.865352
C	-1.093695	0.771588	2.854171
C	-1.384604	-1.557803	2.244452
C	-1.044418	0.403451	4.201258
H	-1.001375	1.816969	2.577875
C	-1.337159	-1.919136	3.590137
H	-1.540991	-2.326507	1.488992
C	-1.163340	-0.937378	4.570377
H	-0.916502	1.168312	4.961660
H	-1.438804	-2.962586	3.873880
H	-1.124954	-1.218438	5.618640
C	-0.984464	1.982212	-0.094647
C	0.325289	2.483181	0.009082
C	-2.047260	2.875481	-0.303022
C	0.562515	3.854649	-0.079407
H	1.162544	1.809643	0.166230
C	-1.801596	4.246334	-0.401656
H	-3.063797	2.505609	-0.388248
C	-0.500024	4.737725	-0.288425
H	1.576846	4.231248	0.015629
H	-2.630231	4.929073	-0.564820
H	-0.313528	5.805047	-0.363053
C	-2.984765	-0.135624	-0.506032
C	-4.063678	-0.263881	0.383562
C	-3.216037	-0.256325	-1.888240
C	-5.348407	-0.508248	-0.104832
H	-3.904378	-0.173287	1.453146
C	-4.501841	-0.498568	-2.370601
H	-2.395577	-0.144863	-2.592167
C	-5.569053	-0.627865	-1.478534
H	-6.177048	-0.604545	0.590559
H	-4.669526	-0.587523	-3.439906
H	-6.569863	-0.820674	-1.853426

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```
=====================================================
 SCF Energy=     -1649.54758210  Predicted Change= -8.612871D-08
 Zero-point correction (ZPE)=            -1649.0264          0.52108
 Internal Energy (U)=                          -1648.9932          0.55432
 Enthalpy (H)=                                       -1648.9923          0.55526
 Gibbs Free Energy (G)=                        -1649.0967 0.45083
-----------------------------------------------------------------------------------------------------
 Frequencies --    10.9344               19.6510               25.7879
SCF Energy (M06) =  -1648.571688
SCF Energy (M06/def2-tzvp) = -1650.135281
```

2π-Insertion TS $RhPPh_3$ (Mono)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) freq
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)]
#Atoms= 63
Charge = 1 Multiplicity = 1

SCF Energy= -1649.54358952 Predicted Change= -1.344592D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.01233 II	0.00180	[NO]	0.01233 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.742227	-1.791741	-0.495476
Rh	-1.146339	0.134138	-0.282880
C	-2.933590	-1.297717	-0.335382
C	-4.332978	-1.809022	-0.088907
C	-4.820924	0.389357	0.204734
C	-3.462309	0.705147	-0.411464
C	-2.654469	1.786482	0.205602
C	-1.724026	2.489472	-0.540536
C	-1.501558	2.298908	-2.037156
C	-0.976766	0.873651	-2.218602
H	0.054328	0.825509	-2.564213
H	-1.604610	0.214797	-2.824867
H	-0.771792	3.034366	-2.387055
H	-2.427078	2.479820	-2.599910
H	-3.554084	0.783599	-1.493446
H	-4.402376	-2.153019	0.957131
H	-4.542732	-2.656020	-0.748870
H	-5.536480	1.170969	-0.070254
H	-4.766872	0.330524	1.301328
H	-1.178414	3.286713	-0.042511
O	-5.295678	-0.815780	-0.346305

C	-1.137002	-3.147084	-0.640574
H	-0.769047	-3.300964	-1.661101
H	-0.286581	-3.273342	0.036799
H	-1.871588	-3.933075	-0.428229
C	-2.866449	2.131866	1.665945
H	-2.087509	2.813485	2.017025
H	-3.835029	2.626360	1.812075
H	-2.856356	1.243379	2.307627
P	1.123807	-0.045535	0.062257
C	1.336216	-1.181676	1.489269
C	0.526658	-0.987911	2.624441
C	2.236104	-2.257948	1.467976
C	0.624863	-1.846817	3.718478
H	-0.171237	-0.153840	2.661109
C	2.326114	-3.119224	2.564426
H	2.868577	-2.425895	0.602607
C	1.524088	-2.916320	3.688431
H	0.001759	-1.681691	4.592688
H	3.027529	-3.948016	2.537881
H	1.599192	-3.587235	4.539068
C	1.897944	1.550166	0.555662
C	2.384973	1.785667	1.849242
C	1.986534	2.573829	-0.405405
C	2.940387	3.025897	2.177019
H	2.342318	1.006125	2.602073
C	2.545393	3.806529	-0.075494
H	1.636380	2.403227	-1.419996
C	3.019391	4.037069	1.219994
H	3.317117	3.194542	3.181680
H	2.617209	4.585438	-0.829265
H	3.454398	4.998443	1.476829
C	2.200418	-0.670754	-1.283745
C	1.653896	-1.418813	-2.337622
C	3.586171	-0.432154	-1.258038
C	2.476341	-1.927319	-3.344166
H	0.584088	-1.593798	-2.373096
C	4.404853	-0.945255	-2.263889
H	4.024885	0.154564	-0.456792
C	3.851898	-1.692410	-3.307270
H	2.042290	-2.500939	-4.157962
H	5.474019	-0.756860	-2.235049
H	4.491611	-2.085333	-4.092070

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1649.54358952 Predicted Change= -1.344592D-08

Zero-point correction (ZPE)= -1649.0212 0.52237

Internal Energy (U)= -1648.9902 0.55338

Enthalpy (H)= -1648.9892 0.55433

Gibbs Free Energy (G)= -1649.0855 0.45803

Frequencies -- -220.6489 12.1668 16.7544

SCF Energy (M06) = -1648.576519

SCF Energy (M06/def2-tzvp) = -1650.1385

Metallacycle $RhPPh_3$ (Mono)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)]
#Atoms= 63

Charge = 1 Multiplicity = 1

SCF Energy= -1649.58752318 Predicted Change= -4.112610D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00128 ll	0.00180	[YES]	0.00128 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.889462	-1.196564	0.219269
Rh	0.910546	0.533114	-0.125955
C	3.215608	-1.065578	0.350039
C	4.268773	-2.168660	0.469871
C	5.401019	-0.237042	-0.009512
C	3.980590	0.252322	0.360432
C	3.312393	1.291837	-0.512716
C	2.494011	2.253964	0.020275
C	2.129170	2.407587	1.498811
C	1.113764	1.295239	1.783930
H	0.141671	1.635168	2.143824
H	1.493253	0.492495	2.418147
H	1.688118	3.396620	1.651921
H	3.010060	2.340701	2.146985
H	4.028479	0.612854	1.395413
H	4.294494	-2.786868	-0.442808
H	4.115054	-2.830369	1.328747
H	6.199426	0.409030	0.362135
H	5.517310	-0.361131	-1.096737
H	2.093199	3.006066	-0.661334
O	5.502432	-1.486682	0.656899
C	1.181035	-2.525809	0.240619

H	0.451939	-2.595227	1.055011
H	0.641500	-2.722595	-0.690878
H	1.902246	-3.340586	0.381134
C	3.623795	1.290288	-1.991911
H	4.660566	1.606401	-2.164408
H	3.518833	0.289315	-2.425666
H	2.973275	1.977820	-2.540112
P	-1.309866	-0.126698	-0.010307
C	-1.800146	-1.442251	-1.186287
C	-1.125170	-1.525779	-2.418278
C	-2.808332	-2.372491	-0.893602
C	-1.468272	-2.507165	-3.347075
H	-0.329546	-0.822014	-2.656572
C	-3.143474	-3.358117	-1.824467
H	-3.330773	-2.334688	0.056296
C	-2.479228	-3.425559	-3.049920
H	-0.944237	-2.559036	-4.296873
H	-3.925103	-4.073971	-1.588073
H	-2.743170	-4.193901	-3.770480
C	-2.050309	1.441932	-0.630472
C	-2.099796	2.556680	0.230249
C	-2.490221	1.585485	-1.957661
C	-2.581210	3.782276	-0.228433
H	-1.793051	2.462067	1.267715
C	-2.970172	2.815310	-2.409909
H	-2.477572	0.737423	-2.633851
C	-3.013478	3.914949	-1.550383
H	-2.626240	4.630101	0.448916
H	-3.318193	2.910164	-3.434284
H	-3.390481	4.869281	-1.905978
C	-2.131659	-0.465385	1.587539
C	-1.404727	-1.013688	2.655835
C	-3.503288	-0.198951	1.751617
C	-2.040425	-1.302772	3.864353
H	-0.342863	-1.207413	2.548984
C	-4.132894	-0.490209	2.961392
H	-4.076610	0.239035	0.939987
C	-3.403415	-1.043311	4.017350
H	-1.469563	-1.725902	4.685558
H	-5.192063	-0.281815	3.080022
H	-3.896440	-1.266450	4.958904

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1649.58752318 Predicted Change= -4.112610D-09

Zero-point correction (ZPE)= -1649.0626 0.52489

Internal Energy (U)= -1649.0317 0.55580

Enthalpy (H)= -1649.0307 0.55675

Gibbs Free Energy (G)= -1649.1270 0.46052

Frequencies -- 14.7697 15.7728 22.9073

SCF Energy (M06) = -1648.615978

SCF Energy (M06/def2-tzvp) = -1650.172595

Reductive Elimination TS $RhPPh_3$ (Mono)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) freq
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)]
#Atoms= 63
Charge = 1 Multiplicity = 1

SCF Energy= -1649.55171239 Predicted Change= -7.244992D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00116 ll	0.00180	[YES]	0.00116 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.659265	0.779538	-1.494126
Rh	0.759819	-0.612932	-0.276454
C	2.936645	0.975058	-1.093621
C	3.713781	2.281515	-1.119378
C	4.665301	0.925728	0.479669
C	3.829241	-0.032918	-0.395371
C	3.051177	-1.167934	0.255593
C	2.441652	-2.114493	-0.544973
C	2.405154	-2.021788	-2.065308
C	1.324678	-0.999515	-2.418090
H	0.321774	-1.429226	-2.518303
H	1.525521	-0.421743	-3.318402
H	2.156492	-2.996772	-2.499065
H	3.378759	-1.726119	-2.471620
H	4.534036	-0.453944	-1.130962
H	3.137140	3.101287	-0.661090
H	3.993517	2.598368	-2.133059
H	5.633562	0.521770	0.783809
H	4.110553	1.244177	1.376356
H	2.078028	-3.028605	-0.078744
O	4.909052	2.027533	-0.386465

C	0.887428	1.858160	-2.221838
H	0.035420	1.451054	-2.772843
H	0.494033	2.603459	-1.520450
H	1.523473	2.384558	-2.945044
C	3.196700	-1.390735	1.741806
H	2.569759	-2.218088	2.085259
H	4.241129	-1.633074	1.983543
H	2.933095	-0.498308	2.318766
P	-1.385170	0.155539	0.036502
C	-1.779045	1.836229	0.625818
C	-0.732644	2.642954	1.109135
C	-3.088470	2.342752	0.601903
C	-0.998923	3.927114	1.582924
H	0.286218	2.263121	1.109879
C	-3.345929	3.631626	1.070291
H	-3.903363	1.737648	0.218229
C	-2.305595	4.422269	1.562839
H	-0.187465	4.543495	1.958663
H	-4.360709	4.017661	1.048860
H	-2.510974	5.425468	1.924564
C	-1.107946	-0.942675	1.478417
C	-0.867298	-0.460250	2.784659
C	-0.954222	-2.326891	1.216565
C	-0.504823	-1.339805	3.798228
H	-0.985790	0.597153	2.998778
C	-0.577792	-3.199679	2.246441
H	-1.203684	-2.727904	0.238455
C	-0.356217	-2.708944	3.531057
H	-0.344288	-0.963863	4.804418
H	-0.484883	-4.262294	2.041876
H	-0.080329	-3.388723	4.331920
C	-2.821460	-0.472795	-0.894461
C	-2.825893	-0.355461	-2.294291
C	-3.921026	-1.060987	-0.245676
C	-3.917255	-0.811884	-3.033451
H	-1.979165	0.092028	-2.807592
C	-5.007279	-1.520307	-0.991456
H	-3.929948	-1.162265	0.835712
C	-5.006899	-1.395278	-2.382904
H	-3.914963	-0.715690	-4.115128
H	-5.853268	-1.975467	-0.484955
H	-5.854214	-1.754209	-2.959591

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1649.55171239 Predicted Change= -7.244992D-09

Zero-point correction (ZPE)= -1649.0280 0.52362

Internal Energy (U)= -1648.9977 0.55398

Enthalpy (H)= -1648.9967 0.55493

Gibbs Free Energy (G)= -1649.0906 0.46105

Frequencies -- -402.2206 24.5631 29.2993

SCF Energy (M06) = -1648.595291

SCF Energy (M06/def2-tzvp) = -1650.152517

Product-Catalyst Complex $RhPPh_3$ (Mono)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=(gdiis,maxcycle=250) freq b3lyp geom=connectivity gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C29H31OPRh(1+) C1[X(C29H31OPRh)]
#Atoms= 63

Charge = 1 Multiplicity = 1

SCF Energy= -1649.62738467 Predicted Change= -1.754522D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00063 ll	0.00180	[YES]	0.00063 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.028510	-1.152285	0.207174
Rh	-0.951667	-0.061549	-0.094766
C	-3.249487	0.177432	-0.093942
C	-3.851770	1.211949	0.860653
C	-3.613359	2.300100	-1.120362
C	-3.189795	0.854416	-1.475117
C	-1.755709	0.661577	-1.962285
C	-1.319797	-0.678122	-2.130454
C	-2.293626	-1.846439	-2.186760
C	-2.854322	-2.264057	-0.815699
H	-2.187823	-3.013603	-0.372793
H	-3.824637	-2.769156	-0.940711
H	-1.798260	-2.709792	-2.640765
H	-3.114971	-1.578788	-2.866105
H	-3.919929	0.426523	-2.178735
H	-3.086292	1.685324	1.500243
H	-4.630098	0.796125	1.506032
H	-4.180751	2.797225	-1.909357
H	-2.738976	2.918900	-0.866899
H	-0.387622	-0.817137	-2.675244
O	-4.460070	2.167681	0.010722
C	-1.034260	1.793228	-2.654784

H	-1.601238	2.095995	-3.547562
H	-0.919999	2.681342	-2.027207
H	-0.042958	1.472907	-2.989419
C	-3.279688	-1.666020	1.609620
H	-3.285398	-0.875808	2.362773
H	-4.252347	-2.177344	1.646659
H	-2.521633	-2.401827	1.899256
P	1.364948	0.063529	0.020108
C	0.952644	-0.524445	1.705368
C	0.050378	0.293882	2.429807
C	1.294624	-1.790757	2.216647
C	-0.473494	-0.146515	3.653674
H	-0.159714	1.308907	2.091827
C	0.773209	-2.211513	3.436843
H	1.976252	-2.430682	1.665181
C	-0.112390	-1.394637	4.154727
H	-1.142701	0.498271	4.215909
H	1.061394	-3.178670	3.838591
H	-0.508176	-1.733015	5.107673
C	2.295288	1.624905	0.202348
C	2.252453	2.574476	-0.831765
C	3.070740	1.881900	1.345923
C	2.978570	3.760533	-0.725061
H	1.654367	2.390161	-1.718651
C	3.789584	3.073427	1.448916
H	3.114801	1.156446	2.152638
C	3.744696	4.012035	0.415521
H	2.942258	4.489184	-1.529485
H	4.385815	3.266315	2.335893
H	4.305307	4.938350	0.499296
C	2.465457	-1.147863	-0.785601
C	1.922156	-2.369616	-1.222280
C	3.831151	-0.889016	-0.984245
C	2.737525	-3.323227	-1.829798
H	0.863572	-2.571484	-1.080931
C	4.639628	-1.844637	-1.601382
H	4.263048	0.052238	-0.660413
C	4.096621	-3.060185	-2.022024
H	2.312410	-4.266682	-2.159688
H	5.694941	-1.637786	-1.752295
H	4.729637	-3.800278	-2.502640

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```
=====================================================
 SCF Energy=     -1649.62738467  Predicted Change= -1.754522D-09
 Zero-point correction (ZPE)=            -1649.1003          0.52700
 Internal Energy (U)=                          -1649.0700          0.55733
 Enthalpy (H)=                                       -1649.0691          0.55827
 Gibbs Free Energy (G)=                        -1649.1630 0.46429
-----------------------------------------------------------------------------------------------------
 Frequencies --    19.7262               26.4524               32.4598
SCF Energy (M06) =  -1648.672528
SCF Energy (M06/def2-tzvp) = -1650.227608
```

Substrate-Catalyst Complex $RhPPh_3$ (Bis)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=maxcycle=250 freq=noraman b3lyp gen pseudo=read geom=connectivity gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)]
#Atoms= 97

Charge = 1 Multiplicity = 1

SCF Energy= -2685.86570695 Predicted Change= -3.316737D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.05085 ll	0.00180	[NO]	0.05085 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.246541	0.533959	-0.919595
Rh	0.384846	0.130371	-1.167587
C	-5.228361	0.768580	-0.028570
C	-6.335280	-0.226712	0.091511
C	-0.346752	1.334894	-2.748582
C	0.861305	1.071467	-3.000988
H	-4.299888	-0.369267	-1.527263
C	-3.033647	1.366777	-1.202117
H	-3.141658	2.409195	-0.867461
H	-2.140747	0.957321	-0.684995
C	-1.640762	2.034123	-3.005563
H	-1.594772	3.027923	-2.530190
H	-1.732569	2.181940	-4.087649
H	-6.202742	-1.089569	-0.557773
C	-7.042923	-0.524092	1.408032
C	-7.785997	0.172878	0.306069
H	-8.022026	1.224888	0.434898
H	-7.285463	-1.560733	1.625957
H	-6.771835	0.060140	2.282895
H	-8.537113	-0.381214	-0.249248
O	-2.794473	1.334420	-2.608231
C	2.144273	1.070906	-3.731664

H	2.093062	1.753029	-4.589314
H	2.969752	1.383000	-3.083400
H	2.380007	0.069905	-4.109698
C	-5.267484	1.978457	0.875156
H	-4.515540	2.724275	0.608185
H	-6.245935	2.471264	0.840095
H	-5.092882	1.696526	1.921793
P	1.197225	1.607332	0.335857
P	0.553243	-1.991247	-0.070239
C	0.253547	-2.975715	-1.598055
C	-0.815019	-3.877209	-1.728767
C	1.107909	-2.765059	-2.698766
C	-1.022978	-4.549954	-2.933914
H	-1.481608	-4.058638	-0.892576
C	0.898379	-3.444121	-3.898813
H	1.948519	-2.081899	-2.606792
C	-0.171332	-4.334184	-4.019508
H	-1.850780	-5.247593	-3.022107
H	1.569190	-3.280028	-4.737326
H	-0.338020	-4.860587	-4.954750
C	-0.773899	-2.489816	1.099544
C	-2.067823	-1.975280	0.905921
C	-0.539681	-3.366983	2.168495
C	-3.107680	-2.331064	1.764203
H	-2.269925	-1.296899	0.081534
C	-1.582391	-3.717891	3.029166
H	0.451553	-3.775628	2.333419
C	-2.864055	-3.201620	2.830825
H	-4.101022	-1.923574	1.598963
H	-1.389953	-4.397779	3.854224
H	-3.671409	-3.478136	3.503063
C	2.110322	-2.658856	0.647833
C	2.707937	-3.829629	0.154101
C	2.706023	-1.992245	1.732999
C	3.882232	-4.318036	0.730902
H	2.258722	-4.365142	-0.675132
C	3.874339	-2.489571	2.309824
H	2.255365	-1.091815	2.137841
C	4.467562	-3.650555	1.807609
H	4.334186	-5.224943	0.339541
H	4.321678	-1.967278	3.150682
H	5.379658	-4.034063	2.255783
C	3.006683	1.877965	0.148672
C	3.821784	0.824872	-0.297411

C	3.599699	3.110549	0.475748
C	5.202220	0.998788	-0.410360
H	3.373394	-0.129131	-0.554807
C	4.980258	3.279230	0.360028
H	2.987629	3.940438	0.814439
C	5.782975	2.225545	-0.083047
H	5.821635	0.175732	-0.755008
H	5.426992	4.236210	0.613818
H	6.856624	2.361845	-0.175168
C	0.445464	3.273584	0.077777
C	0.812095	4.035444	-1.046095
C	-0.515962	3.787312	0.961050
C	0.234963	5.283764	-1.273781
H	1.556849	3.659361	-1.740265
C	-1.098541	5.035301	0.724415
H	-0.806156	3.225548	1.842193
C	-0.725701	5.785840	-0.390441
H	0.537516	5.866265	-2.139408
H	-1.836985	5.421826	1.420997
H	-1.175099	6.758195	-0.569752
C	0.921153	1.265374	2.123644
C	-0.300604	0.702270	2.526367
C	1.882593	1.581243	3.097747
C	-0.560317	0.465022	3.876549
H	-1.047724	0.438208	1.785169
C	1.620417	1.337020	4.447145
H	2.835443	2.011554	2.808831
C	0.400902	0.780676	4.839121
H	-1.507424	0.022424	4.170422
H	2.371960	1.583194	5.191832
H	0.202422	0.590898	5.889997

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.86570695 Predicted Change= -3.316737D-07
Zero-point correction (ZPE)= -2685.0681 0.79752
Internal Energy (U)= -2685.0172 0.84846
Enthalpy (H)= -2685.0162 0.84940
Gibbs Free Energy (G)= -2685.1626 0.70309

Frequencies -- 7.0325 14.3236 15.7476
SCF Energy (M06) = -2684.330841
SCF Energy (M06/def2-tzvp) = -2686.18237

Ox.-Add. TS $RhPPh_3$ (Bis)

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)] #Atoms= 97
Charge = 1 Multiplicity = 1

SCF Energy= -2685.84024310 Predicted Change= -4.611699D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00023 II	0.00180	[YES]	0.00023 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.270682	-1.232355	0.032277
P	2.379469	-0.130638	-0.215704
P	-1.141245	0.755129	0.322435
C	3.773214	-1.316362	-0.542917
C	4.247652	-2.114357	0.514612
C	4.342840	-1.477093	-1.814755
C	5.259373	-3.050072	0.302445
H	3.846418	-1.983814	1.516452
C	5.356571	-2.417714	-2.024927
H	4.009157	-0.862676	-2.644550
C	5.814893	-3.207302	-0.970942
H	5.621527	-3.649194	1.133331
H	5.790902	-2.523305	-3.015054
H	6.605432	-3.933629	-1.135482
C	3.036438	0.741842	1.268995
C	2.206647	0.978067	2.372194
C	4.389394	1.123892	1.345692
C	2.703181	1.604253	3.517443
H	1.171004	0.662186	2.332916
C	4.882333	1.755284	2.486490

H	5.065825	0.907765	0.524659
C	4.039379	1.999040	3.574352
H	2.045404	1.780860	4.363674
H	5.927958	2.046209	2.530373
H	4.427450	2.485273	4.464777
C	2.495910	1.023892	-1.652168
C	3.317088	2.160847	-1.673766
C	1.739516	0.711811	-2.794718
C	3.383047	2.961632	-2.815551
H	3.892906	2.438574	-0.798271
C	1.811247	1.510276	-3.937447
H	1.081089	-0.152470	-2.787153
C	2.634175	2.638574	-3.949283
H	4.020829	3.841168	-2.816686
H	1.219419	1.255260	-4.811849
H	2.688620	3.264464	-4.835348
C	-0.461577	2.459861	0.625448
C	-0.584980	3.110349	1.863137
C	0.191653	3.131471	-0.422265
C	-0.059512	4.390553	2.050701
H	-1.106532	2.634244	2.685137
C	0.711673	4.411860	-0.232739
H	0.277859	2.668278	-1.398520
C	0.591760	5.045096	1.005612
H	-0.172400	4.878169	3.015000
H	1.207018	4.913286	-1.059048
H	0.993967	6.043622	1.151219
C	-2.124266	1.016092	-1.220215
C	-2.729810	2.254805	-1.497673
C	-2.287710	-0.034578	-2.134500
C	-3.468012	2.434983	-2.667358
H	-2.619365	3.083632	-0.806389
C	-3.022425	0.148725	-3.306870
H	-1.854885	-1.004916	-1.919553
C	-3.609960	1.385024	-3.578103
H	-3.926463	3.399085	-2.868796
H	-3.139391	-0.676655	-4.003303
H	-4.174703	1.531646	-4.494777
C	-2.387473	0.596580	1.680227
C	-3.756765	0.808931	1.470055
C	-1.944276	0.280001	2.976567
C	-4.656821	0.723516	2.536359
H	-4.130850	1.025782	0.476150
C	-2.843001	0.203929	4.042108

H	-0.888810	0.096310	3.159626
C	-4.204661	0.427006	3.823242
H	-5.714634	0.892410	2.355123
H	-2.480408	-0.030068	5.039310
H	-4.906929	0.367270	4.649703
C	-0.335139	-3.033735	1.162686
C	0.899039	-3.377253	0.464628
C	0.958039	-4.264295	-0.745979
C	0.998799	-2.907708	-1.368598
C	-5.883615	-1.504160	-0.694800
C	-6.576852	-0.896337	-1.477069
H	1.867459	-4.856504	-0.829313
H	0.064703	-4.859212	-0.929755
H	1.975997	-2.585366	-1.700216
H	0.163431	-2.634201	-2.011571
H	1.828271	-3.281961	1.016673
C	-1.485310	-2.845143	0.397345
H	-1.502703	-3.205507	-0.628523
C	-2.870453	-2.692229	0.957737
H	-2.894665	-2.082493	1.870159
C	-5.084067	-2.242357	0.275777
H	-5.262822	-1.846414	1.288096
O	-3.695157	-2.131702	-0.045972
H	-3.242919	-3.699192	1.228599
H	-5.375061	-3.306161	0.287667
C	-7.405752	-0.163052	-2.429796
H	-6.807727	0.577009	-2.974844
H	-7.860341	-0.836320	-3.166023
H	-8.216314	0.372509	-1.921455
C	-0.304931	-2.995563	2.671054
H	-0.488211	-4.003631	3.068450
H	0.672467	-2.668907	3.039062
H	-1.070732	-2.333486	3.079850

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.84024310 Predicted Change= -4.611699D-10
Zero-point correction (ZPE)= -2685.0426 0.79761
Internal Energy (U)= -2684.9929 0.84734
Enthalpy (H)= -2684.9919 0.84828
Gibbs Free Energy (G)= -2685.1302 0.70995

Frequencies -- -262.2775 15.2013 19.1212

SCF Energy (M06) = -2684.321356
SCF Energy (M06/def2-tzvp) = -2686.172375

Alkyne Coord. Complex $RhPPh_3$ (Bis)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

#b3lyp gen pseudo=read geom=check guess=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(nofreeze,maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)]
#Atoms= 97
Charge = 1 Multiplicity = 1

SCF Energy= -2685.86472214 Predicted Change= -7.010565D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.07604 ll	0.00180	[NO]	0.07604 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.098381	-3.220798	-1.611925
Rh	0.181756	-0.841132	0.046100
C	5.185627	-2.872161	-0.454992
C	5.369516	-2.459885	0.945474
C	3.272263	-1.349918	1.384102
C	2.172372	-1.868755	0.484231
C	1.119142	-2.686903	0.988032
C	0.112190	-3.081334	0.083626
C	0.333123	-3.115705	-1.433982
C	0.362824	-1.651517	-1.855263
H	-0.485533	-1.335602	-2.461331
H	1.294760	-1.295153	-2.296232
H	-0.492512	-3.655630	-1.904003
H	1.262350	-3.644972	-1.680862
H	2.518654	-2.099291	-0.519664
H	5.887308	-1.487535	0.976459
H	6.009686	-3.185639	1.458517
H	2.872573	-0.965405	2.325955
H	3.808902	-0.527234	0.895888
H	-0.750757	-3.611683	0.475843
O	4.182626	-2.398450	1.731059

C	5.014312	-3.681338	-2.997267
H	4.292546	-3.095397	-3.579432
H	5.987113	-3.593976	-3.495759
H	4.710844	-4.733620	-3.048774
C	0.945077	-2.933003	2.469711
H	-0.010718	-3.419307	2.684335
H	1.753640	-3.583652	2.822404
H	1.006331	-2.007756	3.053177
P	-2.247668	-0.590477	-0.105159
P	1.071895	1.449825	-0.123384
C	1.656615	1.756943	1.604505
C	2.898229	2.336845	1.903542
C	0.830088	1.343089	2.664198
C	3.300440	2.497987	3.231433
H	3.557444	2.660709	1.105562
C	1.232002	1.511494	3.990363
H	-0.142671	0.902809	2.460726
C	2.471906	2.086425	4.276979
H	4.265661	2.947354	3.447035
H	0.574425	1.195495	4.795365
H	2.789906	2.213696	5.307637
C	2.550182	1.777814	-1.180713
C	3.309341	0.711206	-1.684020
C	2.979359	3.092351	-1.445100
C	4.467141	0.944626	-2.429365
H	3.005794	-0.307731	-1.484386
C	4.133720	3.324011	-2.193002
H	2.412801	3.937301	-1.068179
C	4.880019	2.251414	-2.688035
H	5.043564	0.101797	-2.799471
H	4.450690	4.344785	-2.386720
H	5.778488	2.435669	-3.269943
C	-0.009289	2.908910	-0.488512
C	-0.682439	3.596289	0.532785
C	-0.191587	3.328369	-1.817659
C	-1.512825	4.678222	0.231098
H	-0.549185	3.307273	1.569364
C	-1.015755	4.413383	-2.114570
H	0.331914	2.825224	-2.625707
C	-1.681413	5.090875	-1.090746
H	-2.015561	5.206627	1.036326
H	-1.133012	4.732505	-3.146302
H	-2.319710	5.938705	-1.322054
C	-3.085112	0.334908	-1.457632

C	-2.342111	0.873498	-2.514536
C	-4.489757	0.424107	-1.495114
C	-2.984284	1.496271	-3.588511
H	-1.260423	0.805960	-2.499361
C	-5.126849	1.059637	-2.558137
H	-5.084877	-0.012118	-0.698026
C	-4.374439	1.593597	-3.609624
H	-2.395951	1.903523	-4.405791
H	-6.210807	1.127576	-2.573692
H	-4.874439	2.077355	-4.443828
C	-2.761951	0.195570	1.479483
C	-3.448539	1.418234	1.531098
C	-2.383729	-0.419981	2.688993
C	-3.770166	1.995855	2.761874
H	-3.734001	1.922378	0.614656
C	-2.716294	0.155197	3.916183
H	-1.834106	-1.357924	2.674173
C	-3.412400	1.366134	3.954745
H	-4.307764	2.939526	2.784947
H	-2.434423	-0.343462	4.839427
H	-3.672809	1.815063	4.908799
C	-3.192909	-2.187217	-0.185223
C	-3.218931	-2.863734	-1.418935
C	-3.867599	-2.754141	0.904958
C	-3.886615	-4.080027	-1.551887
H	-2.738761	-2.428139	-2.291054
C	-4.535957	-3.974957	0.768487
H	-3.896921	-2.244882	1.861422
C	-4.543851	-4.643574	-0.454834
H	-3.902032	-4.582386	-2.515050
H	-5.059521	-4.394598	1.622922
H	-5.066761	-5.589803	-0.558065

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.86472214 Predicted Change= -7.010565D-06
Zero-point correction (ZPE)= -2685.0658 0.79888
Internal Energy (U)= -2685.0156 0.84904
Enthalpy (H)= -2685.0147 0.84998
Gibbs Free Energy (G)= -2685.1562 0.70843

Frequencies -- 10.5158 14.6076 17.7091
SCF Energy (M06) = -2684.33231

SCF Energy (M06/def2-tzvp) = -2686.182407

2π-Insertion TS $RhPPh_3$ (Bis)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=(gdiis,modredundant,maxcycle=250) freq b3lyp geom=check guess=read gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

Modredundant Input: B 3 6 F

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)]
#Atoms= 97

Charge = 1 Multiplicity = 1

SCF Energy= -2685.82853253 Predicted Change= -1.834560D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00137 II	0.00180	[YES]	0.00137 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.038256	-2.057225	-1.343349
Rh	-0.143954	-0.981227	0.368704
C	0.673070	-3.207984	-1.262152
C	1.241262	-4.242212	-2.191117
C	2.330863	-4.970125	-0.262246
C	1.425580	-4.038174	0.513942
C	1.917932	-2.929934	1.358807
C	1.100998	-2.321251	2.268112
C	-0.336827	-2.726628	2.574371
C	-1.214535	-2.503318	1.341134
H	-2.236094	-2.233970	1.608688
H	-1.236439	-3.363235	0.672083
H	-0.696873	-2.112596	3.406331
H	-0.387137	-3.772992	2.916191
H	0.539563	-4.543583	0.891143
H	2.100496	-3.822799	-2.746798
H	0.508093	-4.600821	-2.921758
H	2.541432	-5.894119	0.287238
H	3.289164	-4.490959	-0.511349
H	1.542820	-1.550100	2.894002
O	1.654299	-5.380496	-1.446957

C	-0.411764	-1.475005	-2.665297
H	-1.502669	-1.487036	-2.759527
H	-0.067051	-0.443309	-2.786953
H	-0.006251	-2.059019	-3.500767
C	3.371676	-2.535224	1.248769
H	4.015843	-3.376486	1.535830
H	3.649849	-2.258524	0.225372
H	3.605849	-1.695001	1.904100
P	-2.174700	0.053646	0.016412
P	1.732936	0.962177	-0.150575
C	2.913042	0.755025	-1.558987
C	3.086329	-0.512707	-2.135339
C	3.678257	1.830126	-2.047271
C	4.003089	-0.703482	-3.172446
H	2.495058	-1.349891	-1.781484
C	4.591685	1.636400	-3.083435
H	3.560500	2.821116	-1.621195
C	4.756328	0.369423	-3.649105
H	4.123880	-1.690664	-3.610200
H	5.174844	2.476931	-3.448950
H	5.466197	0.221864	-4.457931
C	2.830422	1.041288	1.341407
C	2.235737	1.034167	2.615869
C	4.229243	1.106155	1.256725
C	3.015270	1.105235	3.771743
H	1.154500	0.979320	2.713054
C	5.009559	1.163836	2.414319
H	4.717265	1.108063	0.288470
C	4.407334	1.165789	3.673297
H	2.536094	1.106964	4.746968
H	6.091493	1.209992	2.328100
H	5.016698	1.213077	4.571104
C	1.214748	2.732492	-0.355658
C	0.705224	3.146284	-1.598831
C	1.327963	3.679403	0.673801
C	0.342733	4.475080	-1.811096
H	0.614977	2.436345	-2.415588
C	0.946456	5.007738	0.462821
H	1.741929	3.395695	1.635332
C	0.460387	5.410960	-0.780031
H	-0.032017	4.778977	-2.783757
H	1.051822	5.728843	1.268724
H	0.181067	6.447186	-0.948023
C	-2.430173	1.578022	-1.000874

C	-2.415293	1.470070	-2.403259
C	-2.798557	2.803746	-0.423711
C	-2.755533	2.558631	-3.203877
H	-2.170930	0.528418	-2.878373
C	-3.141307	3.891006	-1.230314
H	-2.843327	2.916608	0.652379
C	-3.122703	3.773189	-2.619429
H	-2.749490	2.451322	-4.284843
H	-3.432287	4.828027	-0.764597
H	-3.401762	4.617248	-3.243643
C	-3.616027	-0.956967	-0.525344
C	-4.891333	-0.360631	-0.541681
C	-3.477337	-2.281217	-0.963554
C	-6.002892	-1.087112	-0.963884
H	-5.017810	0.671941	-0.230006
C	-4.592989	-3.000537	-1.399023
H	-2.501872	-2.751638	-0.968644
C	-5.855751	-2.408731	-1.394634
H	-6.982429	-0.617975	-0.964466
H	-4.470508	-4.024520	-1.739853
H	-6.722457	-2.970674	-1.730303
C	-2.489914	0.572706	1.753897
C	-1.612299	1.500941	2.348090
C	-3.506624	0.000920	2.535528
C	-1.758095	1.852103	3.691518
H	-0.837232	1.978305	1.754743
C	-3.644042	0.353539	3.879197
H	-4.196180	-0.713356	2.098517
C	-2.771211	1.275884	4.460667
H	-1.084707	2.581669	4.132480
H	-4.438629	-0.092085	4.470538
H	-2.884710	1.549125	5.505611

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.82853253 Predicted Change= -1.834560D-08
Zero-point correction (ZPE)= -2685.0286 0.79990
Internal Energy (U)= -2684.9807 0.84778
Enthalpy (H)= -2684.9798 0.84873
Gibbs Free Energy (G)= -2685.1109 0.71755

Frequencies -- -231.7512 19.6821 25.1923
SCF Energy (M06) = -2684.296381

SCF Energy (M06/def2-tzvp) = -2686.137843

Metallacycle $RhPPh_3$ (Bis)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=maxcycle=250 freq=noraman b3lyp gen pseudo=read geom=connectivity gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)]
#Atoms= 97

Charge = 1 Multiplicity = 1

SCF Energy= -2685.88261381 Predicted Change= -2.166814D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.08690 ll	0.00180	[NO]	0.08690 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.483066	2.272581	0.922497
Rh	-0.319126	0.917659	-0.579723
C	-0.099217	3.534831	0.697879
C	-0.060556	4.671702	1.726072
C	1.062581	5.442778	-0.100994
C	0.419299	4.129095	-0.608062
C	1.298919	3.157990	-1.368189
C	0.794400	2.382367	-2.366058
C	-0.630335	2.459800	-2.904730
C	-1.598910	2.009788	-1.808481
H	-2.406997	1.382526	-2.187713
H	-2.037940	2.832545	-1.243018
H	-0.704135	1.799558	-3.775695
H	-0.860491	3.472557	-3.267152
H	-0.435420	4.412456	-1.234414
H	0.720676	4.493749	2.486106
H	-1.011688	4.831351	2.243308
H	1.063195	6.244576	-0.843084
H	2.092499	5.281707	0.249779
H	1.498298	1.751908	-2.904585
O	0.226161	5.841763	0.974595
C	-0.926518	1.809571	2.286596

H	-2.005483	1.627718	2.346679
H	-0.441874	0.876229	2.587930
H	-0.680267	2.563599	3.044625
C	2.772960	3.142558	-1.060527
H	3.272654	2.296948	-1.538107
H	3.237771	4.062747	-1.440360
H	2.973326	3.100714	0.013792
P	-2.140724	-0.435652	0.022808
P	1.945939	-0.696329	0.073011
C	3.249768	0.337003	0.880301
C	2.866995	1.087991	2.005806
C	4.578786	0.418992	0.438131
C	3.794070	1.878205	2.687543
H	1.837941	1.058841	2.350690
C	5.501227	1.223159	1.111514
H	4.900865	-0.134227	-0.437014
C	5.115044	1.949551	2.239202
H	3.482775	2.441988	3.562622
H	6.525358	1.277693	0.753200
H	5.836688	2.569488	2.763241
C	1.956015	-2.243381	1.104326
C	2.469587	-2.284517	2.409171
C	1.386115	-3.411145	0.564721
C	2.417578	-3.466376	3.154794
H	2.927608	-1.403477	2.845975
C	1.338235	-4.587725	1.310855
H	0.990475	-3.409529	-0.446685
C	1.853006	-4.619946	2.609707
H	2.834041	-3.483782	4.158264
H	0.903661	-5.482674	0.874203
H	1.820110	-5.538823	3.188012
C	2.708427	-1.348491	-1.480941
C	3.822469	-2.208116	-1.449051
C	2.150491	-1.026056	-2.726185
C	4.377581	-2.696939	-2.630856
H	4.249309	-2.506880	-0.496562
C	2.702649	-1.519246	-3.911388
H	1.266926	-0.397925	-2.775351
C	3.822118	-2.349446	-3.865563
H	5.240377	-3.355498	-2.587570
H	2.255192	-1.258415	-4.866500
H	4.254545	-2.733707	-4.784868
C	-2.363025	-1.117879	1.718451
C	-1.263164	-1.660072	2.401514

C	-3.624191	-1.132278	2.338248
C	-1.419133	-2.210837	3.673072
H	-0.283910	-1.661986	1.940844
C	-3.773871	-1.678579	3.614485
H	-4.491380	-0.724194	1.832905
C	-2.675006	-2.218180	4.284311
H	-0.556071	-2.631267	4.180221
H	-4.754395	-1.682255	4.081660
H	-2.796526	-2.642388	5.276850
C	-1.979302	-1.901849	-1.079385
C	-2.143384	-3.213743	-0.608215
C	-1.687673	-1.697740	-2.441064
C	-2.018353	-4.295801	-1.482520
H	-2.373210	-3.393340	0.436207
C	-1.560774	-2.781733	-3.309445
H	-1.582232	-0.689762	-2.833201
C	-1.723867	-4.083950	-2.830590
H	-2.157107	-5.305742	-1.107325
H	-1.341095	-2.609561	-4.359092
H	-1.628277	-4.928258	-3.506985
C	-3.799859	0.266746	-0.361726
C	-4.146060	1.537234	0.130676
C	-4.751790	-0.466152	-1.086971
C	-5.419783	2.058013	-0.092270
H	-3.418216	2.128045	0.677388
C	-6.024927	0.062981	-1.313197
H	-4.508494	-1.450537	-1.472240
C	-6.361765	1.322345	-0.816348
H	-5.674219	3.040688	0.294236
H	-6.752125	-0.514140	-1.876937
H	-7.352297	1.731045	-0.993459

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.88261381 Predicted Change= -2.166814D-06
Zero-point correction (ZPE)= -2685.0806 0.80193
Internal Energy (U)= -2685.0323 0.85026
Enthalpy (H)= -2685.0314 0.85120
Gibbs Free Energy (G)= -2685.1667 0.71583

Frequencies -- 9.3911 17.5414 19.5034
SCF Energy (M06) = -2684.352451
SCF Energy (M06/def2-tzvp) = -2686.193405

Reductive Elimination TS $RhPPh_3$ (Bis)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=(gdiis,modredundant,maxcycle=250) freq b3lyp geom=check guess=read gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

Modredundant Input: B 1 10 F

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)]
#Atoms= 97

Charge = 1 Multiplicity = 1

SCF Energy= -2685.86019668 Predicted Change= -5.232804D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00240 II	0.00180	[NO]	0.00240 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.102889	-2.941977	0.125242
Rh	-0.117271	-1.018814	-0.590821
C	-1.003799	-3.712142	0.149241
C	-1.280246	-4.837673	1.148719
C	-3.310334	-4.096527	0.338945
C	-2.266039	-3.603168	-0.681587
C	-2.469588	-2.275588	-1.377926
C	-1.576976	-1.881141	-2.337282
C	-0.419729	-2.754194	-2.801651
C	0.748884	-2.561208	-1.836316
H	1.509431	-1.884498	-2.237243
H	1.267983	-3.484675	-1.589437
H	-0.126806	-2.459649	-3.815622
H	-0.727468	-3.804782	-2.851411
H	-2.232831	-4.386163	-1.459837
H	-1.091318	-4.516788	2.184488
H	-0.684505	-5.741495	0.963524
H	-4.228544	-4.483194	-0.110580
H	-3.573593	-3.308436	1.062390
H	-1.821672	-1.000834	-2.926932
O	-2.653753	-5.182403	0.977652

C	1.280307	-3.308484	0.997114
H	1.436059	-2.585098	1.803225
H	1.146801	-4.293403	1.457465
H	2.205832	-3.354036	0.417781
C	-3.796484	-1.586526	-1.197238
H	-4.594220	-2.287216	-1.480733
H	-3.987018	-1.298532	-0.158660
H	-3.887923	-0.702729	-1.828154
P	1.999590	-0.091824	-0.015952
P	-1.393297	1.115075	0.087673
C	-2.412371	0.753707	1.587002
C	-2.476192	-0.556102	2.086903
C	-3.117791	1.768959	2.259112
C	-3.240832	-0.850668	3.219234
H	-1.916119	-1.346062	1.594012
C	-3.884988	1.471465	3.385553
H	-3.057812	2.795866	1.912716
C	-3.950251	0.161266	3.867033
H	-3.276585	-1.869429	3.595187
H	-4.426254	2.265914	3.891358
H	-4.544884	-0.066323	4.747052
C	-2.587114	1.597663	-1.242885
C	-2.114396	1.658650	-2.565368
C	-3.926426	1.929875	-0.991324
C	-2.957523	2.046277	-3.608476
H	-1.078114	1.414379	-2.780464
C	-4.771123	2.308834	-2.037162
H	-4.322847	1.879813	0.016392
C	-4.291083	2.368019	-3.346590
H	-2.573766	2.094009	-4.623808
H	-5.807270	2.556698	-1.825081
H	-4.950686	2.662883	-4.157470
C	-0.653632	2.760735	0.534139
C	-0.098549	2.951558	1.811226
C	-0.654342	3.837330	-0.365565
C	0.438522	4.185577	2.177228
H	-0.100644	2.145881	2.535892
C	-0.117236	5.071933	0.004900
H	-1.086254	3.728225	-1.353412
C	0.429940	5.251509	1.275257
H	0.853005	4.314132	3.173248
H	-0.138227	5.896123	-0.702485
H	0.838115	6.215920	1.564174
C	2.340323	0.236909	1.763435

C	1.351994	-0.044140	2.718749
C	3.589559	0.713930	2.203272
C	1.593803	0.165284	4.078756
H	0.389297	-0.430023	2.398326
C	3.825413	0.932442	3.560495
H	4.387868	0.896618	1.490944
C	2.828048	0.660411	4.500837
H	0.817752	-0.062102	4.804011
H	4.793233	1.304589	3.883904
H	3.018393	0.822756	5.557813
C	3.518529	-1.021927	-0.554672
C	4.233189	-1.830457	0.346830
C	3.969129	-0.947086	-1.884026
C	5.359170	-2.542207	-0.070203
H	3.926309	-1.897170	1.384343
C	5.092402	-1.663581	-2.299315
H	3.465506	-0.307724	-2.600565
C	5.790543	-2.465001	-1.395025
H	5.900382	-3.153399	0.646389
H	5.426327	-1.583570	-3.329829
H	6.668189	-3.017402	-1.717667
C	2.198814	1.494509	-0.946638
C	2.846497	2.622474	-0.424788
C	1.742595	1.532639	-2.276444
C	3.054447	3.749236	-1.222800
H	3.176273	2.639766	0.606819
C	1.959632	2.656546	-3.074583
H	1.217663	0.675034	-2.690572
C	2.622706	3.767222	-2.549403
H	3.555252	4.615796	-0.801125
H	1.611870	2.663339	-4.103966
H	2.794882	4.643086	-3.168221

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.86019668 Predicted Change= -5.232804D-08
Zero-point correction (ZPE)= -2685.0575 0.80267
Internal Energy (U)= -2685.0104 0.84973
Enthalpy (H)= -2685.0095 0.85068
Gibbs Free Energy (G)= -2685.1380 0.72216

Frequencies -- -288.1092 21.3697 27.1699
SCF Energy (M06) = -2684.346903

SCF Energy (M06/def2-tzvp) = -2686.187807

Product-Catalyst Complex $RhPPh_3$ (Bis)

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

opt=maxcycle=250 freq=noraman b3lyp gen pseudo=read geom=connectivity gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C47H46OP2Rh(1+) C1[X(C47H46OP2Rh)]
#Atoms= 97

Charge = 1 Multiplicity = 1

SCF Energy= -2685.93408968 Predicted Change= -1.738538D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.03032 II	0.00180	[NO]	0.03032 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.966202	-2.597454	-1.705566
Rh	0.053839	-1.068167	-0.269949
C	1.999556	-3.049870	-0.422775
C	3.289931	-3.112512	0.388366
C	1.611144	-3.798394	1.793417
C	0.946703	-3.794674	0.399949
C	-0.437807	-3.177291	0.328581
C	-0.994930	-2.961618	-0.933618
C	-0.404244	-3.527020	-2.213247
C	0.868963	-2.843473	-2.720741
H	0.604048	-1.891794	-3.199658
H	1.308233	-3.453135	-3.526623
H	-1.158968	-3.474202	-3.004587
H	-0.202871	-4.597744	-2.059204
H	0.889602	-4.843074	0.057836
H	3.658988	-2.120424	0.668442
H	4.086509	-3.623334	-0.166575
H	1.320380	-4.648942	2.414725
H	1.377940	-2.868573	2.334766
H	-2.064909	-2.790955	-0.965583
O	3.000374	-3.896678	1.540398
C	-1.304710	-3.319812	1.558498

H	-1.415304	-4.388738	1.795790
H	-0.878867	-2.835536	2.441931
H	-2.304795	-2.920577	1.390803
C	3.241601	-2.048851	-2.317014
H	3.844296	-1.479600	-1.604576
H	3.859848	-2.881619	-2.683354
H	3.034177	-1.403118	-3.173986
P	1.456435	0.968022	0.054230
P	-1.988937	0.015691	0.037308
C	2.936427	0.422376	1.023434
C	2.731723	-0.236806	2.249691
C	4.254504	0.635232	0.590820
C	3.810585	-0.642826	3.035364
H	1.721861	-0.444226	2.591407
C	5.334514	0.215452	1.373117
H	4.447466	1.129799	-0.354434
C	5.117563	-0.416460	2.597963
H	3.630612	-1.149096	3.979099
H	6.347617	0.388129	1.021066
H	5.959059	-0.739585	3.203483
C	0.931484	2.506184	0.957395
C	1.194468	2.700168	2.322665
C	0.261580	3.520189	0.251974
C	0.793763	3.872769	2.965115
H	1.736896	1.953749	2.890710
C	-0.134922	4.691844	0.897236
H	0.064551	3.411746	-0.808447
C	0.126837	4.872029	2.256060
H	1.017181	4.007089	4.019727
H	-0.644176	5.465930	0.330361
H	-0.176989	5.787539	2.755532
C	2.132867	1.681936	-1.507293
C	1.849357	1.071322	-2.735694
C	2.922084	2.846895	-1.498449
C	2.349070	1.597535	-3.929483
H	1.228418	0.181796	-2.754279
C	3.425359	3.369700	-2.689141
H	3.136855	3.351503	-0.561665
C	3.140644	2.745977	-3.907180
H	2.117695	1.112538	-4.873956
H	4.035717	4.267895	-2.666065
H	3.530090	3.158139	-4.833630
C	-2.138520	1.513340	-1.037992
C	-1.606435	1.442201	-2.335782

C	-2.816532	2.678916	-0.651270
C	-1.758067	2.502467	-3.230827
H	-1.066706	0.551992	-2.644770
C	-2.970082	3.737684	-1.548084
H	-3.209859	2.780201	0.352606
C	-2.444291	3.653441	-2.838717
H	-1.336171	2.429963	-4.229055
H	-3.498780	4.632692	-1.232379
H	-2.565271	4.480044	-3.532877
C	-2.366044	0.523989	1.766955
C	-1.401353	0.320059	2.762420
C	-3.613809	1.062336	2.137029
C	-1.659672	0.661485	4.091221
H	-0.450113	-0.122031	2.485712
C	-3.868431	1.410392	3.463062
H	-4.398944	1.186626	1.398112
C	-2.891469	1.212886	4.442664
H	-0.900532	0.493788	4.849979
H	-4.835180	1.825648	3.732771
H	-3.095831	1.478730	5.475785
C	-3.529608	-0.909963	-0.453027
C	-4.315511	-1.583949	0.496969
C	-3.909209	-0.979870	-1.804636
C	-5.446234	-2.305238	0.106474
H	-4.063777	-1.535253	1.550700
C	-5.038069	-1.701811	-2.192145
H	-3.335895	-0.457769	-2.562986
C	-5.810200	-2.368857	-1.238455
H	-6.043512	-2.811553	0.859395
H	-5.318384	-1.734496	-3.241167
H	-6.691109	-2.927238	-1.541272

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2685.93408968 Predicted Change= -1.738538D-06
Zero-point correction (ZPE)= -2685.1291 0.80491
Internal Energy (U)= -2685.0817 0.85238
Enthalpy (H)= -2685.0807 0.85333
Gibbs Free Energy (G)= -2685.2111 0.72296

Frequencies -- 18.6188 23.3449 26.8201
SCF Energy (M06) = -2684.422435
SCF Energy (M06/def2-tzvp) = -2686.261487

5. RhCOF

5.a. Additional Figures

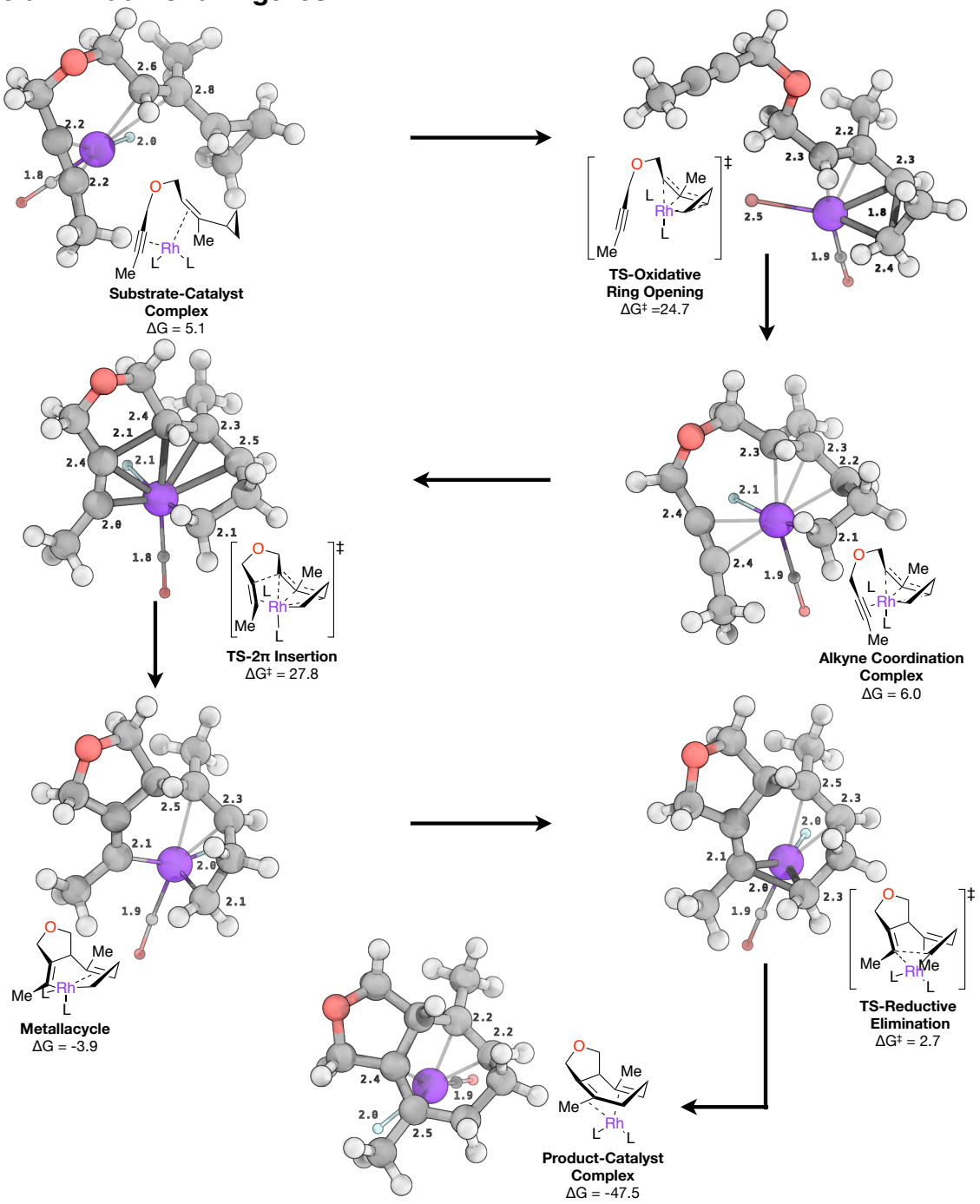


Figure S10. Computed geometries for RhCOF.

Substrate-Catalyst Complex RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)

opt=(maxcycle=250,gdiis) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq
---
Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.628689018 Predicted Change= -4.741596D-09
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00056 II	0.00180	[YES]	0.00056 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.855446	1.567329	0.251048
Rh	-0.528677	-0.569261	-0.254884
C	1.931136	0.784472	-0.052319
C	2.598797	0.027586	1.047084
C	-1.918952	0.919924	0.453391
C	-1.850894	0.062390	1.360708
H	0.581471	1.668719	1.299911
C	0.201756	2.616387	-0.633654
H	0.841908	3.506331	-0.688091
H	0.041133	2.259417	-1.661041
C	-2.126416	2.220513	-0.228327
H	-2.345709	2.054840	-1.294363
H	-2.977574	2.745400	0.219730
C	-1.802679	-1.764608	-0.812450
O	-2.607290	-2.499511	-1.188537
F	0.825738	-1.540784	-1.331638
H	2.301658	0.359945	2.039615
C	2.890205	-1.465189	0.926114
C	4.025368	-0.491706	0.934247
H	4.565574	-0.324419	0.007516
H	2.713129	-2.063915	1.815881
H	2.583045	-1.930554	-0.003733
H	4.643299	-0.414571	1.824940
O	-1.019608	3.097254	-0.079428
C	-2.142576	-0.649539	2.616826
H	-2.819771	-0.057809	3.244854
H	-2.613227	-1.619522	2.418939

H	-1.224077	-0.841434	3.182358
C	2.518482	0.718193	-1.436268
H	1.980127	1.352522	-2.143723
H	3.564948	1.043557	-1.419091
H	2.460057	-0.311183	-1.803876

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.628689018 Predicted Change= -4.741596D-09
Zero-point correction (ZPE)= -826.3727 0.25589
Internal Energy (U)= -826.3538 0.27483
Enthalpy (H)= -826.3529 0.27578
Gibbs Free Energy (G)= -826.4203 0.20831

Frequencies -- 46.8868 56.0439 65.4770
SCF Energy (M06) = -826.1566785

Oxidative-Addition TS RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
opt=(maxcycle=250,modredundant,gdiis)
Modredundant Input: B 8 10 F
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) Freq=Noraman
Geom=AllCheck Guess=Read SCRF=Check
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.594193996 Predicted Change= -7.056730D-09

==========

Optimization completed on the basis of negligible forces. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00255 II	0.00180	[NO]	0.00255 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.378606	-0.414138	-0.532811
Rh	1.542212	-0.517158	-0.209265
C	-4.605479	-0.094731	0.341466
C	-3.655844	0.295302	1.394122
C	-1.615711	-0.042194	0.220023
C	-0.383928	0.674975	-0.260077
C	0.568936	1.228868	0.602973
C	1.783109	1.804332	0.003948
C	1.873546	2.580529	-1.263907
C	2.382804	1.200241	-1.582728
H	3.460504	1.086544	-1.616286
H	1.836415	0.659893	-2.353364
H	2.596591	3.393306	-1.276121
H	0.926218	2.853699	-1.724436
H	-0.392484	0.989903	-1.302604
H	-3.415314	-0.582640	2.017605
H	-4.109252	1.048747	2.048397
H	-1.332480	-0.873900	0.881089

H	-2.145701	-0.472817	-0.639469
H	2.610145	1.954650	0.691574
O	-2.461055	0.889784	0.904100
C	-6.321199	-0.799749	-1.579966
H	-6.336471	-0.063097	-2.392515
H	-6.062068	-1.772379	-2.015523
H	-7.341168	-0.874699	-1.183342
C	0.424976	1.273872	2.103324
H	1.402231	1.238561	2.595302
H	-0.079975	2.203241	2.397545
H	-0.179992	0.441682	2.467575
C	3.230271	-1.358369	0.077115
O	4.260879	-1.808094	0.324637
F	0.549715	-2.078414	0.427857

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.594193996 Predicted Change= -7.056730D-09
Zero-point correction (ZPE)= -826.3407 0.25347
Internal Energy (U)= -826.3213 0.27279
Enthalpy (H)= -826.3204 0.27374
Gibbs Free Energy (G)= -826.3920 0.20212

Frequencies -- -214.6704 17.4949 24.5594
SCF Energy (M06) = -826.1191431

Alkyne Coordination Complex RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/genecp gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Opt=(Maxcycle=250,Nofreeze,gdiis) Freq=Noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/GenECP Freq

---

Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.629986251 Predicted Change= -3.802705D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00510 ll	0.00180	[NO]	0.00510 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.113149	2.082189	0.301236
Rh	0.413863	-0.198746	-0.129239
F	-0.532698	0.226803	-1.964463
C	-0.093921	2.141079	0.080008
C	-1.485607	2.456519	-0.291998
C	-2.755589	0.542942	0.315448
C	-1.664685	-0.385258	0.788624
C	-1.365908	-1.603757	0.128529
C	-0.153720	-2.257281	0.481749
C	0.521331	-2.107461	1.846530
C	1.129331	-0.701148	1.788544
C	2.091029	-0.552739	-0.964999
O	3.072612	-0.789239	-1.514469
H	2.219823	-0.706911	1.848709
H	0.725110	0.006328	2.518247
H	1.284436	-2.883935	1.962060
H	-0.201442	-2.242492	2.662076
H	-1.398069	-0.268432	1.836547
H	-1.621265	2.093987	-1.319545
H	-1.622025	3.543080	-0.256582
H	-3.687992	0.344907	0.859997
H	-2.940537	0.405952	-0.755602

H	0.142266	-3.097905	-0.142153
O	-2.464752	1.913501	0.581376
C	2.514245	2.357292	0.638852
H	3.181043	2.109006	-0.194183
H	2.640284	3.420020	0.876156
H	2.830348	1.774110	1.510322
C	-2.091663	-2.015678	-1.130327
H	-1.748251	-2.994796	-1.476698
H	-3.172640	-2.069444	-0.960138
H	-1.871502	-1.265428	-1.901707

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.629986251 Predicted Change= -3.802705D-07
Zero-point correction (ZPE)= -826.3742 0.25577
Internal Energy (U)= -826.3559 0.27404
Enthalpy (H)= -826.3550 0.27498
Gibbs Free Energy (G)= -826.4191 0.21085

Frequencies -- 56.7557 68.5071 76.1503
SCF Energy (M06) = -826.1577661

2π-Insertion TS RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
opt=(maxcycle=250,modredundant,gdiis)
Modredundant Input: B 4 7 F
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) Freq=Noraman
Geom=AllCheck Guess=Read SCRF=Check
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.602346179 Predicted Change= -2.510173D-09

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00044 ll	0.00180	[YES]	0.00044 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.110311	1.865460	0.250760
Rh	0.732368	-0.037953	-0.144062
F	0.222411	0.127514	-2.143157
C	-1.093744	1.425958	0.284019
C	-2.511774	1.872770	0.097709
C	-2.942283	-0.346669	-0.095087
C	-1.539051	-0.613414	0.429229
C	-0.819615	-1.775199	-0.146483
C	0.233097	-2.346657	0.545654
C	0.681732	-1.945238	1.946651
C	1.060465	-0.453720	1.904721
C	2.537713	0.223910	-0.430906
O	3.659329	0.401679	-0.625180
H	2.091668	-0.283243	2.220680
H	0.403139	0.188730	2.498806
H	1.541952	-2.562978	2.223314
H	-0.106955	-2.169159	2.680687
H	-1.519116	-0.585517	1.517400

H	-2.657907	2.152526	-0.958805
H	-2.715255	2.747306	0.724581
H	-3.619496	-1.139839	0.240305
H	-2.954515	-0.308078	-1.193030
H	0.714827	-3.205856	0.082738
O	-3.423477	0.859287	0.462163
C	0.897974	3.121084	0.330908
H	1.427065	3.297360	-0.612289
H	0.250903	3.982404	0.536744
H	1.649919	3.058553	1.125813
C	-1.199248	-2.278311	-1.520007
H	-0.611288	-3.164637	-1.776163
H	-2.260389	-2.549274	-1.572784
H	-0.973081	-1.485624	-2.245644

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.602346179 Predicted Change= -2.510173D-09
Zero-point correction (ZPE)= -826.3463 0.25600
Internal Energy (U)= -826.3292 0.27307
Enthalpy (H)= -826.3283 0.27402
Gibbs Free Energy (G)= -826.3900 0.21230

Frequencies -- -222.1335 63.8127 74.5511
SCF Energy (M06) = -826.1243671

Metallacycle RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/genecp gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Opt=(Maxcycle=250,Nofreeze,gdiis) Freq=Noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/GenECP Freq

---

Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.653997823 Predicted Change= -6.152748D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00080 ll	0.00180	[YES]	0.00080 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.309599	1.339273	0.034829
Rh	1.105123	-0.130345	-0.172438
F	2.034837	-1.656474	-1.111313
C	-1.586063	0.935687	0.132341
C	-2.860319	1.752580	-0.063828
C	-3.363309	-0.467801	-0.485066
C	-2.050914	-0.500167	0.319638
C	-0.983095	-1.525679	-0.020084
C	-0.023804	-1.857370	0.901444
C	0.200239	-1.164053	2.239941
C	1.194911	-0.045791	1.917625
C	2.524072	1.058593	-0.432873
O	3.424082	1.760996	-0.552527
H	2.234474	-0.305289	2.132099
H	0.939016	0.927041	2.335730
H	0.605488	-1.873225	2.971666
H	-0.729219	-0.755213	2.645266
H	-2.350218	-0.637770	1.370021
H	-2.814279	2.362075	-0.979443
H	-3.088159	2.422180	0.775983
H	-4.086110	-1.235548	-0.193913
H	-3.179604	-0.544965	-1.567475

H	0.682901	-2.639241	0.632090
O	-3.924356	0.798333	-0.151527
C	0.050150	2.800374	-0.095673
H	0.709485	3.116960	0.724091
H	0.586651	3.009065	-1.030279
H	-0.831681	3.452663	-0.068837
C	-1.045898	-2.266430	-1.336532
H	-0.081693	-2.732822	-1.551365
H	-1.832504	-3.033303	-1.308950
H	-1.284645	-1.588748	-2.163276

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.653997823 Predicted Change= -6.152748D-09
Zero-point correction (ZPE)= -826.3954 0.25850
Internal Energy (U)= -826.3781 0.27582
Enthalpy (H)= -826.3772 0.27677
Gibbs Free Energy (G)= -826.4405 0.21341

Frequencies -- 42.1506 47.8021 80.7261
SCF Energy (M06) = -826.1760336

Reductive Elimination TS RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant,gdiis)
Modredundant Input: B 1 11 F
Modredundant Input: B 2 11 F
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant) Geom=AllCheck Guess=Read SCRF=Check
Modredundant Input: B 1 11 F
Modredundant Input: B 2 11 A
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.632891090 Predicted Change= -1.443962D-08

==========

Optimization completed on the basis of negligible forces. {Found 4 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00383 II	0.00180	[NO]	0.00383 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.224156	1.347255	0.278873
Rh	1.112999	-0.230056	-0.094132
F	1.772941	-1.725431	-1.176233
C	-1.504310	0.951054	0.113494
C	-2.636673	1.777246	-0.473354
C	-3.105310	-0.447520	-0.853891
C	-2.045955	-0.461054	0.265769
C	-0.968117	-1.538605	0.260194
C	-0.093303	-1.612339	1.315406
C	-0.067364	-0.590778	2.444218
C	0.638499	0.667725	1.916884
C	2.566919	0.800985	-0.690216
O	3.486585	1.384710	-1.058091

H	1.717943	0.662061	2.103485
H	0.254455	1.588879	2.357205
H	0.478036	-0.993250	3.304767
H	-1.082493	-0.353856	2.783425
H	-2.609813	-0.537699	1.211542
H	-2.326277	2.295974	-1.394912
H	-3.033621	2.535624	0.216670
H	-3.905925	-1.180853	-0.723212
H	-2.645286	-0.590890	-1.843400
H	0.572817	-2.470163	1.378110
O	-3.687810	0.848515	-0.748235
C	0.182752	2.787714	0.046989
H	0.281959	2.989651	-1.027301
H	-0.555953	3.492990	0.449768
H	1.146012	3.019391	0.510721
C	-1.014569	-2.632981	-0.777453
H	-0.083419	-3.200697	-0.779240
H	-1.860441	-3.304566	-0.571863
H	-1.150083	-2.229201	-1.784618

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.632891090 Predicted Change= -1.443962D-08
Zero-point correction (ZPE)= -826.3757 0.25714
Internal Energy (U)= -826.3587 0.27409
Enthalpy (H)= -826.3578 0.27503
Gibbs Free Energy (G)= -826.4202 0.21262

Frequencies -- -370.3819 47.4754 56.6043
SCF Energy (M06) = -826.1646759

Product-Catalyst Complex RhCOF

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/genecp gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Opt=(Maxcycle=250,Nofreeze,gdiis) Freq=Noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/GenECP Freq

---

Pointgroup= C1 Stoichiometry= C12H16FO2Rh C1[X(C12H16FO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -826.715575239 Predicted Change= -2.872117D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00293 ll	0.00180	[NO]	0.00293 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.331957	-1.264476	0.614230
Rh	-0.777161	-0.378415	-0.314326
C	1.543198	-0.040256	0.033534
C	2.338627	0.154375	-1.252867
C	1.687646	2.242695	-0.629755
C	1.191903	1.370299	0.551115
C	-0.316556	1.413002	0.811788
C	-0.833778	0.468135	1.720406
C	0.056422	-0.327214	2.668165
C	0.786328	-1.506009	2.009068
H	0.101851	-2.360781	1.948416
H	1.621948	-1.841472	2.644820
H	-0.550408	-0.714325	3.493038
H	0.787359	0.356318	3.123625
H	1.766520	1.627310	1.455190
H	1.725290	-0.072831	-2.138679
H	3.241610	-0.463366	-1.291936
H	2.075910	3.215857	-0.318938
H	0.881809	2.397814	-1.362311
H	-1.852653	0.631349	2.066935
C	-2.588730	-0.105713	-0.670443
O	-3.709764	0.071623	-0.864882

F	-0.491245	-1.598594	-1.828699
O	2.750669	1.516062	-1.223992
C	-1.093388	2.670202	0.485368
H	-0.718472	3.508735	1.091270
H	-1.015897	2.964292	-0.565180
H	-2.154601	2.541962	0.721493
C	1.799518	-2.509269	-0.114454
H	1.265903	-2.585810	-1.069236
H	2.878605	-2.475430	-0.312572
H	1.592529	-3.409695	0.471093

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -826.715575239 Predicted Change= -2.872117D-08
Zero-point correction (ZPE)= -826.4548 0.26072
Internal Energy (U)= -826.4382 0.27736
Enthalpy (H)= -826.4372 0.27830
Gibbs Free Energy (G)= -826.4984 0.21710

Frequencies -- 52.4112 65.7164 77.3922
SCF Energy (M06) = -826.249231

6. RhCOBr

6.a. Additional Figures

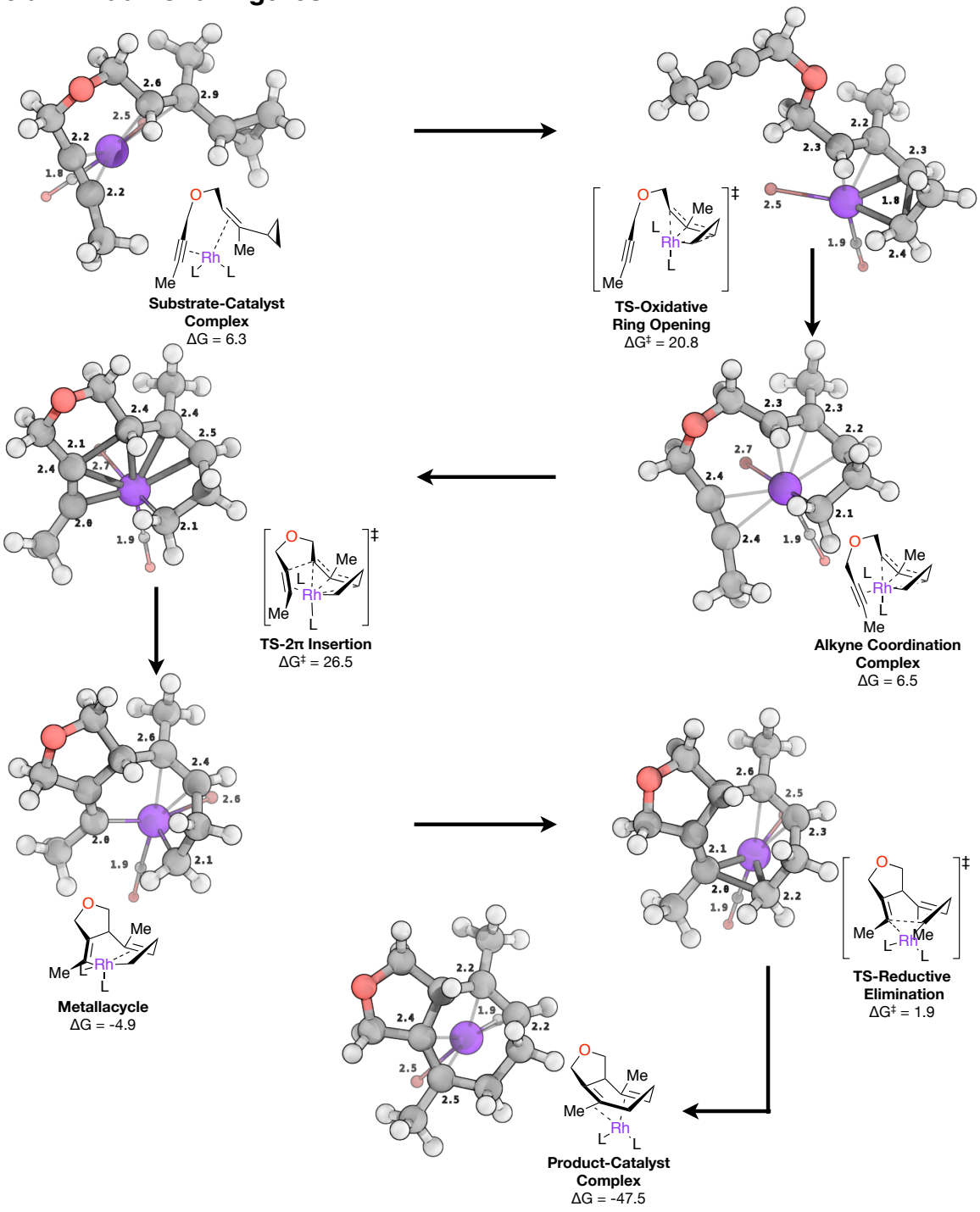


Figure S11. Computed geometries for RhCOBr.

Substrate-Catalyst Complex RhCOBr

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

```
=====================================================
 #b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,gdiis) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq
---------------------------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C12H16BrO2Rh   C1[X(C12H16BrO2Rh)]
#Atoms= 32
 Charge = 0   Multiplicity = 1
---------------------------------------------------------------------------------------------------
 SCF Energy= -3298.23120857      Predicted Change= -2.219370D-08
=====================================================
 Optimization completed. {Found  2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00002 II  0.00045   [ YES ]      0.00000 II  0.00030   [ YES ]
 Displ      0.00157 II  0.00180   [ YES ]      0.00157 II  0.00180   [ YES ]
---------------------------------------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
       Type        X           Y        Z
---------------------------------------------------------------------------------------------------
      C       -0.407162     -1.898071     -0.254468
      Rh       0.664778      0.398999      0.085965
      C       -1.647767     -1.336762     -0.149225
      C       -2.284008     -1.245471      1.192000
      C        2.275898     -1.052172      0.124065
      C        2.164564     -0.662039      1.305343
      H        0.021397     -2.337366      0.643633
      C        0.268909     -2.371596     -1.532424
      H       -0.280365     -3.223070     -1.954170
      H        0.304634     -1.587330     -2.303453
      C        2.572246     -1.903397     -1.053986
      H        2.705489     -1.273896     -1.946761
      H        3.500002     -2.462106     -0.886590
      C        1.767627      1.863282      0.062778
      O        2.489576      2.760772      0.036292
      Br      -1.082742      2.044032     -0.696315
      H       -1.675786     -1.672362      1.986432
      C       -3.164099     -0.080162      1.613746
      C       -3.791036     -1.416323      1.373986
      H       -4.401774     -1.543640      0.485260
      H       -3.044245      0.267146      2.636177
      H       -3.319334      0.715317      0.893040
      H       -4.115995     -2.009604      2.224261
      O        1.573165     -2.885754     -1.280212
      C        2.430032     -0.480448      2.741833
```

H	3.229635	-1.155214	3.071520
H	2.734742	0.549730	2.958124
H	1.533688	-0.688299	3.336445
C	-2.463286	-0.979932	-1.364819
H	-1.841551	-0.846235	-2.251728
H	-3.173400	-1.794192	-1.567160
H	-3.029598	-0.056521	-1.224066

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3298.23120857 Predicted Change= -2.219370D-08
Zero-point correction (ZPE)= -3297.9768 0.25434
Internal Energy (U)= -3297.9571 0.27410
Enthalpy (H)= -3297.9561 0.27504
Gibbs Free Energy (G)= -3298.0269 0.20425

Frequencies -- 28.5472 51.7631 61.1623
SCF Energy (M06) = -3297.63319

Oxidative-Addition TS RhCOBr

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant,gdiis)
Modredundant Input: B 8 10 F
#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16BrO2Rh C1[X(C12H16BrO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -3298.20582794 Predicted Change= -1.619851D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00565 ll	0.00180	[NO]	0.00565 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.419151	-0.320525	-0.700044
Rh	1.503474	-0.012903	-0.283898
C	-4.756909	0.119407	0.212104
C	-3.937399	0.649992	1.310564
C	-1.778491	0.250684	0.388826
C	-0.566932	0.992270	-0.102965
C	0.381519	1.566212	0.742511
C	1.506247	2.294311	0.140726
C	1.436124	3.183794	-1.056390
C	2.053907	1.902725	-1.530556
H	3.132686	1.897535	-1.633383
H	1.510673	1.358617	-2.301346
H	2.075469	4.063584	-1.030376
H	0.436324	3.397588	-1.428979
H	-0.633797	1.345519	-1.131100
H	-3.753028	-0.145944	2.051970
H	-4.470858	1.458460	1.823271
H	-1.517146	-0.471768	1.173827

H	-2.226291	-0.315364	-0.437160
H	2.353015	2.472679	0.796438
O	-2.704077	1.221904	0.889448
C	-6.228325	-0.852013	-1.793805
H	-6.104001	-0.255636	-2.705876
H	-5.952446	-1.886582	-2.030942
H	-7.294375	-0.842342	-1.535729
C	0.314761	1.498505	2.247694
H	1.314745	1.530172	2.690974
H	-0.260184	2.354096	2.625811
H	-0.182643	0.587454	2.584977
C	3.258393	-0.721681	-0.290918
O	4.330879	-1.133659	-0.228113
Br	0.666247	-2.287300	0.301882

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3298.20582794 Predicted Change= -1.619851D-09
Zero-point correction (ZPE)= -3297.9533 0.25248
Internal Energy (U)= -3297.9333 0.27246
Enthalpy (H)= -3297.9324 0.27340
Gibbs Free Energy (G)= -3298.0069 0.19887

Frequencies -- -208.3443 15.1042 19.7752
SCF Energy (M06) = -3297.604664

Alkyne Coordination Complex RhCOBr

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/genecp gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Opt=(Maxcycle=250,Nofreeze,gdiis) Freq=Noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/GenECP Freq

---

Pointgroup= C1 Stoichiometry= C12H16BrO2Rh C1[X(C12H16BrO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -3298.23573790 Predicted Change= -2.020953D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00360 ll	0.00180	[NO]	0.00360 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.148014	-1.299815	1.686451
Rh	-0.501681	0.296120	0.023723
Br	0.546382	-1.529433	-1.662146
C	0.083531	-1.302820	1.699226
C	1.508321	-1.657677	1.876303
C	2.640942	0.273688	1.081970
C	1.470719	1.173555	0.783017
C	1.209863	1.741483	-0.488505
C	-0.055968	2.362631	-0.672151
C	-0.860590	2.984078	0.471396
C	-1.379469	1.771619	1.247002
C	-2.116096	-0.033021	-0.955455
O	-3.061920	-0.231275	-1.575167
H	-2.467383	1.687196	1.243327
H	-0.999911	1.664826	2.265821
H	-1.677312	3.582591	0.055592
H	-0.238338	3.659691	1.073339
H	1.077550	1.669841	1.666923
H	1.841586	-2.173806	0.964453
H	1.581777	-2.350005	2.722369
H	3.512829	0.866109	1.388591
H	2.917892	-0.325226	0.205067

H	-0.308244	2.655780	-1.688704
O	2.370753	-0.578326	2.192957
C	-2.570005	-1.546982	1.955501
H	-3.067675	-1.980388	1.081120
H	-2.674711	-2.245911	2.793539
H	-3.091253	-0.620256	2.218606
C	2.128838	1.544894	-1.669911
H	1.636005	1.832044	-2.602168
H	3.013914	2.181781	-1.537119
H	2.452470	0.507488	-1.774573

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3298.23573790 Predicted Change= -2.020953D-07
Zero-point correction (ZPE)= -3297.9812 0.25444
Internal Energy (U)= -3297.9621 0.27356
Enthalpy (H)= -3297.9612 0.27451
Gibbs Free Energy (G)= -3298.0286 0.20709

Frequencies -- 55.8645 62.8419 72.0193
SCF Energy (M06) = -3297.635783

2π-Insertion TS RhCOBr

 Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004
===
 #b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,modredundant,gdiis)
 #b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,modredundant) geom=connectivity
 ===
 CARD - FULL OPTIMIZATION - Following PARTIAL OPT
 #B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 Opt=(Maxcycle=250,Nofreeze) Freq=Noraman Geom=AllCheck Guess=Read
 SCRF=Check
 ===
 CARD - FULL OPTIMIZATION - Continued from Checkpoint File
 #B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,readfc,nofreeze) Freq=Noraman Geom=AllCheck
Guess=Read
 SCRF=Check
 ===
 CARD - TRANSITION STRUCTURE OPTIMIZATION - Following PARTIAL OPT
 %chk=025-COBr-TS-2Pi-Insertion-Yne-Boat.chk %mem=1800MB
 #B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze) Freq=Noraman
 Geom=AllCheck Guess=Read SCRF=Check
 ===
 CARD - TRANSITION STRUCTURE OPTIMIZATION - Continued from
Checkpoint File
 #B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,readfc,ts,noeigentest,nofreeze) Freq=Noraman
 Geom=AllCheck Guess=Read SCRF=Check
 Modredundant Input: B   4   7 F
 #B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
 opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) Freq=Noraman
 Geom=AllCheck Guess=Read SCRF=Check
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq
---
 Pointgroup= C1   Stoichiometry= C12H16BrO2Rh   C1[X(C12H16BrO2Rh)]
#Atoms= 32
 Charge = 0   Multiplicity = 1

 SCF Energy= -3298.21036002   Predicted Change= -6.887141D-09
===
 Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00104 II	0.00180	[YES]	0.00104 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.033336	-0.578089	1.857157
Rh	-0.561297	0.431832	0.153226
Br	-1.034554	-1.814980	-1.207122
C	1.168122	-0.630067	1.410562
C	2.412575	-1.458129	1.495375
C	3.035633	-0.319303	-0.362105
C	1.841920	0.597282	-0.128045
C	1.137718	1.089926	-1.337382
C	0.360308	2.231479	-1.274644
C	0.233967	3.141821	-0.060140
C	-0.258687	2.288423	1.116462
C	-2.403662	0.542791	0.348409
O	-3.544715	0.601289	0.482921
H	-1.181437	2.671093	1.555233
H	0.478650	2.141099	1.910595
H	-0.484310	3.933211	-0.295551
H	1.192282	3.643453	0.143995
H	2.094927	1.388657	0.575709
H	2.224403	-2.428404	1.006780
H	2.674628	-1.633936	2.543726
H	3.857798	0.252820	-0.805845
H	2.774499	-1.147003	-1.036044
H	-0.111319	2.553779	-2.200802
O	3.501389	-0.803802	0.879831
C	-0.886806	-1.059607	2.971563
H	-1.651177	-1.743802	2.586536
H	-0.290537	-1.585293	3.727140
H	-1.401775	-0.224440	3.459675
C	1.317400	0.371042	-2.657034
H	0.689424	0.828597	-3.426174
H	2.361800	0.439833	-2.989237
H	1.035631	-0.683124	-2.584723

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -3298.21036002 Predicted Change= -6.887141D-09

Zero-point correction (ZPE)=	-3297.9555	0.25479	
Internal Energy (U)=	-3297.9376	0.27268	
Enthalpy (H)=	-3297.9367	0.27363	
Gibbs Free Energy (G)=	-3298.0016	0.20872	

Frequencies -- -223.7547 51.5862 61.8346

SCF Energy (M06) = -3297.605466

Metallacycle RhCOBr

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/genecp gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Opt=(Maxcycle=250,Nofreeze,gdiis) Freq=Noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/GenECP Freq

---

Pointgroup= C1 Stoichiometry= C12H16BrO2Rh C1[X(C12H16BrO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -3298.26486842 Predicted Change= -3.611484D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00311 ll	0.00180	[NO]	0.00311 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.134686	1.336854	-0.206633
Rh	0.640676	0.362322	0.084833
Br	2.736577	-1.008159	-0.603276
C	-2.259096	0.609833	-0.144217
C	-3.657668	0.985981	-0.629978
C	-3.536352	-1.317505	-0.547696
C	-2.359443	-0.831535	0.321200
C	-1.038801	-1.578351	0.265264
C	-0.145801	-1.503783	1.301470
C	-0.280510	-0.601617	2.524629
C	0.359862	0.729891	2.122865
C	1.711130	1.869937	-0.197054
O	2.390414	2.785099	-0.324652
H	1.374368	0.865992	2.502601
H	-0.253683	1.608921	2.316431
H	0.239206	-1.055480	3.376337
H	-1.328541	-0.463220	2.807054
H	-2.729551	-0.838837	1.357222
H	-3.638751	1.354418	-1.667633
H	-4.149063	1.746306	-0.009781
H	-4.068859	-2.179980	-0.137024
H	-3.213852	-1.553061	-1.573313

H	0.740278	-2.131647	1.254094
O	-4.433091	-0.212063	-0.537333
C	-1.142671	2.786638	-0.629118
H	-0.748881	3.431923	0.167614
H	-0.520443	2.959880	-1.515994
H	-2.154438	3.142041	-0.861463
C	-0.786564	-2.519575	-0.889485
H	0.237052	-2.900235	-0.873071
H	-1.483468	-3.367877	-0.844446
H	-0.946953	-2.022925	-1.853061

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3298.26486842 Predicted Change= -3.611484D-08
Zero-point correction (ZPE)= -3298.0072 0.25761
Internal Energy (U)= -3297.9893 0.27547
Enthalpy (H)= -3297.9884 0.27641
Gibbs Free Energy (G)= -3298.0543 0.21051

Frequencies -- 25.7565 41.4384 78.4475
SCF Energy (M06) = -3297.657258

Reductive Elimination TS RhCOBr

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant,gdiis)

#b3lyp/gen pseudo=read gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant) geom=connectivity

==========

CARD - FULL OPTIMIZATION - Following PARTIAL OPT

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) Opt=(Maxcycle=250,Nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

==========

CARD - FULL OPTIMIZATION - Continued from Checkpoint File

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,readfc,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

==========

CARD - TRANSITION STRUCTURE OPTIMIZATION - Following PARTIAL OPT

%chk=035-COBr-TS-ReductiveElim-Yne-Boat.chk %mem=1800MB

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

==========

CARD - TRANSITION STRUCTURE OPTIMIZATION - Continued from Checkpoint File

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,readfc,ts,noeigentest,nofreeze) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

Modredundant Input: B 1 11 F

Modredundant Input: B 2 11 F

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,modredundant) Geom=AllCheck Guess=Read SCRF=Check

Modredundant Input: B 1 11 F

Modredundant Input: B 2 11 A

#B3LYP/ChkBas GenChk gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) Freq=Noraman Geom=AllCheck Guess=Read SCRF=Check

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16BrO2Rh C1[X(C12H16BrO2Rh)] #Atoms= 32

Charge = 0 Multiplicity = 1

SCF Energy= -3298.24205820 Predicted Change= -1.792834D-09

==========

Optimization completed. {Found 4 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00087 II	0.00180	[YES]	0.00087 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.151005	1.370179	-0.006373
Rh	0.693475	0.388016	0.186787
Br	2.585591	-1.088530	-0.570557
C	-2.168554	0.508368	-0.205893
C	-3.380819	0.738736	-1.095218
C	-3.054839	-1.534651	-0.917038
C	-2.255823	-0.935311	0.257488
C	-0.918093	-1.554734	0.638826
C	-0.253849	-1.092993	1.744608
C	-0.753970	0.069510	2.593077
C	-0.424981	1.378886	1.865190
C	1.747635	1.769289	-0.492801
O	2.415207	2.615699	-0.892661
H	0.538212	1.807454	2.162358
H	-1.174571	2.156703	2.008753
H	-0.260185	0.053756	3.570926
H	-1.832359	-0.015632	2.772105
H	-2.924599	-0.990830	1.133976
H	-3.088190	1.115893	-2.088299
H	-4.107114	1.446502	-0.671234
H	-3.594194	-2.453055	-0.670236
H	-2.408215	-1.720833	-1.788042
H	0.622314	-1.639428	2.085570
O	-4.023707	-0.531661	-1.207053
C	-1.210455	2.786266	-0.538446
H	-0.934691	2.809835	-1.600507
H	-2.216626	3.215555	-0.446572
H	-0.520343	3.450504	-0.010204
C	-0.477392	-2.811706	-0.067783
H	0.513488	-3.127597	0.262734
H	-1.198014	-3.616135	0.139309
H	-0.436100	-2.678202	-1.152645

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3298.24205820 Predicted Change= -1.792834D-09
Zero-point correction (ZPE)= -3297.9858 0.25622
Internal Energy (U)= -3297.9684 0.27364
Enthalpy (H)= -3297.9674 0.27458
Gibbs Free Energy (G)= -3298.0318 0.21022

Frequencies -- -382.3534 38.0302 52.3138
SCF Energy (M06) = -3297.646242

Product-Catalyst Complex RhCOBr

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

#B3LYP/genecp gfprint gfinput scf=(direct,xqc,tight,maxcycle=250)
Opt=(Maxcycle=250,Nofreeze,gdiis) Freq=Noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/GenECP Freq

---

Pointgroup= C1 Stoichiometry= C12H16BrO2Rh C1[X(C12H16BrO2Rh)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -3298.32265463 Predicted Change= -3.125961D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00206 ll	0.00180	[NO]	0.00206 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.849482	-1.325046	1.243914
Rh	-0.482575	0.504504	0.137728
C	1.383916	-1.060335	0.012178
C	1.387583	-2.061494	-1.142734
C	2.432155	-0.209749	-1.947331
C	2.232383	0.139647	-0.452943
C	1.464350	1.428436	-0.168073
C	1.090631	1.666720	1.168851
C	1.672931	0.882526	2.336132
C	1.077477	-0.520933	2.511277
H	0.113448	-0.437202	3.027354
H	1.717619	-1.122134	3.177321
H	1.512328	1.443297	3.262371
H	2.762791	0.812194	2.207288
H	3.216703	0.144009	0.042722
H	0.419414	-2.080120	-1.665859
H	1.627758	-3.078225	-0.817288
H	3.380249	0.147833	-2.356549
H	1.606419	0.190568	-2.554431
H	0.742654	2.670086	1.407367
C	-1.602341	1.951222	-0.170732
O	-2.291401	2.854675	-0.353332

Br	-2.375916	-1.020230	-0.451220
O	2.437468	-1.626315	-1.999579
C	1.528241	2.565264	-1.165033
H	2.566757	2.915107	-1.265036
H	1.180297	2.280409	-2.161845
H	0.924959	3.413521	-0.826599
C	0.150654	-2.647788	1.484576
H	-0.368269	-3.014856	0.597827
H	0.888913	-3.399739	1.801031
H	-0.592424	-2.557045	2.282055

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3298.32265463 Predicted Change= -3.125961D-08
Zero-point correction (ZPE)= -3298.0630 0.25964
Internal Energy (U)= -3298.0456 0.27696
Enthalpy (H)= -3298.0447 0.27791
Gibbs Free Energy (G)= -3298.1086 0.21397

Frequencies -- 41.6867 60.3645 80.3334
SCF Energy (M06) = -3297.728667

7. RhCSCl

7.a. Additional Figures

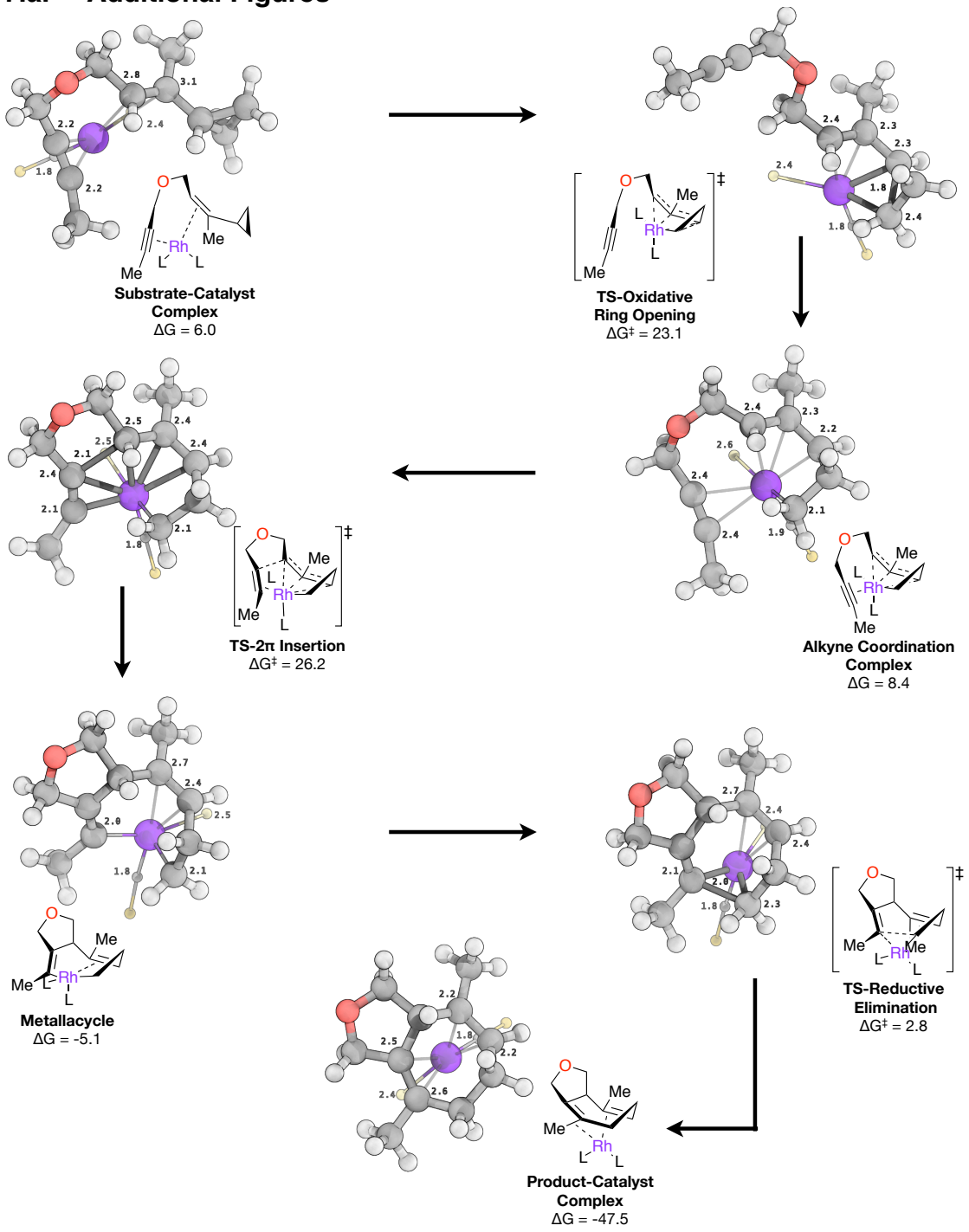


Figure S12. Computed geometries for RhCSCl.

Substrate-Catalyst Complex RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

```
=====================================================================
 # b3lyp/gen pseudo=read gfprint gfinput
 scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq
---------------------------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C12H16ClORhS   C1[X(C12H16ClORhS)]
#Atoms= 32
 Charge = 0   Multiplicity = 1
---------------------------------------------------------------------------------------------------
 SCF Energy= -1509.94221211      Predicted Change= -1.035736D-08
=====================================================================
 Optimization completed. {Found  1 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 II  0.00045   [ YES ]      0.00000 II  0.00030   [ YES ]
 Displ      0.00208 II  0.00180   [ NO ]       0.00208 II  0.00180   [ YES ]
---------------------------------------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
       Type        X           Y        Z
---------------------------------------------------------------------------------------------------
       C         1.518911      1.431894     -0.132251
       Rh       -0.660125     -0.286708      0.016777
       C         2.366412      0.373095     -0.225771
       C         2.952721     -0.194164      1.019519
       C        -1.337761      1.732240      0.354940
       C        -1.454216      1.151192      1.455731
       H         1.344661      1.862152      0.852058
       C         1.040260      2.319359     -1.268420
       H         1.875895      2.914540     -1.658273
       H         0.628316      1.742488     -2.110342
       C        -1.227097      2.808742     -0.662070
       H        -1.629000      2.452482     -1.622735
       H        -1.818123      3.674918     -0.343596
       C        -2.274743     -0.997438     -0.213731
       Cl        0.293094     -2.247642     -0.947189
       H         2.667653      0.351838      1.916534
       C         3.182321     -1.683507      1.221226
       C         4.361699     -0.779356      1.046044
       H         4.910435     -0.829859      0.110400
       H         2.967380     -2.076109      2.211277
       H         2.898877     -2.347552      0.412093
       H         4.977248     -0.539268      1.908711
       O         0.096119      3.289568     -0.821252
       C        -1.806643      0.895952      2.862362
```

H	-2.173415	1.814593	3.336296
H	-2.587802	0.131127	2.934054
H	-0.940427	0.535372	3.427458
C	2.846006	-0.151267	-1.555186
H	2.184681	0.138972	-2.374015
H	3.845779	0.252076	-1.768130
H	2.908608	-1.242035	-1.562879
S	-3.694620	-1.592560	-0.447877

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1509.94221211 Predicted Change= -1.035736D-08
Zero-point correction (ZPE)= -1509.6897 0.25241
Internal Energy (U)= -1509.6699 0.27230
Enthalpy (H)= -1509.6689 0.27325
Gibbs Free Energy (G)= -1509.7401 0.20208

Frequencies -- 28.8555 46.5056 56.7809
SCF Energy (M06) = -1509.470701

Oxidative-Addition TS RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClORhS C1[X(C12H16ClORhS)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1509.91173116 Predicted Change= -1.011479D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.01490 II	0.00180	[NO]	0.01490 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.647480	-0.673757	-0.618868
Rh	1.399450	-0.224133	-0.207466
C	-4.977380	-0.166429	0.251585
C	-4.147577	0.442068	1.300562
C	-2.008310	0.061995	0.329609
C	-0.804403	0.800217	-0.185622
C	0.114568	1.437109	0.623881
C	1.278447	2.103485	0.008176
C	1.247563	2.905070	-1.251270
C	1.895956	1.600761	-1.604841
H	2.977065	1.601429	-1.676648
H	1.382599	0.989296	-2.344728
H	1.877480	3.791898	-1.265591
H	0.260893	3.078356	-1.676299
H	-0.790122	0.995191	-1.257050
H	-3.919645	-0.310684	2.074227
H	-4.691816	1.259250	1.787241
H	-1.728362	-0.641057	1.127474
H	-2.456569	-0.527203	-0.479774
H	2.090004	2.346545	0.686604

O	-2.942668	1.028746	0.819955
C	-6.465974	-1.286876	-1.661781
H	-6.363012	-0.751317	-2.613377
H	-6.180044	-2.331561	-1.833657
H	-7.528063	-1.272769	-1.388151
C	0.004502	1.487597	2.127795
H	0.992064	1.536182	2.596115
H	-0.564018	2.379010	2.422513
H	-0.520399	0.614438	2.519667
C	3.134967	-0.773064	-0.119741
Cl	0.580682	-2.326378	0.499848
S	4.631699	-1.186352	0.025214

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1509.91173116 Predicted Change= -1.011479D-08
Zero-point correction (ZPE)= -1509.6612 0.25050
Internal Energy (U)= -1509.6411 0.27062
Enthalpy (H)= -1509.6401 0.27157
Gibbs Free Energy (G)= -1509.7149 0.19678

Frequencies -- -204.7763 17.0950 20.5724
SCF Energy (M06) = -1509.438094

Alkyne Coordination Complex RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClORhS C1[X(C12H16ClORhS)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1509.94049865 Predicted Change= -1.796601D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00142 ll	0.00180	[YES]	0.00142 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.382486	2.290575	-0.508599
Rh	-0.323915	-0.106254	-0.108973
Cl	0.155930	0.097184	2.393548
C	0.774500	2.077841	-0.150536
C	2.159150	2.159595	0.359430
C	3.093818	0.009319	-0.060952
C	1.916194	-0.673988	-0.701057
C	1.265036	-1.805071	-0.186828
C	0.006641	-2.170994	-0.768331
C	-0.364658	-1.855967	-2.218405
C	-0.693680	-0.361478	-2.167378
C	-2.120990	-0.199364	0.327729
H	-1.729574	-0.133684	-2.420154
H	-0.017053	0.291040	-2.724427
H	-1.232735	-2.454685	-2.511174
H	0.452360	-2.106852	-2.907681
H	1.777997	-0.410563	-1.746131
H	2.145641	1.875568	1.421031
H	2.486658	3.201998	0.275063
H	4.034262	-0.380049	-0.472225
H	3.104310	-0.143651	1.025692

H	-0.541203	-2.965021	-0.266922
O	3.119042	1.403483	-0.361749
C	-1.642342	2.883099	-0.971941
H	-2.428208	2.775213	-0.217278
H	-1.499308	3.950805	-1.175352
H	-1.989456	2.403066	-1.892845
C	1.736535	-2.513505	1.061084
H	0.968996	-3.193143	1.439142
H	2.630590	-3.103708	0.819351
H	1.978435	-1.814556	1.864203
S	-3.603436	-0.308169	0.781991

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1509.94049865 Predicted Change= -1.796601D-08
Zero-point correction (ZPE)= -1509.6882 0.25226
Internal Energy (U)= -1509.6689 0.27159
Enthalpy (H)= -1509.6679 0.27254
Gibbs Free Energy (G)= -1509.7361 0.20436

Frequencies -- 45.8672 53.5271 55.5839
SCF Energy (M06) = -1509.469082

2π-Insertion TS RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClORhS C1[X(C12H16ClORhS)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1509.91958447 Predicted Change= -8.355967D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00035 II	0.00180	[YES]	0.00035 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.014660	1.795371	-0.615929
Rh	-0.517636	-0.120427	-0.058276
Cl	-0.358978	0.465051	2.403558
C	1.245480	1.469753	-0.494022
C	2.602241	2.019424	-0.195572
C	3.219252	-0.141092	0.152851
C	1.883579	-0.579334	-0.420612
C	1.207588	-1.723687	0.207019
C	0.216321	-2.411177	-0.479830
C	-0.155665	-2.190397	-1.940612
C	-0.609890	-0.730868	-2.077383
C	-2.324998	0.001372	0.054707
H	-1.618182	-0.638070	-2.481475
H	0.070085	-0.096122	-2.651786
H	-0.966295	-2.878724	-2.198066
H	0.690650	-2.443492	-2.596772
H	1.910203	-0.616910	-1.507919
H	2.629400	2.332087	0.861153
H	2.795638	2.892317	-0.827889
H	3.989290	-0.879932	-0.097178

H	3.168525	-0.039859	1.245990
H	-0.245275	-3.248683	0.039218
O	3.618380	1.072732	-0.451079
C	-0.880996	2.949525	-0.876293
H	-1.479437	3.161758	0.016367
H	-0.303301	3.844385	-1.137182
H	-1.573148	2.731565	-1.696911
C	1.609581	-2.168452	1.595902
H	0.980859	-2.999403	1.926811
H	2.652258	-2.512648	1.596338
H	1.499377	-1.358517	2.322462
S	-3.869649	0.121195	0.193504

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1509.91958447 Predicted Change= -8.355967D-10
Zero-point correction (ZPE)= -1509.6668 0.25276
Internal Energy (U)= -1509.6488 0.27073
Enthalpy (H)= -1509.6479 0.27168
Gibbs Free Energy (G)= -1509.7126 0.20692

Frequencies -- -221.3057 53.1375 55.5049
SCF Energy (M06) = -1509.44328

Metallacycle RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClORhS C1[X(C12H16ClORhS)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1509.97310803 Predicted Change= -1.175539D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00169 ll	0.00180	[YES]	0.00169 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.569420	1.370747	-0.012667
Rh	0.811473	-0.142884	-0.056871
C	-1.869158	1.035826	0.031840
C	-3.070233	1.930735	-0.275694
C	-3.738722	-0.261367	-0.550875
C	-2.452037	-0.343215	0.291477
C	-1.483459	-1.486832	0.053475
C	-0.577857	-1.843124	1.008984
C	-0.316683	-1.099400	2.312997
C	0.843573	-0.144160	2.027588
H	1.825963	-0.559074	2.259649
H	0.726793	0.857729	2.438793
H	-0.056931	-1.811727	3.106459
H	-1.199187	-0.540371	2.635701
H	-2.788227	-0.378746	1.339014
H	-2.948842	2.447671	-1.240294
H	-3.260597	2.690815	0.492939
H	-4.525296	-0.951796	-0.233254
H	-3.534268	-0.422436	-1.620500
H	0.051199	-2.708552	0.817277
O	-4.205343	1.062230	-0.313454

C	-0.139476	2.806563	-0.201362
H	0.491402	3.138211	0.633545
H	0.452091	2.941896	-1.115147
H	-0.993655	3.493050	-0.253065
C	-1.607095	-2.293794	-1.218339
H	-2.559985	-2.840403	-1.234572
H	-1.594447	-1.648644	-2.104745
H	-0.787055	-3.009304	-1.312084
C	2.269449	0.933160	-0.191234
Cl	2.170927	-2.035656	-0.872185
S	3.574277	1.763058	-0.273305

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1509.97310803 Predicted Change= -1.175539D-08
Zero-point correction (ZPE)= -1509.7177 0.25535
Internal Energy (U)= -1509.6996 0.27346
Enthalpy (H)= -1509.6987 0.27440
Gibbs Free Energy (G)= -1509.7650 0.20805

Frequencies -- 33.6445 38.1898 65.6135
SCF Energy (M06) = -1509.494316

Reductive Elimination TS RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16ClORhS C1[X(C12H16ClORhS)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1509.94972487 Predicted Change= -2.778480D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00035 II	0.00180	[YES]	0.00035 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.445557	-1.402887	0.220434
Rh	-0.844851	0.250395	0.114251
Cl	-1.768665	2.150847	-0.991411
C	1.725960	-1.081638	-0.056933
C	2.707742	-1.956468	-0.823825
C	3.406710	0.228616	-1.027564
C	2.442097	0.240096	0.174235
C	1.525385	1.435837	0.379694
C	0.738791	1.484950	1.492788
C	0.689477	0.373021	2.531997
C	-0.200508	-0.764871	2.016707
C	-2.367712	-0.643759	-0.277885
H	-1.246116	-0.665789	2.326522
H	0.128820	-1.754010	2.334255
H	0.281260	0.763343	3.471082
H	1.698257	0.002453	2.747593
H	3.081052	0.138195	1.068443
H	2.264723	-2.331826	-1.760191
H	3.059516	-2.825583	-0.250252
H	4.295493	0.850778	-0.892467

H	2.896434	0.528827	-1.955446
H	0.161382	2.387175	1.681721
O	3.837070	-1.127198	-1.096811
C	-0.083664	-2.791213	-0.066264
H	-0.347299	-2.889609	-1.126815
H	0.658132	-3.565759	0.168308
H	-0.986547	-3.010865	0.509548
C	1.630980	2.607278	-0.562737
H	0.911925	3.387011	-0.306281
H	2.645743	3.027540	-0.518880
H	1.439439	2.313296	-1.599423
S	-3.719879	-1.346471	-0.588401

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1509.94972487 Predicted Change= -2.778480D-10
Zero-point correction (ZPE)= -1509.6952 0.25446
Internal Energy (U)= -1509.6778 0.27190
Enthalpy (H)= -1509.6768 0.27285
Gibbs Free Energy (G)= -1509.7410 0.20864

Frequencies -- -383.5338 39.4106 48.8380
SCF Energy (M06) = -1509.482293

Product-Catalyst Complex RhCSCl

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C12H16ClORhS C1[X(C12H16ClORhS)]
#Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -1510.03125987 Predicted Change= -5.186987D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00155 ll	0.00180	[YES]	0.00155 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.743611	-0.902404	0.962116
Rh	-0.639311	-0.306246	0.019740
C	1.882534	0.005263	-0.043918
C	2.578446	-0.306746	-1.366364
C	1.875081	1.842288	-1.557809
C	1.535268	1.506419	-0.084627
C	0.079725	1.732830	0.318870
C	-0.326010	1.234659	1.572122
C	0.662238	0.769224	2.631846
C	1.276714	-0.612910	2.376073
H	0.544876	-1.383792	2.648357
H	2.133682	-0.770629	3.050627
H	0.159066	0.745894	3.603770
H	1.461295	1.520049	2.719884
H	2.211453	2.079996	0.570326
H	1.913624	-0.863870	-2.045451
H	3.502001	-0.878437	-1.235466
H	2.225525	2.867130	-1.702569
H	1.002611	1.667003	-2.205704
H	-1.282656	1.588978	1.950695
C	-2.404316	-0.002846	-0.148207

Cl	-0.741999	-2.372310	-1.141609
O	2.929172	0.962255	-1.906781
C	-0.698770	2.839736	-0.358614
H	-0.218913	3.808219	-0.151991
H	-0.750110	2.722644	-1.444451
H	-1.722093	2.887098	0.024554
C	2.237869	-2.320701	0.760169
H	2.078971	-2.671698	-0.261231
H	3.311593	-2.380298	0.991469
H	1.716540	-3.013806	1.426671
S	-3.937014	0.236185	-0.283510

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1510.03125987 Predicted Change= -5.186987D-08
Zero-point correction (ZPE)= -1509.7735 0.25769
Internal Energy (U)= -1509.7560 0.27518
Enthalpy (H)= -1509.7551 0.27612
Gibbs Free Energy (G)= -1509.8195 0.21168

Frequencies -- 40.8001 57.0536 63.4771
SCF Energy (M06) = -1509.565524

8. RhDiEt

8.a. Additional Figures

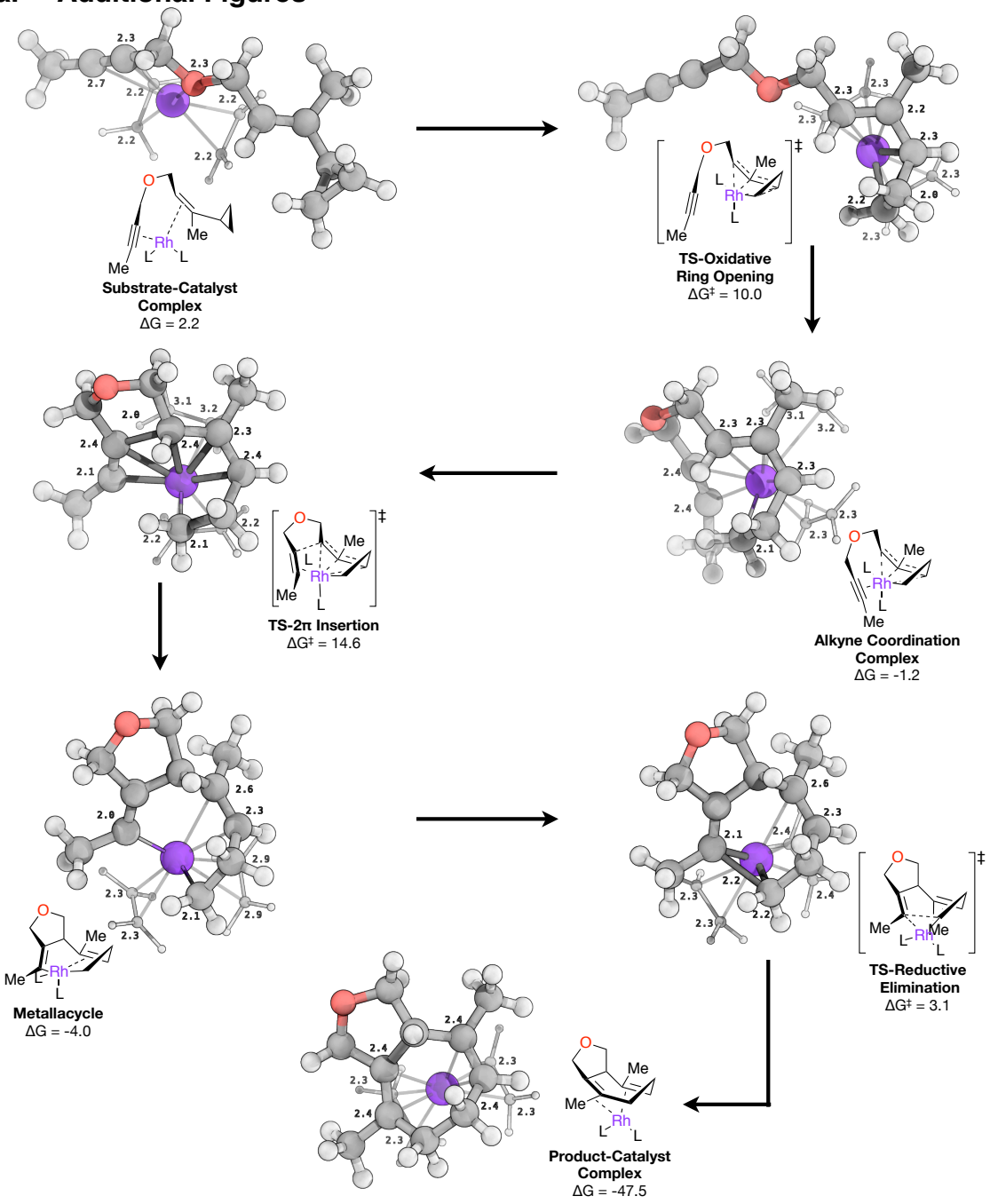


Figure S13. Computed geometries for RhDiEth.

Substrate-Catalyst Complex RhDiEt

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput

scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)] #Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.430457367 Predicted Change= -4.890011D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.01216 ll	0.00180	[NO]	0.01216 ll	0.00180	[NO]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
Rh	1.387873	-0.402414	0.012597
C	-3.320370	0.150692	0.471869
C	-4.379523	-0.568215	-0.298948
C	-5.657171	0.161968	-0.699127
C	-4.701451	-0.324221	-1.753428
C	2.261311	1.777522	-0.065885
C	3.380573	1.396420	-0.373527
H	-6.602876	-0.353806	-0.561952
H	-5.695236	1.232190	-0.515283
H	-4.983840	-1.187375	-2.349146
H	-4.142051	0.424401	-2.306425
H	-4.546558	-1.585370	0.054529
C	2.873402	-1.853604	-0.570986
H	3.544183	-1.369171	-1.275473
C	2.969204	-1.624601	0.808001
H	3.702106	-0.933767	1.218398
C	-0.133259	-1.834884	-0.556431
H	-0.891151	-1.232528	-1.050655
C	-0.024099	-1.821880	0.836130
H	-0.704856	-1.224541	1.437271
C	-2.377693	0.893229	-0.142531
H	-2.381360	0.948645	-1.228953
C	-1.352893	1.754812	0.506915
H	-1.474520	2.801919	0.197124
C	0.966995	2.415276	0.217420
H	0.939524	2.804723	1.243637

O	-0.006733	1.372257	0.048224
H	-1.362797	1.713997	1.599626
H	0.766699	3.239321	-0.479985
C	4.756467	1.071860	-0.735367
H	5.392867	1.942990	-0.540178
H	5.150613	0.237268	-0.145078
H	4.840074	0.822034	-1.798591
C	-3.455224	-0.015798	1.967305
H	-4.408235	0.407704	2.307430
H	-3.483059	-1.081598	2.227882
H	-2.655874	0.453104	2.546498
H	0.278705	-2.648375	-1.145160
H	0.468651	-2.633216	1.363325
H	2.418157	-2.767569	-0.940353
H	2.592795	-2.351881	1.520394

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.430457367 Predicted Change= -4.890011D-07
Zero-point correction (ZPE)= -770.0755 0.35489
Internal Energy (U)= -770.0535 0.37694
Enthalpy (H)= -770.0525 0.37788
Gibbs Free Energy (G)= -770.1290 0.30142

Frequencies -- 16.1854 25.7061 37.1956
SCF Energy (M06) = -769.902515

Oxidative-Addition TS RhDiEt

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)] #Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.412236073 Predicted Change= -1.535604D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00281 II	0.00180	[NO]	0.00281 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	1.239980	-0.536294	0.041697
C	1.312771	1.692183	-0.252051
C	2.413427	1.392194	0.641333
C	2.379916	1.463361	2.135651
C	2.165794	-0.014768	1.986458
C	-4.553067	0.298162	0.034175
C	-5.395508	-0.459303	0.456526
H	3.319451	1.767601	2.594810
H	1.539518	2.020093	2.548919
H	3.045242	-0.634302	2.135446
H	1.237012	-0.415251	2.409683
H	3.402041	1.333849	0.193622
C	-0.479987	-1.564095	-1.092401
H	-1.338151	-0.967148	-0.793908
C	0.394109	-1.141981	-2.062910
H	0.250020	-0.201411	-2.584657
C	2.247483	-2.556489	0.211851
H	2.368212	-2.750760	1.274358
C	3.118949	-1.726509	-0.464731
H	3.942790	-1.240980	0.050201

C	0.018065	1.419368	0.201214
H	-0.160700	1.307899	1.270525
C	-1.250354	1.716741	-0.551106
H	-1.504689	2.782285	-0.399741
C	-3.575420	1.234594	-0.497123
H	-3.581077	1.218088	-1.599134
O	-2.261532	0.887233	-0.020739
H	-1.144385	1.569505	-1.638071
H	-3.808933	2.264810	-0.184868
C	-6.415576	-1.368553	0.970593
H	-6.083588	-1.844814	1.900519
H	-7.345169	-0.829525	1.187253
H	-6.646297	-2.160662	0.249036
C	1.642115	2.270037	-1.606451
H	1.744072	3.359774	-1.518457
H	2.590018	1.879553	-1.988539
H	0.861665	2.076647	-2.345441
H	1.109112	-1.822590	-2.516053
H	-0.465740	-2.594656	-0.747903
H	1.633391	-3.271698	-0.326852
H	3.193042	-1.740622	-1.547353

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.412236073 Predicted Change= -1.535604D-09
Zero-point correction (ZPE)= -770.0596 0.35261
Internal Energy (U)= -770.0379 0.37432
Enthalpy (H)= -770.0369 0.37526
Gibbs Free Energy (G)= -770.1110 0.30121

Frequencies -- -221.3047 23.4057 34.9129
SCF Energy (M06) = -769.8898058

Alkyne Coordination Complex RhDiEt

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)] #Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.431727035 Predicted Change= -7.447566D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00464 ll	0.00180	[NO]	0.00464 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.326025	-1.616700	-0.341814
C	-0.140112	-2.211165	-0.835189
C	0.467340	-1.857286	-2.196518
C	1.017786	-0.445972	-2.003581
C	-0.240407	2.049015	-0.132839
C	0.983955	2.151262	-0.272441
H	1.257672	-2.572262	-2.440797
H	-0.286209	-1.921861	-2.991013
H	2.105813	-0.377543	-2.059167
H	0.556651	0.338416	-2.605756
H	0.184900	-3.133052	-0.359355
C	-1.669215	-0.349910	-0.876573
H	-1.424042	-0.149347	-1.915791
C	-2.815266	0.505963	-0.404268
H	-3.731708	0.210402	-0.929447
C	-1.644681	2.508238	0.049764
H	-1.916442	2.435279	1.114051
O	-2.606536	1.864150	-0.753573
H	-3.002682	0.407131	0.674545
H	-1.679740	3.565102	-0.233635
C	2.301565	2.743656	-0.545781

H	2.165992	3.805537	-0.781415
H	2.974583	2.670726	0.313717
H	2.785970	2.270667	-1.406824
C	-2.075649	-2.255824	0.803352
H	-2.964759	-2.761757	0.405580
H	-1.466715	-3.009575	1.309178
H	-2.423190	-1.531065	1.544002
Rh	0.458319	-0.195187	-0.029976
C	0.178879	-0.629794	3.111078
C	-0.434978	0.525326	2.828190
C	2.288875	-1.459210	0.616676
C	2.644623	-0.130525	0.688073
H	-0.360356	-1.571934	3.153528
H	-1.505138	0.568712	2.646581
H	2.596069	-2.061727	-0.232339
H	3.246846	0.312387	-0.096922
H	2.609739	0.412782	1.627633
H	1.959769	-2.009757	1.491547
H	0.092145	1.474970	2.846070
H	1.232633	-0.664439	3.374741

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.431727035 Predicted Change= -7.447566D-08
Zero-point correction (ZPE)= -770.0772 0.35450
Internal Energy (U)= -770.0554 0.37629
Enthalpy (H)= -770.0544 0.37724
Gibbs Free Energy (G)= -770.1263 0.30534

Frequencies -- 41.5354 53.8898 70.6854
SCF Energy (M06) = -769.9118042

2π-Insertion TS RhDiEt

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)]
#Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.409597250 Predicted Change= -1.408120D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00105 II	0.00180	[YES]	0.00105 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.722362	-0.006941	-0.099948
C	-0.697560	-1.809491	0.249932
C	0.344336	-2.365700	-0.474154
C	0.629509	-2.086872	-1.946796
C	0.841553	-0.577154	-2.085249
C	-1.286023	1.219314	-0.416590
C	-0.156084	1.808644	-0.593566
H	1.528175	-2.636384	-2.239301
H	-0.187916	-2.461881	-2.578409
H	1.817692	-0.300883	-2.486816
H	0.059075	-0.042485	-2.627885
H	0.925752	-3.146213	0.012073
C	0.278489	1.156941	2.706828
H	-0.779178	0.917768	2.782033
C	1.229448	0.261810	3.000600
H	0.992155	-0.748432	3.322907
C	2.637314	1.024413	-0.180469
H	2.787365	1.445031	-1.170150
C	2.877473	-0.332652	0.052304
H	3.212404	-0.978801	-0.753624

C	-1.565056	-0.780238	-0.373947
H	-1.615913	-0.860560	-1.458333
C	-2.975731	-0.619747	0.196843
H	-3.573336	-1.497826	-0.068374
C	-2.731126	1.593629	-0.179529
H	-2.840550	1.948814	0.858837
O	-3.571942	0.493915	-0.417693
H	-2.965481	-0.516270	1.291532
H	-3.020055	2.400156	-0.859867
C	0.389368	3.140661	-0.960053
H	-0.423644	3.852616	-1.143412
H	1.032099	3.544384	-0.170664
H	0.991816	3.075797	-1.873285
C	-1.005469	-2.306886	1.646354
H	-1.923459	-2.908248	1.638351
H	-0.199494	-2.943746	2.019667
H	-1.158671	-1.492316	2.359233
H	2.283072	0.528881	2.991065
H	0.519599	2.184026	2.446651
H	2.664294	1.737242	0.638321
H	3.080813	-0.699703	1.053620

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.409597250 Predicted Change= -1.408120D-09
Zero-point correction (ZPE)= -770.0550 0.35458
Internal Energy (U)= -770.0344 0.37511
Enthalpy (H)= -770.0335 0.37605
Gibbs Free Energy (G)= -770.1027 0.30682

Frequencies -- -222.1580 38.7417 66.4517
SCF Energy (M06) = -769.8881467

Metallacycle RhDiEt

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)] #Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.445989720 Predicted Change= -1.961152D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00125 ll	0.00180	[YES]	0.00125 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.923285	0.184950	-0.089836
C	0.907120	-1.614454	0.002783
C	-0.116695	-1.744636	0.913900
C	-0.213934	-1.061795	2.277232
C	-1.076823	0.160310	2.003100
C	1.923610	0.686630	0.029109
C	0.744987	1.330623	-0.051836
H	-0.672325	-1.739303	3.007093
H	0.769640	-0.774391	2.655208
H	-2.139348	0.026834	2.211459
H	-0.703843	1.101101	2.404597
H	-0.891526	-2.474653	0.691819
C	-2.816499	-1.616952	-1.286252
H	-2.217927	-2.521121	-1.339258
C	-3.434209	-1.247416	-0.152685
H	-3.355618	-1.833895	0.758906
C	-2.178406	1.717614	-1.191699
H	-1.470059	2.232759	-1.833363
C	-2.297509	2.014901	0.145458
H	-1.701813	2.788111	0.613324
C	2.128248	-0.782466	0.319901

H	2.371683	-0.886087	1.386592
C	3.453588	-1.033707	-0.435796
H	4.018186	-1.893491	-0.067978
C	3.322363	1.253803	-0.220066
H	3.637821	1.982725	0.535171
O	4.201925	0.136194	-0.143431
H	3.381958	1.734339	-1.209159
H	3.293153	-1.143376	-1.519157
C	0.713415	2.838647	-0.158093
H	1.705752	3.220644	-0.422687
H	0.020481	3.227414	-0.908890
H	0.450512	3.299188	0.803341
C	0.911549	-2.425616	-1.268934
H	1.067878	-1.798818	-2.154527
H	1.741170	-3.144196	-1.243372
H	-0.013121	-2.991890	-1.398911
H	-3.155959	1.669887	0.713253
H	-2.946494	1.146409	-1.703245
H	-2.966273	-1.091248	-2.225729
H	-4.116339	-0.402160	-0.121162

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.445989720 Predicted Change= -1.961152D-08
Zero-point correction (ZPE)= -770.0888 0.35714
Internal Energy (U)= -770.0682 0.37769
Enthalpy (H)= -770.0673 0.37863
Gibbs Free Energy (G)= -770.1366 0.30930

Frequencies -- 37.1740 58.0310 72.5422
SCF Energy (M06) = -769.920197

Reductive Elimination TS RhDiEt

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)]
#Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.428476711 Predicted Change= -1.410029D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00118 ll	0.00180	[YES]	0.00118 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.892895	-1.647738	0.266367
C	-0.036487	-1.574217	1.279744
C	0.046287	-0.604183	2.454254
C	-0.585230	0.701094	2.004383
C	1.755591	0.732657	0.069328
C	0.564792	1.353516	0.223467
H	-0.500330	-1.015270	3.310998
H	1.084018	-0.455996	2.768993
H	-1.663352	0.764494	2.167670
H	-0.109791	1.607498	2.368786
H	-0.760587	-2.381325	1.351894
C	2.095453	-0.727742	0.281791
H	2.593845	-0.820010	1.260890
C	3.216603	-0.898233	-0.767995
H	3.893446	-1.730676	-0.564191
C	3.030605	1.373026	-0.468210
H	3.465142	2.105774	0.224183
O	3.956683	0.306056	-0.632057
H	2.842701	1.885240	-1.425438
H	2.808801	-1.003492	-1.785634
C	0.510348	2.865714	0.160424

H	1.150047	3.309521	0.933477
H	0.887426	3.227934	-0.805537
H	-0.488842	3.281580	0.297746
C	0.894615	-2.795477	-0.709347
H	0.937260	-2.458338	-1.750767
H	1.792212	-3.405536	-0.540219
H	0.026762	-3.446514	-0.579196
Rh	-1.018268	0.047501	-0.100122
C	-1.885344	1.630003	-1.487807
C	-2.572028	1.702010	-0.293725
C	-2.280078	-1.504690	-1.336948
C	-2.940841	-1.427001	-0.140273
H	-1.069207	2.303995	-1.716427
H	-2.320999	2.440482	0.459750
H	-1.567784	-2.297494	-1.536959
H	-2.760486	-2.137597	0.659244
H	-3.821559	-0.806110	-0.017574
H	-2.643452	-0.970997	-2.208946
H	-3.550856	1.247915	-0.186641
H	-2.298898	1.096477	-2.336882

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.428476711 Predicted Change= -1.410029D-08
Zero-point correction (ZPE)= -770.0714 0.35704
Internal Energy (U)= -770.0521 0.37632
Enthalpy (H)= -770.0512 0.37726
Gibbs Free Energy (G)= -770.1172 0.31119

Frequencies -- -316.9295 45.8613 49.6956
SCF Energy (M06) = -769.9108324

Reductive Elimination TS Rh-Mono-Et

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcall,ts,noeigentest)

Pointgroup= C1 Stoichiometry= C13H20ORh(1+) C1[X(C13H20ORh)]
#Atoms= 35
Charge = 1 Multiplicity = 1

SCF Energy= -691.817574094 Predicted Change= -9.180737D-10

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00050 ll	0.00180	[YES]	0.00050 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.760655	0.083520	-0.218485
C	0.541092	-1.796164	-0.288800
C	-0.584911	-2.242285	0.384564
C	-0.979088	-1.822947	1.799198
C	-1.212169	-0.311756	1.759735
C	1.263445	1.224491	0.061986
C	0.167600	1.904853	0.005177
H	-1.892611	-2.351243	2.084278
H	-0.205771	-2.110709	2.523639
H	-2.242327	-0.011729	1.953027
H	-0.523297	0.294139	2.352226
H	-1.176974	-3.018906	-0.094237
C	-2.595639	1.200991	-0.584186
H	-2.424465	1.855104	-1.434944
C	-2.848674	-0.158985	-0.784519
H	-2.858735	-0.576609	-1.789137
C	1.417493	-0.770501	0.330797
H	1.357721	-0.742218	1.417865
C	2.885883	-0.752458	-0.103157
H	3.394040	-1.626213	0.316939
C	2.753473	1.501816	0.007802
H	3.018192	1.755227	-1.031574

O	3.484240	0.389320	0.453467
H	2.988918	-0.771029	-1.197218
H	2.996978	2.351577	0.652261
C	-0.292215	3.317924	0.051991
H	0.553494	3.992647	0.227182
H	-0.776942	3.610986	-0.885139
H	-1.017839	3.465040	0.859454
C	0.895922	-2.361205	-1.648223
H	1.794799	-2.986834	-1.582957
H	0.085132	-2.984157	-2.033880
H	1.100436	-1.574603	-2.383289
H	-3.372934	-0.742171	-0.033072
H	-2.915538	1.696120	0.328473

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -691.817574094 Predicted Change= -9.180737D-10
Zero-point correction (ZPE)= -691.5165 0.30100
Internal Energy (U)= -691.5001 0.31742
Enthalpy (H)= -691.4992 0.31836
Gibbs Free Energy (G)= -691.5589 0.25859

Frequencies -- -213.0195 72.5718 86.4542
SCF Energy (M06) = -691.3586927

Ethylene

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= CS Stoichiometry= C2H4 CS[SG(C2H4)] #Atoms= 6

Charge = 0 Multiplicity = 1

SCF Energy= -78.5858248474 Predicted Change= -2.375630D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ll	0.00045	[YES]	0.00003 ll	0.00030	[YES]
Displ	0.00015 ll	0.00180	[YES]	0.00015 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.665618	0.000000
H	-0.923772	1.239626	0.000000
H	0.923772	1.239626	0.000000
C	0.000000	-0.665618	0.000000
H	0.923772	-1.239626	0.000000
H	-0.923772	-1.239627	0.000000

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -78.5858248474 Predicted Change= -2.375630D-08

Zero-point correction (ZPE)=	-78.5345	0.05123
Internal Energy (U)=	-78.5315	0.05427
Enthalpy (H)=	-78.5306	0.05522
Gibbs Free Energy (G)=	-78.5567	0.02905

Frequencies -- 835.2126 956.4483 975.8595

SCF Energy (M06) = -78.5098784606

Product-Catalyst Complex RhDiEt

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C15H24ORh(1+) C1[X(C15H24ORh)] #Atoms= 41
Charge = 1 Multiplicity = 1

SCF Energy= -770.505795816 Predicted Change= -5.237088D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00343 ll	0.00180	[NO]	0.00343 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.893516	-0.098964	-0.122378
C	-0.474002	1.760910	0.443459
C	0.208188	1.403611	1.589156
C	-0.389076	0.530543	2.677698
C	-0.460907	-0.966597	2.343795
C	-1.508677	-0.489100	0.032375
C	-0.920180	-1.339913	0.942744
H	0.196024	0.651927	3.593344
H	-1.396008	0.906379	2.905396
H	0.520882	-1.425744	2.517769
H	-1.139977	-1.466841	3.051405
H	1.055043	2.021148	1.878005
C	1.971388	-1.996625	-0.783885
H	1.677179	-2.749725	-0.059197
C	1.133651	-1.626690	-1.810123
H	0.154966	-2.079673	-1.916563
C	2.942468	0.806877	0.121019
H	2.868087	1.575464	0.882295
C	2.524050	1.049821	-1.173271
H	2.098734	2.006789	-1.457833
C	-1.771159	1.023192	0.148891

H	-2.500588	1.214980	0.951565
C	-2.465331	1.311526	-1.201270
H	-3.169596	2.144515	-1.164115
C	-2.339822	-0.957433	-1.168863
H	-2.967175	-1.821386	-0.930566
O	-3.196745	0.128805	-1.469079
H	-1.717756	-1.213914	-2.040414
H	-1.729165	1.499198	-1.998232
C	-1.009919	-2.839386	0.735946
H	-0.190174	-3.363047	1.237644
H	-1.941127	-3.206520	1.189905
H	-1.021658	-3.141210	-0.314034
C	-0.143710	3.026376	-0.307642
H	-0.911022	3.779542	-0.077865
H	0.818699	3.440964	0.005383
H	-0.141141	2.899599	-1.393691
H	1.495481	-1.087856	-2.679978
H	3.032174	-1.768498	-0.818940
H	2.873991	0.434864	-1.996359
H	3.618122	-0.010689	0.354552

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -770.505795816 Predicted Change= -5.237088D-08
Zero-point correction (ZPE)= -770.1460 0.35973
Internal Energy (U)= -770.1264 0.37931
Enthalpy (H)= -770.1255 0.38025
Gibbs Free Energy (G)= -770.1923 0.31341

Frequencies -- 33.2757 63.1107 92.2130
SCF Energy (M06) = -769.9936668

9. RhCOT

9.a. Additional Figures

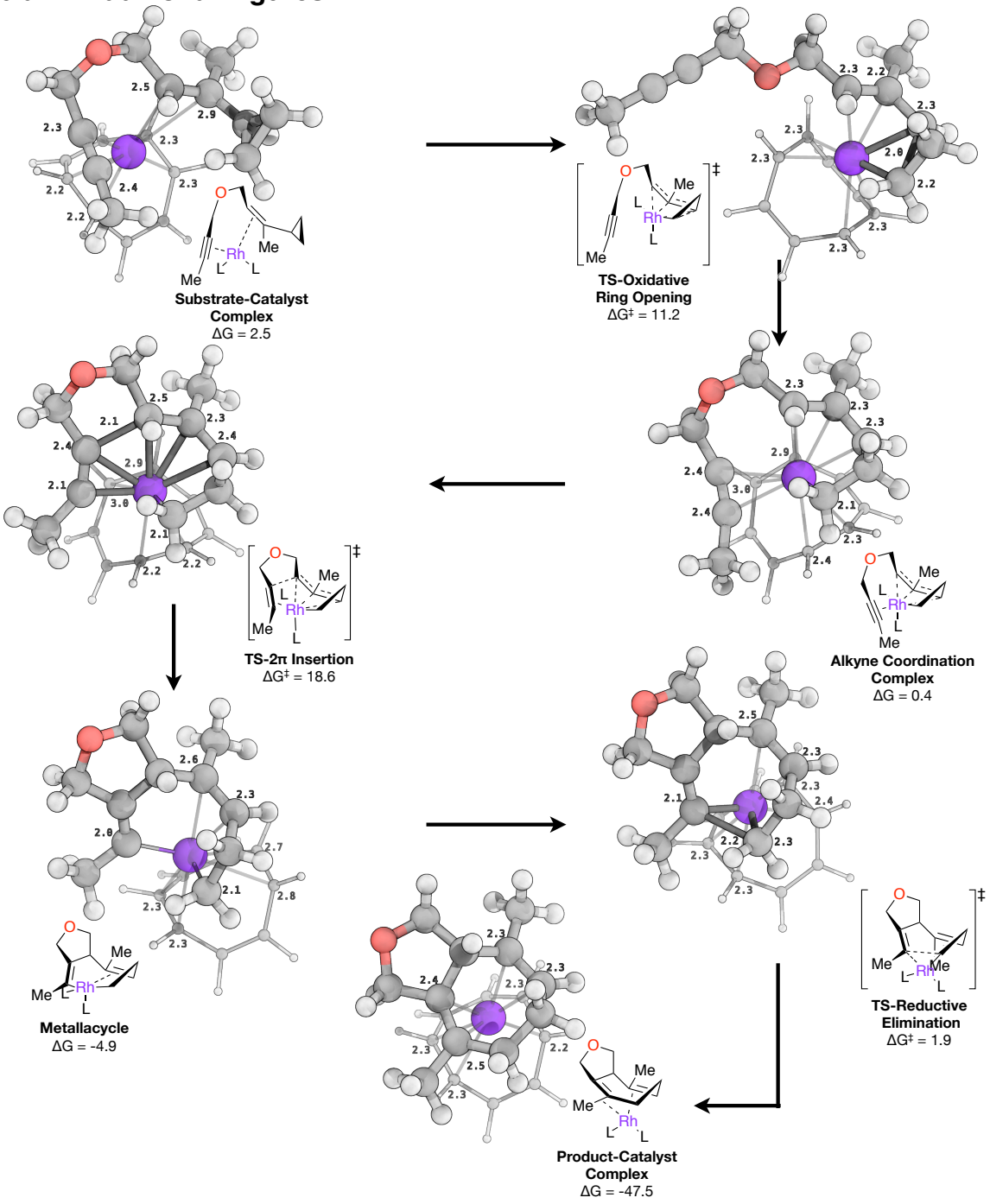


Figure S14. Computed geometries for RhCOT.

Substrate-Catalyst Complex RhCOT

Supporting Information: 000-COT-VCP-Complex-BisCoord2.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

```
=====================================================================
 # b3lyp/gen pseudo=read gfprint gfinput
 scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq
---------------------------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C19H24ORh(1+)   C1[X(C19H24ORh)]
#Atoms= 45
 Charge = 1   Multiplicity = 1
---------------------------------------------------------------------------------------------------
 SCF Energy= -922.824614402      Predicted Change= -3.565694D-08
=====================================================================
 Optimization completed. {Found  2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 II  0.00045   [ YES ]      0.00000 II  0.00030   [ YES ]
 Displ      0.00152 II  0.00180   [ YES ]      0.00152 II  0.00180   [ YES ]
---------------------------------------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
       Type        X           Y        Z
---------------------------------------------------------------------------------------------------
       C         2.116199     -0.941262     -0.647197
       C         2.568830     -1.754615      0.512437
       C         3.966153     -1.500943      1.096125
       C         2.746342     -1.227793      1.918559
       C        -0.012938      2.344124      0.324553
       C        -0.064871      2.028358      1.514255
       H         4.576209     -2.370131      1.322531
       H         4.515019     -0.650103      0.702704
       H         2.503477     -1.909861      2.728129
       H         2.493626     -0.191822      2.122950
       H         2.312632     -2.809274      0.433995
       C         1.908066      0.411513     -0.576839
       H         2.176402      0.912702      0.348967
       C         1.858660      1.358266     -1.771501
       H         2.833657      1.371694     -2.272782
       C         0.335094      3.010799     -0.960670
       H        -0.397901      2.754877     -1.739475
       O         1.649489      2.704658     -1.372395
       H         1.107696      1.057627     -2.517807
       H         0.308233      4.095004     -0.808492
       C        -0.040220      1.909675      2.975366
       H         0.371055      2.833814      3.399251
       H        -1.040044      1.763857      3.396211
       H         0.589707      1.074609      3.298571
```

C	2.124915	-1.685829	-1.958672
H	3.168014	-1.927725	-2.205243
H	1.600912	-2.646573	-1.891392
H	1.715158	-1.112677	-2.793081
Rh	-0.496249	0.124743	0.075836
C	-0.994685	-2.088054	-0.135332
C	-1.191918	-1.483872	-1.374451
C	-2.420111	0.069524	1.120742
C	-2.597249	0.685468	-0.139189
C	-2.093229	-2.351117	0.829427
H	-0.062593	-2.623983	0.032680
H	-0.402311	-1.578258	-2.115501
C	-2.511501	-1.035535	-1.887070
H	-2.386059	0.728700	1.984940
C	-2.757307	-1.347647	1.409759
H	-2.658393	1.772981	-0.147221
C	-3.158521	-0.013180	-1.320952
H	-2.319677	-3.390952	1.059265
H	-2.906155	-1.544011	-2.765122
H	-3.548071	-1.537644	2.133737
H	-4.105542	0.349202	-1.717396

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.824614402 Predicted Change= -3.565694D-08
Zero-point correction (ZPE)= -922.4443 0.38027
Internal Energy (U)= -922.4213 0.40326
Enthalpy (H)= -922.4204 0.40420
Gibbs Free Energy (G)= -922.4963 0.32829

Frequencies -- 26.6787 41.2744 61.2722
SCF Energy (M06) = -922.2023053

Oxidative-Addition TS RhCOT

Supporting Information: 015-COT-VCP-Opening-TS-Linear.log

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H24ORh(1+) C1[X(C19H24ORh)]
#Atoms= 45
Charge = 1 Multiplicity = 1

SCF Energy= -922.815406945 Predicted Change= -1.365868D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00042 II	0.00180	[YES]	0.00042 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	1.042665	0.014611	-0.310882
C	1.128956	-2.065383	0.481834
C	2.209156	-2.009512	-0.479119
C	2.140383	-2.408953	-1.917348
C	1.930263	-0.932970	-2.106583
C	-4.641163	-0.370779	0.124845
C	-5.441055	0.382292	-0.380229
H	3.067469	-2.817109	-2.318095
H	1.289451	-3.037568	-2.178140
H	2.817278	-0.369834	-2.381085
H	1.011072	-0.636334	-2.622663
H	3.206539	-1.852590	-0.076372
C	-0.461084	1.475384	0.632613
H	-1.418438	0.963245	0.544914
C	-0.294684	2.726699	-0.151607
C	0.391808	1.090516	1.657077
H	0.041146	0.312202	2.332328
C	1.575615	1.858126	2.113741
C	1.883886	1.994410	-1.083906
H	2.215656	1.822207	-2.107352

C	2.731655	1.581752	-0.060541
C	2.644711	2.066706	1.337435
H	3.665631	1.098353	-0.345046
H	-1.113320	3.443172	-0.104098
C	0.770897	2.965249	-0.925262
H	1.564062	2.213519	3.143259
H	3.516337	2.593114	1.724262
H	0.831377	3.877343	-1.516956
C	-0.176598	-1.868864	0.005024
H	-0.384660	-2.024841	-1.053231
C	-1.428168	-1.929250	0.837397
H	-1.771546	-2.979846	0.871848
C	-3.714882	-1.297631	0.757274
H	-3.688013	-1.134215	1.847130
O	-2.396367	-1.113392	0.211969
H	-1.261376	-1.617828	1.880695
H	-4.031016	-2.339958	0.592240
C	-6.411187	1.284844	-0.993566
H	-6.017590	1.709079	-1.924732
H	-7.339388	0.754921	-1.236892
H	-6.663616	2.115731	-0.324713
C	1.488104	-2.316153	1.926448
H	1.544724	-3.398925	2.099686
H	2.463752	-1.888171	2.174333
H	0.745822	-1.914928	2.619464

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.815406945 Predicted Change= -1.365868D-10
Zero-point correction (ZPE)= -922.4371 0.37820
Internal Energy (U)= -922.4142 0.40111
Enthalpy (H)= -922.4133 0.40205
Gibbs Free Energy (G)= -922.4905 0.32488

Frequencies -- -227.6317 17.9266 32.7448
SCF Energy (M06) = -922.1849636

Alkyne Coordination Complex RhCOT

Supporting Information: 020-COT-Open-VCP-Complex-Ene.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H24ORh(1+) C1[X(C19H24ORh)]
#Atoms= 45
Charge = 1 Multiplicity = 1

SCF Energy= -922.834487984 Predicted Change= -1.232560D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00201 II	0.00180	[NO]	0.00201 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	0.029356	-0.030859	0.387148
C	1.465215	-1.818513	0.067568
C	0.650939	-2.044007	1.200185
C	0.930846	-1.417322	2.568046
C	0.594983	0.057253	2.373785
C	0.980206	1.996159	-0.372741
C	0.162269	2.405945	0.454466
H	0.292108	-1.885457	3.322175
H	1.971246	-1.587243	2.871427
H	-0.274219	0.395646	2.942294
H	1.423153	0.758238	2.491179
H	-0.020529	-2.898171	1.160345
C	-1.449529	0.447873	-2.123087
H	-0.759409	1.007004	-2.755354
C	-2.556676	1.224881	-1.531231
C	-1.318120	-0.896624	-2.075566
H	-0.534617	-1.351288	-2.680267
C	-2.253598	-1.832995	-1.417310
C	-2.213432	0.500492	0.857868
H	-2.158306	1.025308	1.809315

C	-2.087616	-0.883052	0.913901
C	-2.573845	-1.831722	-0.115916
H	-1.950326	-1.314798	1.903414
H	-3.114007	1.854587	-2.224029
C	-2.880760	1.249856	-0.232308
H	-2.668520	-2.612562	-2.055702
H	-3.243218	-2.605009	0.260004
H	-3.700275	1.891593	0.090929
C	2.209586	-0.609174	0.044707
H	2.615656	-0.235177	0.980686
C	2.996424	-0.125740	-1.148208
H	4.003813	-0.558959	-1.125046
C	2.031442	2.013253	-1.422174
H	1.607997	1.676296	-2.382274
O	3.192793	1.277920	-1.107730
H	2.529900	-0.415884	-2.101088
H	2.357234	3.051265	-1.544868
C	-0.602497	3.264075	1.366893
H	-0.159991	4.266934	1.364895
H	-1.646585	3.352068	1.052413
H	-0.575406	2.890168	2.395893
C	1.401442	-2.772280	-1.101385
H	2.234946	-3.481503	-1.012666
H	0.474085	-3.350193	-1.099097
H	1.508245	-2.277707	-2.069356

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.834487984 Predicted Change= -1.232560D-07
Zero-point correction (ZPE)= -922.4531 0.38137
Internal Energy (U)= -922.4307 0.40369
Enthalpy (H)= -922.4298 0.40463
Gibbs Free Energy (G)= -922.5021 0.33237

Frequencies -- 57.3766 66.0326 76.1570
SCF Energy (M06) = -922.2096651

2π-Insertion TS RhCOT

Supporting Information: 025-COT-TS-2Pi-Insertion-Ene2.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H24ORh(1+) C1[X(C19H24ORh)]
#Atoms= 45
Charge = 1 Multiplicity = 1

SCF Energy= -922.811300380 Predicted Change= -2.206133D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00161 ll	0.00180	[YES]	0.00161 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.302417	-1.752168	-0.294494
C	0.613689	-2.340497	0.753095
C	0.761246	-1.950389	2.220399
C	0.399295	-0.466610	2.332219
C	1.623004	1.407142	-0.025738
C	0.550636	1.866587	0.510184
H	0.080826	-2.565010	2.816052
H	1.776816	-2.167293	2.580139
H	-0.431633	-0.263397	3.010225
H	1.232113	0.199547	2.567496
H	0.012362	-3.217104	0.521908
C	2.164307	-0.580316	-0.041530
H	2.545354	-0.529586	0.976284
C	3.288963	-0.300655	-1.036330
H	4.065259	-1.064661	-0.922228
C	2.848106	1.898513	-0.753584
H	2.574867	2.133316	-1.795902
O	3.872881	0.937105	-0.715753
H	2.930041	-0.315005	-2.075459

H	3.217616	2.809685	-0.273361
C	0.004163	3.143084	1.040196
H	0.742640	3.946289	0.934872
H	-0.909632	3.432263	0.515192
H	-0.236827	3.045719	2.105251
C	1.238133	-2.356705	-1.681199
H	2.165205	-2.905259	-1.892535
H	0.410096	-3.065650	-1.762161
H	1.124730	-1.602810	-2.464765
Rh	-0.195683	-0.078488	0.391946
C	-1.691368	-0.458742	-2.114126
C	-1.650541	0.888129	-2.011265
C	-2.228589	-0.704508	0.924401
C	-2.158776	0.705635	1.014280
C	-2.685305	-1.346810	-1.476742
H	-1.011397	-0.935807	-2.818650
H	-0.928315	1.427649	-2.624752
C	-2.613952	1.712071	-1.253982
H	-2.157779	-1.249027	1.864328
C	-2.904969	-1.458146	-0.157719
H	-2.024992	1.111765	2.015664
C	-2.826007	1.632851	0.065339
H	-3.236029	-2.001118	-2.151820
H	-3.154508	2.461953	-1.830891
H	-3.628594	-2.195558	0.188253
H	-3.542238	2.313425	0.524901

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.811300380 Predicted Change= -2.206133D-08
Zero-point correction (ZPE)= -922.4297 0.38150
Internal Energy (U)= -922.4087 0.40252
Enthalpy (H)= -922.4078 0.40346
Gibbs Free Energy (G)= -922.4773 0.33392

Frequencies -- -228.5597 54.8829 62.2199
SCF Energy (M06) = -922.1822673

Metallacycle RhCOT

Supporting Information: 030-COT-Metallacycle-Ene.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H24ORh(1+) C1[X(C19H24ORh)]
#Atoms= 45
Charge = 1 Multiplicity = 1

SCF Energy= -922.854101296 Predicted Change= -8.951722D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00316 ll	0.00180	[NO]	0.00316 ll	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
Rh	-0.466152	0.042607	0.077661
C	1.490353	-1.583899	-0.102151
C	0.553371	-1.866459	0.867506
C	0.518786	-1.299919	2.286327
C	-0.365916	-0.064346	2.164955
C	2.341445	0.773470	0.081772
C	1.113415	1.314450	0.116464
H	0.098170	-2.041578	2.974332
H	1.519441	-1.041593	2.641213
H	-1.395149	-0.197354	2.497739
H	0.066862	0.856330	2.553665
H	-0.186868	-2.629928	0.636357
C	-2.411571	-1.413116	-1.091022
H	-1.892396	-2.299901	-1.455272
C	-2.724822	-0.397638	-2.118259
C	-2.851576	-1.424206	0.191435
H	-2.647491	-2.314090	0.788008
C	-3.731347	-0.418664	0.819962
C	-1.829732	1.611531	-0.891938
H	-1.164247	2.420643	-1.175201

C	-2.216353	1.552761	0.439931
C	-3.436694	0.880526	0.944220
H	-1.800627	2.308496	1.102338
H	-3.128920	-0.784342	-3.052982
C	-2.467667	0.918973	-2.029376
H	-4.650554	-0.799602	1.262950
H	-4.123787	1.534180	1.480574
H	-2.666904	1.548424	-2.895320
C	2.675084	-0.695596	0.203467
H	3.011001	-0.886706	1.232732
C	3.948799	-0.760546	-0.669219
H	4.604447	-1.603403	-0.438544
C	3.668091	1.477302	-0.197273
H	3.987388	2.146493	0.611078
O	4.631388	0.432034	-0.309301
H	3.616555	2.064612	-1.126999
H	3.708770	-0.773478	-1.743589
C	0.935958	2.817148	0.107554
H	1.845586	3.311241	0.467957
H	0.735653	3.213826	-0.896605
H	0.125369	3.152052	0.762939
C	1.443092	-2.280666	-1.438729
H	1.513183	-1.570319	-2.270306
H	2.300786	-2.959939	-1.532195
H	0.533181	-2.874320	-1.558971

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.854101296 Predicted Change= -8.951722D-08
Zero-point correction (ZPE)= -922.4703 0.38375
Internal Energy (U)= -922.4491 0.40498
Enthalpy (H)= -922.4481 0.40592
Gibbs Free Energy (G)= -922.5186 0.33541

Frequencies -- 37.7177 63.8244 83.9586
SCF Energy (M06) = -922.2211138

Reductive Elimination TS RhCOT

Supporting Information: 035-COT-TS-ReductiveElim-Ene.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H24ORh(1+) C1[X(C19H24ORh)]
#Atoms= 45
Charge = 1 Multiplicity = 1

SCF Energy= -922.834789935 Predicted Change= -6.503556D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00137 II	0.00180	[YES]	0.00137 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.549676	-0.006106	0.162134
C	1.399192	-1.604145	0.320110
C	0.605902	-1.532894	1.447054
C	0.823389	-0.535394	2.580150
C	0.152021	0.762488	2.161821
C	2.201519	0.774428	-0.022197
C	1.016032	1.358260	0.254581
H	0.370182	-0.916334	3.502472
H	1.890106	-0.387896	2.776843
H	-0.897859	0.841974	2.449566
H	0.672846	1.673391	2.444705
H	-0.091544	-2.348199	1.624168
C	-1.979475	-1.520485	-0.922507
H	-1.378502	-2.407678	-1.110021
C	-2.430523	-0.780896	-2.129228
C	-2.518251	-1.370757	0.342521
H	-2.295076	-2.136894	1.083151
C	-3.619979	-0.439059	0.677564
C	-1.728474	1.407907	-1.203325

H	-1.024493	2.163558	-1.542121
C	-2.251187	1.536519	0.080511
C	-3.499885	0.884580	0.549983
H	-1.917337	2.386237	0.672507
H	-2.826981	-1.378652	-2.948617
C	-2.309684	0.545512	-2.259332
H	-4.539715	-0.881391	1.057715
H	-4.319832	1.548674	0.819948
H	-2.602356	1.040449	-3.183977
C	2.588624	-0.674812	0.178568
H	3.201924	-0.748168	1.091636
C	3.574719	-0.851248	-0.998659
H	4.288260	-1.667007	-0.863356
C	3.383186	1.424424	-0.729777
H	3.887875	2.181551	-0.115565
O	4.302859	0.368306	-0.983879
H	3.066779	1.908593	-1.667637
H	3.046010	-0.987738	-1.955104
C	0.869109	2.858233	0.117527
H	1.025507	3.172996	-0.922943
H	-0.107070	3.232830	0.430960
H	1.620267	3.381421	0.722628
C	1.289349	-2.763273	-0.636347
H	1.187893	-2.435511	-1.676440
H	2.208579	-3.362031	-0.581737
H	0.453572	-3.422192	-0.387872

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.834789935 Predicted Change= -6.503556D-09
Zero-point correction (ZPE)= -922.4521 0.38260
Internal Energy (U)= -922.4317 0.40306
Enthalpy (H)= -922.4307 0.40400
Gibbs Free Energy (G)= -922.4992 0.33558

Frequencies -- -348.0643 44.4661 59.1036
SCF Energy (M06) = -922.2104806

Product-Catalyst Complex RhCOT

Supporting Information: 040-COT-Product-Complex-Ene-Boat2.log

---

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C19H24ORh(1+) C1[X(C19H24ORh)]
#Atoms= 45
Charge = 1 Multiplicity = 1

SCF Energy= -922.911959486 Predicted Change= -1.809687D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00233 II	0.00180	[NO]	0.00233 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.238907	-1.394492	0.981526
C	0.739000	-0.657721	2.047246
C	1.440812	0.571122	2.603523
C	1.291824	1.845503	1.759474
C	1.828618	0.582780	-0.429274
C	1.360129	1.684208	0.251076
H	1.058922	0.775833	3.607451
H	2.505469	0.329218	2.725987
H	0.339239	2.331138	2.003479
H	2.068137	2.571926	2.046470
H	0.063931	-1.174073	2.727766
C	2.330633	-0.758352	0.135290
H	3.240542	-0.605474	0.737134
C	2.725789	-1.497495	-1.164310
H	3.541125	-2.211400	-1.034541
C	2.263127	0.604673	-1.899372
H	2.791439	1.524223	-2.167329
O	3.175827	-0.469475	-2.028808
H	1.413068	0.484428	-2.590527
H	1.859447	-2.016448	-1.602502

C	1.167685	2.991966	-0.489024
H	0.380320	3.599284	-0.031585
H	2.095914	3.577178	-0.422144
H	0.939346	2.865538	-1.550031
C	0.985799	-2.877040	0.858349
H	1.919103	-3.406785	1.097987
H	0.231927	-3.218577	1.572255
H	0.691092	-3.188487	-0.147433
Rh	-0.434279	-0.004167	0.181746
C	-1.527916	0.375400	-1.841815
C	-1.852145	1.416285	-0.987262
C	-2.073420	-1.542793	0.293471
C	-2.390737	-0.497262	1.166503
C	-2.367902	-0.826518	-2.054528
H	-0.741607	0.554265	-2.573986
H	-1.313261	2.352658	-1.111851
C	-3.078995	1.477430	-0.155690
H	-1.653303	-2.443015	0.736012
C	-2.624621	-1.699417	-1.074705
H	-2.195575	-0.654067	2.226435
C	-3.318070	0.611828	0.835844
H	-2.746560	-0.990230	-3.062244
H	-3.764647	2.300380	-0.351220
H	-3.218675	-2.591660	-1.266758
H	-4.200544	0.716862	1.465142

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -922.911959486 Predicted Change= -1.809687D-07
Zero-point correction (ZPE)= -922.5265 0.38544
Internal Energy (U)= -922.5058 0.40610
Enthalpy (H)= -922.5049 0.40705
Gibbs Free Energy (G)= -922.5743 0.33762

Frequencies -- 23.0851 57.0532 75.2880
SCF Energy (M06) = -922.2913007

10. RhdnCOT

10.a. Additional Figures

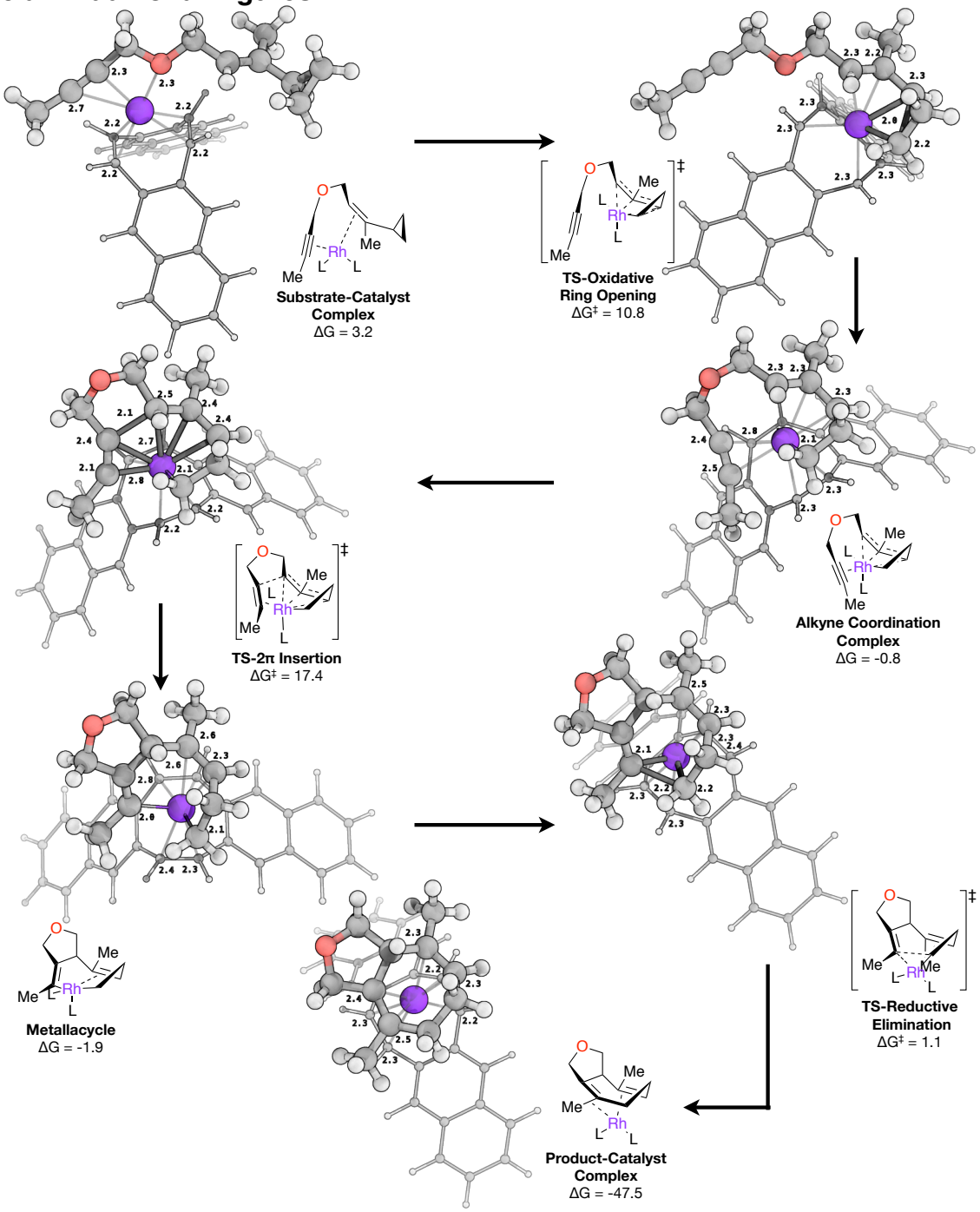


Figure S15. Computed geometries for RhdnCOT.

Substrate-Catalyst Complex RhdnCOT

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)]
#Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.43332309 Predicted Change= -1.436827D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00374 II	0.00180	[NO]	0.00374 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.973396	-0.176332	-2.179885
C	-3.910920	0.823315	-3.290017
C	-5.196365	1.341138	-3.923901
C	-4.298756	2.276344	-3.160366
C	-2.381884	-0.727229	3.396131
C	-1.439552	-0.594462	4.161405
C	-4.103110	0.202085	-0.893269
C	-4.295112	-0.685933	0.287251
C	-3.614548	-0.875077	2.609068
O	-3.281056	-0.385855	1.301059
C	-0.412135	-0.464285	5.190340
C	-3.917921	-1.607452	-2.661556
H	-5.238661	1.413705	-5.006640
H	-6.133066	1.053793	-3.454048
H	-3.711155	2.999182	-3.718978
H	-4.658001	2.648940	-2.205789
H	-3.119970	0.610805	-4.009258
H	-4.141230	1.263880	-0.659958
H	-5.262321	-0.485191	0.769738
H	-3.920576	-1.928753	2.559639
H	-4.241393	-1.753175	0.052819
H	-4.438171	-0.287580	3.036206
H	-0.789970	-0.882908	6.130476
H	0.500628	-1.010159	4.928197
H	-0.156185	0.586061	5.366749

H	-4.796581	-1.830840	-3.279360
H	-3.043164	-1.755638	-3.307591
H	-3.873990	-2.349015	-1.860312
Rh	-1.032660	-0.277166	1.525647
C	0.987939	-0.967540	1.848165
C	0.941300	0.435413	2.045731
C	-0.481725	-0.671734	-0.535182
C	-0.538119	0.726617	-0.340748
C	1.500444	-1.640149	0.624920
C	1.390848	1.456608	1.061648
C	0.762817	-1.484979	-0.581348
C	0.642116	1.606843	-0.138731
C	1.168872	-2.135371	-1.727078
C	2.341910	-2.936700	-1.738343
C	3.083684	-3.094703	-0.521149
C	2.620857	-2.443287	0.652988
C	2.792350	-3.601434	-2.909659
C	3.926245	-4.382746	-2.880612
C	4.658856	-4.538980	-1.677923
C	4.245731	-3.911120	-0.523859
C	0.980706	2.588394	-1.046000
C	2.098320	3.436634	-0.824651
C	2.853000	3.285325	0.385378
C	2.456549	2.292411	1.320498
C	2.480502	4.441178	-1.752929
C	3.561765	5.255666	-1.499101
C	4.307150	5.106255	-0.303406
C	3.959213	4.144584	0.619110
H	0.990161	-1.585027	2.746797
H	0.923070	0.776991	3.080323
H	-1.359034	-1.119594	-1.001582
H	-1.451132	1.217353	-0.676706
H	0.590327	-2.041509	-2.643597
H	3.168512	-2.587391	1.581902
H	2.229218	-3.481732	-3.831741
H	4.264397	-4.883915	-3.782809
H	5.550891	-5.158379	-1.670538
H	4.806392	-4.030975	0.399675
H	0.390344	2.724377	-1.949473
H	3.011160	2.200324	2.251966
H	1.906907	4.555837	-2.669182
H	3.848149	6.018587	-2.217028
H	5.157154	5.756075	-0.117225
H	4.529645	4.029389	1.537236

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.43332309 Predicted Change= -1.436827D-08
Zero-point correction (ZPE)= -1536.8646 0.56868
Internal Energy (U)= -1536.8306 0.60270
Enthalpy (H)= -1536.8296 0.60365
Gibbs Free Energy (G)= -1536.9333 0.50001

Frequencies -- 13.3944 21.1444 22.3200
SCF Energy (M06) = -1536.322608

Oxidative-Addition TS RhdnCOT

Using Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)]
#Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.41546254 Predicted Change= -2.111574D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00700 II	0.00180	[NO]	0.00700 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Rh	-0.291566	-1.481555	-1.035460
C	-0.257460	-3.640527	-0.448571
C	0.144720	-3.628441	-1.839071
C	-0.749420	-3.808694	-3.023663
C	-0.691564	-2.307054	-3.050429
C	-4.817332	-0.991488	2.460525
C	-5.592122	-0.063952	2.495116
C	-1.539256	-3.169159	-0.136038
C	-2.149332	-3.146348	1.238284
C	-3.908451	-2.128349	2.457260
O	-3.092405	-2.095202	1.275632
C	-6.534279	1.050932	2.532878
C	0.745040	-4.141872	0.563287
H	-0.288029	-4.323907	-3.865634
H	-1.727881	-4.231465	-2.795815
H	0.021165	-1.881920	-3.750866
H	-1.651470	-1.782405	-2.989110
H	1.211062	-3.706653	-2.034319
H	-2.294709	-3.124927	-0.920284
H	-2.649463	-4.117002	1.414107
H	-3.263514	-2.109701	3.351490

H	-1.397148	-3.030890	2.034081
H	-4.470859	-3.075644	2.483325
H	-6.501564	1.622163	1.597639
H	-7.561720	0.693630	2.668153
H	-6.306602	1.738883	3.355440
H	0.678949	-5.236144	0.624580
H	1.767674	-3.885567	0.271691
H	0.563427	-3.748295	1.565169
C	-0.707313	0.075827	0.602205
C	-0.729957	1.397031	-0.077433
C	0.430513	-0.611387	1.002035
C	1.845402	-0.194282	0.829649
C	0.456214	0.392938	-2.072488
C	1.586001	-0.326452	-1.682593
C	2.412036	-0.085740	-0.476063
C	-0.151941	1.555810	-1.371875
C	-0.240837	2.774346	-2.016287
C	-0.853615	3.896390	-1.400676
C	-1.436725	3.735186	-0.101206
C	-1.376425	2.460829	0.519824
C	-0.926691	5.164244	-2.036810
C	-1.544245	6.225431	-1.413061
C	-2.120617	6.066107	-0.127986
C	-2.070365	4.848123	0.512711
C	2.647102	-0.007974	1.938490
C	4.019505	0.333097	1.816845
C	4.589819	0.432701	0.505714
C	3.757975	0.193419	-0.618233
C	4.849007	0.554293	2.947964
C	6.181501	0.864352	2.788240
C	6.745565	0.962269	1.491740
C	5.968256	0.749047	0.375040
H	-1.649921	-0.249065	1.040508
H	0.273896	-1.399137	1.736522
H	0.183266	0.309123	-3.123862
H	2.070160	-0.912632	-2.463326
H	0.167665	2.888454	-3.018111
H	-1.850486	2.328522	1.489703
H	-0.485155	5.284787	-3.022743
H	-1.592144	7.192319	-1.905275
H	-2.603653	6.912896	0.350709
H	-2.512016	4.724246	1.498186
H	2.225688	-0.122097	2.935004
H	4.198242	0.243121	-1.611869

H	4.415581	0.478488	3.941887
H	6.807659	1.036233	3.658736
H	7.797770	1.207935	1.382819
H	6.399576	0.824343	-0.619852

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.41546254 Predicted Change= -2.111574D-09
Zero-point correction (ZPE)= -1536.8484 0.56698
Internal Energy (U)= -1536.8149 0.60051
Enthalpy (H)= -1536.8140 0.60146
Gibbs Free Energy (G)= -1536.9163 0.49913

Frequencies -- -226.1564 12.9518 18.3679
SCF Energy (M06) = -1536.309758

Alkyne Coordination Complex RhdnCOT

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)]
#Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.43419288 Predicted Change= -1.865573D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00489 ll	0.00180	[NO]	0.00489 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.088079	-2.781175	0.299609
C	2.254448	-2.239352	-0.997948
C	1.781005	-2.951944	-2.265700
C	0.262899	-2.816537	-2.208353
C	-1.782771	-2.864385	0.474326
C	-2.247360	-2.378303	-0.559017
C	1.005423	-3.676547	0.486516
C	0.565994	-4.206244	1.828861
C	-1.717776	-3.600372	1.761586
O	-0.779508	-4.653663	1.795734
C	-3.123406	-2.051612	-1.689339
C	2.971783	-2.301491	1.426533
Rh	0.127659	-1.760627	-0.428291
H	2.203905	-2.455422	-3.143633
H	2.125184	-3.993394	-2.284162
H	-0.156570	-2.192068	-3.000009
H	-0.295619	-3.750979	-2.127934
H	2.988468	-1.444397	-1.105999
H	0.739143	-4.347537	-0.325638
H	1.157514	-5.091703	2.092231
H	-1.534291	-2.894752	2.587980

H	0.696574	-3.464432	2.630679
H	-2.694978	-4.065292	1.927447
H	-4.048225	-2.633390	-1.600238
H	-3.386480	-0.989996	-1.699185
H	-2.657472	-2.309908	-2.646547
H	3.841345	-2.969877	1.481412
H	3.343883	-1.289031	1.249995
H	2.484920	-2.335185	2.403581
C	0.676157	0.113791	1.528066
C	-0.678409	0.034421	1.537691
C	0.670307	0.227263	-1.502939
C	-0.719811	0.136038	-1.481253
C	1.535773	1.048780	0.762057
C	-1.642053	0.870517	0.787238
C	1.537680	1.093413	-0.668112
C	-1.655362	0.923058	-0.639588
C	-2.588339	1.580969	1.502604
C	-3.547184	2.410334	0.866846
C	-3.556033	2.471861	-0.563752
C	-2.610000	1.694615	-1.280132
C	-4.501056	3.168192	1.596577
C	-5.418862	3.955929	0.937647
C	-5.427117	4.017345	-0.478362
C	-4.518088	3.289564	-1.213959
C	2.424233	1.932435	-1.319949
C	3.306095	2.791806	-0.616626
C	3.306429	2.746476	0.814362
C	2.423282	1.845143	1.463354
C	4.198529	3.674121	-1.280906
C	5.050121	4.479909	-0.557791
C	5.050454	4.435475	0.858700
C	4.199350	3.586126	1.531129
H	1.190189	-0.454592	2.300359
H	-1.118665	-0.598972	2.306989
H	1.134411	-0.085668	-2.436439
H	-1.163704	-0.239675	-2.400666
H	-2.597322	1.517452	2.588636
H	-2.636555	1.720997	-2.367847
H	-4.492989	3.120855	2.682450
H	-6.142243	4.536243	1.502705
H	-6.156396	4.644497	-0.982553
H	-4.523334	3.336489	-2.299958
H	2.448183	1.945758	-2.407774
H	2.445641	1.791507	2.549791

H	4.196842	3.707085	-2.367374
H	5.726941	5.155614	-1.072258
H	5.727734	5.077718	1.413823
H	4.198898	3.551825	2.617518

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.43419288 Predicted Change= -1.865573D-07
Zero-point correction (ZPE)= -1536.8638 0.57036
Internal Energy (U)= -1536.8312 0.60293
Enthalpy (H)= -1536.8303 0.60387
Gibbs Free Energy (G)= -1536.9257 0.50848

Frequencies -- 21.6814 33.0368 47.6321
SCF Energy (M06) = -1536.337561

2π-Insertion TS RhdnCOT

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)]
#Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.41075495 Predicted Change= -3.933960D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00069 II	0.00180	[YES]	0.00069 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.069367	-1.642731	-0.324795
C	2.611016	-2.162652	0.875807
C	3.004579	-1.644938	2.254820
C	2.591433	-0.171805	2.311583
C	3.227564	1.542432	-0.342416
C	2.255171	1.986070	0.368340
C	3.880366	-0.409122	-0.331352
C	4.780735	-0.154834	-1.538030
C	4.244423	2.032647	-1.337329
O	5.325607	1.137219	-1.429272
C	1.747371	3.265955	0.924978
C	2.823709	-2.396121	-1.615295
Rh	1.599698	0.003219	0.496610
C	-0.118299	-0.638226	-1.542718
C	-0.152864	0.717695	-1.538892
C	-0.235668	-0.692512	1.481154
C	-0.250791	0.721425	1.463854
C	-0.994461	-1.576937	-0.797859
C	-1.091667	1.584562	-0.789186
C	-1.035335	-1.609642	0.632898

C	-1.139998	1.579329	0.637761
C	-1.900423	2.455369	-1.495236
C	-2.822655	3.316709	-0.846748
C	-2.877223	3.307205	0.584307
C	-2.002892	2.441581	1.290303
C	-3.677754	4.194484	-1.564394
C	-4.550745	5.022277	-0.893626
C	-4.604450	5.013111	0.522631
C	-3.784269	4.176368	1.246682
C	-1.722809	-2.505989	-1.516658
C	-2.553452	-3.467624	-0.885079
C	-2.594000	-3.501125	0.545990
C	-1.801814	-2.572510	1.266859
C	-3.325856	-4.405499	-1.619417
C	-4.106842	-5.332350	-0.964402
C	-4.146746	-5.365874	0.451898
C	-3.404962	-4.471921	1.191910
H	2.476100	-2.231305	3.011570
H	4.078263	-1.797191	2.434984
H	1.905206	0.059115	3.128516
H	3.419703	0.539829	2.326456
H	2.031255	-3.081934	0.826654
H	4.435632	-0.248411	0.590172
H	5.617367	-0.861334	-1.518982
H	3.759759	2.154726	-2.320810
H	4.238336	-0.277204	-2.486780
H	4.632760	3.003748	-1.015248
H	2.404176	4.094490	0.635150
H	0.732896	3.479814	0.579949
H	1.722392	3.223565	2.020335
H	3.728101	-2.953115	-1.893295
H	2.013030	-3.119659	-1.498148
H	2.582117	-1.739360	-2.454701
H	0.514616	-1.100268	-2.297025
H	0.473712	1.223886	-2.273029
H	0.058246	-1.135169	2.431599
H	0.048328	1.188268	2.401130
H	-1.842700	2.480058	-2.581294
H	-2.020900	2.462886	2.378065
H	-3.635774	4.200533	-2.650516
H	-5.204633	5.687664	-1.449578
H	-5.298988	5.671421	1.036087
H	-3.824451	4.168346	2.332896
H	-1.669044	-2.502650	-2.603294

H	-1.809550	-2.620798	2.353901
H	-3.294925	-4.379124	-2.705604
H	-4.697972	-6.043898	-1.533299
H	-4.768142	-6.102416	0.952599
H	-3.434748	-4.495969	2.278222

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.41075495 Predicted Change= -3.933960D-09
Zero-point correction (ZPE)= -1536.8400 0.57065
Internal Energy (U)= -1536.8087 0.60199
Enthalpy (H)= -1536.8078 0.60294
Gibbs Free Energy (G)= -1536.9008 0.50988

Frequencies -- -233.9919 20.8584 28.7426
SCF Energy (M06) = -1536.309851

Metallacycle RhdnCOT

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)] #Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.44782399 Predicted Change= -3.002060D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00185 ll	0.00180	[NO]	0.00185 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.045896	-2.820318	0.926355
C	-1.194210	-3.353062	-0.013818
C	-1.529022	-3.630481	-1.474333
C	-1.086335	-2.350219	-2.179273
C	-3.624971	-1.170355	-0.178145
C	-2.670301	-0.463325	-0.790323
C	-3.476583	-2.484760	0.558141
C	-4.539363	-2.298220	1.662140
C	-5.080476	-0.743484	0.044067
O	-5.616966	-1.694743	0.961237
C	-2.965147	0.764237	-1.606076
C	-1.657407	-2.772426	2.382424
Rh	-0.756727	-1.132799	-0.525614
C	0.715934	-0.337895	1.482588
C	-0.143833	0.714020	1.485444
C	1.007680	-0.164653	-1.604158
C	0.093282	0.875323	-1.555940
C	1.987239	-0.550565	0.747633
C	-0.059731	1.991700	0.752369
C	2.100312	-0.522812	-0.687179
C	0.046745	2.059332	-0.669728

C	0.040224	3.297884	-1.291203
C	-0.003954	4.509981	-0.558183
C	-0.110696	4.441292	0.868178
C	-0.164427	3.163570	1.480505
C	0.026934	5.781597	-1.189406
C	-0.038412	6.934219	-0.438060
C	-0.143587	6.866434	0.973699
C	-0.181917	5.647180	1.613999
C	3.085258	-0.948341	1.492358
C	4.331890	-1.273429	0.904543
C	4.437626	-1.264681	-0.525687
C	3.295290	-0.921237	-1.280074
C	5.467430	-1.634034	1.676926
C	6.652566	-1.966083	1.059085
C	6.757165	-1.958607	-0.356129
C	5.674101	-1.617709	-1.133089
H	-0.985049	-4.515053	-1.823227
H	-2.596300	-3.822445	-1.611650
H	-0.123446	-2.449573	-2.687590
H	-1.828075	-1.917473	-2.852729
H	-0.214056	-3.686741	0.331666
H	-3.867029	-3.281201	-0.092741
H	-4.905501	-3.233310	2.093281
H	-5.688482	-0.777749	-0.867797
H	-5.136406	0.273253	0.460017
H	-4.175670	-1.646767	2.472127
H	-4.043522	0.964243	-1.603329
H	-2.460074	1.660089	-1.235536
H	-2.677262	0.623576	-2.655384
H	-1.828913	-1.785516	2.824942
H	-2.278914	-3.481094	2.946003
H	-0.612783	-3.056320	2.535575
H	0.537763	-1.082471	2.255800
H	-0.930532	0.673334	2.238383
H	1.079159	-0.656159	-2.571901
H	-0.446621	1.014856	-2.488327
H	0.076758	3.352582	-2.377155
H	-0.284329	3.111534	2.560415
H	0.106057	5.831998	-2.272254
H	-0.009733	7.903628	-0.926588
H	-0.194324	7.784881	1.550876
H	-0.263943	5.594426	2.696446
H	2.994500	-1.008727	2.574561
H	3.366507	-0.942106	-2.365270

H	5.388760	-1.641084	2.760715
H	7.518061	-2.237185	1.656293
H	7.700508	-2.223931	-0.823714
H	5.750872	-1.610042	-2.217096

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.44782399 Predicted Change= -3.002060D-08
Zero-point correction (ZPE)= -1536.8753 0.57246
Internal Energy (U)= -1536.8435 0.60426
Enthalpy (H)= -1536.8426 0.60520
Gibbs Free Energy (G)= -1536.9379 0.50984

Frequencies -- 18.8989 23.8572 26.8118
SCF Energy (M06) = -1536.340605

Reductive Elimination TS RhdnCOT

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)]
#Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.43660713 Predicted Change= -4.854606D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00094 II	0.00180	[YES]	0.00094 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.186012	-0.878048	-1.599188
C	2.351998	-1.973169	-1.660367
C	2.470994	-3.190654	-0.750439
C	1.752253	-2.852901	0.548300
C	3.883851	-0.760668	0.838204
C	2.665465	-1.038664	1.347649
C	4.331607	-0.858449	-0.605288
C	5.364029	0.289878	-0.640870
C	5.059195	-0.156405	1.594857
O	6.034655	0.151964	0.604395
C	2.462443	-1.024949	2.847737
C	3.164535	0.178562	-2.674479
Rh	1.170107	-0.771018	-0.066016
C	-0.034336	0.489535	1.414479
C	-0.602142	-0.783648	1.377330
C	-0.131473	0.510577	-1.521728
C	-0.727873	-0.738019	-1.551626
C	-0.497997	1.691366	0.686917
C	-1.836938	-1.197626	0.661581
C	-0.575373	1.695193	-0.737178

C	-1.896316	-1.184251	-0.761831
C	-2.909813	-1.677666	1.386473
C	-4.100885	-2.114773	0.749250
C	-4.159573	-2.102347	-0.682724
C	-3.024843	-1.652682	-1.406460
C	-5.222934	-2.584248	1.481298
C	-6.354701	-3.016281	0.825194
C	-6.413039	-3.003478	-0.590473
C	-5.338578	-2.559020	-1.329018
C	-0.964176	2.845210	-1.394016
C	-1.334055	4.019017	-0.685693
C	-1.246974	4.016451	0.745214
C	-0.798936	2.839373	1.396297
C	-1.763553	5.199533	-1.346968
C	-2.096027	6.324358	-0.624400
C	-2.009295	6.321961	0.790202
C	-1.591962	5.193965	1.460842
H	2.001354	-4.057836	-1.228670
H	3.520509	-3.445830	-0.570413
H	0.691559	-3.111383	0.557777
H	2.221488	-3.231918	1.452423
H	1.684277	-2.051292	-2.514741
H	4.916061	-1.785646	-0.723863
H	6.110732	0.194411	-1.432475
H	5.508643	-0.850904	2.316848
H	4.754608	0.748704	2.144272
H	4.874571	1.273064	-0.722279
H	3.171830	-1.697837	3.346091
H	2.638645	-0.020266	3.255106
H	1.461490	-1.333269	3.154918
H	3.068730	1.188872	-2.262435
H	4.112418	0.150148	-3.228537
H	2.357668	0.012360	-3.392786
H	0.621818	0.695111	2.256082
H	-0.324867	-1.444591	2.196068
H	0.524792	0.742431	-2.357656
H	-0.468920	-1.377100	-2.394268
H	-2.853601	-1.724400	2.471977
H	-3.057155	-1.675039	-2.493651
H	-5.177211	-2.594627	2.567213
H	-7.210267	-3.369646	1.393037
H	-7.312678	-3.347016	-1.092373
H	-5.381621	-2.549442	-2.415030
H	-0.991522	2.863560	-2.481372

H	-0.703802	2.846395	2.480023
H	-1.828675	5.201938	-2.431924
H	-2.427077	7.221854	-1.138473
H	-2.274801	7.217230	1.344519
H	-1.524571	5.189878	2.545674

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.43660713 Predicted Change= -4.854606D-09
Zero-point correction (ZPE)= -1536.8650 0.57159
Internal Energy (U)= -1536.8340 0.60255
Enthalpy (H)= -1536.8331 0.60349
Gibbs Free Energy (G)= -1536.9257 0.51088

Frequencies -- -333.1046 20.5632 28.7384
SCF Energy (M06) = -1536.336923

Product-Catalyst Complex RhdnCOT

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C35H32ORh(1+) C1[X(C35H32ORh)]
#Atoms= 69
Charge = 1 Multiplicity = 1

SCF Energy= -1537.51325222 Predicted Change= -9.269183D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00239 II	0.00180	[NO]	0.00239 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.203879	-0.068157	-1.507528
C	2.680256	-1.268230	-1.965315
C	3.232743	-2.622881	-1.548549
C	2.838910	-3.081670	-0.136792
C	3.430873	-0.784562	0.884903
C	2.853410	-2.030530	0.959539
C	4.139108	-0.116883	-0.308802
C	4.547587	1.239204	0.310943
C	3.775537	0.074213	2.106926
O	4.808440	0.939699	1.671194
C	2.431496	-2.580766	2.306701
C	3.138019	1.192205	-2.335566
H	2.895226	-3.379829	-2.262114
H	4.327521	-2.589693	-1.635740
H	1.835192	-3.523594	-0.166844
H	3.504696	-3.898410	0.183811
H	2.129621	-1.239598	-2.903952
H	5.057316	-0.669061	-0.564850
H	5.455368	1.664765	-0.120876
H	4.168124	-0.518105	2.938597
H	2.909760	0.648719	2.474297

H	3.732011	1.973722	0.228204
H	1.578374	-3.259782	2.210035
H	3.258996	-3.168808	2.728592
H	2.176953	-1.805967	3.033726
H	4.149999	1.428125	-2.694949
H	2.506044	1.059020	-3.217216
H	2.784227	2.062998	-1.776588
Rh	1.302942	-0.547287	-0.261647
C	0.080314	0.575986	1.360340
C	-0.332860	-0.748869	1.347228
C	-0.105346	0.642261	-1.545259
C	-0.514100	-0.695916	-1.567987
C	-0.575387	1.720203	0.685421
C	-1.524926	-1.309392	0.660060
C	-0.681792	1.744731	-0.735589
C	-1.599799	-1.304716	-0.764425
C	-2.516769	-1.928595	1.394310
C	-3.641457	-2.526229	0.767636
C	-3.711864	-2.528475	-0.664375
C	-2.657201	-1.928387	-1.398821
C	-4.684560	-3.140505	1.509793
C	-5.750827	-3.726478	0.864163
C	-5.820078	-3.729428	-0.551460
C	-4.822169	-3.145749	-1.299712
C	-1.238066	2.843480	-1.360486
C	-1.754777	3.936871	-0.617630
C	-1.643115	3.912974	0.811562
C	-1.023549	2.795241	1.428084
C	-2.355912	5.060931	-1.243347
C	-2.829620	6.111204	-0.488654
C	-2.719049	6.087704	0.924081
C	-2.136871	5.014047	1.560499
H	0.796818	0.843254	2.136223
H	0.082064	-1.380620	2.129160
H	0.447424	0.973495	-2.421470
H	-0.229059	-1.263306	-2.453049
H	-2.446007	-1.962847	2.479359
H	-2.696086	-1.956811	-2.485657
H	-4.630349	-3.138735	2.595367
H	-6.546104	-4.190673	1.439845
H	-6.667548	-4.195787	-1.045025
H	-4.873929	-3.147256	-2.385404
H	-1.288782	2.881257	-2.446606
H	-0.910700	2.792110	2.510058

H	-2.439350	5.078630	-2.326940
H	-3.291547	6.965103	-0.975293
H	-3.097390	6.923829	1.504641
H	-2.051054	4.995156	2.643857

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1537.51325222 Predicted Change= -9.269183D-08
Zero-point correction (ZPE)= -1536.9385 0.57469
Internal Energy (U)= -1536.9075 0.60571
Enthalpy (H)= -1536.9065 0.60666
Gibbs Free Energy (G)= -1536.9993 0.51386

Frequencies -- 20.1360 24.3004 32.8143
SCF Energy (M06) = -1536.417344

11. RhNHC-H_2

11.a. Additional Figures

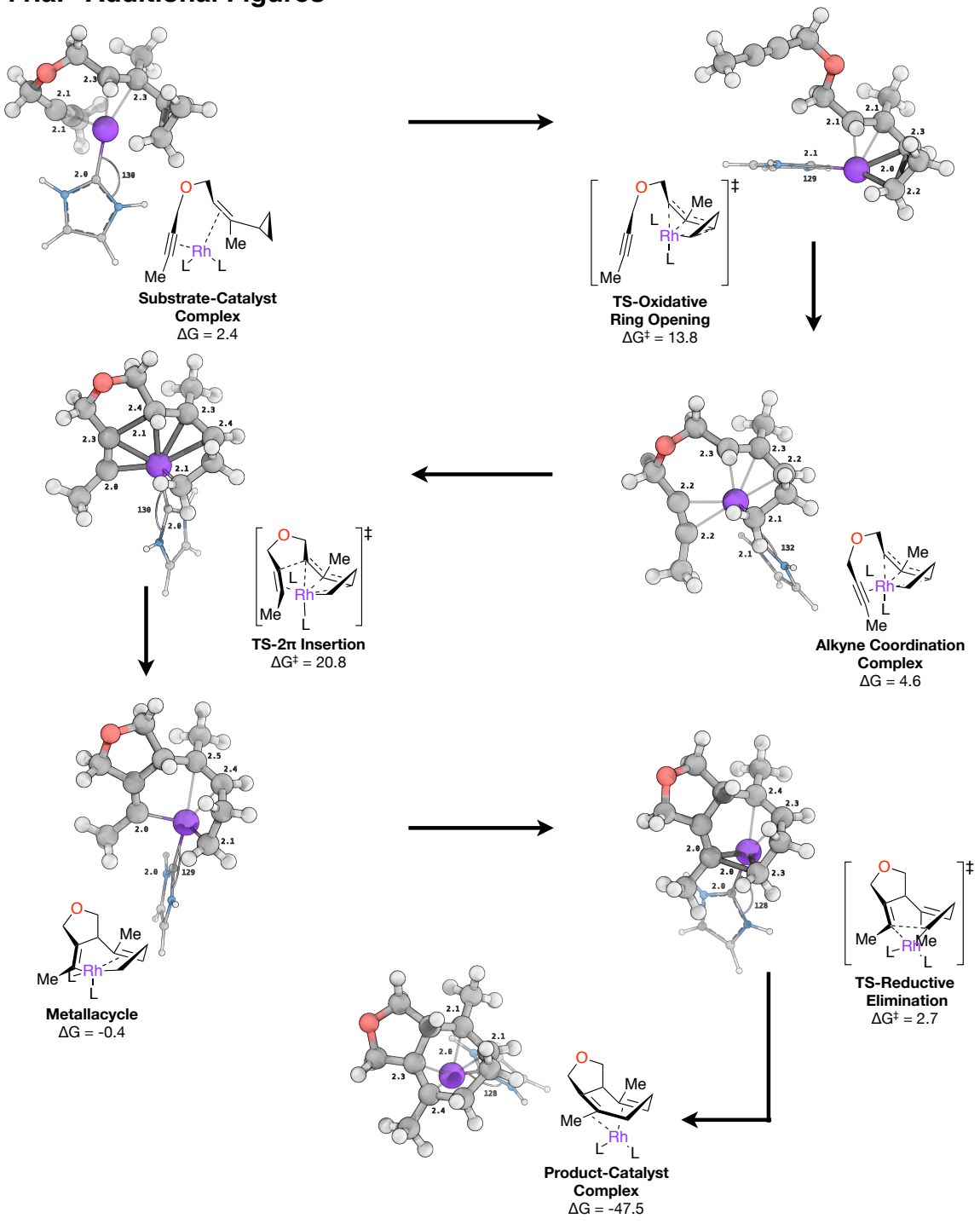


Figure S16. Computed geometries for RhNHC-H_2.

Substrate-Catalyst Complex RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

```
 ---------------------------------------------------------------------
 # opt=maxcycle=250 freq=noraman b3lyp/gen geom=connectivity gfinput
 gfprint pseudo=read scf=(direct,tight,maxcycle=300,xqc)
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas
Freq
 ---------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C14H20N2ORh(1+)   C1[X(C14H20N2ORh)]
#Atoms= 38
 Charge = 1   Multiplicity = 1
 ---------------------------------------------------------------------
 SCF Energy= -839.463890959      Predicted Change= -2.970332D-08
 =====================================================================
 Optimization completed. {Found  1 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 II  0.00045   [ YES ]      0.00000 II  0.00030   [ YES ]
 Displ      0.00201 II  0.00180   [ NO ]       0.00201 II  0.00180   [ YES ]
 ---------------------------------------------------------------------
      Atomic         Coordinates (Angstroms)
       Type        X           Y        Z
 ---------------------------------------------------------------------
       Rh      -0.015556      0.169472     -0.034533
       C        2.091257      0.787603      0.555541
       C        1.611412      2.205027      0.473807
       C        1.970036      3.156037     -0.625021
       C        0.555027      2.637164     -0.627759
       C        0.122647     -1.937616     -0.071452
       C       -0.285338     -1.634135      1.080854
       H        2.114946      4.197116     -0.353439
       H        2.633335      2.796306     -1.406165
       H       -0.232883      3.316109     -0.318935
       H        0.292873      1.992581     -1.473562
       H        1.421367      2.660791      1.441179
       C        2.202047      0.030783     -0.598502
       H        2.086859      0.522759     -1.565392
       C        2.761928     -1.363762     -0.752149
       H        3.754761     -1.310124     -1.212977
       C        0.849071     -2.766841     -1.074276
       H        1.175751     -3.689405     -0.566301
       O        1.959540     -2.109383     -1.663991
       H        2.866754     -1.889334      0.205112
       H        0.198472     -3.051393     -1.906402
       C       -0.802989     -1.825836      2.447239
       H       -0.788370     -2.890826      2.709395
       H       -0.197632     -1.282317      3.179966
```

H	-1.833282	-1.462970	2.536178
C	2.572252	0.344511	1.916233
H	3.559093	0.782428	2.119568
H	1.895218	0.690388	2.704837
H	2.667923	-0.739885	1.994975
C	-2.047927	0.257910	-0.146086
N	-2.898488	-0.746313	-0.474500
N	-2.878447	1.321364	0.022222
C	-4.220444	-0.329238	-0.517249
C	-4.209353	0.990288	-0.196938
H	-5.034424	-0.989795	-0.771240
H	-5.011050	1.706510	-0.109389
H	-2.570551	-1.685162	-0.655639
H	-2.554652	2.238304	0.294636

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.463890959 Predicted Change= -2.970332D-08
Zero-point correction (ZPE)= -839.1440 0.31983
Internal Energy (U)= -839.1243 0.33954
Enthalpy (H)= -839.1234 0.34049
Gibbs Free Energy (G)= -839.1925 0.27138

Frequencies -- 30.8383 47.0309 65.9560
SCF Energy (M06) = -838.9275505

Oxidative-Addition TS RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C14H20N2ORh(1+) C1[X(C14H20N2ORh)] #Atoms= 38
Charge = 1 Multiplicity = 1

SCF Energy= -839.426481449 Predicted Change= -2.496024D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00210 II	0.00180	[NO]	0.00210 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.968385	-0.325610	-0.575050
Rh	-1.677110	-0.016580	-0.477266
C	4.261056	-0.669217	0.345340
C	3.425222	-1.091817	1.472277
C	1.319032	-0.457058	0.544866
C	0.060201	-1.112330	0.030669
C	-1.028503	-1.470289	0.902591
C	-2.151995	-2.120507	0.272171
C	-2.135948	-3.023194	-0.927175
C	-2.410833	-1.739422	-1.656229
H	-3.461534	-1.530086	-1.857585
H	-1.723971	-1.477602	-2.465650
H	-2.924055	-3.775877	-0.934022
H	-1.168269	-3.476393	-1.142653
H	0.256174	-1.757111	-0.826776
H	3.364654	-0.287688	2.223770
H	3.856995	-1.969711	1.962827
H	1.105381	0.315040	1.299178
H	1.852100	0.026189	-0.287560
H	-3.091184	-2.088265	0.821181

O	2.103110	-1.499321	1.095219
C	5.851011	0.065805	-1.671309
H	5.562349	-0.426341	-2.607556
H	5.834567	1.149203	-1.838879
H	6.886532	-0.221315	-1.454252
C	-1.040537	-1.235861	2.389797
H	-2.062125	-1.168989	2.775741
H	-0.543443	-2.078536	2.887649
H	-0.499057	-0.327947	2.665601
C	-0.953215	1.895719	-0.058142
N	-1.480124	2.819763	0.790029
N	0.063802	2.578407	-0.648945
C	-0.817570	4.036101	0.731906
C	0.168783	3.882293	-0.190305
H	-1.097254	4.884827	1.336035
H	0.915439	4.572003	-0.551186
H	0.668171	2.163446	-1.344470
H	-2.262654	2.620964	1.397785

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.426481449 Predicted Change= -2.496024D-09
Zero-point correction (ZPE)= -839.1088 0.31766
Internal Energy (U)= -839.0885 0.33794
Enthalpy (H)= -839.0875 0.33888
Gibbs Free Energy (G)= -839.1619 0.26457

Frequencies -- -205.3511 17.1268 27.2039
SCF Energy (M06) = -838.8789072

Alkyne Coordination Complex RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

opt=maxcycle=250 freq=noraman b3lyp/gen geom=connectivity gfinput gfprint pseudo=read scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C14H20N2ORh(1+) C1[X(C14H20N2ORh)] #Atoms= 38

Charge = 1 Multiplicity = 1

SCF Energy= -839.478084463 Predicted Change= -2.907883D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00053 II	0.00180	[YES]	0.00053 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.015777	2.188053	0.216430
Rh	-0.070606	-0.031067	0.028501
C	-1.172597	1.881145	-0.025640
C	-2.602666	2.121383	-0.381395
C	-3.380160	-0.123984	-0.464086
C	-2.223118	-0.835592	0.185105
C	-1.397017	-1.819645	-0.411732
C	-0.243393	-2.221662	0.313485
C	-0.121324	-2.062341	1.835100
C	0.059940	-0.558026	2.022291
H	1.027068	-0.242500	2.417664
H	-0.738449	-0.030240	2.546152
H	0.742912	-2.628509	2.195301
H	-1.003625	-2.453354	2.357024
H	-2.312639	-0.836306	1.268608
H	-2.676467	2.215263	-1.477644
H	-2.902682	3.078113	0.058019
H	-4.319467	-0.640578	-0.235144
H	-3.285569	-0.066681	-1.558119
H	0.439841	-2.909065	-0.178485
O	-3.534261	1.176743	0.094063

C	1.151069	3.070970	0.548495
H	1.561432	2.824502	1.533944
H	1.962745	2.983545	-0.180354
H	0.818455	4.114773	0.570261
C	-1.571366	-2.259970	-1.847959
H	-0.668086	-2.743196	-2.229905
H	-2.392481	-2.984745	-1.912602
H	-1.826230	-1.427909	-2.512879
C	1.992182	-0.047081	-0.216598
N	3.006706	-0.452866	0.586752
N	2.637604	0.329630	-1.352475
C	4.250525	-0.338479	-0.024707
C	4.014942	0.159588	-1.263310
H	5.169422	-0.616782	0.466747
H	4.686444	0.403171	-2.071455
H	2.157774	0.687671	-2.166614
H	2.864034	-0.806610	1.521639

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.478084463 Predicted Change= -2.907883D-09
Zero-point correction (ZPE)= -839.1580 0.32002
Internal Energy (U)= -839.1386 0.33945
Enthalpy (H)= -839.1376 0.34039
Gibbs Free Energy (G)= -839.2061 0.27194

Frequencies -- 19.9637 47.0288 57.7685
SCF Energy (M06) = -838.9320662

2π-Insertion TS RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C14H20N2ORh(1+) C1[X(C14H20N2ORh)] #Atoms= 38
Charge = 1 Multiplicity = 1

SCF Energy= -839.455116675 Predicted Change= -7.850273D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.02652 II	0.00180	[NO]	0.02652 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.306655	1.866815	0.036805
Rh	0.187346	-0.086777	-0.035659
C	-1.530665	1.444368	-0.065905
C	-2.906090	2.002607	-0.337715
C	-3.505057	-0.187562	-0.399007
C	-2.145611	-0.503230	0.219001
C	-1.422946	-1.700068	-0.287581
C	-0.510491	-2.371256	0.508847
C	-0.214397	-2.014131	1.962093
C	0.344107	-0.588755	1.967350
H	1.384174	-0.538634	2.290096
H	-0.255211	0.149160	2.507201
H	0.520042	-2.719899	2.359752
H	-1.116194	-2.112863	2.581814
H	-2.216167	-0.461971	1.304948
H	-2.983237	2.245114	-1.410929
H	-3.057143	2.920633	0.238450
H	-4.249552	-0.900427	-0.030621
H	-3.476078	-0.242890	-1.496695
H	-0.057881	-3.273699	0.104700

O	-3.908470	1.089087	0.036342
C	-1.717850	-2.201086	-1.687612
H	-2.732727	-2.613401	-1.747605
H	-1.647965	-1.403846	-2.436663
H	-1.021635	-2.995222	-1.969755
C	0.415099	3.168700	0.115951
H	0.890369	3.286044	1.097982
H	1.202448	3.233179	-0.642317
H	-0.267518	4.015240	-0.021853
C	2.176500	0.017441	-0.217638
N	2.943789	-0.602876	-1.153197
N	3.082321	0.729938	0.500705
C	4.290728	-0.285560	-1.024705
C	4.379345	0.561895	0.030700
H	5.048085	-0.683945	-1.681126
H	5.229951	1.050273	0.479273
H	2.821458	1.321276	1.276712
H	2.563115	-1.232369	-1.845515

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.455116675 Predicted Change= -7.850273D-08
Zero-point correction (ZPE)= -839.1350 0.32006
Internal Energy (U)= -839.1165 0.33857
Enthalpy (H)= -839.1156 0.33951
Gibbs Free Energy (G)= -839.1825 0.27260

Frequencies -- -213.7773 14.2458 53.9326
SCF Energy (M06) = -838.9050431

Metallacycle RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

opt=maxcycle=250 freq=noraman b3lyp/gen geom=connectivity gfinput gfprint pseudo=read scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C14H20N2ORh(1+) C1[X(C14H20N2ORh)] #Atoms= 38

Charge = 1 Multiplicity = 1

SCF Energy= -839.502136388 Predicted Change= -5.605600D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00284 ll	0.00180	[NO]	0.00284 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.332751	1.185309	-0.185780
Rh	-0.496107	-0.587480	0.241678
C	1.670092	1.169681	-0.267139
C	2.617152	2.369688	-0.352040
C	3.886697	0.557279	0.256740
C	2.563481	-0.062388	-0.249100
C	1.954284	-1.228264	0.503528
C	1.198823	-2.176255	-0.134838
C	0.783658	-2.182740	-1.604661
C	-0.576331	-1.483342	-1.602446
H	-1.425531	-2.175929	-1.548531
H	-0.719475	-0.751396	-2.401747
H	0.721321	-3.211497	-1.978103
H	1.502003	-1.647315	-2.229988
H	2.744401	-0.351570	-1.292250
H	2.499148	3.021200	0.528721
H	2.472006	2.977329	-1.251899
H	4.776687	-0.003741	-0.036799
H	3.885526	0.684969	1.349561
H	0.860705	-3.028956	0.457571
O	3.924715	1.813727	-0.403888

C	-0.501541	2.433771	-0.323985
H	-1.153831	2.385402	-1.203724
H	-1.141503	2.613011	0.546568
H	0.141491	3.313517	-0.446338
C	2.286317	-1.380060	1.971273
H	1.714918	-2.190676	2.432027
H	3.352138	-1.609576	2.098548
H	2.092827	-0.456652	2.529398
C	-2.383032	0.105530	0.189353
N	-3.153836	0.476435	1.245780
N	-3.221212	0.235435	-0.868155
C	-4.439527	0.829595	0.858132
C	-4.481703	0.675205	-0.490217
H	-5.193199	1.148482	1.560774
H	-5.280783	0.832458	-1.197480
H	-2.942216	0.028911	-1.817382
H	-2.820944	0.487673	2.200345

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.502136388 Predicted Change= -5.605600D-08
Zero-point correction (ZPE)= -839.1795 0.32254
Internal Energy (U)= -839.1612 0.34090
Enthalpy (H)= -839.1602 0.34184
Gibbs Free Energy (G)= -839.2264 0.27571

Frequencies -- 30.2498 46.7792 60.2230
SCF Energy (M06) = -838.9495075

Reductive Elimination TS RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcall,ts,noeigentest)

Pointgroup= C1 Stoichiometry= C14H20N2ORh(1+) C1[X(C14H20N2ORh)]
#Atoms= 38
Charge = 1 Multiplicity = 1

SCF Energy= -839.456784412 Predicted Change= -8.136552D-11

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00025 ll	0.00180	[YES]	0.00025 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.321852	0.857870	0.862110
Rh	0.458458	-0.720653	-0.185072
C	-1.602206	1.059318	0.459890
C	-2.320681	2.390400	0.326009
C	-3.361030	0.875695	-1.066272
C	-2.555849	0.010359	-0.072387
C	-1.844658	-1.248821	-0.549812
C	-1.263265	-2.083799	0.382086
C	-1.182603	-1.751877	1.868166
C	-0.039186	-0.750542	2.031992
H	0.940487	-1.225891	2.159783
H	-0.158781	-0.046964	2.854340
H	-0.976794	-2.656581	2.450583
H	-2.127015	-1.338792	2.238186
H	-3.265796	-0.256302	0.727864
H	-1.711631	3.117454	-0.235714
H	-2.571275	2.845894	1.293667
H	-4.353718	0.482581	-1.295843
H	-2.810224	1.035018	-2.006367
H	-0.945312	-3.077132	0.064284
O	-3.533850	2.099725	-0.360097
C	0.512738	1.995206	1.410900

H	1.457726	1.648597	1.834799
H	0.750241	2.725231	0.626888
H	-0.027300	2.531394	2.202216
C	-2.028109	-1.690688	-1.982815
H	-1.471839	-2.608947	-2.195096
H	-3.089755	-1.891394	-2.182462
H	-1.711187	-0.921954	-2.696725
C	2.323508	0.067274	-0.304871
N	2.768913	1.049436	-1.131724
N	3.459000	-0.353095	0.312739
C	4.141696	1.233683	-1.041482
C	4.582406	0.338456	-0.120626
H	4.672406	1.966715	-1.628384
H	5.573215	0.134967	0.253933
H	3.471651	-1.098491	0.995033
H	2.154256	1.576575	-1.736406

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.456784412 Predicted Change= -8.136552D-11
Zero-point correction (ZPE)= -839.1356 0.32116
Internal Energy (U)= -839.1176 0.33909
Enthalpy (H)= -839.1167 0.34003
Gibbs Free Energy (G)= -839.1818 0.27497

Frequencies -- -436.1592 33.5564 42.5757
SCF Energy (M06) = -838.9168352

Product-Catalyst Complex RhNHC-H_2

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

opt=maxcycle=250 freq=noraman b3lyp/gen geom=connectivity gfinput gfprint pseudo=read scf=(direct,tight,maxcycle=300,xqc)

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C14H20N2ORh(1+) C1[X(C14H20N2ORh)] #Atoms= 38

Charge = 1 Multiplicity = 1

SCF Energy= -839.535885725 Predicted Change= -3.717090D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00408 II	0.00180	[NO]	0.00408 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.871524	-1.350816	-0.296652
Rh	-0.259064	-0.347474	-0.388251
C	2.008853	0.020731	-0.322426
C	2.586019	0.833779	-1.483667
C	2.192049	2.353396	0.158860
C	1.818771	1.013880	0.841375
C	0.361380	0.850580	1.266570
C	-0.021815	-0.454102	1.719858
C	1.005178	-1.495992	2.142444
C	1.708788	-2.189463	0.961666
H	1.138701	-3.085442	0.688805
H	2.701418	-2.552743	1.267387
H	0.518784	-2.256707	2.759608
H	1.743297	-1.006054	2.792793
H	2.510894	0.822092	1.674987
H	1.819625	1.085007	-2.240924
H	3.413386	0.330616	-1.990878
H	2.693176	3.059583	0.823362
H	1.302201	2.839984	-0.269916
H	-0.980674	-0.512267	2.234113
O	3.097237	2.004854	-0.874819

C	-0.453898	2.057605	1.664453
H	-0.006602	2.514071	2.559935
H	-0.483054	2.833400	0.894124
H	-1.480602	1.776729	1.915510
C	2.182139	-2.168256	-1.534649
H	2.184099	-1.576372	-2.453487
H	3.171381	-2.637672	-1.437117
H	1.460244	-2.984582	-1.656562
C	-2.269924	-0.042901	-0.348689
N	-3.242806	-0.892083	0.075851
N	-2.975426	1.021166	-0.815848
C	-4.516986	-0.380670	-0.127210
C	-4.346244	0.841165	-0.694773
H	-5.412171	-0.918690	0.142254
H	-5.062940	1.580379	-1.016277
H	-2.535474	1.845902	-1.199794
H	-3.043058	-1.796933	0.478946

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -839.535885725 Predicted Change= -3.717090D-08
Zero-point correction (ZPE)= -839.2113 0.32458
Internal Energy (U)= -839.1934 0.34248
Enthalpy (H)= -839.1924 0.34342
Gibbs Free Energy (G)= -839.2575 0.27831

Frequencies -- 34.4555 45.3352 52.7331
SCF Energy (M06) = -838.9971722

12. Substrate and Product

12.a. Additional Figures

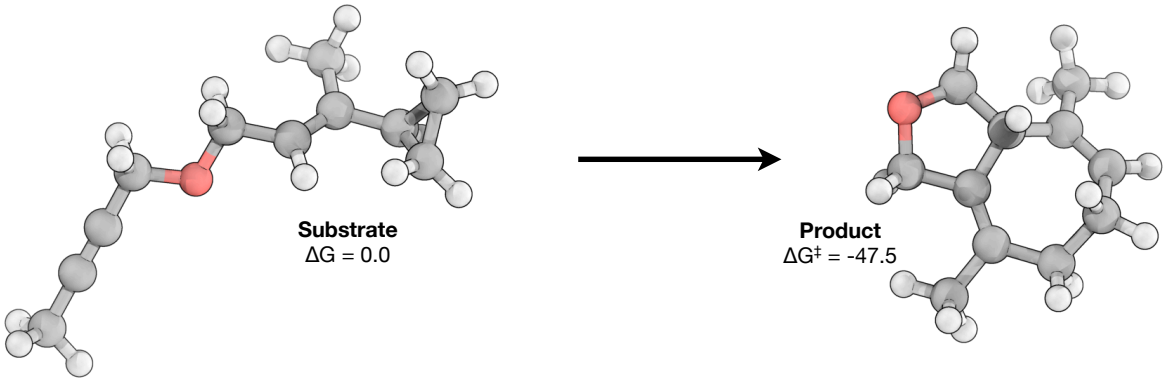


Figure S17. Computed geometries for the substrate and product.

Substrate

Supporting Information: SM-VCP-Linear.output

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

b3lyp/6-31+G* 5D gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(gdiis,maxcycle=250) freq=noraman geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31+G(d) Freq

---

Pointgroup= C1 Stoichiometry= C11H16O C1[X(C11H16O)] #Atoms= 28
Charge = 0 Multiplicity = 1

SCF Energy= -503.909332222 Predicted Change= -1.355676D-06

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.01064 II	0.00180	[NO]	0.01064 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.205750	-0.371089	0.345458
C	3.329212	0.591144	0.595869
C	4.545544	0.619446	-0.317538
C	3.607306	1.802672	-0.256352
C	-3.617219	-0.183469	-0.185615
C	-4.612708	0.391851	0.194214

H	5.531549	0.705667	0.132984
H	4.511839	0.002916	-1.213072
H	3.945911	2.706616	0.243659
H	2.977024	1.986828	-1.121502
H	3.567307	0.703367	1.655169
C	1.112175	-0.010671	-0.348427
H	1.036033	1.015205	-0.704366
C	-0.066184	-0.860752	-0.716155
H	-0.122558	-0.971169	-1.815038
C	-2.432242	-0.895732	-0.659086
H	-2.424433	-1.923209	-0.255436
O	-1.252051	-0.208331	-0.257370
H	-0.006624	-1.872589	-0.290010
H	-2.459220	-0.982025	-1.759429
C	-5.806613	1.101328	0.651252
H	-6.402305	0.483353	1.334218
H	-5.531865	2.018870	1.186003
H	-6.448262	1.386134	-0.191577
C	2.444689	-1.737551	0.947860
H	3.310199	-2.222416	0.475888
H	2.684723	-1.643087	2.015832
H	1.588829	-2.410874	0.856757

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -503.909332222 Predicted Change= -1.355676D-06
Zero-point correction (ZPE)= -503.6673 0.24202
Internal Energy (U)= -503.6527 0.25663
Enthalpy (H)= -503.6517 0.25757
Gibbs Free Energy (G)= -503.7119 0.19739

Frequencies -- 17.8485 32.7582 42.0991
SCF Energy (M06) = -503.505363

Product

Supporting Information: Product.output

Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004

==========

b3lyp/6-31+G* 5D gfprint gfinput scf=(direct,xqc,tight,maxcycle=250) opt=(gdiis,maxcycle=250) freq=noraman geom=connectivity

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31+G(d) Freq

---

Pointgroup= C1 Stoichiometry= C11H16O C1[X(C11H16O)] #Atoms= 28

Charge = 0 Multiplicity = 1

SCF Energy= -503.991118055 Predicted Change= -2.890105D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00031 ll	0.00180	[YES]	0.00031 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.374295	-1.056837	0.115239
C	-0.673694	-2.186788	-0.064168
C	0.647588	-2.239054	-0.789584
C	1.781127	-1.522977	-0.033491
C	0.537412	0.702681	-0.061109
C	1.646245	-0.023054	0.158852
H	0.942243	-3.283136	-0.948600
H	0.553419	-1.790480	-1.790440
H	1.912479	-1.996744	0.952951
H	2.726517	-1.704308	-0.569279
H	-1.055444	-3.117778	0.355530
C	-0.860850	0.244179	-0.496375
H	-0.849539	0.118581	-1.592314
C	-1.692729	1.513595	-0.211548
H	-2.560254	1.632988	-0.865796
C	0.457544	2.220698	0.078243
H	1.226069	2.759491	-0.484777
O	-0.807812	2.598281	-0.464855
H	0.519739	2.535568	1.134955
H	-2.031262	1.543281	0.836118
C	2.932017	0.625638	0.629685

H	3.336593	0.089346	1.499812
H	3.705054	0.579014	-0.151607
H	2.809850	1.673604	0.917043
C	-2.681258	-1.054750	0.873798
H	-3.500597	-0.630449	0.277012
H	-2.965477	-2.074314	1.155092
H	-2.621535	-0.460895	1.795885

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -503.991118055 Predicted Change= -2.890105D-09
Zero-point correction (ZPE)= -503.7431 0.24798
Internal Energy (U)= -503.7316 0.25950
Enthalpy (H)= -503.7306 0.26044
Gibbs Free Energy (G)= -503.7799 0.21119

Frequencies -- 65.3949 111.9348 118.3282
SCF Energy (M06) = -503.594655

13. Dispersion Corrections

13.a B3LYP/6-31G*/LANL2DZ Geometries w/ M06 SP Corrections

Table S1. Comparison of both M06/6-31G*/LANL2DZ and M06/def2-tzvp single point corrections using the B3LYP/6-31G*/LANL2DZ geometries.

	Pdt-Cat-Comp	Sub-Cat-Comp	Ox-Ring-TS	Alkyne-Comp	2π-Insert	Metalla-cycle	Red-Elim	Pdt-Cat-Comp	Sub-Cat-Comp	FES
RhCOCl	n-1	Cycle n							n+1	$\Delta G_{Exp.}$ = 27.7
M06/6-31Gd/LANL2DZ// B3LYP/6-31Gd/LANL2DZ	**0.0**	6.4	21.3	6.0	**26.5**	-5.2	2.1	-47.5	-41.1	26.5
M06/def2-tzvp//B3LYP/ 6-31Gd/LANL2DZ	**0.0**	8.6	21.6	8.8	**30.5**	1.0	8.0	-40.5	-31.9	30.5
RhCOD	n-1	Cycle n							n+1	$\Delta G_{Exp.}$ = 21.4
M06/6-31Gd/LANL2DZ// B3LYP/6-31Gd/LANL2DZ	**0.0**	2.4	13.8	4.6	**20.8**	-0.4	2.7	-47.5	-45.1	20.8
M06/def2-tzvp//B3LYP/ 6-31Gd/LANL2DZ	**0.0**	4.9	14.8	7.0	**24.3**	5.7	8.6	-40.5	-35.5	24.3
RhNHC-IPr	n-1	Cycle n							n+1	$\Delta G_{Exp.}$ = 20.3
M06/6-31Gd/LANL2DZ// B3LYP/6-31Gd/LANL2DZ	3.9	**0.0**	18.2	4.2	**19.5**	-12.2	4.0	-43.6	-47.5	19.5
M06/def2-tzvp//B3LYP/ 6-31Gd/LANL2DZ	0.7	**0.0**	16.4	1.9	**18.6**	-9.7	6.5	-39.7	-40.5	18.6
Rh(PPh3)3	n-1	Cycle n							n+1	$\Delta G_{Exp.}$ = 30.7
M06/6-31Gd/LANL2DZ// B3LYP/6-31Gd/LANL2DZ	11.7	**0.0**	19.5	11.6	**38.5**	3.7	11.1	-35.8	-47.5	38.5
M06/def2-tzvp//B3LYP/ 6-31Gd/LANL2DZ	14.3	**0.0**	21.6	14.4	**41.1**	12.1	19.6	-26.2	-40.5	41.1

13.b B3LYP-D3/6-31G*/LANL2DZ Geometries w/ M06 SP Corrections

Table S2. Comparison of the M06/6-31G*/LANL2DZ//B3LYP/6-31G*/LANL2DZ energies and B3LYP-D3/6-31G*/LANL2DZ, M06/6-31G*/LANL2DZ, and M06/def2-tzvp single point corrections using the B3LYP-D2/6-31G*/LANL2DZ geometries.

	Pdt-Cat-Comp	Sub-Cat-Comp	Ox-Ring-TS	Alkyne-Comp	2π-Insert	Metalla-cycle	Red-Elim	Pdt-Cat-Comp	Sub-Cat-Comp	FES
RhCOCl	n-1	Cycle n							n+1	$\Delta G_{Exp.}$ = 27.7
M06/6-31Gd/LANL2DZ// B3LYP/6-31Gd/LANL2DZ	**0.0**	6.4	21.3	6.0	**26.5**	-5.2	2.1	-47.5	-41.1	26.5
B3LYP-D3/6-31Gd/LANL2DZ	0.0	3.5	17.9	**-1.1**	**17.2**	-15.1	-1.0	-49.7	-46.1	18.4
M06/6-31Gd/LANL2DZ// B3LYP-D3/6-31Gd/LANL2DZ	**0.0**	6.5	21.3	5.8	**26.1**	-5.1	2.0	-47.2	-40.7	26.1
M06/def2-tzvp//B3LYP-D3/6-31Gd/LANL2DZ	**0.0**	8.6	21.7	8.5	**30.0**	1.0	8.0	-40.2	-31.5	30.0
RhNHC-IPr	n-1	Cycle n							n+1	$\Delta G_{Exp.}$ = 20.3
M06/6-31Gd/LANL2DZ// B3LYP/6-31Gd/LANL2DZ	3.9	**0.0**	18.2	4.2	**19.5**	-12.2	4.0	-43.6	-47.5	19.5
B3LYP-D3/6-31Gd/LANL2DZ	6.0	0.0	19.7	-1.5	11.5	**-19.6**	**3.2**	-43.6	-49.7	22.8
M06/6-31Gd/LANL2DZ// B3LYP-D3/6-31Gd/LANL2DZ	0.5	**0.0**	17.8	1.2	**16.2**	-14.1	1.8	-46.7	-47.2	16.2
M06/def2-tzvp//B3LYP-D3/6-31Gd/LANL2DZ	**0.0**	2.1	**18.6**	1.3	17.8	-8.9	7.7	-40.2	-38.0	18.6

Substrate-Catalyst Complex RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.05274116 Predicted Change = -1.055911D-07

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000058 II	0.000450	YES	0.000011 II	0.000300	YES
Disp	0.006558 II	0.001800	NO!	0.000950 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	0.759926	1.642741	0.008078
Rh	-0.607832	-0.519439	-0.094752
C	1.87733	0.864978	-0.08037
C	2.507169	0.363159	1.169137
C	-1.989097	1.083163	0.349238
C	-1.870898	0.443368	1.415404
H	0.428806	1.943997	0.999579
C	0.133304	2.467158	-1.103279
H	0.784447	3.313449	-1.356455
H	-0.018089	1.879694	-2.021616
C	-2.200753	2.193105	-0.612118
H	-2.436558	1.78273	-1.605871
H	-3.043528	2.812652	-0.285724
C	-1.917635	-1.785653	-0.330649
O	-2.755445	-2.560232	-0.485609
Cl	0.815922	-2.018202	-1.311958
H	2.032778	0.735326	2.074876
C	3.085038	-1.040313	1.271982
C	4.012275	0.133555	1.266449
H	4.612515	0.308937	0.37851
H	2.908997	-1.565682	2.20664
H	3.013303	-1.666768	0.389723
H	4.492989	0.432967	2.193853
O	-1.08728	3.071788	-0.683082

C -2.07657 0.003374 2.804223
H -2.744279 0.695058 3.332053
H -2.517394 -0.999577 2.834181
H -1.12293 -0.041711 3.341835
C 2.592521 0.653213 -1.389267
H 1.917591 0.730688 -2.243009
H 3.368846 1.425051 -1.488987
H 3.070411 -0.326152 -1.445902
Statistical Thermodynamic Analysis for 000-COCl-Complex-Alkyne-Bent-Yne-original.log
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -1187.05274116
Zero-point correction (ZPE)= 0.255251 -1186.797490
Internal Energy (U)= 0.274522 -1186.778219
Enthalpy (H)= 0.275467 -1186.777275
Gibbs Free Energy (G)= 0.206755 -1186.845986
Entropy (S) [Cal/Mol-Kelvin]= 144.615
Entropy (S): electronic= 0.000
Entropy (S): translational= 43.277
Entropy (S): rotational= 33.184
Entropy (S): vibrational= 68.154
Frequencies: 33.4174 52.4257 72.4635 75.9198 80.6365

SCF Energy (M06) = -1186.544998
SCF Energy (M06/def2-tzvp) = -1187.910435

Oxidative-Addition TS RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300 ,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.02488391 Predicted Change = -2.220996D-09

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000004 II	0.000450	YES	0.000001 II	0.000300	YES
Disp	0.001126 II	0.001800	YES	0.000220 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-5.227507	-0.706951	-0.717077
Rh	1.447062	-0.302686	-0.110736
C	-4.64231	0.019653	0.052833
C	-3.895547	0.88204	0.976843
C	-1.708758	0.214037	0.306362
C	-0.433649	0.796073	-0.240395
C	0.498554	1.48939	0.58042
C	1.684707	1.988176	-0.064194
C	1.814552	2.372745	-1.504205
C	2.187686	0.931052	-1.766812
H	3.248534	0.712059	-1.831065
H	1.566981	0.393147	-2.488786
H	2.598143	3.107562	-1.696345
H	0.877858	2.697104	-1.961091
H	-0.507677	1.069333	-1.291298
H	-3.776315	0.368848	1.947057
H	-4.445584	1.811115	1.162504
H	-1.544933	-0.303591	1.264224
H	-2.111819	-0.524839	-0.399527
H	2.532042	2.212586	0.580456
O	-2.622318	1.293919	0.484394
C	-5.95211	-1.575911	-1.6407
H	-5.717341	-2.632732	-1.465054

H -7.036075 -1.451086 -1.528433
H -5.698099 -1.344817 -2.682325
C 0.325423 1.706279 2.064726
H 1.294073 1.749291 2.572378
H -0.198184 2.655406 2.232151
H -0.268544 0.915453 2.52766
C 0.887754 -1.570281 1.263107
O 0.619776 -2.29156 2.11358
Cl 3.344513 -1.712392 -0.506388
Statistical Thermodynamic Analysis for 015-COCl-VCP-Opening-TS-LI-original.log
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -1187.02488391
Zero-point correction (ZPE)= 0.253053 -1186.771831
Internal Energy (U)= 0.272487 -1186.752397
Enthalpy (H)= 0.273431 -1186.751453
Gibbs Free Energy (G)= 0.201761 -1186.823123
Entropy (S) [Cal/Mol-Kelvin]= 150.842
Entropy (S): electronic= 0.000
Entropy (S): translational= 43.277
Entropy (S): rotational= 34.035
Entropy (S): vibrational= 73.530
Frequencies: -204.5505 17.8831 21.7399 50.0962 52.3506

SCF Energy (M06) = -1186.516373
SCF Energy (M06/def2-tzvp) = -1187.884649

Alkyne Coordination Complex RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.06221427 Predicted Change = -1.946806D-08

Optimization completed. ---------- Optimization step: 1
Optimization completed on the basis of negligible forces.

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000004 II	0.000450	YES	0.000001 II	0.000300	YES
Disp	0.003258 II	0.001800	NO!	0.000451 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-1.110763	2.026067	-0.473383
Rh	-0.440149	-0.208173	0.018882
C	0.109997	2.093073	-0.335165
C	1.505649	2.513363	-0.092524
C	2.742215	0.516191	-0.451063
C	1.641684	-0.415391	-0.885342
C	1.336935	-1.632896	-0.22801
C	0.119495	-2.274941	-0.580331
C	-0.545056	-2.118284	-1.949975
C	-1.113821	-0.698231	-1.912914
H	-2.203097	-0.665193	-1.973857
H	-0.679145	0.003868	-2.628582
H	-1.330759	-2.871969	-2.060477
H	0.179265	-2.280286	-2.758814
H	1.372361	-0.293659	-1.931645
H	1.706109	2.385179	0.980611
H	1.589349	3.575464	-0.347951
H	3.689189	0.241878	-0.933492
H	2.881792	0.485288	0.636806
H	-0.184032	-3.116276	0.03872
O	2.483775	1.851979	-0.878837
C	-2.529406	2.302768	-0.727284
H	-2.90912	1.677967	-1.54279

H -3.133861 2.101641 0.163807
H -2.662466 3.353546 -1.008905
C 2.143418 -2.13685 0.94337
H 3.093051 -2.539459 0.566885
H 2.355359 -1.345086 1.66403
H 1.615546 -2.933449 1.473593
C -2.144882 -0.555859 0.821733
O -3.145919 -0.773831 1.339064
Cl 0.399501 0.30877 2.373875
Statistical Thermodynamic Analysis for 020-COCl-OpenVCP-Complex-Yne-SqrPyr-LI-original.log
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -1187.06221427
Zero-point correction (ZPE)= 0.255088 -1186.807126
Internal Energy (U)= 0.273871 -1186.788343
Enthalpy (H)= 0.274816 -1186.787399
Gibbs Free Energy (G)= 0.208830 -1186.853385
Entropy (S) [Cal/Mol-Kelvin]= 138.879
Entropy (S): electronic= 0.000
Entropy (S): translational= 43.277
Entropy (S): rotational= 32.667
Entropy (S): vibrational= 62.935
Frequencies: 52.7203 66.0891 71.9870 80.5668 95.9677

SCF Energy (M06) = -1186.548207
SCF Energy (M06/def2-tzvp) = -1187.912694

2π-Insertion TS RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest) EmpiricalDispersion=GD3
freq=noraman

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.03506338 Predicted Change = -5.281016D-10

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000002 II	0.000450	YES	0.000001 II	0.000300	YES
Disp	0.000221 II	0.001800	YES	0.000045 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-0.174475	1.766689	-0.63198
Rh	-0.717504	-0.10144	-0.013559
Cl	-0.418997	0.557302	2.407813
C	1.050502	1.392221	-0.573135
C	2.421815	1.955363	-0.358184
C	2.970687	-0.192648	0.096168
C	1.610247	-0.59096	-0.457825
C	0.946224	-1.741972	0.207371
C	-0.04742	-2.446864	-0.443786
C	-0.48667	-2.213836	-1.883743
C	-0.930469	-0.74899	-2.009371
C	-2.550072	0.102731	0.181359
O	-3.683662	0.253338	0.306813
H	-1.956071	-0.65024	-2.369008
H	-0.275724	-0.129856	-2.629382
H	-1.313708	-2.894214	-2.107636
H	0.328582	-2.4735	-2.575588
H	1.647876	-0.680715	-1.542998
H	2.478735	2.343187	0.672323
H	2.603694	2.77675	-1.05873
H	3.701243	-0.980133	-0.117931
H	2.92131	-0.035943	1.182814
H	-0.476593	-3.294366	0.086756

O	3.413293	0.972311	-0.568637
C	-1.030466	2.956291	-0.851414
H	-1.557857	3.201864	0.077251
H	-0.433996	3.822321	-1.16239
H	-1.783804	2.756929	-1.621793
C	1.406761	-2.172582	1.58219
H	0.786142	-2.99275	1.952588
H	2.445719	-2.524688	1.539005
H	1.338063	-1.351834	2.300716

Statistical Thermodynamic Analysis for 025-COCl-TS-2Pi-Insertion-Yne-Boat-original.log
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

==========

SCF Energy=	-1187.03506338	
Zero-point correction (ZPE)=	0.255664	-1186.779399
Internal Energy (U)=	0.273147	-1186.761917
Enthalpy (H)=	0.274091	-1186.760972
Gibbs Free Energy (G)=	0.210924	-1186.824139
Entropy (S) [Cal/Mol-Kelvin]=	132.945	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	43.277	
Entropy (S): rotational=	32.763	
Entropy (S): vibrational=	56.906	

Frequencies: -215.7116 61.6608 72.2993 78.8215 84.3116

SCF Energy (M06) = -1186.517855
SCF Energy (M06/def2-tzvp) = -1187.880505

Metallacycle RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.08820016 Predicted Change = -6.869148D-09

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000007 II	0.000450	YES	0.000002 II	0.000300	YES
Disp	0.000626 II	0.001800	YES	0.000142 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-0.648283	1.355973	-0.059061
Rh	0.966156	0.103605	-0.07296
Cl	2.634463	-1.530872	-0.862995
C	-1.863634	0.796416	0.028076
C	-3.216062	1.424043	-0.294941
C	-3.395132	-0.865847	-0.574294
C	-2.157112	-0.662464	0.317668
C	-0.956855	-1.57653	0.150838
C	-0.013324	-1.671901	1.138482
C	0.057648	-0.79648	2.384794
C	1.013524	0.330513	1.999104
C	2.215977	1.461556	-0.377938
O	3.009985	2.275987	-0.521118
H	2.058476	0.13097	2.24538
H	0.709419	1.326815	2.319552
H	0.430489	-1.375501	3.238616
H	-0.923839	-0.39237	2.645054
H	-2.521744	-0.744604	1.353017
H	-3.185082	1.976065	-1.246549
H	-3.577568	2.108823	0.483432
H	-4.029557	-1.705211	-0.27531
H	-3.115353	-0.989714	-1.631906
H	0.773889	-2.413121	1.024015
O	-4.140007	0.332558	-0.376875

C -0.4691 2.837377 -0.291138
H 0.130543 3.285055 0.512514
H 0.058361 3.043299 -1.231286
H -1.42452 3.375761 -0.320311
C -0.892433 -2.472557 -1.061934
H 0.060529 -3.003394 -1.11242
H -1.716263 -3.198798 -1.03952
H -1.001752 -1.890434 -1.984148
Statistical Thermodynamic Analysis for 030-COCl-Metallacycle-Yne-TrigPyr-original.log
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -1187.08820016
Zero-point correction (ZPE)= 0.258165 -1186.830035
Internal Energy (U)= 0.275731 -1186.812469
Enthalpy (H)= 0.276676 -1186.811525
Gibbs Free Energy (G)= 0.212452 -1186.875749
Entropy (S) [Cal/Mol-Kelvin]= 135.171
Entropy (S): electronic= 0.000
Entropy (S): translational= 43.277
Entropy (S): rotational= 33.012
Entropy (S): vibrational= 58.882
Frequencies: 36.2613 51.1408 82.3776 89.6075 99.4554

SCF Energy (M06) = -1186.569141
SCF Energy (M06/def2-tzvp) = -1187.928284

Reductive Elimination TS RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300 ,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.06557212 Predicted Change = -5.745308D-10

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000003 II	0.000450	YES	0.000001 II	0.000300	YES
Disp	0.000251 II	0.001800	YES	0.000064 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-0.560833	1.405362	0.153342
Rh	1.023537	0.034327	0.051761
Cl	2.327315	-1.694247	-0.9473
C	-1.755206	0.808179	-0.028555
C	-2.938158	1.395286	-0.778951
C	-3.0736	-0.899435	-0.912548
C	-2.119146	-0.634656	0.268744
C	-0.925011	-1.556605	0.467284
C	-0.101412	-1.37375	1.547312
C	-0.280141	-0.235509	2.544831
C	0.289983	1.044259	1.922561
C	2.291643	1.241963	-0.600624
O	3.091124	1.970846	-0.98859
H	1.3479	1.207211	2.15448
H	-0.242646	1.947326	2.220279
H	0.250977	-0.467475	3.474121
H	-1.338485	-0.102574	2.796418
H	-2.743979	-0.671635	1.177542
H	-2.622128	1.847456	-1.732878
H	-3.478788	2.163555	-0.208192
H	-3.773126	-1.722985	-0.74684
H	-2.5122	-1.085547	-1.841204
H	0.660578	-2.12287	1.749807

O -3.831793 0.303434 -1.004677
C -0.348161 2.853161 -0.233637
H -0.18557 2.934989 -1.315746
H -1.214125 3.476538 0.0236
H 0.528328 3.282554 0.260033
C -0.812709 -2.775203 -0.411328
H 0.070061 -3.366059 -0.163908
H -1.712509 -3.39435 -0.289622
H -0.735946 -2.501213 -1.46749
Statistical Thermodynamic Analysis for 035-COCl-TS-ReductiveElim-Yne-Boat-original.log
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -1187.06557212
Zero-point correction (ZPE)= 0.257003 -1186.808569
Internal Energy (U)= 0.274018 -1186.791554
Enthalpy (H)= 0.274962 -1186.790610
Gibbs Free Energy (G)= 0.212333 -1186.853239
Entropy (S) [Cal/Mol-Kelvin]= 131.814
Entropy (S): electronic= 0.000
Entropy (S): translational= 43.277
Entropy (S): rotational= 32.952
Entropy (S): vibrational= 55.585
Frequencies: -384.6088 45.7534 52.0262 85.6661 90.6302

SCF Energy (M06) = -1186.557697
SCF Energy (M06/def2-tzvp) = -1187.917041

Product-Catalyst Complex RhCOCl

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C12H16ClO2Rh C1[X(C12H16ClO2Rh)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1187.14716493 Predicted Change = -6.629254D-08

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000030	0.000450	YES	0.000006	0.000300	YES
Disp	0.002449	0.001800	NO!	0.000464	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	1.351578	-0.927149	1.075556
Rh	-0.811816	-0.238874	-0.001878
C	1.602207	-0.096323	0.017386
C	2.320121	-0.546012	-1.253735
C	1.82163	1.640487	-1.58708
C	1.40995	1.42772	-0.110807
C	-0.040392	1.770989	0.218142
C	-0.524621	1.374551	1.480299
C	0.400272	0.935031	2.606666
C	0.918672	-0.50158	2.465886
H	0.137064	-1.196555	2.796246
H	1.770053	-0.667512	3.145314
H	-0.126788	1.021619	3.56181
H	1.248189	1.632685	2.658888
H	2.111676	1.974159	0.538883
H	1.633951	-1.080968	-1.928172
H	3.181034	-1.188597	-1.045992
H	2.257486	2.623204	-1.782605
H	0.956634	1.490704	-2.251383
H	-1.476212	1.799772	1.794718
C	-2.601391	0.148411	-0.319947
O	-3.70647	0.407976	-0.507958
Cl	-0.977408	-2.323887	-1.12686
O	2.808142	0.655573	-1.841608

C	-0.734889	2.860003	-0.568423
H	-0.218901	3.817787	-0.406878
H	-0.744275	2.666778	-1.644386
H	-1.771455	2.977632	-0.237706
C	1.72642	-2.390309	0.971179
H	1.581478	-2.781323	-0.03681
H	2.779933	-2.519315	1.259024
H	1.117052	-2.997953	1.645995

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========

SCF Energy=	-1187.14716493	
Zero-point correction (ZPE)=	0.260594	-1186.886571
Internal Energy (U)=	0.277471	-1186.869694
Enthalpy (H)=	0.278415	-1186.868750
Gibbs Free Energy (G)=	0.216399	-1186.930765
Entropy (S) [Cal/Mol-Kelvin]=	130.522	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	43.277	
Entropy (S): rotational=	32.754	
Entropy (S): vibrational=	54.491	

Frequencies: 51.9793 67.3197 82.9041 98.0489 110.4367

SCF Energy (M06) = -1186.640203
SCF Energy (M06/def2-tzvp) = -1187.997835

Substrate-Catalyst Complex RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.46469581 Predicted Change = -5.939265D-08

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000020 II	0.000450	YES	0.000003 II	0.000300	YES
Disp	0.002126 II	0.001800	NO!	0.000316 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
Rh	-0.384113	-0.810838	-0.461072
C	-1.843559	-2.382758	-1.510485
C	-3.115804	-1.948174	-0.850672
C	-4.286942	-2.925207	-0.78703
C	-3.612501	-2.477843	0.476691
C	1.325531	-1.274056	-1.542599
C	0.724531	-0.397271	-2.221967
H	-5.276177	-2.544526	-1.023611
H	-4.099796	-3.941742	-1.122515
H	-4.132879	-1.771811	1.114235
H	-3.013153	-3.205239	1.015533
H	-3.406116	-0.923814	-1.088092
C	-0.859429	-3.059652	-0.822032
H	-1.025372	-3.276813	0.233729
C	0.299899	-3.841806	-1.403814
H	0.124878	-4.908625	-1.225165
C	2.221791	-2.428052	-1.292334
H	2.701029	-2.706929	-2.245815
O	1.529553	-3.542812	-0.742821
H	0.396394	-3.70054	-2.487404
H	3.002431	-2.167196	-0.574338
C	0.507126	0.549916	-3.327475
H	1.240062	0.36863	-4.122141

H	-0.49594	0.444482	-3.748832
H	0.622018	1.58597	-2.991429
C	-1.863205	-2.227265	-3.01468
H	-2.507701	-2.99947	-3.453963
H	-2.29317	-1.257932	-3.289924
H	-0.873667	-2.30516	-3.467545
C	0.306169	0.878135	0.356915
N	1.537814	1.319021	0.729577
N	-0.552847	1.857681	0.754355
C	1.440482	2.557366	1.363767
C	2.776826	0.576119	0.652801
C	0.127083	2.899191	1.37546
C	-1.986404	1.68406	0.695725
H	2.312209	3.059105	1.751081
C	3.022929	-0.416727	1.619443
C	3.703902	0.917239	-0.349809
H	-0.386726	3.760873	1.771207
C	-2.679872	2.099925	-0.457919
C	-2.620076	1.082701	1.802076
C	2.0107	-0.811189	2.686593
C	4.270208	-1.055144	1.578529
C	4.932538	0.24699	-0.344808
C	3.406209	1.979149	-1.399699
C	-1.958748	2.781062	-1.611515
C	-4.064616	1.898606	-0.479084
C	-4.007586	0.907439	1.72776
C	-1.839122	0.596069	3.017278
C	1.702339	-2.319531	2.631832
H	1.074987	-0.283575	2.485939
C	2.485186	-0.382035	4.087439
H	4.498883	-1.820323	2.31363
C	5.217975	-0.723554	0.614101
H	5.676678	0.48902	-1.096486
C	4.088631	3.315235	-1.043983
H	2.323351	2.146552	-1.406554
C	3.813564	1.528283	-2.813869
H	-0.916088	2.449109	-1.586396
C	-1.965909	4.311501	-1.419957
C	-2.531352	2.39804	-2.985226
H	-4.639141	2.210289	-1.344669
C	-4.721447	1.309771	0.601546
H	-4.533901	0.450831	2.559951
H	-0.837419	1.035299	2.982994
C	-1.670835	-0.933839	2.971249

C	-2.474353	1.037822	4.347504
H	2.580969	-2.918795	2.894247
H	1.379024	-2.627027	1.631569
H	0.912486	-2.569485	3.348562
H	2.660838	0.698566	4.134151
H	3.418356	-0.88621	4.36209
H	1.731384	-0.63935	4.84054
H	6.18049	-1.226788	0.60497
H	5.176925	3.193315	-1.003215
H	3.759413	3.693915	-0.070714
H	3.860408	4.076699	-1.798208
H	3.418125	0.533671	-3.041714
H	4.901877	1.492598	-2.930084
H	3.43184	2.235012	-3.55881
H	-1.490004	4.598285	-0.475953
H	-2.99185	4.69629	-1.410457
H	-1.424999	4.803478	-2.236051
H	-3.525405	2.827557	-3.149654
H	-2.611877	1.310485	-3.094603
H	-1.881827	2.777705	-3.781015
H	-5.797952	1.168435	0.565734
H	-1.171335	-1.256072	2.044948
H	-2.639811	-1.4401	3.020367
H	-1.05961	-1.280066	3.811031
H	-3.45056	0.568956	4.511987
H	-2.611684	2.123591	4.380332
H	-1.828139	0.74904	5.183301

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

==========

SCF Energy= -1773.46469581
Zero-point correction (ZPE)= 0.824376 -1772.640320
Internal Energy (U)= 0.869496 -1772.595200
Enthalpy (H)= 0.870440 -1772.594256
Gibbs Free Energy (G)= 0.748652 -1772.716044
Entropy (S) [Cal/Mol-Kelvin]= 256.324
Entropy (S): electronic= 0.000
Entropy (S): translational= 45.322
Entropy (S): rotational= 37.500
Entropy (S): vibrational= 173.502
Frequencies: 20.9548 35.2894 38.1276 42.2949 50.4673

SCF Energy (M06) = -1772.050888
SCF Energy (M06/def2-tzvp) = -1773.754571

Oxidative-Addition TS RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest) EmpiricalDispersion=GD3
freq=noraman

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.42702389 Predicted Change = -6.868792D-09

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000011 ll 0.000450		YES	0.000001 ll 0.000300		YES
Disp	0.001717 ll 0.001800		YES	0.000252 ll 0.001200		YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-3.612771	3.802827	-0.969239
Rh	-0.512066	-0.575215	-1.123696
C	-2.506734	4.17289	-0.645534
C	-1.168978	4.602353	-0.218382
C	-0.163361	2.413628	-0.186191
C	-0.765592	1.514149	-1.233153
C	0.00897	1.050011	-2.350017
C	-0.699865	0.197406	-3.28168
C	-2.155762	0.243956	-3.628978
C	-2.205548	-0.813832	-2.560607
H	-2.178311	-1.841181	-2.917521
H	-2.884418	-0.637049	-1.722256
H	-2.395681	-0.0635	-4.646404
H	-2.651775	1.180381	-3.373682
H	-1.832642	1.675388	-1.370935
H	-1.14552	4.684194	0.880801
H	-0.937478	5.591364	-0.626649
H	0.858584	2.110474	0.031602
H	-0.740566	2.34987	0.744135
H	-0.082416	-0.423743	-3.928255
O	-0.102368	3.760205	-0.659889

C	-4.953668	3.367753	-1.353087
H	-5.006165	3.123093	-2.420841
H	-5.262401	2.48123	-0.785165
H	-5.68888	4.157796	-1.159832
C	1.432996	1.448595	-2.632659
H	1.94474	0.697401	-3.240461
H	1.434389	2.397381	-3.184437
H	2.008789	1.594145	-1.717753
C	0.51341	-0.655104	0.677471
N	1.750523	-0.453672	1.209952
N	-0.184381	-1.272823	1.67155
C	1.820239	-0.966737	2.506119
C	2.862834	0.147892	0.511753
C	0.597926	-1.478865	2.800568
C	-1.547221	-1.682174	1.430276
H	2.729221	-0.922059	3.082504
C	3.501174	-0.598575	-0.497539
C	3.268306	1.451706	0.873844
H	0.219282	-1.965533	3.685338
C	-2.590975	-0.807884	1.798732
C	-1.764459	-2.903671	0.758493
C	3.143408	-2.04623	-0.816426
C	4.555124	0.017753	-1.183708
C	4.325407	2.016531	0.149977
C	2.653281	2.215988	2.044654
C	-2.316562	0.477	2.567531
C	-3.892154	-1.189852	1.456462
C	-3.086527	-3.226863	0.425424
C	-0.614836	-3.826285	0.367002
C	2.841244	-2.256456	-2.310445
H	2.239251	-2.313077	-0.262494
C	4.26535	-2.990327	-0.340362
H	5.074901	-0.529491	-1.963993
C	4.956902	1.313445	-0.873615
H	4.66318	3.017819	0.394402
C	3.537446	2.057018	3.300719
H	1.673433	1.776028	2.264529
C	2.43594	3.714789	1.756893
H	-1.273545	0.757569	2.383859
C	-2.472295	0.230917	4.082614
C	-3.19468	1.653765	2.112355
H	-4.726091	-0.550431	1.725946
C	-4.136807	-2.379006	0.768252
H	-3.295897	-4.152839	-0.100307

H	0.276104	-3.520431	0.925131
C	-0.292589	-3.678075	-1.130563
C	-0.890956	-5.298692	0.720256
H	3.715868	-2.047925	-2.935722
H	2.024465	-1.605743	-2.640684
H	2.547597	-3.295587	-2.495346
H	4.45352	-2.872127	0.732364
H	5.20362	-2.788462	-0.868953
H	3.991398	-4.035033	-0.527298
H	5.774191	1.773448	-1.42145
H	4.525971	2.497606	3.128905
H	3.689172	1.007749	3.572762
H	3.082196	2.567814	4.156471
H	1.875646	3.891979	0.834739
H	3.388069	4.251061	1.6832
H	1.880164	4.166898	2.586065
H	-1.801143	-0.560962	4.433051
H	-3.498552	-0.069876	4.322135
H	-2.244633	1.143314	4.644731
H	-4.248116	1.501858	2.372346
H	-3.128801	1.820511	1.032739
H	-2.871843	2.573219	2.612841
H	-5.155861	-2.650987	0.508337
H	0.052084	-2.653506	-1.381585
H	-1.165721	-3.90028	-1.752772
H	0.525813	-4.342418	-1.427931
H	-1.711437	-5.715725	0.126531
H	-1.149724	-5.408918	1.778117
H	-0.000792	-5.904673	0.52079

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========

SCF Energy=		-1773.42702389
Zero-point correction (ZPE)=	0.821359	-1772.605665
Internal Energy (U)=	0.866974	-1772.560050
Enthalpy (H)=	0.867918	-1772.559106
Gibbs Free Energy (G)=	0.742437	-1772.684587
Entropy (S) [Cal/Mol-Kelvin]=	264.097	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	45.322	
Entropy (S): rotational=	37.664	
Entropy (S): vibrational=	181.111	

Frequencies: -215.5961 20.1889 24.8402 27.6334 30.7810

SCF Energy (M06) = -1772.016297
SCF Energy (M06/def2-tzvp) = -1773.722056

Alkyne Coordination Complex RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.46843464 Predicted Change = -4.917293D-07

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000039 II	0.000450	YES	0.000007 II	0.000300	YES
Disp	0.048627 II	0.001800	NO!	0.006813 II	0.001200	NO!

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	1.144342	1.605477	-1.819112
Rh	0.495256	-0.482726	-1.142271
C	2.073675	0.838975	-2.106727
C	3.373918	0.295615	-2.567068
C	2.806073	-1.955389	-3.085052
C	1.335992	-1.919	-2.748681
C	0.744218	-2.670915	-1.708332
C	-0.59632	-2.378858	-1.335248
C	-1.59783	-1.736044	-2.302299
C	-1.109681	-0.298175	-2.42138
H	-1.787553	0.446123	-2.014912
H	-0.719259	0.010411	-3.39359
H	-2.599132	-1.77648	-1.868187
H	-1.618153	-2.262719	-3.265118
H	0.721657	-1.592545	-3.584144
H	3.942238	-0.071808	-1.696128
H	3.9417	1.116232	-3.018406
H	2.992655	-2.655235	-3.907418
H	3.416897	-2.274663	-2.227722
H	-0.993347	-2.907635	-0.476355
O	3.272301	-0.696833	-3.566589
C	0.312346	2.814738	-1.774866
H	-0.042251	3.02472	-0.763472

H	0.884845	3.678109	-2.130073
H	-0.564706	2.69539	-2.417556
C	1.575841	-3.576726	-0.829273
H	0.989325	-3.957149	0.008973
H	1.940275	-4.43214	-1.409726
H	2.45106	-3.058171	-0.425008
C	-0.393883	0.379989	0.528346
N	0.429126	0.840126	1.523736
N	-1.649012	0.726512	0.945163
C	-0.295611	1.50379	2.510771
C	1.850796	0.560653	1.589913
C	-1.596495	1.432996	2.148579
C	-2.91316	0.296988	0.380127
H	0.180963	1.934537	3.375657
C	2.272731	-0.747568	1.947276
C	2.761184	1.605148	1.329354
H	-2.491531	1.795172	2.627275
C	-3.653459	1.201731	-0.403668
C	-3.391533	-0.989596	0.714057
C	1.299944	-1.833755	2.424466
C	3.651791	-0.995576	1.925026
C	4.127291	1.294973	1.335255
C	2.323733	3.05203	1.14159
C	-3.185536	2.627654	-0.66212
C	-4.885565	0.766275	-0.9084
C	-4.62801	-1.372395	0.180259
C	-2.655102	-1.907533	1.684873
C	1.948247	-3.216512	2.612066
H	0.510808	-1.932377	1.668857
C	0.636732	-1.448899	3.766581
H	4.025609	-1.977861	2.185744
C	4.568241	0.005094	1.606058
H	4.852542	2.076472	1.1354
C	2.479857	3.821555	2.471552
H	1.262448	3.055846	0.879903
C	3.089864	3.78495	0.025563
H	-2.124519	2.683623	-0.405185
C	-3.937351	3.612069	0.257227
C	-3.334767	3.051536	-2.134631
H	-5.479654	1.439183	-1.517966
C	-5.363901	-0.510062	-0.630398
H	-5.028505	-2.353602	0.409562
H	-1.583516	-1.712515	1.586377
C	-2.881877	-3.40572	1.414974

C	-3.062416	-1.584505	3.139059
H	2.624969	-3.21987	3.474086
H	2.513445	-3.554643	1.741394
H	1.167017	-3.9578	2.811294
H	0.011661	-0.559127	3.693594
H	1.402484	-1.271121	4.53011
H	-9.2e-05	-2.269339	4.114974
H	5.631339	-0.218142	1.601897
H	3.531951	3.852551	2.776023
H	1.916936	3.354991	3.286437
H	2.127676	4.853089	2.360576
H	3.09761	3.209202	-0.903523
H	4.128888	3.981249	0.310523
H	2.623241	4.756409	-0.169895
H	-3.795186	3.365494	1.314798
H	-5.013406	3.589108	0.052019
H	-3.582277	4.636069	0.095834
H	-4.386443	3.15474	-2.421926
H	-2.876314	2.328031	-2.817661
H	-2.859824	4.025753	-2.29478
H	-6.32123	-0.829838	-1.031545
H	-2.757959	-3.664103	0.358306
H	-3.886004	-3.724183	1.715389
H	-2.170132	-3.998273	2.000177
H	-4.138614	-1.737925	3.276416
H	-2.829837	-0.551034	3.409457
H	-2.532438	-2.241372	3.837549

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

==========

SCF Energy=		-1773.46843464
Zero-point correction (ZPE)=	0.824947	-1772.643488
Internal Energy (U)=	0.869460	-1772.598975
Enthalpy (H)=	0.870404	-1772.598031
Gibbs Free Energy (G)=	0.749981	-1772.718453
Entropy (S) [Cal/Mol-Kelvin]=	253.451	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	45.322	
Entropy (S): rotational=	37.510	
Entropy (S): vibrational=	170.619	

Frequencies: 7.7469 25.9229 34.8329 42.3040 47.7786

SCF Energy (M06) = -1772.050255
SCF Energy (M06/def2-tzvp) = -1773.757274

2π-Insertion TS RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest) EmpiricalDispersion=GD3
freq=noraman

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.44857974 Predicted Change = -7.298505D-10

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000013 ll 0.000450		YES	0.000001 ll 0.000300		YES
Disp	0.000403 ll 0.001800		YES	0.000087 ll 0.001200		YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-1.015259	-2.345414	0.370204
Rh	-0.556759	-0.690703	-0.699632
C	-1.912008	-2.564396	-0.539606
C	-3.150773	-3.395764	-0.740957
C	-3.38379	-2.111412	-2.597644
C	-1.938176	-1.683322	-2.376926
C	-1.588302	-0.273122	-2.693856
C	-0.282379	0.078017	-2.994245
C	0.86811	-0.919298	-3.082969
C	0.9628	-1.634952	-1.73386
H	1.90944	-1.496322	-1.223466
H	0.698687	-2.695631	-1.752683
H	1.793794	-0.375648	-3.282745
H	0.718517	-1.61552	-3.92084
H	-1.270473	-2.410947	-2.836848
H	-3.963737	-2.977093	-0.122054
H	-2.96689	-4.425661	-0.420348
H	-3.600828	-2.149615	-3.669611
H	-4.091514	-1.418901	-2.117672
H	-0.086585	1.104876	-3.290781
O	-3.533503	-3.421205	-2.096541
C	-2.696745	0.759263	-2.723364

H	-3.407459	0.535927	-3.528517
H	-3.258652	0.788431	-1.783051
H	-2.29514	1.75897	-2.89742
C	-0.488286	-3.031554	1.581458
H	-0.171274	-2.321537	2.348311
H	-1.233829	-3.707735	2.015324
H	0.389874	-3.625176	1.307299
C	0.5322	0.325282	0.645542
N	-0.166558	1.097043	1.538251
N	1.831989	0.443087	1.038167
C	0.681015	1.661063	2.486528
C	-1.535629	1.495818	1.289195
C	1.932222	1.247428	2.177356
C	3.001581	-0.003941	0.313849
H	0.31301	2.308257	3.266333
C	-1.744178	2.624691	0.466435
C	-2.593068	0.770119	1.873731
H	2.886585	1.447799	2.63664
C	3.670119	-1.156805	0.75825
C	3.440215	0.767148	-0.787093
C	-0.599068	3.522799	0.010483
C	-3.068573	2.966103	0.169658
C	-3.897847	1.148851	1.532764
C	-2.331488	-0.294166	2.927432
C	3.171529	-1.978175	1.93955
C	4.832792	-1.533174	0.071766
C	4.598219	0.336029	-1.442007
C	2.708507	2.030812	-1.234342
C	-0.607896	3.8146	-1.497752
H	0.34472	3.020592	0.230612
C	-0.613972	4.832067	0.825901
H	-3.269379	3.831416	-0.454307
C	-4.133235	2.224582	0.678164
H	-4.739454	0.612825	1.958318
C	-2.357033	0.352636	4.329013
H	-1.32146	-0.67719	2.763724
C	-3.305909	-1.479724	2.864272
H	2.14029	-1.674934	2.148964
C	4.011143	-1.691518	3.199967
C	3.154083	-3.486009	1.629498
H	5.38063	-2.413541	0.391545
C	5.290939	-0.797281	-1.015811
H	4.96998	0.89337	-2.294339
H	1.637704	1.86242	-1.080491

C	2.895667	2.36829	-2.722779
C	3.133406	3.245067	-0.380787
H	-1.523199	4.324826	-1.816477
H	-0.510393	2.890797	-2.073826
H	0.235534	4.46383	-1.757203
H	-0.568295	4.63033	1.901752
H	-1.526278	5.407219	0.632447
H	0.245516	5.457003	0.558849
H	-5.153472	2.505305	0.432229
H	-3.344634	0.777122	4.541709
H	-1.621105	1.159676	4.413066
H	-2.132713	-0.393465	5.099469
H	-3.354199	-1.899084	1.855394
H	-4.31872	-1.191472	3.165259
H	-2.979253	-2.268484	3.55013
H	3.978306	-0.631286	3.473603
H	5.060553	-1.961444	3.036374
H	3.639582	-2.273506	4.050777
H	4.166081	-3.894978	1.539682
H	2.627182	-3.696042	0.691939
H	2.656119	-4.031052	2.439029
H	6.192057	-1.106383	-1.537529
H	2.684187	1.513309	-3.372548
H	3.913403	2.710144	-2.940056
H	2.217266	3.182027	-3.000462
H	4.203845	3.442764	-0.506343
H	2.940026	3.089108	0.683546
H	2.584624	4.140812	-0.693988

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -1773.44857974
Zero-point correction (ZPE)= 0.824517 -1772.624063
Internal Energy (U)= 0.868337 -1772.580243
Enthalpy (H)= 0.869281 -1772.579299
Gibbs Free Energy (G)= 0.750918 -1772.697662
Entropy (S) [Cal/Mol-Kelvin]= 249.117
Entropy (S): electronic= 0.000
Entropy (S): translational= 45.322
Entropy (S): rotational= 37.539
Entropy (S): vibrational= 166.256
Frequencies: -200.7708 29.5658 35.6020 37.3312 41.1009

SCF Energy (M06) = -1772.027394

SCF Energy (M06/def2-tzvp) = -1773.731815

Metallacycle RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.50000197 Predicted Change = -2.101462D-08

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000023 II	0.000450	YES	0.000003 II	0.000300	YES
Disp	0.001693 II	0.001800	YES	0.000295 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-0.995519	-1.90583	-0.091242
Rh	-0.521069	-0.151198	-0.928549
C	-2.029196	-2.557629	-0.636735
C	-2.782492	-3.761111	-0.078599
C	-4.208324	-2.571871	-1.470755
C	-2.783046	-2.16359	-1.888872
C	-2.505009	-0.749795	-2.360565
C	-1.375256	-0.465705	-3.082211
C	-0.20679	-1.413868	-3.344143
C	0.781051	-1.066072	-2.230597
H	1.501729	-0.295653	-2.510143
H	1.295697	-1.908388	-1.766143
H	0.20904	-1.250362	-4.345942
H	-0.520434	-2.458473	-3.27673
H	-2.494783	-2.865824	-2.68471
H	-2.983697	-3.648846	0.996424
H	-2.249593	-4.708812	-0.228657
H	-4.888931	-2.739882	-2.30938
H	-4.655441	-1.831837	-0.788306
H	-1.286643	0.531629	-3.515831
O	-4.005499	-3.82063	-0.817805
C	-0.189934	-2.440112	1.056326
H	0.84454	-2.588067	0.737048

H	-0.168779	-1.760862	1.912537
H	-0.57259	-3.408684	1.400352
C	-3.565669	0.299454	-2.127408
H	-4.502608	0.014235	-2.622599
H	-3.785614	0.410495	-1.058833
H	-3.25765	1.276259	-2.510091
C	0.680887	0.452689	0.579691
N	1.988356	0.392541	0.954549
N	0.089706	1.261406	1.506385
C	2.198763	1.153702	2.105095
C	3.065277	-0.236782	0.216058
C	1.0063	1.699196	2.452789
C	-1.271554	1.724746	1.345204
H	3.176052	1.23815	2.550671
C	3.637142	-1.419975	0.721008
C	3.536736	0.407138	-0.950719
H	0.724448	2.352225	3.26352
C	-1.502017	2.77998	0.433308
C	-2.302275	1.114252	2.085295
C	3.231594	-2.036106	2.056066
C	4.681539	-1.993551	-0.018157
C	4.577775	-0.214295	-1.646823
C	2.98978	1.758579	-1.407018
C	-0.371536	3.506815	-0.28824
C	-2.829951	3.172344	0.228173
C	-3.609997	1.556799	1.848532
C	-2.027937	0.060389	3.146964
C	3.10336	-3.570609	2.000697
H	2.256186	-1.629535	2.34119
C	4.244763	-1.64155	3.152196
H	5.147477	-2.905913	0.338772
C	5.138555	-1.407273	-1.192762
H	4.963727	0.239802	-2.552241
C	3.653001	2.906143	-0.615712
H	1.919561	1.780361	-1.182415
C	3.13519	2.016914	-2.915464
H	0.582568	3.1163	0.077534
C	-0.385016	5.015241	0.0243
C	-0.420199	3.261156	-1.806549
H	-3.047329	3.973913	-0.471037
C	-3.873744	2.563506	0.922045
H	-4.429925	1.112591	2.403592
H	-0.985569	-0.257004	3.04636
C	-2.914727	-1.184242	2.972141

C	-2.188593	0.667256	4.555241
H	4.081847	-4.053353	1.907439
H	2.487659	-3.904748	1.159983
H	2.648318	-3.939066	2.926251
H	4.332966	-0.555769	3.261471
H	5.241094	-2.029391	2.912501
H	3.942377	-2.05688	4.119937
H	5.946906	-1.87068	-1.750894
H	4.731904	2.928197	-0.805389
H	3.501221	2.800301	0.46235
H	3.23487	3.87232	-0.921889
H	2.736197	1.193872	-3.518305
H	4.180979	2.167504	-3.20392
H	2.593077	2.929168	-3.185982
H	-0.34471	5.195001	1.103565
H	-1.28604	5.501858	-0.364174
H	0.481492	5.502169	-0.436349
H	-1.363173	3.61234	-2.239809
H	-0.326912	2.191788	-2.046419
H	0.401316	3.78165	-2.310113
H	-4.89655	2.887728	0.752923
H	-2.848637	-1.568348	1.950495
H	-3.966239	-0.964098	3.185828
H	-2.599218	-1.9727	3.66385
H	-3.215932	1.011675	4.718545
H	-1.522162	1.525111	4.700829
H	-1.955995	-0.080161	5.321597

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

==========

SCF Energy=	-1773.50000197	
Zero-point correction (ZPE)=	0.826708	-1772.673294
Internal Energy (U)=	0.870596	-1772.629406
Enthalpy (H)=	0.871541	-1772.628461
Gibbs Free Energy (G)=	0.752786	-1772.747216
Entropy (S) [Cal/Mol-Kelvin]=	249.940	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	45.322	
Entropy (S): rotational=	37.622	
Entropy (S): vibrational=	166.996	

Frequencies: 21.2904 33.6974 35.6208 44.6674 47.0461

SCF Energy (M06) = -1772.077571
SCF Energy (M06/def2-tzvp) = -1773.776229

Reductive Elimination TS RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest) EmpiricalDispersion=GD3
freq=noraman

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.46270865 Predicted Change = -2.295727D-08

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000027 II	0.000450	YES	0.000003 II	0.000300	YES
Disp	0.002752 II	0.001800	NO!	0.000473 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-0.417935	-1.896238	-1.031906
Rh	-0.445187	0.162663	-1.014847
C	-1.618735	-2.34765	-1.459077
C	-2.339834	-3.586717	-0.988367
C	-3.890373	-1.896733	-1.467225
C	-2.62422	-1.584113	-2.291077
C	-2.260489	-0.121911	-2.511035
C	-1.112699	0.214196	-3.197287
C	-0.071113	-0.795582	-3.662491
C	0.771584	-1.133942	-2.439132
H	1.577751	-0.424764	-2.234432
H	1.220816	-2.126086	-2.452348
H	0.553583	-0.363803	-4.452283
H	-0.545514	-1.693621	-4.072834
H	-2.746629	-2.078329	-3.269674
H	-2.06493	-3.873315	0.033572
H	-2.150416	-4.450805	-1.644242
H	-4.819414	-1.824647	-2.039321
H	-3.955817	-1.235494	-0.590919
H	-0.992684	1.2464	-3.524429
O	-3.733981	-3.257704	-1.055326
C	0.454567	-2.718342	-0.117033

H	0.032246	-2.764376	0.893327
H	0.559497	-3.74769	-0.482192
H	1.451192	-2.28861	-0.04336
C	-3.32587	0.913918	-2.237882
H	-2.989345	1.91584	-2.517517
H	-4.22761	0.68374	-2.82117
H	-3.617955	0.935433	-1.182482
C	0.585582	0.36039	0.717257
N	-0.106866	0.819632	1.797671
N	1.890186	0.3695	1.113961
C	0.747486	1.141727	2.845732
C	-1.525758	1.096451	1.733578
C	2.002435	0.862668	2.413964
C	3.02021	0.018358	0.283124
H	0.384275	1.545041	3.777396
C	-1.925063	2.353502	1.23594
C	-2.43994	0.105113	2.145184
H	2.959821	0.969849	2.895295
C	3.73012	-1.169277	0.564928
C	3.383033	0.896247	-0.759597
C	-0.914537	3.387671	0.753763
C	-3.299901	2.603588	1.144807
C	-3.801246	0.410226	2.035879
C	-1.968239	-1.224533	2.717108
C	3.432933	-2.046757	1.779607
C	4.796721	-1.493967	-0.282841
C	4.453627	0.51367	-1.577495
C	2.741275	2.267569	-0.950481
C	-0.812596	3.349975	-0.780723
H	0.070011	3.126184	1.154335
C	-1.232788	4.812778	1.239769
H	-3.647837	3.556416	0.759471
C	-4.227184	1.643335	1.541085
H	-4.539893	-0.322544	2.340953
C	-1.726867	-1.101852	4.236802
H	-1.007681	-1.459541	2.245773
C	-2.930817	-2.388908	2.429312
H	2.413986	-1.830629	2.120272
C	4.405491	-1.703901	2.929382
C	3.512424	-3.556618	1.482155
H	5.366464	-2.398784	-0.100029
C	5.145451	-0.673376	-1.35195
H	4.765395	1.165065	-2.387542
H	1.819215	2.30533	-0.366138

C	2.362234	2.562074	-2.411986
C	3.6788	3.358868	-0.394145
H	-1.777641	3.5695	-1.247979
H	-0.485423	2.355984	-1.148841
H	-0.072875	4.068315	-1.148682
H	-1.344977	4.842002	2.328156
H	-2.154057	5.203309	0.794633
H	-0.421054	5.492945	0.960699
H	-5.289867	1.855982	1.467415
H	-2.655734	-0.83326	4.752358
H	-0.978377	-0.33877	4.471921
H	-1.375544	-2.056034	4.644874
H	-3.224359	-2.441283	1.3773
H	-3.845438	-2.312969	3.028033
H	-2.453507	-3.336966	2.700312
H	4.364334	-0.646913	3.209771
H	5.437495	-1.923039	2.633512
H	4.172797	-2.300334	3.818392
H	4.543898	-3.879339	1.305814
H	2.919638	-3.839878	0.608128
H	3.142238	-4.121839	2.34399
H	5.974286	-0.94832	-1.997811
H	1.664904	1.813322	-2.802662
H	3.239007	2.585719	-3.067211
H	1.879672	3.542698	-2.483542
H	4.623878	3.383827	-0.948032
H	3.913285	3.179185	0.660829
H	3.210301	4.346306	-0.477458

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========

SCF Energy=		-1773.46270865
Zero-point correction (ZPE)=	0.825142	-1772.637567
Internal Energy (U)=	0.868615	-1772.594093
Enthalpy (H)=	0.869559	-1772.593149
Gibbs Free Energy (G)=	0.751755	-1772.710954
Entropy (S) [Cal/Mol-Kelvin]=	247.941	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	45.322	
Entropy (S): rotational=	37.524	
Entropy (S): vibrational=	165.095	

Frequencies: -445.0464 28.1326 33.8346 36.3392 43.6721

SCF Energy (M06) = -1772.051172

SCF Energy (M06/def2-tzvp) = -1773.748738

Product-Catalyst Complex RhNHC-IPr

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300
,xqc) opt=(maxcycle=250) EmpiricalDispersion=GD3 freq=noraman

---

Pointgroup=C1 Stoichiometry=C38H52N2ORh(1+)
C1[X(C38H52N2ORh)]
Charge = 1 Multiplicity = 1 Basis = Nuclear

SCF Energy = -1773.53954754 Predicted Change = -3.568075D-08

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000014 II	0.000450	YES	0.000002 II	0.000300	YES
Disp	0.003217 II	0.001800	NO!	0.000619 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-0.358007	-3.327546	-0.846456
Rh	-0.175274	-1.03519	-0.192988
C	-1.389661	-2.596766	-1.39133
C	-2.86622	-2.746275	-1.015486
C	-2.833767	-1.191348	-2.664096
C	-1.356457	-1.647287	-2.605199
C	-0.344847	-0.563111	-2.257095
C	0.985669	-0.994991	-1.980984
C	1.493244	-2.370341	-2.387654
C	1.021077	-3.503742	-1.461797
H	1.737735	-3.603009	-0.638399
H	1.041189	-4.466731	-1.994063
H	2.586857	-2.359031	-2.399911
H	1.174046	-2.566603	-3.420543
H	-1.097949	-2.174113	-3.536134
H	-3.127393	-2.145978	-0.127222
H	-3.155754	-3.784891	-0.834004
H	-3.187772	-0.980625	-3.675145
H	-2.995199	-0.302895	-2.033984
H	1.745697	-0.221405	-1.930923
O	-3.576628	-2.287381	-2.153186
C	-0.621508	0.869271	-2.640163
H	-0.717349	0.950236	-3.732647

H	-1.545892	1.242517	-2.197793
H	0.194863	1.523683	-2.324072
C	-0.637514	-4.303172	0.281268
H	-1.542338	-4.063948	0.844131
H	-0.752472	-5.317502	-0.125945
H	0.197812	-4.334369	0.988114
C	0.341463	0.781353	0.510933
N	1.548401	1.348307	0.780439
N	-0.574821	1.635023	1.05608
C	1.393021	2.530307	1.499845
C	2.820557	0.757292	0.438111
C	0.060725	2.71045	1.674092
C	-2.004018	1.409971	1.031645
H	2.240343	3.115237	1.819209
C	3.295211	-0.304468	1.229094
C	3.516717	1.257023	-0.679399
H	-0.492031	3.485041	2.17805
C	-2.818439	2.307191	0.312852
C	-2.52842	0.284608	1.715834
C	2.553332	-0.800651	2.464719
C	4.498852	-0.905309	0.840817
C	4.724223	0.631328	-1.01192
C	3.015469	2.455486	-1.478569
C	-2.273264	3.539093	-0.405687
C	-4.199447	2.05971	0.30214
C	-3.911472	0.087699	1.661347
C	-1.640882	-0.67991	2.511786
C	1.957174	-2.197844	2.222317
H	1.718071	-0.121682	2.659248
C	3.447125	-0.787618	3.718028
H	4.892158	-1.734955	1.420325
C	5.204309	-0.446146	-0.269075
H	5.295639	0.99041	-1.861662
C	3.784803	3.727949	-1.068039
H	1.96002	2.612611	-1.2285
C	3.099611	2.245911	-3.001217
H	-1.194111	3.408066	-0.542197
C	-2.505086	4.80622	0.445863
C	-2.890201	3.748657	-1.802591
H	-4.855922	2.735957	-0.234837
C	-4.740873	0.965351	0.963347
H	-4.35764	-0.756863	2.172019
H	-0.781817	-0.982825	1.870189
C	-2.329107	-1.987583	2.924536

C	-1.026495	-0.004447	3.754034
H	2.741288	-2.943365	2.046948
H	1.312065	-2.18891	1.330265
H	1.360142	-2.524693	3.081573
H	3.864492	0.208893	3.896185
H	4.281956	-1.49075	3.627951
H	2.864372	-1.077483	4.599574
H	6.139837	-0.921286	-0.549878
H	4.850845	3.625728	-1.300382
H	3.697047	3.924379	0.006014
H	3.401339	4.601149	-1.607303
H	2.582416	1.333782	-3.316984
H	4.136924	2.17942	-3.34568
H	2.639103	3.093945	-3.519482
H	-2.067747	4.725874	1.446017
H	-3.578227	4.986779	0.574929
H	-2.070941	5.683397	-0.046173
H	-3.94078	4.051327	-1.740979
H	-2.839573	2.846204	-2.418159
H	-2.354605	4.548034	-2.325492
H	-5.812192	0.790028	0.938338
H	-2.797155	-2.495814	2.076754
H	-3.098744	-1.810856	3.683509
H	-1.589436	-2.66673	3.360273
H	-1.825266	0.285851	4.445948
H	-0.452864	0.890768	3.505879
H	-0.361162	-0.700586	4.276249

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

==========

SCF Energy=		-1773.53954754
Zero-point correction (ZPE)=	0.827913	-1772.711635
Internal Energy (U)=	0.871339	-1772.668209
Enthalpy (H)=	0.872283	-1772.667265
Gibbs Free Energy (G)=	0.753971	-1772.785577
Entropy (S) [Cal/Mol-Kelvin]=	249.008	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	45.322	
Entropy (S): rotational=	37.488	
Entropy (S): vibrational=	166.199	

Frequencies: 22.3874 27.4320 32.0410 39.0786 42.4319

SCF Energy (M06) = -1772.130582
SCF Energy (M06/def2-tzvp) = -1773.827285

Product

Using: Gaussian 09, Revision D.01

==========

b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(m
axcycle=250) EmpiricalDispersion=GD3 freq=noraman

Pointgroup=C1 Stoichiometry=C11H16O C1[X(C11H16O)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -503.999209550 Predicted Change = -1.536180D-08

Optimization completed. ---------- Optimization step: 1

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.000020 II	0.000450	YES	0.000004 II	0.000300	YES
Disp	0.001748 II	0.001800	YES	0.000402 II	0.001200	YES

Atomic Type:	Coordinates (Angstroms) X	Y	Z
C	-1.386434	-1.042255	0.106706
C	-0.701912	-2.178174	-0.073282
C	0.62255	-2.240497	-0.791082
C	1.756135	-1.546445	-0.015066
C	0.546263	0.692525	-0.066112
C	1.641943	-0.04417	0.16347
H	0.904833	-3.285196	-0.964296
H	0.54298	-1.772969	-1.78375
H	1.858243	-2.016321	0.975934
H	2.708676	-1.747774	-0.529748
H	-1.093189	-3.105565	0.343855
C	-0.858589	0.255419	-0.492885
H	-0.858531	0.150085	-1.59049
C	-1.66638	1.533399	-0.179357
H	-2.55703	1.656578	-0.801477
C	0.488795	2.212792	0.053413
H	1.257612	2.728403	-0.532096
O	-0.779629	2.60394	-0.462636
H	0.592031	2.533226	1.106051
H	-1.972273	1.557046	0.879547
C	2.93586	0.590899	0.626831
H	3.343535	0.043508	1.487948
H	3.700583	0.542983	-0.16186
H	2.827171	1.637345	0.924117

C -2.693645 -1.019922 0.860779
H -3.49906 -0.567356 0.266453
H -3.005938 -2.032981 1.13381
H -2.620131 -0.433959 1.786603
Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
==========
SCF Energy= -503.999209550
Zero-point correction (ZPE)= 0.248925 -503.750285
Internal Energy (U)= 0.260334 -503.738875
Enthalpy (H)= 0.261279 -503.737931
Gibbs Free Energy (G)= 0.212266 -503.786944
Entropy (S) [Cal/Mol-Kelvin]= 103.156
Entropy (S): electronic= 0.000
Entropy (S): translational= 41.195
Entropy (S): rotational= 30.615
Entropy (S): vibrational= 31.345
Frequencies: 63.4359 115.3932 124.3408 164.1437 197.7355

SCF Energy (M06) = -503.5947979
SCF Energy (M06/def2-tzvp) = -503.7883521

Substrate

Using: Gaussian 09, Revision D.01
==========
b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(m
axcycle=250) EmpiricalDispersion=GD3 freq=noraman

Pointgroup=C1 Stoichiometry=C11H16O C1[X(C11H16O)]
Charge = 0 Multiplicity = 1 Basis = Nuclear

SCF Energy = -503.905916409 Predicted Change = -2.587229D-08

Optimization completed. ---------- Optimization step: 1
Optimization completed on the basis of negligible forces.
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.000004 II 0.000450 YES 0.000001 II 0.000300 YES
Disp 0.019337 II 0.001800 NO! 0.003483 II 0.001200 NO!

Atomic Coordinates (Angstroms)
Type: X Y Z

C 2.234134 -0.380519 0.345283

C	3.338375	0.602667	0.588924
C	4.503939	0.692172	-0.381073
C	3.54332	1.847824	-0.233865
C	-3.621938	-0.194368	-0.178686
C	-4.620858	0.392844	0.163798
H	5.509544	0.788089	0.020417
H	4.437884	0.103428	-1.2929
H	3.884308	2.743857	0.277687
H	2.863565	2.041674	-1.058258
H	3.623218	0.680492	1.63958
C	1.091746	-0.019975	-0.256375
H	0.954257	1.020372	-0.543657
C	-0.073488	-0.890559	-0.618122
H	-0.095734	-1.056542	-1.712924
C	-2.430453	-0.925354	-0.603142
H	-2.432552	-1.936717	-0.15689
O	-1.261967	-0.217734	-0.217019
H	-0.01952	-1.885595	-0.149048
H	-2.447735	-1.068394	-1.699439
C	-5.819494	1.113701	0.584098
H	-6.417521	0.521314	1.287623
H	-5.554255	2.053602	1.083684
H	-6.458761	1.362032	-0.272162
C	2.561361	-1.774577	0.827289
H	3.406395	-2.186604	0.259727
H	2.877058	-1.748484	1.879024
H	1.725715	-2.473786	0.744914

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

==========

SCF Energy=		-503.905916409
Zero-point correction (ZPE)=	0.242739	-503.663177
Internal Energy (U)=	0.257281	-503.648635
Enthalpy (H)=	0.258225	-503.647691
Gibbs Free Energy (G)=	0.198125	-503.707792
Entropy (S) [Cal/Mol-Kelvin]=	126.492	
Entropy (S): electronic=	0.000	
Entropy (S): translational=	41.195	
Entropy (S): rotational=	32.018	
Entropy (S): vibrational=	53.279	

Frequencies: 20.2278 26.5908 43.1312 58.1385 71.4467

SCF Energy (M06) = -503.5054512
SCF Energy (M06/def2-tzvp) = -503.7102041

Appendix III.

Computational Data for Chapter 4

Palladium-Catalyzed Completely Linear-Selective Negishi Cross-Coupling of Allylzinc Halides with Aryl and Vinyl Electrophiles

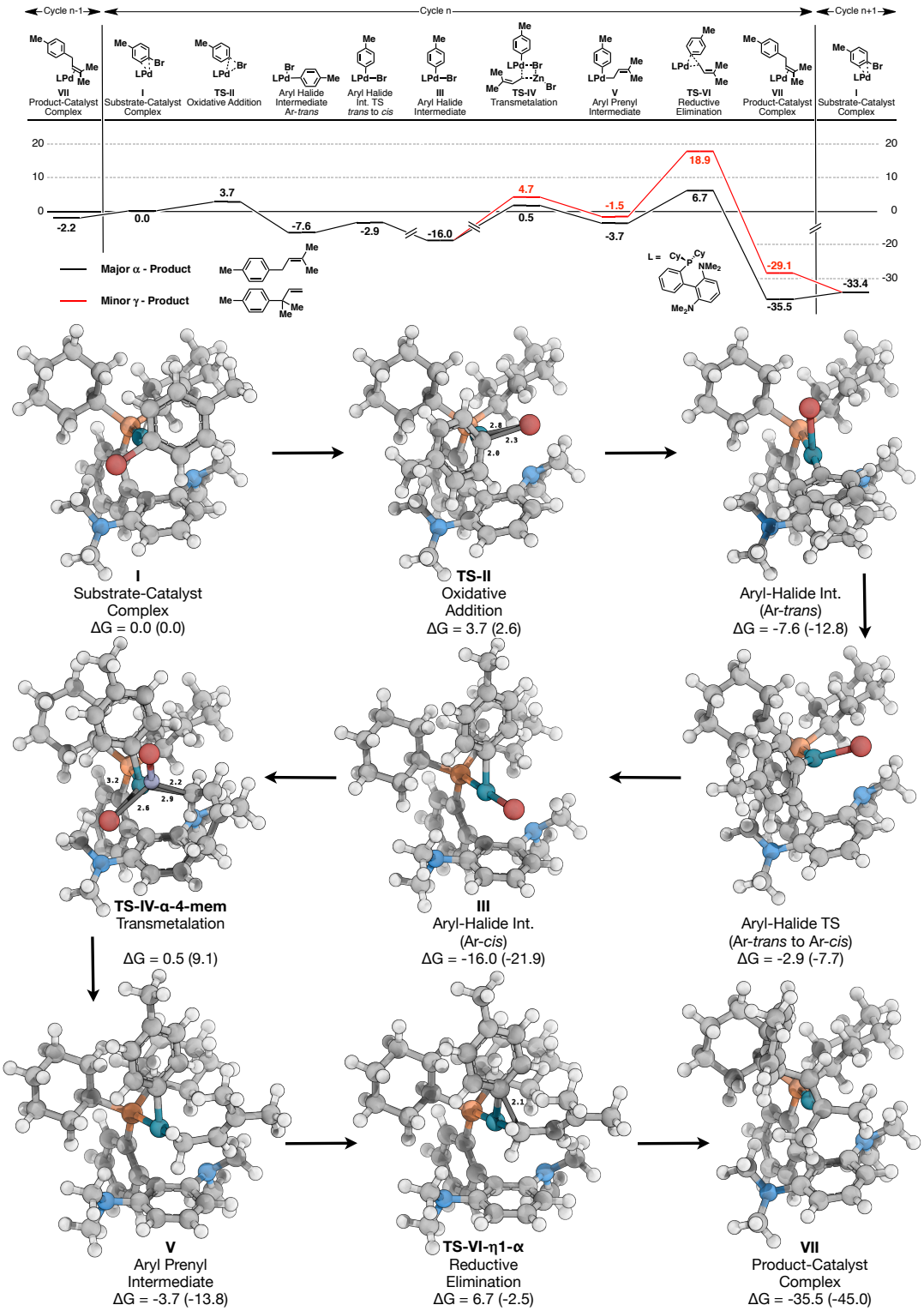
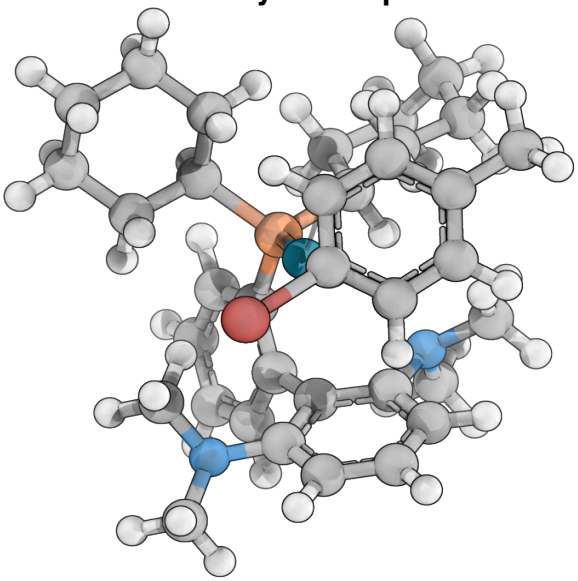


Figure A3.1. Reaction coordinate of Pd(0)-catalyzed cross-coupling of prenylZnBr with p-bromotoluene (above) and all structures (below).[1] All

(1) (a) The B3LYP hybrid functional with the 6-31G* (for H, C, N, and P) and LANL2DZ+ECP (for Zn, Br and Pd) basis sets were used. (b) M. J.

energies are displayed in kcal/mol, solvation energies in parentheses and distances in Å. Computed structures are rendered in Pymol.[2]

I Substrate-Catalyst Complex:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) iop(1/8=18)
freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd
C1[X(C35H48BrN2PPd)] #Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.40661501 Predicted Change= -3.929247D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.02082 II	0.00180	[NO]	0.02082 II	0.00180	[NO]

Frisch,; et al. Gaussian, Inc.: Pittsburgh, PA, 2004. (c) The B3LYP hybrid functional and PCM solvation model with tetrahydrofuran with the 6-31++G(d,p) (for H, C, N, and P) and LANL2DZ+ECP (for Zn, Br and Pd) basis sets were used. (d) M. J. Frisch,; et al. Gaussian, Inc.: Wallingford, CT, 2010.

(2) *The PyMOL Molecular Graphics System, version 1.3*; Schrödinger, LLC.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.886710	4.287479	-0.122124
H	3.226395	5.315168	-0.220653
C	3.681545	3.331744	0.508026
H	4.655657	3.596789	0.910798
C	3.211714	2.026637	0.627225
H	3.838730	1.308253	1.142633
C	1.958247	1.620879	0.125078
P	1.403834	-0.146644	0.394273
Pd	-0.875674	-0.678074	0.332087
C	2.473788	-1.082347	-0.868412
H	2.358333	-0.442949	-1.753523
C	2.142344	-0.555551	2.089547
H	3.230222	-0.407380	2.056081
C	1.157052	2.594077	-0.526883
C	-0.196995	2.377091	-1.147885
C	1.644637	3.913174	-0.623094
H	1.017251	4.654572	-1.108077
C	-0.339948	1.697749	-2.383062
N	0.802633	1.092861	-3.005368
C	0.513897	-0.038491	-3.879488
H	1.452140	-0.561939	-4.095036
H	-0.163800	-0.732670	-3.375997
H	0.071091	0.249658	-4.850739
C	1.704563	2.039782	-3.667046
H	1.254741	2.479586	-4.575880
H	1.977765	2.848268	-2.988389
H	2.621950	1.515724	-3.959425
C	-1.591524	1.651509	-3.017341
H	-1.695586	1.143610	-3.969190
C	-2.694217	2.282160	-2.453539
H	-3.656899	2.247000	-2.958226
C	-2.567985	2.969540	-1.251710
H	-3.437530	3.446494	-0.814265
C	-1.330497	3.036941	-0.591921
N	-1.191677	3.805180	0.596070
C	-0.934480	3.068159	1.832249
H	-1.856056	2.622874	2.244725
H	-0.226386	2.261610	1.654289
H	-0.508613	3.748413	2.579734
C	-2.151770	4.876749	0.805557
H	-2.275009	5.458415	-0.112499

H	-3.147642	4.527932	1.135904
H	-1.763884	5.542522	1.585451
C	1.877959	-2.464160	-1.216446
H	1.904957	-3.119125	-0.335301
H	0.819528	-2.352468	-1.476574
C	2.651666	-3.141221	-2.361066
H	2.227777	-4.134541	-2.559318
H	2.520732	-2.556508	-3.283631
C	4.150773	-3.252220	-2.048877
H	4.294068	-3.932532	-1.195935
H	4.687337	-3.697265	-2.896904
C	4.742781	-1.878767	-1.703802
H	5.803748	-1.974567	-1.437724
H	4.701075	-1.231400	-2.592357
C	3.977388	-1.201520	-0.551457
H	4.121364	-1.796120	0.361547
H	4.411308	-0.213837	-0.362524
C	1.886801	-2.033423	2.459772
H	0.805446	-2.225540	2.422606
H	2.345949	-2.700985	1.722245
C	2.426710	-2.376481	3.859575
H	2.195564	-3.423538	4.095486
H	3.524059	-2.293246	3.857598
C	1.851728	-1.445936	4.935654
H	0.768327	-1.616169	5.020561
H	2.284609	-1.682073	5.916358
C	2.104148	0.024604	4.578126
H	1.643989	0.684587	5.324886
H	3.185749	0.225481	4.608752
C	1.561459	0.369741	3.180877
H	0.466764	0.268809	3.181612
H	1.782211	1.417568	2.949396
C	-2.481871	-3.593858	-1.434816
C	-2.289608	-4.744505	-2.394753
H	-3.201437	-4.946241	-2.970201
H	-2.016603	-5.663960	-1.867113
H	-1.493262	-4.531692	-3.120779
C	-2.133651	-3.707171	-0.089184
H	-1.729325	-4.644819	0.285650
C	-2.319094	-2.644169	0.815298
H	-2.167208	-2.796271	1.877766
C	-2.880344	-1.433362	0.342599
Br	-3.794642	-0.218191	1.670691
C	-3.217759	-1.295558	-1.026242

H	-3.659298	-0.371464	-1.380893
C	-3.005228	-2.366006	-1.889232
H	-3.266662	-2.252137	-2.939325

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

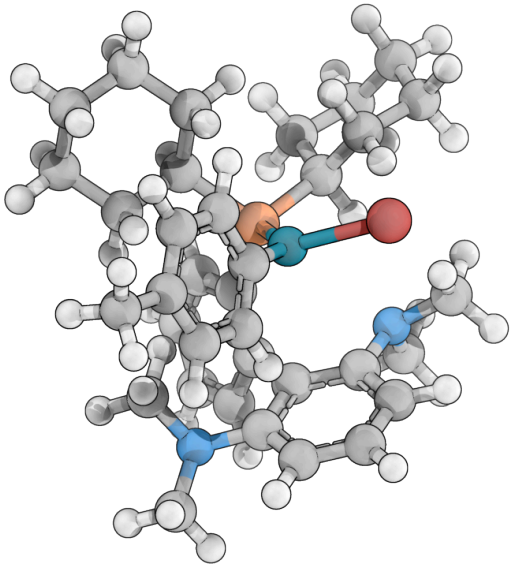
==========

SCF Energy= -1953.40661501 Predicted Change= -3.929247D-08
Zero-point correction (ZPE)= -1952.6449 0.76168
Internal Energy (U)= -1952.6017 0.80486
Enthalpy (H)= -1952.6008 0.80580
Gibbs Free Energy (G)= -1952.7257 0.68081

Frequencies -- 7.0878 18.4940 26.8622

$\Delta G_{Solvation}$ = -0.00751849000016591

TS-II Oxidative Addition:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd
C1[X(C35H48BrN2PPd)] #Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.40310422 Predicted Change= -7.374393D-09

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Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00891 II	0.00180	[NO]	0.00891 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.789941	3.643699	2.346027
H	3.124070	4.583172	2.778322
C	3.386627	2.438614	2.712662
H	4.195694	2.416581	3.438031
C	2.931809	1.253025	2.142739

H	3.398303	0.327489	2.459712
C	1.887650	1.216382	1.195114
P	1.351996	-0.440614	0.517472
Pd	-0.831836	-0.743594	-0.401288
C	1.551877	-1.588615	2.008900
H	2.594874	-1.554295	2.351247
C	2.783146	-0.867471	-0.656953
H	2.891612	0.079418	-1.202053
C	1.279947	2.444572	0.826707
C	0.146944	2.637007	-0.144711
C	1.750948	3.632599	1.422574
H	1.273764	4.566492	1.142993
C	-1.089479	3.153113	0.337033
N	-1.272975	3.358873	1.734898
C	-1.406944	2.152443	2.548859
H	-2.399101	1.680721	2.432545
H	-1.266734	2.410664	3.605187
H	-0.651285	1.419622	2.271107
C	-2.233501	4.377298	2.128216
H	-2.080281	5.286817	1.540396
H	-2.071669	4.618784	3.185225
H	-3.289333	4.065588	2.020297
C	-2.105555	3.492295	-0.568903
H	-3.051896	3.871995	-0.200127
C	-1.916807	3.327185	-1.937287
H	-2.710144	3.594340	-2.631109
C	-0.713271	2.830269	-2.421894
H	-0.573561	2.726305	-3.491132
C	0.331163	2.497522	-1.543282
N	1.592550	2.057505	-2.060401
C	1.543946	1.406760	-3.366785
H	1.386074	2.108849	-4.205415
H	0.750015	0.656066	-3.380914
H	2.502131	0.904808	-3.540944
C	2.648219	3.074099	-2.026663
H	2.464257	3.889427	-2.749564
H	3.605606	2.603856	-2.279183
H	2.735708	3.506532	-1.029435
C	0.644978	-1.142963	3.176737
H	-0.397749	-1.126341	2.827685
H	0.892230	-0.120789	3.483536
C	0.758581	-2.086692	4.386006
H	0.079997	-1.749774	5.180406
H	1.776509	-2.026723	4.799771

C	0.452650	-3.540235	4.000903
H	-0.602824	-3.620655	3.701834
H	0.585299	-4.202351	4.866228
C	1.343776	-3.996005	2.838068
H	1.080886	-5.016571	2.530943
H	2.390262	-4.032726	3.176414
C	1.235318	-3.051846	1.627600
H	0.218192	-3.098081	1.212315
H	1.909837	-3.400621	0.838520
C	4.137980	-1.208052	-0.006169
H	4.048709	-2.130335	0.585443
H	4.446168	-0.413942	0.681750
C	5.234276	-1.408510	-1.068973
H	6.180100	-1.675202	-0.579235
H	5.408922	-0.453988	-1.587201
C	4.841496	-2.478354	-2.097290
H	4.777140	-3.455816	-1.595971
H	5.619526	-2.572535	-2.865920
C	3.487235	-2.150417	-2.741848
H	3.190786	-2.946071	-3.437269
H	3.586569	-1.233695	-3.341773
C	2.386161	-1.949277	-1.686316
H	2.210129	-2.906327	-1.177604
H	1.439462	-1.680669	-2.166831
C	-3.538071	-0.027833	-0.755461
H	-3.283600	0.862682	-1.319032
C	-2.764592	-1.193794	-0.882961
C	-3.124790	-2.377481	-0.214971
H	-2.566640	-3.292229	-0.383010
C	-4.219650	-2.353102	0.651871
H	-4.489502	-3.261471	1.186933
C	-4.987928	-1.193303	0.830107
C	-6.204711	-1.199565	1.726342
H	-7.117248	-1.434942	1.161544
H	-6.360599	-0.223052	2.198204
H	-6.113819	-1.947757	2.521118
C	-4.623747	-0.037566	0.121810
H	-5.206882	0.872731	0.247699
Br	-1.786749	-1.512311	-2.906652

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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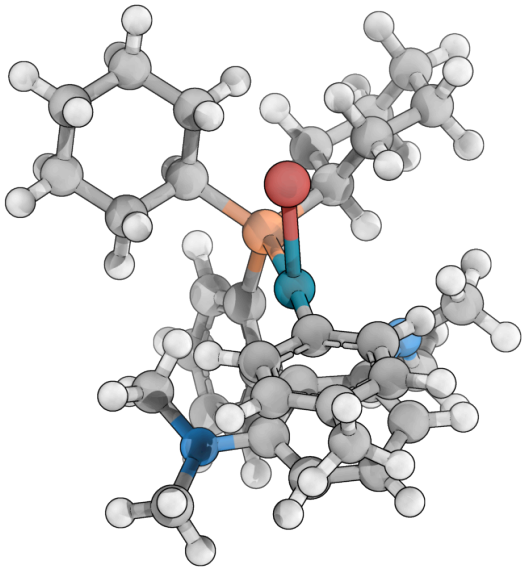
SCF Energy= -1953.40310422 Predicted Change= -7.374393D-09

Zero-point correction (ZPE)=	-1952.6410	0.76202
Internal Energy (U)=	-1952.5987	0.80433
Enthalpy (H)=	-1952.5978	0.80528
Gibbs Free Energy (G)=	-1952.7199	0.68314

Frequencies -- -94.7250 8.1236 19.9197

$\Delta G_{Solvation}$ = -0.00927111999999397

Aryl Halide Intermediate (Ar-*trans*):



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

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b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd
C1[X(C35H48BrN2PPd)] #Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.42433037 Predicted Change= -5.019004D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.02019 II	0.00180	[NO]	0.02019 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.350420	4.305700	1.959891
H	1.244931	5.300398	2.384825
C	2.572394	3.635655	2.020078
H	3.433040	4.096696	2.497062
C	2.679226	2.361160	1.467593
H	3.629833	1.842973	1.539727

C	1.586927	1.727935	0.848309
P	1.685032	0.012614	0.160658
Pd	-0.696419	-0.550017	-0.194593
C	2.810167	0.175077	-1.350065
H	2.372838	1.052463	-1.842350
C	2.688996	-0.900662	1.474587
H	3.601676	-0.310393	1.644194
C	0.347517	2.402591	0.792194
C	-0.921893	1.887204	0.133523
C	0.258345	3.692169	1.351290
H	-0.691783	4.216582	1.306715
C	-1.047157	2.031381	-1.301322
N	0.140932	2.156029	-2.100193
C	0.063377	1.501865	-3.406163
H	1.069037	1.466214	-3.838876
H	-0.297618	0.477755	-3.283066
H	-0.585623	2.025099	-4.129939
C	0.601982	3.542543	-2.240441
H	-0.086582	4.152209	-2.852242
H	0.704356	4.011821	-1.260992
H	1.584603	3.542988	-2.725725
C	-2.300867	2.155664	-1.899558
H	-2.380464	2.251275	-2.976150
C	-3.450221	2.207251	-1.113733
H	-4.421290	2.315872	-1.588693
C	-3.381884	2.097637	0.264400
H	-4.300795	2.086478	0.835076
C	-2.145557	1.923434	0.917978
N	-2.112665	1.846759	2.299040
C	-1.119821	1.043547	3.003834
H	-1.617335	0.473001	3.796483
H	-0.664303	0.325554	2.316566
H	-0.328119	1.653244	3.456490
C	-3.299648	2.175350	3.076112
H	-3.762645	3.093011	2.702727
H	-4.052611	1.371893	3.067481
H	-2.998198	2.352577	4.112255
C	2.647360	-1.025245	-2.311960
H	3.003376	-1.945658	-1.834241
H	1.587281	-1.193553	-2.526515
C	3.433919	-0.807544	-3.615995
H	3.331620	-1.691270	-4.258335
H	2.994928	0.034557	-4.172221
C	4.915321	-0.510086	-3.344471

H	5.386329	-1.395739	-2.892917
H	5.447025	-0.319105	-4.285487
C	5.071652	0.684927	-2.394216
H	6.131962	0.865083	-2.173911
H	4.696640	1.593444	-2.888653
C	4.298647	0.473844	-1.078396
H	4.757847	-0.358760	-0.528754
H	4.403685	1.366893	-0.452651
C	3.118925	-2.319703	1.039801
H	2.227782	-2.908227	0.792854
H	3.728027	-2.275174	0.131214
C	3.922550	-3.024881	2.146950
H	4.185403	-4.037327	1.815304
H	4.872445	-2.491686	2.307412
C	3.146420	-3.081134	3.469282
H	2.254197	-3.709784	3.338650
H	3.755245	-3.554172	4.250576
C	2.715200	-1.675165	3.906614
H	2.116819	-1.724704	4.825632
H	3.608234	-1.078383	4.146831
C	1.909688	-0.964194	2.806261
H	0.969210	-1.506593	2.638941
H	1.647450	0.046579	3.139256
C	-3.412028	-1.324021	0.780203
H	-2.939002	-1.336077	1.759443
C	-2.662493	-1.034914	-0.364879
C	-3.297451	-1.080204	-1.608474
H	-2.735261	-0.903453	-2.521690
C	-4.665886	-1.359093	-1.698145
H	-5.140818	-1.387317	-2.678098
C	-5.430938	-1.621416	-0.555802
C	-6.899601	-1.967450	-0.660130
H	-7.457098	-1.630677	0.221633
H	-7.359216	-1.509808	-1.543541
H	-7.052277	-3.052411	-0.742371
C	-4.779833	-1.598337	0.684847
H	-5.346925	-1.810545	1.590570
Br	-0.340242	-3.062202	-0.476314

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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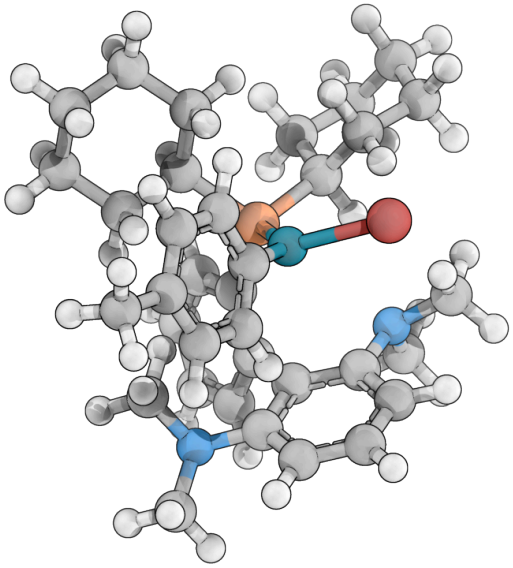
SCF Energy= -1953.42433037 Predicted Change= -5.019004D-07
Zero-point correction (ZPE)= -1952.6610 0.76330

Internal Energy (U)= -1952.6182 0.80603
Enthalpy (H)= -1952.6173 0.80698
Gibbs Free Energy (G)= -1952.7379 0.68641

Frequencies -- 18.1927 27.7029 33.3282

$\Delta G_{Solvation}$ = -0.0157666000000063

Ar-*trans* to Ar-*cis* TS:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd
C1[X(C35H48BrN2PPd)] #Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.41397203 Predicted Change= -1.743349D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00363 II	0.00180	[NO]	0.00363 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.852907	3.465340	2.607518
H	3.208610	4.376642	3.080801
C	3.306954	2.218441	3.034848
H	4.021748	2.136205	3.849280
C	2.830623	1.070044	2.409278

H	3.182449	0.110686	2.771219
C	1.904950	1.116183	1.346425
P	1.325960	-0.491259	0.601483
Pd	-0.892323	-0.675418	-0.702558
C	2.844526	-1.093070	-0.368020
H	3.134943	-0.171829	-0.889012
C	1.171643	-1.628459	2.104819
H	2.142902	-1.673200	2.615709
C	1.438342	2.386181	0.917417
C	0.438718	2.648290	-0.174721
C	1.929270	3.535049	1.570678
H	1.562682	4.502556	1.243909
C	0.751703	2.430983	-1.541367
N	2.015292	1.862993	-1.903270
C	2.059910	1.200336	-3.205698
H	2.982870	0.613133	-3.264183
H	1.208889	0.523889	-3.314759
H	2.067320	1.905584	-4.055783
C	3.154557	2.775267	-1.753624
H	3.138590	3.583257	-2.506584
H	3.163560	3.225745	-0.760882
H	4.084871	2.209730	-1.880201
C	-0.170253	2.797253	-2.535161
H	0.061919	2.626748	-3.578921
C	-1.376201	3.397352	-2.196275
H	-2.077456	3.678295	-2.977543
C	-1.686312	3.644186	-0.863111
H	-2.632587	4.109675	-0.610880
C	-0.793733	3.279198	0.156628
N	-1.100760	3.570133	1.518375
C	-1.414651	2.420253	2.364002
H	-2.409745	1.996057	2.141423
H	-0.671564	1.635594	2.229446
H	-1.397006	2.729371	3.415633
C	-2.015014	4.675816	1.760955
H	-1.729769	5.539251	1.153428
H	-3.074697	4.437558	1.553122
H	-1.945305	4.959133	2.817565
C	2.467626	-2.136440	-1.444146
H	2.107726	-3.056933	-0.966138
H	1.639035	-1.769900	-2.058762
C	3.674460	-2.482884	-2.332979
H	3.382922	-3.247421	-3.063808
H	3.965700	-1.593936	-2.912073

C	4.875656	-2.959629	-1.505246
H	4.626340	-3.914832	-1.019433
H	5.736757	-3.156364	-2.156675
C	5.246488	-1.926948	-0.431906
H	6.074896	-2.294861	0.187460
H	5.605364	-1.009124	-0.920704
C	4.045705	-1.577807	0.467710
H	3.765118	-2.469857	1.045132
H	4.349120	-0.811248	1.188219
C	0.797995	-3.067433	1.682183
H	-0.129305	-3.042467	1.091992
H	1.568209	-3.488898	1.028244
C	0.605077	-3.990368	2.898741
H	0.308664	-4.989332	2.554484
H	1.567583	-4.112335	3.418018
C	-0.431831	-3.430730	3.880817
H	-1.419854	-3.416822	3.397801
H	-0.519557	-4.085511	4.757107
C	-0.059694	-2.006407	4.312554
H	-0.829947	-1.592294	4.975626
H	0.872565	-2.034891	4.896409
C	0.128190	-1.077287	3.101142
H	-0.836718	-0.964760	2.584602
H	0.422370	-0.079951	3.445389
C	-3.355245	-2.102041	-0.046275
H	-2.773075	-3.014210	-0.131515
C	-2.826675	-0.874434	-0.445615
C	-3.603530	0.283565	-0.441650
H	-3.208921	1.221017	-0.821876
C	-4.902421	0.219674	0.075520
H	-5.506814	1.124613	0.098174
C	-5.445872	-0.984938	0.541284
C	-6.845651	-1.039045	1.110049
H	-6.838829	-0.936152	2.203939
H	-7.471198	-0.232888	0.712080
H	-7.336185	-1.991013	0.878691
C	-4.655705	-2.140444	0.466099
H	-5.066382	-3.093657	0.793774
Br	-1.399376	-1.396117	-3.068185

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

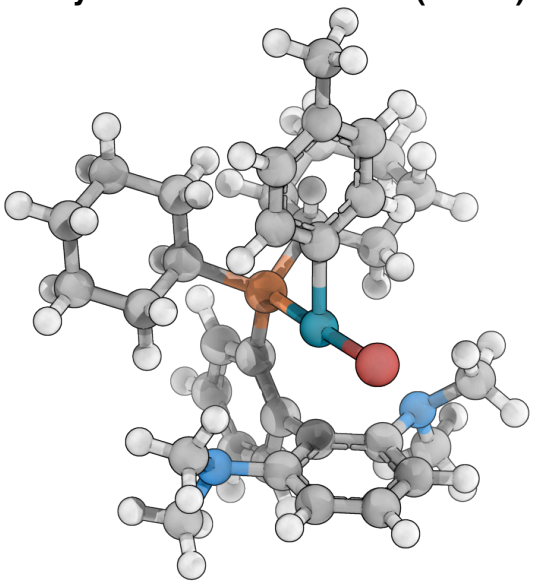
SCF Energy= -1953.41397203 Predicted Change= -1.743349D-09

Zero-point correction (ZPE)=	-1952.6513	0.76258
Internal Energy (U)=	-1952.6090	0.80487
Enthalpy (H)=	-1952.6081	0.80581
Gibbs Free Energy (G)=	-1952.7304	0.68349

Frequencies -- -64.1653 9.7209 22.6338

$\Delta G_{Solvation}$ = -0.0151901799999905

III Aryl Halide Intermediate (Ar-*cis*):



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd
C1[X(C35H48BrN2PPd)] #Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.43608789 Predicted Change= -1.389398D-04

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023 ll	0.00045	[YES]	0.00004 ll	0.00030	[YES]
Displ	0.31456 ll	0.00180	[NO]	0.31456 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.813666	3.314628	0.586672
H	-4.778338	3.807123	0.674528
C	-2.631303	4.039353	0.720968
H	-2.653768	5.107497	0.918400
C	-1.411863	3.377953	0.605051
H	-0.502952	3.955218	0.727217

C	-1.332709	1.995536	0.346717
P	0.329222	1.195264	0.191228
Pd	0.111848	-1.119842	-0.082515
C	1.221817	1.827943	1.722891
H	0.974329	2.896766	1.791298
C	1.192964	2.021279	-1.263541
H	2.170318	1.517529	-1.259553
C	-2.527808	1.255068	0.230177
C	-2.651798	-0.234801	0.026344
C	-3.750928	1.943812	0.351557
H	-4.673600	1.376024	0.266733
C	-2.828343	-1.077587	1.162036
N	-2.557204	-0.563039	2.479864
C	-3.739596	-0.034235	3.163001
H	-4.214240	0.741847	2.560130
H	-3.429899	0.415655	4.113091
H	-4.489802	-0.816223	3.382430
C	-1.833161	-1.495831	3.346696
H	-0.999701	-1.939226	2.796477
H	-2.461320	-2.312287	3.745273
H	-1.434719	-0.939557	4.202942
C	-3.259234	-2.397620	0.987606
H	-3.380127	-3.039739	1.853346
C	-3.512992	-2.900689	-0.282553
H	-3.838168	-3.929515	-0.403811
C	-3.331097	-2.094478	-1.401034
H	-3.507436	-2.505175	-2.389128
C	-2.902672	-0.768934	-1.270950
N	-2.691861	0.049931	-2.434251
C	-2.090666	-0.659491	-3.565181
H	-1.706972	0.080330	-4.277317
H	-2.799547	-1.306951	-4.111559
H	-1.259246	-1.276494	-3.215320
C	-3.872196	0.799803	-2.869127
H	-4.255654	1.418655	-2.057047
H	-4.686462	0.141805	-3.224880
H	-3.586631	1.462491	-3.694008
C	0.675944	1.136075	2.989181
H	0.906611	0.063943	2.930683
H	-0.415976	1.214179	3.029035
C	1.311335	1.724636	4.259831
H	0.929470	1.195593	5.142560
H	1.002553	2.775144	4.368497
C	2.844231	1.646003	4.211739

H	3.152023	0.590423	4.233193
H	3.279281	2.117731	5.102054
C	3.394197	2.304436	2.937998
H	4.484347	2.188873	2.889284
H	3.196000	3.386509	2.974159
C	2.759562	1.711102	1.666333
H	3.048443	0.658958	1.572628
H	3.162126	2.225111	0.786311
C	0.497004	1.665124	-2.593369
H	-0.502944	2.117393	-2.614310
H	0.341609	0.583617	-2.655832
C	1.320085	2.152324	-3.798264
H	0.785341	1.920596	-4.728452
H	2.267154	1.594225	-3.835702
C	1.622911	3.655691	-3.717956
H	0.684322	4.220769	-3.817453
H	2.262800	3.961326	-4.555391
C	2.286305	4.016877	-2.381127
H	2.443685	5.101027	-2.312643
H	3.281174	3.551323	-2.326627
C	1.435353	3.542752	-1.188342
H	0.472402	4.067221	-1.221664
H	1.924405	3.826185	-0.248872
C	2.848013	-1.807505	0.816734
H	2.372064	-2.008520	1.771270
C	2.093742	-1.362454	-0.273185
C	2.726958	-1.154129	-1.500072
H	2.160168	-0.846079	-2.372993
C	4.105405	-1.365668	-1.624038
H	4.580638	-1.198129	-2.589163
C	4.877990	-1.797117	-0.540493
C	6.359057	-2.061008	-0.691429
H	6.898373	-1.876840	0.244479
H	6.803412	-1.426854	-1.466684
H	6.552136	-3.104282	-0.975995
C	4.224010	-2.013909	0.679451
H	4.794766	-2.360695	1.539232
Br	-0.072384	-3.647103	-0.392994

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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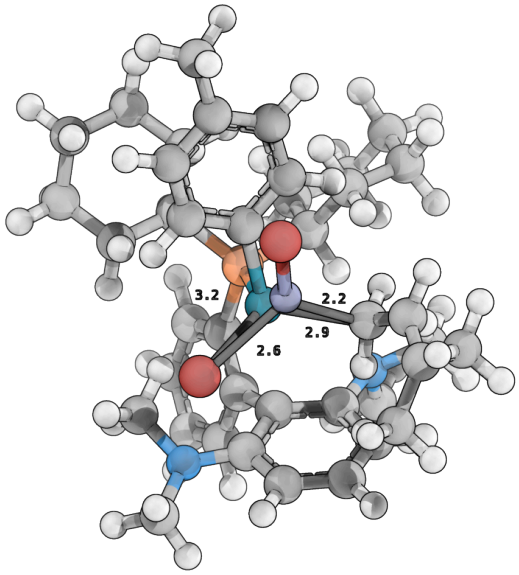
SCF Energy= -1953.43608789 Predicted Change= -1.389398D-04
Zero-point correction (ZPE)= -1952.6725 0.76353

Internal Energy (U)=	-1952.6298	0.80623
Enthalpy (H)=	-1952.6289	0.80718
Gibbs Free Energy (G)=	-1952.7513	0.68471

Frequencies -- 11.8890 18.5342 23.4070

$\Delta G_{Solvation}$ = -0.0167777399999522

TS-IV-a-4-mem Transmetalation:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

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b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn
C1[X(C40H57Br2N2PPdZn)] #Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00311 II	0.00180	[NO]	0.00311 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.004554	-2.651548	-1.665480
H	5.643498	-3.418568	-2.094586
C	5.464856	-1.343193	-1.522539
H	6.467381	-1.069806	-1.839555
C	4.621010	-0.378701	-0.978227

H	4.992821	0.636124	-0.897370
C	3.311318	-0.686255	-0.561371
P	2.203857	0.644041	0.112177
Pd	-0.012339	-0.172776	-0.058016
C	2.876710	0.894170	1.866718
H	2.980571	-0.148702	2.191381
C	2.715941	2.162949	-0.883413
H	3.807934	2.222240	-0.777272
C	2.847028	-2.012796	-0.694003
C	1.492355	-2.535099	-0.278807
C	3.714721	-2.971753	-1.253164
H	3.353439	-3.989322	-1.366254
C	1.272997	-2.892095	1.096041
N	2.161988	-2.398831	2.112864
C	1.545653	-2.203537	3.425976
H	2.224921	-1.606426	4.044446
H	0.600586	-1.665355	3.323277
H	1.354978	-3.145207	3.969231
C	3.395782	-3.184146	2.255192
H	3.199914	-4.190103	2.666186
H	3.899003	-3.293182	1.294660
H	4.073563	-2.660644	2.939207
C	0.238889	-3.760644	1.445479
H	0.073171	-4.021941	2.483431
C	-0.564884	-4.327281	0.454762
H	-1.367274	-5.003586	0.736822
C	-0.368429	-4.029176	-0.880658
H	-1.037602	-4.446680	-1.620195
C	0.665926	-3.154985	-1.287988
N	0.914178	-2.987244	-2.639288
C	1.319579	-1.708669	-3.217864
H	0.613814	-1.434390	-4.009740
H	1.273336	-0.919252	-2.470173
H	2.333388	-1.752923	-3.637690
C	0.290244	-3.883253	-3.605084
H	0.352440	-4.920609	-3.264630
H	-0.761451	-3.626489	-3.798398
H	0.842574	-3.807444	-4.546954
C	1.874103	1.579148	2.817892
H	1.641543	2.591820	2.466020
H	0.931434	1.022062	2.810972
C	2.417604	1.660174	4.255693
H	1.699353	2.198578	4.886798
H	2.497056	0.645358	4.671454

C	3.795265	2.332840	4.313810
H	3.702061	3.385863	4.009545
H	4.173749	2.337496	5.343585
C	4.786402	1.621347	3.384203
H	5.761370	2.124830	3.401487
H	4.956405	0.597260	3.747639
C	4.265985	1.565007	1.935794
H	4.213488	2.589203	1.543764
H	4.985309	1.019607	1.316093
C	2.148679	3.498815	-0.353906
H	1.057136	3.485578	-0.398375
H	2.422690	3.645037	0.696189
C	2.674569	4.682338	-1.186335
H	2.239547	5.614248	-0.804346
H	3.764208	4.768750	-1.056513
C	2.351658	4.512031	-2.676829
H	1.261264	4.533815	-2.812749
H	2.759708	5.351075	-3.254284
C	2.903140	3.182070	-3.208538
H	2.623682	3.043186	-4.260407
H	4.002928	3.205954	-3.177988
C	2.398490	1.985002	-2.383810
H	1.314215	1.886664	-2.510094
H	2.850626	1.061220	-2.761835
C	-1.090620	2.423140	1.096022
H	-0.865766	2.007538	2.071330
C	-0.841791	1.687289	-0.072504
C	-1.169581	2.263101	-1.311207
H	-1.023143	1.708091	-2.230935
C	-1.741393	3.537991	-1.367538
H	-2.010628	3.949817	-2.337713
C	-2.002247	4.274886	-0.206648
C	-2.685689	5.619156	-0.272831
H	-2.405910	6.256854	0.572749
H	-2.441218	6.151204	-1.198587
H	-3.775776	5.494136	-0.244507
C	-1.664248	3.694948	1.022757
H	-1.869629	4.234658	1.944913
Br	-2.119411	-1.081046	-2.219722
C	-2.141770	-1.047271	1.713501
H	-1.435636	-0.488781	2.330762
H	-1.713519	-1.995667	1.392084
C	-3.466033	-1.159009	2.364070
H	-3.721739	-0.331591	3.027147

C	-4.414584	-2.113481	2.200995
C	-4.277025	-3.285837	1.265040
H	-5.087924	-3.281419	0.522369
H	-4.362103	-4.239213	1.808461
H	-3.332492	-3.288165	0.715609
C	-5.722264	-2.034039	2.945336
H	-6.565629	-1.931399	2.246983
H	-5.751226	-1.179966	3.629221
H	-5.908301	-2.947890	3.529380
Br	-4.970761	1.386250	-0.070632
Zn	-2.894431	0.048737	-0.002394

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

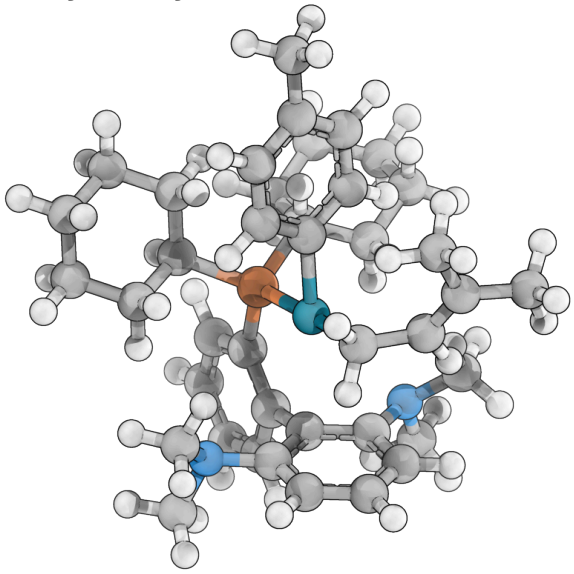
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SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09
Zero-point correction (ZPE)= -2227.2867 0.89270
Internal Energy (U)= -2227.2328 0.94656
Enthalpy (H)= -2227.2319 0.94750
Gibbs Free Energy (G)= -2227.3781 0.80131

Frequencies -- -68.2928 17.3940 18.2056

$\Delta G_{Solvation}$ = -0.0281542599996101

V Aryl Prenyl Intermediate:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)] #Atoms= 101

Charge = 0 Multiplicity = 1

SCF Energy= -2136.14026159 Predicted Change= -1.724614D-05

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00032 ll	0.00045	[YES]	0.00002 ll	0.00030	[YES]
Displ	0.13319 ll	0.00180	[NO]	0.13319 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.167027	-1.217492	0.668217
H	-6.251647	-1.212013	0.736225
C	-4.437351	-2.349445	1.023268
H	-4.940064	-3.247060	1.373192
C	-3.048787	-2.323834	0.919639
H	-2.500003	-3.219344	1.186814

C	-2.346624	-1.186716	0.476197
P	-0.491932	-1.238203	0.348126
Pd	0.585477	0.763429	-0.577697
C	0.154299	-1.564509	2.091609
H	1.227440	-1.708478	1.896679
C	-0.220537	-2.875241	-0.552207
H	-0.896626	-3.616626	-0.103844
C	-3.088326	-0.042875	0.103395
C	-2.533131	1.246517	-0.448596
C	-4.491763	-0.088447	0.211738
H	-5.062475	0.789662	-0.079256
C	-2.280638	2.358128	0.402709
N	-2.308340	2.189177	1.829102
C	-3.631366	2.353904	2.434929
H	-3.573646	2.077194	3.493689
H	-3.998645	3.395027	2.371878
H	-4.358173	1.698483	1.954770
C	-1.310132	2.969081	2.558497
H	-0.334710	2.870424	2.075916
H	-1.556401	4.043343	2.641865
H	-1.234339	2.571635	3.576845
C	-2.002047	3.612203	-0.161598
H	-1.816928	4.460687	0.488498
C	-1.970850	3.786465	-1.542034
H	-1.765402	4.767980	-1.960695
C	-2.202008	2.702606	-2.383059
H	-2.167450	2.837602	-3.459417
C	-2.474931	1.433356	-1.855707
N	-2.694877	0.310214	-2.729460
C	-4.072444	0.199109	-3.210918
H	-4.359275	1.027788	-3.885018
H	-4.182382	-0.741569	-3.762318
H	-4.767613	0.180841	-2.369598
C	-1.742092	0.216545	-3.835079
H	-0.725043	0.329830	-3.450172
H	-1.832850	-0.775583	-4.291450
H	-1.904626	0.964227	-4.632801
C	-0.363884	-2.801190	2.850713
H	-1.433673	-2.677298	3.061852
H	-0.259603	-3.709978	2.244931
C	0.380633	-2.981234	4.186579
H	-0.012720	-3.860016	4.714101
H	1.442682	-3.185032	3.986008
C	0.258351	-1.729663	5.067122

H	-0.794123	-1.596796	5.359163
H	0.827067	-1.860185	5.996768
C	0.738214	-0.478091	4.317867
H	0.589099	0.416781	4.936354
H	1.820991	-0.557224	4.140355
C	0.020209	-0.303557	2.968520
H	-1.042961	-0.084515	3.134174
H	0.432154	0.558739	2.432602
C	1.220441	-3.412190	-0.420920
H	1.926823	-2.669179	-0.808676
H	1.481841	-3.574609	0.630839
C	1.391672	-4.734837	-1.190373
H	2.431704	-5.074762	-1.105097
H	0.769208	-5.512103	-0.721195
C	0.995354	-4.594022	-2.666499
H	1.694693	-3.905471	-3.162833
H	1.087236	-5.559931	-3.179969
C	-0.432771	-4.047400	-2.803730
H	-0.685463	-3.899424	-3.862004
H	-1.145987	-4.789500	-2.414236
C	-0.604475	-2.724405	-2.038879
H	0.040664	-1.957544	-2.488644
H	-1.632884	-2.356984	-2.130859
C	3.231954	0.166220	0.654345
H	2.796100	0.606250	1.547599
C	2.500596	0.129302	-0.540544
C	3.126790	-0.407921	-1.675312
H	2.601664	-0.440031	-2.626787
C	4.429237	-0.915044	-1.605665
H	4.886869	-1.330163	-2.502953
C	5.156898	-0.894998	-0.408969
C	6.576736	-1.411862	-0.346737
H	6.732692	-2.245031	-1.041618
H	7.303153	-0.631073	-0.611937
H	6.832939	-1.761762	0.659678
C	4.532905	-0.345991	0.718085
H	5.073029	-0.310872	1.663559
C	1.427128	2.526881	-1.362217
C	1.821678	3.482583	-0.308813
H	0.987066	3.905246	0.255144
C	3.055879	3.897784	0.054986
C	4.335033	3.450900	-0.606064
H	4.976535	2.909735	0.103797
H	4.164400	2.787170	-1.456210

H	4.916320	4.317194	-0.956883
C	3.238837	4.882764	1.184539
H	3.860506	4.462670	1.990080
H	3.756180	5.793063	0.844774
H	2.281269	5.184881	1.623475
H	2.212398	2.309848	-2.087573
H	0.522577	2.863117	-1.889086

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

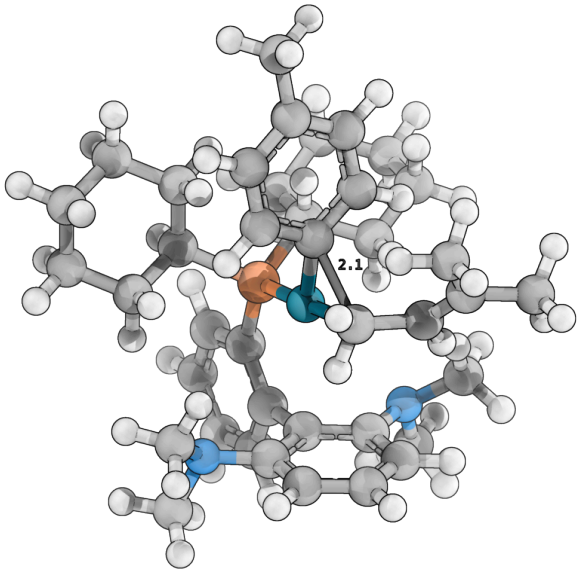
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SCF Energy= -2136.14026159 Predicted Change= -1.724614D-05
Zero-point correction (ZPE)= -2135.2517 0.88846
Internal Energy (U)= -2135.2034 0.93680
Enthalpy (H)= -2135.2025 0.93775
Gibbs Free Energy (G)= -2135.3385 0.80171

Frequencies -- 8.3086 18.6557 21.1872

$\Delta G_{Solvation}$ = -0.00806345000000874

TS-VI-h^1-a Reductive Elimination:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)]
#Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00246 II	0.00180	[NO]	0.00246 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.394518	0.744090	0.160557
H	6.476648	0.659059	0.105930
C	4.793472	1.915501	0.612632
H	5.395440	2.767327	0.917868
C	3.403416	1.990837	0.665757

H	2.960196	2.918580	1.007247
C	2.569888	0.920613	0.286226
P	0.715854	1.139926	0.386585
Pd	-0.799548	-0.468409	-0.478624
C	0.497302	2.850464	-0.382306
H	1.211558	3.535884	0.094483
C	0.334107	1.430498	2.218313
H	-0.728818	1.711161	2.175527
C	3.183584	-0.264581	-0.188366
C	2.463824	-1.483551	-0.703454
C	4.589506	-0.320421	-0.236438
H	5.057280	-1.228212	-0.608812
C	2.163219	-1.584045	-2.084920
N	2.429860	-0.468722	-2.952764
C	1.405376	-0.218714	-3.963424
H	1.563522	0.782150	-4.381162
H	0.416621	-0.246935	-3.498045
H	1.421961	-0.934134	-4.806616
C	3.762558	-0.485415	-3.555713
H	4.529158	-0.575188	-2.784861
H	3.926086	0.458764	-4.087831
H	3.893032	-1.313409	-4.277544
C	1.574758	-2.751915	-2.590293
H	1.343781	-2.821533	-3.648282
C	1.277888	-3.817782	-1.747267
H	0.824163	-4.720542	-2.148023
C	1.580396	-3.734846	-0.391517
H	1.357463	-4.575391	0.256784
C	2.172674	-2.582003	0.146147
N	2.447521	-2.496244	1.552938
C	3.822633	-2.829685	1.929382
H	3.966218	-2.602024	2.991757
H	4.533662	-2.232848	1.358883
H	4.054908	-3.899563	1.772993
C	1.501525	-3.200066	2.414165
H	0.477995	-2.969170	2.109798
H	1.641744	-2.852385	3.443910
H	1.630422	-4.298112	2.417310
C	0.818814	2.804017	-1.890187
H	0.133429	2.093557	-2.371553
H	1.830762	2.416697	-2.053341
C	0.661114	4.186931	-2.542645
H	0.870777	4.116080	-3.618211
H	1.410470	4.875832	-2.124280

C	-0.743442	4.761739	-2.308999
H	-1.481270	4.133908	-2.829904
H	-0.823701	5.766954	-2.743014
C	-1.082311	4.798270	-0.811897
H	-2.108565	5.157186	-0.661398
H	-0.421535	5.521458	-0.310030
C	-0.919846	3.416835	-0.152390
H	-1.663068	2.722105	-0.563659
H	-1.132015	3.503812	0.919549
C	0.417477	0.112236	3.012066
H	1.457474	-0.239819	3.026790
H	-0.164728	-0.657881	2.493261
C	-0.100009	0.284703	4.450468
H	0.013178	-0.658317	5.001709
H	-1.178404	0.500373	4.420267
C	0.620088	1.422661	5.188097
H	1.676485	1.151019	5.332389
H	0.192593	1.560682	6.189707
C	0.542873	2.731696	4.389665
H	1.102375	3.525628	4.901695
H	-0.503464	3.067765	4.340301
C	1.087227	2.550984	2.960676
H	2.152913	2.297005	3.022254
H	1.014155	3.501960	2.418044
C	-3.354007	0.616407	-1.595613
H	-2.849022	0.637631	-2.558579
C	-2.851032	-0.193620	-0.557769
C	-3.566813	-0.229144	0.648178
H	-3.244555	-0.890811	1.447019
C	-4.702220	0.566815	0.831212
H	-5.224850	0.533090	1.786278
C	-5.187414	1.396754	-0.185966
C	-6.437826	2.225244	0.001236
H	-6.319616	3.234992	-0.410488
H	-6.695340	2.324759	1.061340
H	-7.303716	1.774191	-0.503232
C	-4.490432	1.401943	-1.404517
H	-4.846695	2.027956	-2.221750
C	-2.183288	-2.055871	-1.188354
C	-2.422451	-3.075157	-0.145330
H	-1.529377	-3.395855	0.390894
C	-3.592678	-3.641636	0.216221
C	-4.926719	-3.320853	-0.409302
H	-5.627082	-2.938719	0.346369

H	-5.386215	-4.226907	-0.830985
H	-4.861183	-2.570521	-1.199854
C	-3.639033	-4.687405	1.304100
H	-4.301243	-4.378967	2.126446
H	-2.647355	-4.884563	1.725001
H	-4.042099	-5.638615	0.926109
H	-1.227487	-2.249184	-1.712841
H	-2.957634	-1.990442	-1.947485

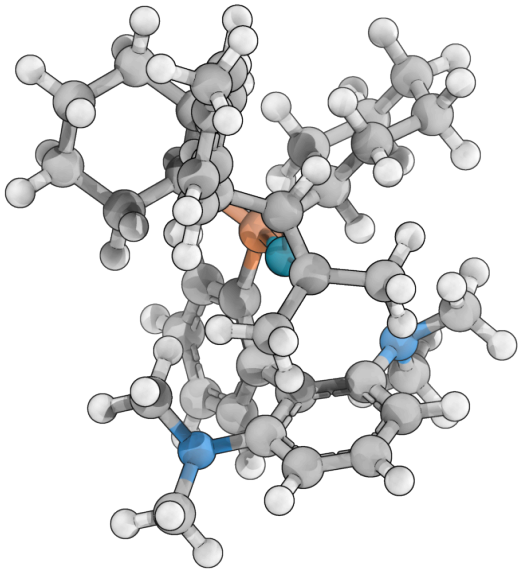
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10
Zero-point correction (ZPE)= -2135.2360 0.88782
Internal Energy (U)= -2135.1882 0.93563
Enthalpy (H)= -2135.1872 0.93657
Gibbs Free Energy (G)= -2135.3218 0.80200

Frequencies -- -320.7174 9.9835 15.8974
$\Delta G_{Solvation}$ = -0.00681763000011415

VII Product-Catalyst Complex:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) iop(1/8=18)
freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)]
#Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.19510844 Predicted Change= -6.272816D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.05684 II	0.00180	[NO]	0.05684 II	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.053959	-0.757535	2.338863
H	-5.924155	-1.183032	2.831773
C	-4.708723	0.578943	2.530895
H	-5.303879	1.219288	3.176804
C	-3.583198	1.090961	1.890974

H	-3.325149	2.127380	2.074711
C	-2.771954	0.312445	1.040399
P	-1.254329	1.086069	0.259561
Pd	0.496482	-0.302998	-0.454501
C	-2.036899	2.176375	-1.087267
H	-2.753169	1.473438	-1.532905
C	-0.673888	2.283199	1.607077
H	-1.502508	2.951364	1.878545
C	-3.130379	-1.046251	0.843158
C	-2.411597	-2.049265	-0.018407
C	-4.266109	-1.548682	1.510111
H	-4.523654	-2.593106	1.364116
C	-2.497346	-2.007707	-1.432484
N	-3.189704	-0.930348	-2.076995
C	-2.758025	-0.630153	-3.437862
H	-3.180512	0.336926	-3.732066
H	-1.668187	-0.557017	-3.474446
H	-3.090515	-1.372999	-4.185807
C	-4.651015	-1.024545	-2.008178
H	-5.044858	-1.852719	-2.624918
H	-4.978799	-1.170953	-0.978710
H	-5.087139	-0.088004	-2.374358
C	-1.949319	-3.049685	-2.199288
H	-2.026561	-3.022870	-3.279999
C	-1.347477	-4.140547	-1.584271
H	-0.938246	-4.946278	-2.188696
C	-1.279144	-4.211127	-0.196741
H	-0.804445	-5.065486	0.272588
C	-1.806390	-3.181941	0.598563
N	-1.790997	-3.292325	2.016825
C	-0.916975	-2.369081	2.736241
H	0.141761	-2.681938	2.688422
H	-0.988632	-1.368054	2.316111
H	-1.218189	-2.328999	3.789892
C	-1.726221	-4.633697	2.573758
H	-2.436930	-5.289364	2.062587
H	-0.722552	-5.095476	2.518590
H	-2.004161	-4.583709	3.633010
C	-1.020269	2.556480	-2.187631
H	-0.238798	3.206514	-1.771784
H	-0.507691	1.654614	-2.540759
C	-1.699781	3.287789	-3.358575
H	-0.945650	3.577517	-4.102121
H	-2.388641	2.597126	-3.867177

C	-2.484553	4.519502	-2.885568
H	-1.781968	5.265469	-2.484568
H	-2.996302	4.996144	-3.731781
C	-3.495408	4.140326	-1.794723
H	-4.020345	5.033473	-1.430877
H	-4.263343	3.480247	-2.224999
C	-2.817158	3.419362	-0.614480
H	-2.136952	4.125279	-0.117776
H	-3.578911	3.139153	0.120596
C	0.486521	3.169216	1.104230
H	1.297672	2.521566	0.745222
H	0.166378	3.770636	0.246534
C	1.012961	4.103512	2.207996
H	1.854197	4.692951	1.820475
H	0.226651	4.823949	2.479617
C	1.436510	3.324825	3.460415
H	2.299381	2.687676	3.216541
H	1.768582	4.015460	4.246330
C	0.287046	2.445191	3.970182
H	0.613175	1.851316	4.834059
H	-0.532023	3.088379	4.325780
C	-0.241539	1.508917	2.870300
H	0.544004	0.794095	2.586951
H	-1.079679	0.920295	3.260027
C	5.759404	-1.147256	0.449478
H	5.266253	-2.035283	0.838276
C	5.007096	0.011871	0.217040
C	3.505980	0.045295	0.468471
C	2.713006	-0.268992	-0.793190
H	2.823206	0.484820	-1.574143
C	2.253692	-1.518100	-1.196472
C	2.397062	-2.775093	-0.362067
H	3.276775	-3.352979	-0.688397
H	1.521489	-3.422009	-0.485299
H	2.509450	-2.567837	0.705349
C	1.987731	-1.786996	-2.667595
H	2.817695	-2.367633	-3.102430
H	1.893568	-0.857677	-3.238702
H	1.073266	-2.374129	-2.812368
H	3.226741	1.044099	0.824751
H	3.252227	-0.653702	1.270989
C	5.678707	1.135634	-0.281466
H	5.121300	2.051637	-0.468764
C	7.049249	1.101784	-0.539766

H	7.543591	1.990823	-0.926448
C	7.801819	-0.055743	-0.304035
C	9.293562	-0.082791	-0.547436
H	9.629253	-1.073369	-0.874211
H	9.588300	0.642662	-1.313478
H	9.853445	0.163159	0.365335
C	7.129923	-1.180232	0.193223
H	7.688165	-2.094508	0.385617

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.19510844 Predicted Change= -6.272816D-08
Zero-point correction (ZPE)= -2135.3035 0.89160
Internal Energy (U)= -2135.2558 0.93923
Enthalpy (H)= -2135.2549 0.94018
Gibbs Free Energy (G)= -2135.3892 0.80588

Frequencies -- 9.6702 13.4988 15.3959

$\Delta G_{Solvation}$ = -0.00707439999996495

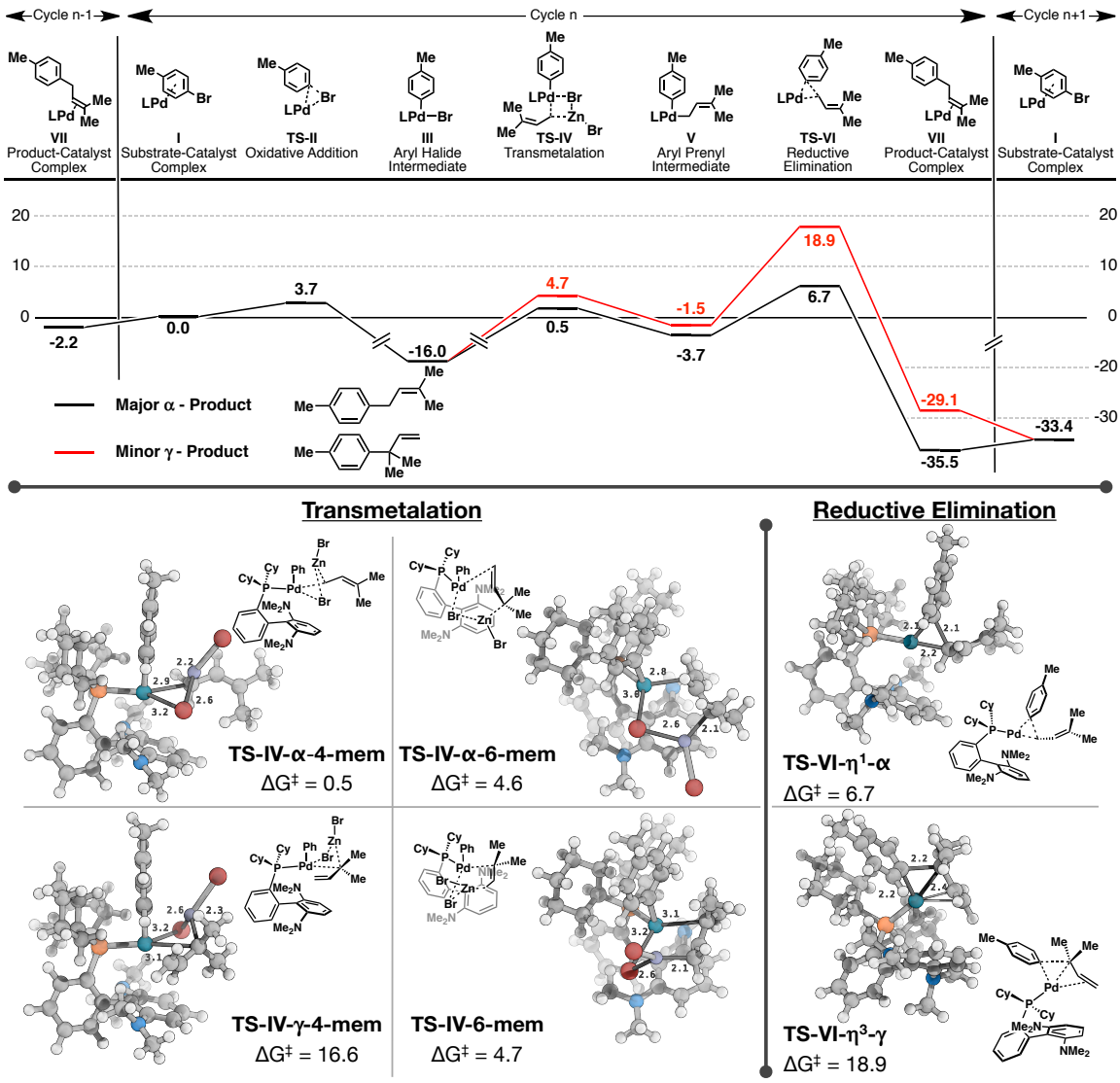
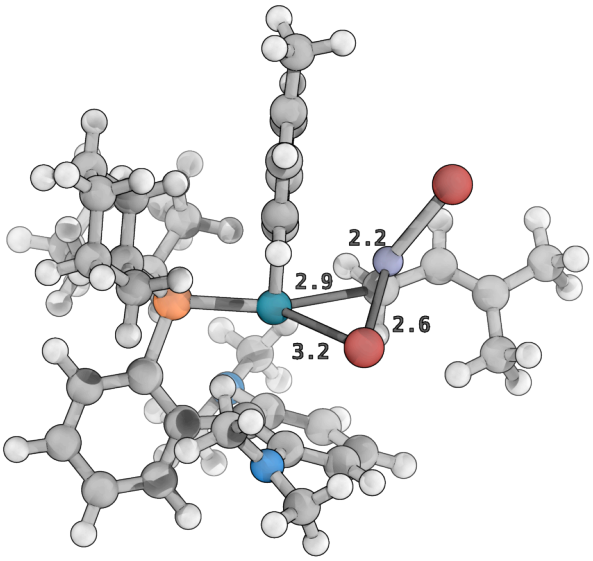


Figure X. Reaction coordinate of Pd(0)-catalyzed cross-coupling of prenylZnBr with p-bromotoluene (above) and transmetalation and reductive elimination transition (below).[1] Energies are displayed in kcal/mol and distances in Å. Computed structures are rendered in Pymol.[2]

TS-IV-a-4-mem:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn
C1[X(C40H57Br2N2PPdZn)] #Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00311 II	0.00180	[NO]	0.00311 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.004554	-2.651548	-1.665480
H	5.643498	-3.418568	-2.094586
C	5.464856	-1.343193	-1.522539
H	6.467381	-1.069806	-1.839555
C	4.621010	-0.378701	-0.978227

H	4.992821	0.636124	-0.897370
C	3.311318	-0.686255	-0.561371
P	2.203857	0.644041	0.112177
Pd	-0.012339	-0.172776	-0.058016
C	2.876710	0.894170	1.866718
H	2.980571	-0.148702	2.191381
C	2.715941	2.162949	-0.883413
H	3.807934	2.222240	-0.777272
C	2.847028	-2.012796	-0.694003
C	1.492355	-2.535099	-0.278807
C	3.714721	-2.971753	-1.253164
H	3.353439	-3.989322	-1.366254
C	1.272997	-2.892095	1.096041
N	2.161988	-2.398831	2.112864
C	1.545653	-2.203537	3.425976
H	2.224921	-1.606426	4.044446
H	0.600586	-1.665355	3.323277
H	1.354978	-3.145207	3.969231
C	3.395782	-3.184146	2.255192
H	3.199914	-4.190103	2.666186
H	3.899003	-3.293182	1.294660
H	4.073563	-2.660644	2.939207
C	0.238889	-3.760644	1.445479
H	0.073171	-4.021941	2.483431
C	-0.564884	-4.327281	0.454762
H	-1.367274	-5.003586	0.736822
C	-0.368429	-4.029176	-0.880658
H	-1.037602	-4.446680	-1.620195
C	0.665926	-3.154985	-1.287988
N	0.914178	-2.987244	-2.639288
C	1.319579	-1.708669	-3.217864
H	0.613814	-1.434390	-4.009740
H	1.273336	-0.919252	-2.470173
H	2.333388	-1.752923	-3.637690
C	0.290244	-3.883253	-3.605084
H	0.352440	-4.920609	-3.264630
H	-0.761451	-3.626489	-3.798398
H	0.842574	-3.807444	-4.546954
C	1.874103	1.579148	2.817892
H	1.641543	2.591820	2.466020
H	0.931434	1.022062	2.810972
C	2.417604	1.660174	4.255693
H	1.699353	2.198578	4.886798
H	2.497056	0.645358	4.671454

C	3.795265	2.332840	4.313810
H	3.702061	3.385863	4.009545
H	4.173749	2.337496	5.343585
C	4.786402	1.621347	3.384203
H	5.761370	2.124830	3.401487
H	4.956405	0.597260	3.747639
C	4.265985	1.565007	1.935794
H	4.213488	2.589203	1.543764
H	4.985309	1.019607	1.316093
C	2.148679	3.498815	-0.353906
H	1.057136	3.485578	-0.398375
H	2.422690	3.645037	0.696189
C	2.674569	4.682338	-1.186335
H	2.239547	5.614248	-0.804346
H	3.764208	4.768750	-1.056513
C	2.351658	4.512031	-2.676829
H	1.261264	4.533815	-2.812749
H	2.759708	5.351075	-3.254284
C	2.903140	3.182070	-3.208538
H	2.623682	3.043186	-4.260407
H	4.002928	3.205954	-3.177988
C	2.398490	1.985002	-2.383810
H	1.314215	1.886664	-2.510094
H	2.850626	1.061220	-2.761835
C	-1.090620	2.423140	1.096022
H	-0.865766	2.007538	2.071330
C	-0.841791	1.687289	-0.072504
C	-1.169581	2.263101	-1.311207
H	-1.023143	1.708091	-2.230935
C	-1.741393	3.537991	-1.367538
H	-2.010628	3.949817	-2.337713
C	-2.002247	4.274886	-0.206648
C	-2.685689	5.619156	-0.272831
H	-2.405910	6.256854	0.572749
H	-2.441218	6.151204	-1.198587
H	-3.775776	5.494136	-0.244507
C	-1.664248	3.694948	1.022757
H	-1.869629	4.234658	1.944913
Br	-2.119411	-1.081046	-2.219722
C	-2.141770	-1.047271	1.713501
H	-1.435636	-0.488781	2.330762
H	-1.713519	-1.995667	1.392084
C	-3.466033	-1.159009	2.364070
H	-3.721739	-0.331591	3.027147

C	-4.414584	-2.113481	2.200995
C	-4.277025	-3.285837	1.265040
H	-5.087924	-3.281419	0.522369
H	-4.362103	-4.239213	1.808461
H	-3.332492	-3.288165	0.715609
C	-5.722264	-2.034039	2.945336
H	-6.565629	-1.931399	2.246983
H	-5.751226	-1.179966	3.629221
H	-5.908301	-2.947890	3.529380
Br	-4.970761	1.386250	-0.070632
Zn	-2.894431	0.048737	-0.002394

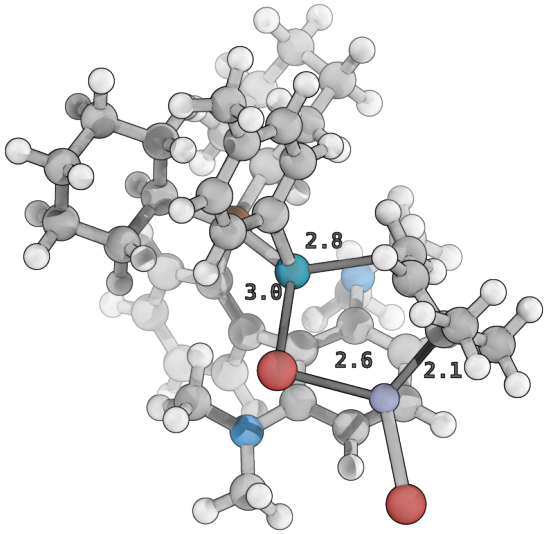
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09
Zero-point correction (ZPE)= -2227.2867 0.89270
Internal Energy (U)= -2227.2328 0.94656
Enthalpy (H)= -2227.2319 0.94750
Gibbs Free Energy (G)= -2227.3781 0.80131

Frequencies -- -68.2928 17.3940 18.2056

TS-IV-a-6-mem



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn
C1[X(C40H57Br2N2PPdZn)] #Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17505355 Predicted Change= -1.703331D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00065 II	0.00180	[YES]	0.00065 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.095916	-4.666571	-2.110210
H	2.011641	-5.645006	-2.575155
C	3.282631	-3.940352	-2.193171
H	4.141432	-4.338224	-2.726479
C	3.358265	-2.685449	-1.594493
H	4.284905	-2.133008	-1.693337
C	2.269793	-2.122008	-0.900109

P	2.423539	-0.426888	-0.150778
Pd	0.230319	0.380124	0.220706
C	3.464113	-0.769181	1.399503
H	2.949194	-1.654203	1.793302
C	3.560046	0.463380	-1.367988
H	4.430521	-0.196491	-1.480134
C	1.068581	-2.859945	-0.809127
C	-0.195376	-2.435610	-0.103824
C	1.012474	-4.126111	-1.424918
H	0.083876	-4.685478	-1.365289
C	-0.297165	-2.611605	1.316632
N	0.890100	-2.877973	2.084965
C	0.860622	-2.384532	3.461405
H	1.873480	-2.447052	3.874689
H	0.542772	-1.340264	3.478504
H	0.201756	-2.966296	4.128923
C	1.288410	-4.292721	2.072508
H	0.570423	-4.928972	2.618952
H	1.371864	-4.661775	1.050422
H	2.268832	-4.390822	2.552483
C	-1.545176	-2.613858	1.944379
H	-1.616380	-2.753124	3.016550
C	-2.708448	-2.498679	1.183301
H	-3.680011	-2.519945	1.669898
C	-2.652278	-2.365005	-0.193859
H	-3.577913	-2.264651	-0.745506
C	-1.411941	-2.353201	-0.877020
N	-1.407780	-2.345374	-2.259876
C	-0.408460	-1.636928	-3.055606
H	-0.920982	-0.967676	-3.754616
H	0.214589	-1.010508	-2.420544
H	0.229325	-2.328782	-3.622048
C	-2.646255	-2.608328	-2.986804
H	-3.182881	-3.450260	-2.541718
H	-3.312058	-1.734293	-3.017326
H	-2.385818	-2.882577	-4.013754
C	3.364137	0.340832	2.465814
H	3.758725	1.285898	2.072651
H	2.310753	0.516712	2.706086
C	4.129347	-0.029058	3.748777
H	4.076509	0.806555	4.458147
H	3.631852	-0.880859	4.234509
C	5.589944	-0.400108	3.462069
H	6.124843	0.483430	3.083111

H	6.096172	-0.698590	4.388539
C	5.669499	-1.525795	2.423373
H	6.715500	-1.765994	2.194116
H	5.223176	-2.439994	2.841427
C	4.935342	-1.150809	1.122884
H	5.464687	-0.310539	0.654818
H	4.988021	-1.993203	0.425603
C	4.105817	1.820923	-0.872475
H	3.282005	2.518877	-0.707505
H	4.619163	1.702672	0.087553
C	5.081221	2.420899	-1.901683
H	5.439677	3.391741	-1.537273
H	5.966771	1.773382	-1.990796
C	4.423928	2.575793	-3.279886
H	5.144204	2.978738	-4.003018
H	3.605173	3.305545	-3.207686
C	3.866667	1.234282	-3.775240
H	3.351320	1.362799	-4.735289
H	4.700527	0.540226	-3.959069
C	2.899376	0.605779	-2.756421
H	2.005360	1.233065	-2.666751
H	2.567571	-0.372383	-3.121861
C	1.330299	2.984311	1.267809
H	1.507779	2.475897	2.207364
C	0.827265	2.305913	0.155002
C	0.642758	3.011337	-1.040328
H	0.239911	2.519373	-1.916460
C	0.941445	4.375327	-1.104427
H	0.775154	4.903968	-2.041272
C	1.435607	5.072823	0.006129
C	1.724680	6.554414	-0.067605
H	2.423042	6.866691	0.716066
H	2.156301	6.832339	-1.035796
H	0.807457	7.145182	0.057588
C	1.624350	4.351756	1.188877
H	2.009813	4.857700	2.072155
Br	-2.126366	1.065738	-1.555697
C	-3.577268	1.554079	2.116529
C	-4.093958	0.544700	3.150416
H	-3.920238	0.912011	4.175893
H	-3.606975	-0.432465	3.069004
H	-5.171540	0.379900	3.037160
C	-4.358333	2.878875	2.203986
H	-5.429087	2.731775	2.018860

H	-3.994517	3.619633	1.480750
H	-4.265986	3.328571	3.206999
C	-2.128788	1.766395	2.122202
H	-1.798446	2.718205	1.701305
C	-1.145915	0.933310	2.568524
H	-1.374632	-0.023062	3.026763
H	-0.129180	1.289059	2.672035
Br	-6.046356	-0.374405	-0.568967
Zn	-3.972573	0.756844	0.200458

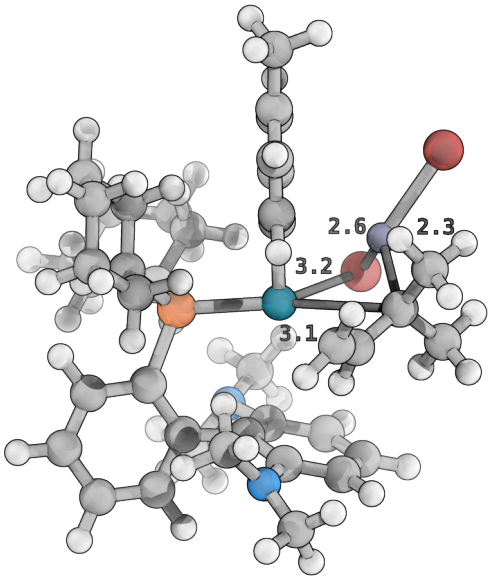
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17505355 Predicted Change= -1.703331D-10
Zero-point correction (ZPE)= -2227.2816 0.89338
Internal Energy (U)= -2227.2282 0.94678
Enthalpy (H)= -2227.2273 0.94772
Gibbs Free Energy (G)= -2227.3716 0.80337

Frequencies -- -69.5245 15.5364 23.4922

TS-IV-g-4-mem:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn
C1[X(C40H57Br2N2PPdZn)] #Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.15420473 Predicted Change= -1.109863D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00122 II	0.00180	[YES]	0.00122 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.825076	-0.360261	-1.338158
H	6.798581	-0.720296	-1.659532
C	5.554469	1.004496	-1.273419
H	6.311329	1.736147	-1.542122
C	4.294192	1.432871	-0.865911

H	4.120500	2.500504	-0.839617
C	3.265416	0.535822	-0.508404
P	1.604635	1.240944	0.010978
Pd	-0.226958	-0.303103	-0.269311
C	1.934635	1.697252	1.818648
H	2.395605	0.767339	2.177045
C	1.531266	2.853692	-0.974081
H	2.490572	3.351690	-0.788138
C	3.549646	-0.850371	-0.555544
C	2.613929	-1.975987	-0.213406
C	4.829977	-1.262045	-0.979553
H	5.030762	-2.327887	-1.027374
C	2.371374	-2.336830	1.146151
N	2.904873	-1.534306	2.206482
C	2.214108	-1.642513	3.493981
H	2.564976	-0.829813	4.139656
H	1.136438	-1.542721	3.356893
H	2.423239	-2.590253	4.020064
C	4.350878	-1.694659	2.413536
H	4.598167	-2.690772	2.820760
H	4.901901	-1.551763	1.485306
H	4.690051	-0.939269	3.131017
C	1.670870	-3.516016	1.440752
H	1.452242	-3.776831	2.467574
C	1.282190	-4.373742	0.419706
H	0.747924	-5.288692	0.661339
C	1.574191	-4.082313	-0.907133
H	1.255950	-4.766724	-1.684392
C	2.252800	-2.897275	-1.251566
N	2.628836	-2.687009	-2.585370
C	2.480507	-1.398980	-3.255783
H	1.932278	-1.539082	-4.196085
H	1.903226	-0.706312	-2.643302
H	3.448859	-0.937609	-3.491647
C	2.685812	-3.818751	-3.495577
H	3.109079	-4.692377	-2.992729
H	1.702889	-4.095858	-3.913696
H	3.343991	-3.561353	-4.332733
C	0.650710	1.931958	2.641210
H	0.098526	2.793801	2.245784
H	-0.003913	1.059003	2.557239
C	0.972235	2.185778	4.125066
H	0.041234	2.398562	4.664675
H	1.381488	1.266624	4.566893

C	1.978401	3.328155	4.312958
H	1.527119	4.274312	3.978512
H	2.218638	3.455429	5.376043
C	3.256605	3.065055	3.506361
H	3.961167	3.900002	3.613083
H	3.763237	2.174540	3.906271
C	2.949294	2.844670	2.013104
H	2.548910	3.780197	1.599740
H	3.881265	2.628917	1.480053
C	0.447632	3.857894	-0.524604
H	-0.547044	3.427295	-0.652202
H	0.557945	4.092167	0.539061
C	0.544825	5.157235	-1.345054
H	-0.243180	5.848373	-1.021108
H	1.503702	5.655069	-1.134560
C	0.432291	4.886725	-2.851442
H	0.532709	5.822392	-3.415821
H	-0.568725	4.489509	-3.071376
C	1.491600	3.874225	-3.308019
H	1.367070	3.641546	-4.373235
H	2.491477	4.321403	-3.201968
C	1.428367	2.572986	-2.488928
H	0.480890	2.059460	-2.690521
H	2.231951	1.899197	-2.808191
C	-2.239080	1.788054	0.565590
H	-1.959336	1.550810	1.585227
C	-1.651659	1.118759	-0.518270
C	-2.050316	1.443533	-1.820896
H	-1.619762	0.921319	-2.671730
C	-3.030018	2.417111	-2.029966
H	-3.336174	2.648670	-3.048524
C	-3.633892	3.091186	-0.957333
C	-4.726958	4.107241	-1.189836
H	-5.714895	3.632378	-1.132084
H	-4.704369	4.901517	-0.436076
H	-4.642281	4.571537	-2.178121
C	-3.222860	2.757830	0.337012
H	-3.684259	3.246024	1.192042
Br	-1.466645	-1.572178	2.433153
C	-2.359474	-2.193371	-1.541082
C	-3.687331	-1.924558	-2.249786
H	-4.549215	-2.161328	-1.621687
H	-3.743466	-2.551843	-3.155976
H	-3.790156	-0.881946	-2.570022

C	-2.325912	-3.560574	-0.843569
H	-1.405279	-3.710513	-0.272177
H	-2.390117	-4.362672	-1.598424
H	-3.172974	-3.702691	-0.161376
C	-1.185000	-1.974475	-2.400846
H	-0.244947	-2.374348	-2.017313
C	-1.178763	-1.431721	-3.638463
H	-0.259179	-1.336720	-4.206106
H	-2.082507	-1.080290	-4.125945
Br	-5.266825	-0.665938	0.823972
Zn	-2.861009	-1.027748	0.351448

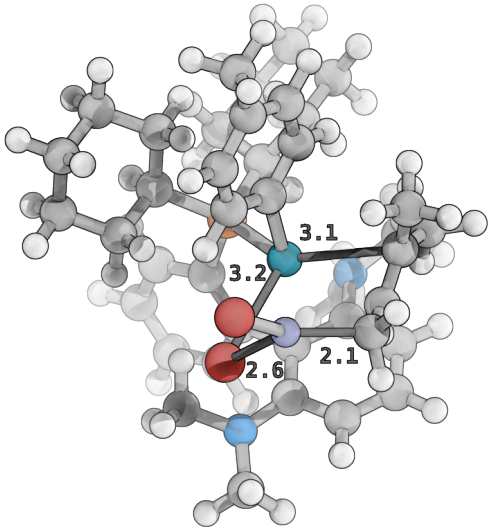
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.15420473 Predicted Change= -1.109863D-09
Zero-point correction (ZPE)= -2227.2620 0.89220
Internal Energy (U)= -2227.2082 0.94599
Enthalpy (H)= -2227.2072 0.94693
Gibbs Free Energy (G)= -2227.3525 0.80162

Frequencies -- -60.7485 17.7116 22.9111

TS-IV-g-6-mem:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk
RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn
C1[X(C40H57Br2N2PPdZn)] #Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17166772 Predicted Change= -1.718430D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.01050 II	0.00180	[NO]	0.01050 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.699844	-2.198171	2.666420
H	-5.365216	-2.905328	3.154121
C	-4.626790	-0.875759	3.095984
H	-5.229895	-0.526584	3.929381
C	-3.762245	0.005928	2.451365
H	-3.723032	1.022629	2.820217
C	-2.948716	-0.386910	1.369424

P	-1.865391	0.909074	0.554013
Pd	0.027169	-0.064446	-0.560712
C	-3.156216	1.789456	-0.527439
H	-3.664375	0.923292	-0.970799
C	-1.446474	2.069726	1.984668
H	-2.403705	2.308999	2.465237
C	-3.016357	-1.735227	0.941428
C	-2.201511	-2.366388	-0.152325
C	-3.899184	-2.609185	1.605899
H	-3.930253	-3.645023	1.280943
C	-2.602519	-2.203479	-1.512370
N	-3.698546	-1.321790	-1.821376
C	-3.668472	-0.730383	-3.157810
H	-4.425290	0.060305	-3.203801
H	-2.690880	-0.285352	-3.351413
H	-3.898080	-1.446092	-3.966464
C	-5.018471	-1.922441	-1.582008
H	-5.232498	-2.742844	-2.289224
H	-5.089714	-2.310229	-0.566583
H	-5.787456	-1.151737	-1.706789
C	-1.996255	-2.949730	-2.529164
H	-2.313356	-2.833555	-3.558499
C	-1.005891	-3.876390	-2.208347
H	-0.518192	-4.441071	-2.999107
C	-0.640935	-4.100603	-0.891845
H	0.139740	-4.818534	-0.679062
C	-1.263615	-3.408390	0.177930
N	-1.014633	-3.836598	1.474054
C	-0.958204	-2.978971	2.658475
H	0.010307	-3.111151	3.149837
H	-1.033012	-1.930526	2.391187
H	-1.759453	-3.227807	3.367210
C	-0.337728	-5.109898	1.683402
H	-0.729435	-5.875024	1.007284
H	0.752342	-5.033443	1.553674
H	-0.535409	-5.436345	2.709185
C	-2.547663	2.615466	-1.676801
H	-1.931512	3.429321	-1.275587
H	-1.882847	1.976516	-2.267055
C	-3.630802	3.214700	-2.591741
H	-3.154234	3.836231	-3.360539
H	-4.147159	2.403250	-3.124198
C	-4.661232	4.031380	-1.802657
H	-4.171925	4.913710	-1.364102

H	-5.443785	4.408435	-2.472928
C	-5.278865	3.185400	-0.682220
H	-5.992359	3.780382	-0.098024
H	-5.850354	2.355740	-1.123781
C	-4.200828	2.613614	0.257535
H	-3.713329	3.448568	0.777918
H	-4.681005	1.994097	1.020914
C	-0.836785	3.422852	1.557460
H	0.103368	3.261810	1.027035
H	-1.506811	3.945190	0.865684
C	-0.576417	4.312768	2.786433
H	-0.124430	5.257143	2.458258
H	-1.533579	4.572836	3.263912
C	0.328618	3.610864	3.807841
H	0.485015	4.252976	4.683702
H	1.316787	3.442371	3.357448
C	-0.270020	2.264166	4.235710
H	0.406847	1.744357	4.924557
H	-1.204816	2.442020	4.788938
C	-0.557874	1.355980	3.027251
H	0.385463	1.053775	2.559135
H	-1.041867	0.434311	3.369654
C	2.165380	1.706943	0.322032
H	2.310134	0.949203	1.083546
C	1.108104	1.618009	-0.592413
C	0.928386	2.631883	-1.532563
H	0.127169	2.590643	-2.258863
C	1.813854	3.716928	-1.566801
H	1.664143	4.492465	-2.315813
C	2.887216	3.817336	-0.675351
C	3.848177	4.982900	-0.723052
H	4.875275	4.642268	-0.901089
H	3.584893	5.686004	-1.519829
H	3.854310	5.536945	0.223867
C	3.048562	2.790943	0.264810
H	3.880373	2.817646	0.965036
Br	1.921003	-1.772179	1.326512
C	3.272871	-1.754313	-2.168098
H	3.391104	-2.842622	-2.113868
H	4.010376	-1.353810	-2.869584
C	1.889344	-1.406608	-2.531908
H	1.124723	-2.151022	-2.306265
C	1.501997	-0.305335	-3.247452
C	2.519027	0.719142	-3.687833

H	2.044110	1.664739	-3.966857
H	3.068304	0.358012	-4.571450
H	3.259381	0.930461	-2.910086
C	0.156563	-0.215907	-3.922906
H	0.279942	-0.327767	-5.012339
H	-0.325081	0.760405	-3.772155
H	-0.522541	-1.001962	-3.584147
Br	5.920409	-0.229087	0.719113
Zn	3.860252	-1.162386	-0.266214

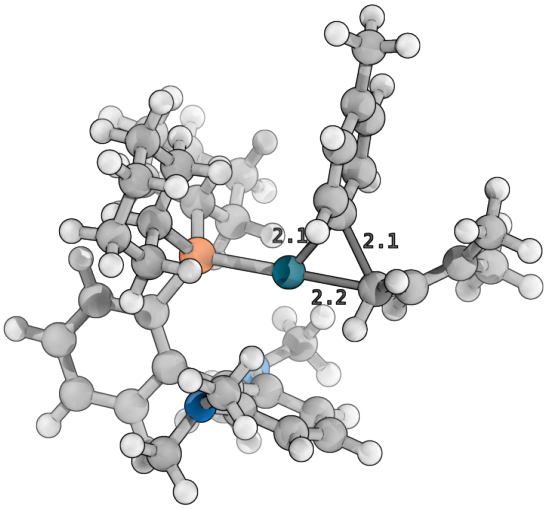
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17166772 Predicted Change= -1.718430D-08
Zero-point correction (ZPE)= -2227.2787 0.89292
Internal Energy (U)= -2227.2250 0.94664
Enthalpy (H)= -2227.2240 0.94758
Gibbs Free Energy (G)= -2227.3715 0.80015

Frequencies -- -54.0448 12.8572 17.7196

TS-VI-h^1-a:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)]
#Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00246 II	0.00180	[NO]	0.00246 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.394518	0.744090	0.160557
H	6.476648	0.659059	0.105930
C	4.793472	1.915501	0.612632
H	5.395440	2.767327	0.917868
C	3.403416	1.990837	0.665757
H	2.960196	2.918580	1.007247
C	2.569888	0.920613	0.286226

P	0.715854	1.139926	0.386585
Pd	-0.799548	-0.468409	-0.478624
C	0.497302	2.850464	-0.382306
H	1.211558	3.535884	0.094483
C	0.334107	1.430498	2.218313
H	-0.728818	1.711161	2.175527
C	3.183584	-0.264581	-0.188366
C	2.463824	-1.483551	-0.703454
C	4.589506	-0.320421	-0.236438
H	5.057280	-1.228212	-0.608812
C	2.163219	-1.584045	-2.084920
N	2.429860	-0.468722	-2.952764
C	1.405376	-0.218714	-3.963424
H	1.563522	0.782150	-4.381162
H	0.416621	-0.246935	-3.498045
H	1.421961	-0.934134	-4.806616
C	3.762558	-0.485415	-3.555713
H	4.529158	-0.575188	-2.784861
H	3.926086	0.458764	-4.087831
H	3.893032	-1.313409	-4.277544
C	1.574758	-2.751915	-2.590293
H	1.343781	-2.821533	-3.648282
C	1.277888	-3.817782	-1.747267
H	0.824163	-4.720542	-2.148023
C	1.580396	-3.734846	-0.391517
H	1.357463	-4.575391	0.256784
C	2.172674	-2.582003	0.146147
N	2.447521	-2.496244	1.552938
C	3.822633	-2.829685	1.929382
H	3.966218	-2.602024	2.991757
H	4.533662	-2.232848	1.358883
H	4.054908	-3.899563	1.772993
C	1.501525	-3.200066	2.414165
H	0.477995	-2.969170	2.109798
H	1.641744	-2.852385	3.443910
H	1.630422	-4.298112	2.417310
C	0.818814	2.804017	-1.890187
H	0.133429	2.093557	-2.371553
H	1.830762	2.416697	-2.053341
C	0.661114	4.186931	-2.542645
H	0.870777	4.116080	-3.618211
H	1.410470	4.875832	-2.124280
C	-0.743442	4.761739	-2.308999
H	-1.481270	4.133908	-2.829904

H	-0.823701	5.766954	-2.743014
C	-1.082311	4.798270	-0.811897
H	-2.108565	5.157186	-0.661398
H	-0.421535	5.521458	-0.310030
C	-0.919846	3.416835	-0.152390
H	-1.663068	2.722105	-0.563659
H	-1.132015	3.503812	0.919549
C	0.417477	0.112236	3.012066
H	1.457474	-0.239819	3.026790
H	-0.164728	-0.657881	2.493261
C	-0.100009	0.284703	4.450468
H	0.013178	-0.658317	5.001709
H	-1.178404	0.500373	4.420267
C	0.620088	1.422661	5.188097
H	1.676485	1.151019	5.332389
H	0.192593	1.560682	6.189707
C	0.542873	2.731696	4.389665
H	1.102375	3.525628	4.901695
H	-0.503464	3.067765	4.340301
C	1.087227	2.550984	2.960676
H	2.152913	2.297005	3.022254
H	1.014155	3.501960	2.418044
C	-3.354007	0.616407	-1.595613
H	-2.849022	0.637631	-2.558579
C	-2.851032	-0.193620	-0.557769
C	-3.566813	-0.229144	0.648178
H	-3.244555	-0.890811	1.447019
C	-4.702220	0.566815	0.831212
H	-5.224850	0.533090	1.786278
C	-5.187414	1.396754	-0.185966
C	-6.437826	2.225244	0.001236
H	-6.319616	3.234992	-0.410488
H	-6.695340	2.324759	1.061340
H	-7.303716	1.774191	-0.503232
C	-4.490432	1.401943	-1.404517
H	-4.846695	2.027956	-2.221750
C	-2.183288	-2.055871	-1.188354
C	-2.422451	-3.075157	-0.145330
H	-1.529377	-3.395855	0.390894
C	-3.592678	-3.641636	0.216221
C	-4.926719	-3.320853	-0.409302
H	-5.627082	-2.938719	0.346369
H	-5.386215	-4.226907	-0.830985
H	-4.861183	-2.570521	-1.199854

C	-3.639033	-4.687405	1.304100
H	-4.301243	-4.378967	2.126446
H	-2.647355	-4.884563	1.725001
H	-4.042099	-5.638615	0.926109
H	-1.227487	-2.249184	-1.712841
H	-2.957634	-1.990442	-1.947485

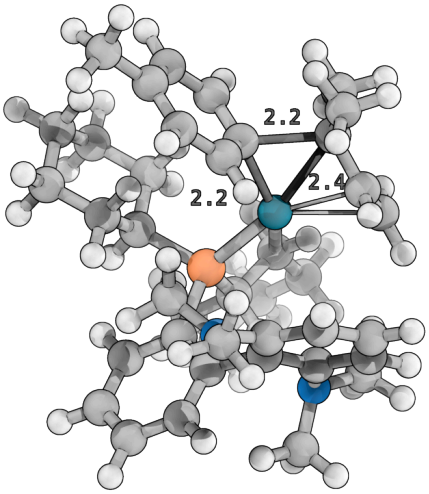
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10
Zero-point correction (ZPE)= -2135.2360 0.88782
Internal Energy (U)= -2135.1882 0.93563
Enthalpy (H)= -2135.1872 0.93657
Gibbs Free Energy (G)= -2135.3218 0.80200

Frequencies -- -320.7174 9.9835 15.8974

TS-VI- h3-g:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)]
#Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.11180380 Predicted Change= -5.083163D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00213 II	0.00180	[NO]	0.00213 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.736981	-0.915160	4.078125
H	-3.192691	-1.365575	4.956044
C	-2.440612	0.445148	4.045108
H	-2.660588	1.083768	4.896617
C	-1.845017	0.986877	2.908644
H	-1.608005	2.042982	2.925389
C	-1.528916	0.219287	1.768768

P	-0.673109	1.074747	0.322638
Pd	0.577895	-0.196488	-1.247086
C	-2.151356	1.975696	-0.474188
H	-2.886512	1.161643	-0.522376
C	0.302525	2.438242	1.207427
H	-0.395754	3.030843	1.813060
C	-1.853073	-1.162132	1.801106
C	-1.615877	-2.162207	0.705613
C	-2.440405	-1.695547	2.965949
H	-2.660162	-2.758809	2.983087
C	-2.458891	-2.208157	-0.430391
N	-3.518883	-1.247965	-0.565958
C	-3.944509	-0.961908	-1.931566
H	-4.515410	-1.782160	-2.404075
H	-4.597912	-0.082269	-1.914708
H	-3.074281	-0.732040	-2.549411
C	-4.683304	-1.521370	0.282245
H	-4.380755	-1.656892	1.320554
H	-5.366988	-0.665889	0.236335
H	-5.235114	-2.421575	-0.044521
C	-2.298731	-3.224694	-1.385512
H	-2.951375	-3.266943	-2.249932
C	-1.328608	-4.204892	-1.210168
H	-1.209895	-4.989132	-1.954141
C	-0.524599	-4.204675	-0.075386
H	0.221024	-4.981921	0.049772
C	-0.666509	-3.208136	0.908173
N	0.053608	-3.312705	2.117106
C	0.558349	-4.615003	2.509288
H	0.769412	-4.596698	3.585216
H	-0.191728	-5.388571	2.322105
H	1.494428	-4.903277	1.995714
C	0.897692	-2.222611	2.598107
H	1.962301	-2.450417	2.436320
H	0.681359	-1.299419	2.067333
H	0.741121	-2.057522	3.672438
C	-1.856714	2.422391	-1.922610
H	-1.075382	3.194067	-1.928903
H	-1.459024	1.574759	-2.490946
C	-3.111866	2.988579	-2.609064
H	-2.857936	3.331574	-3.620825
H	-3.853645	2.185350	-2.729427
C	-3.736616	4.132915	-1.798448
H	-3.039693	4.984160	-1.777058

H	-4.653625	4.491631	-2.283760
C	-4.032197	3.687619	-0.359917
H	-4.437494	4.524017	0.224789
H	-4.810432	2.910054	-0.373078
C	-2.775371	3.130621	0.335117
H	-2.048599	3.947069	0.450515
H	-3.041330	2.793918	1.342649
C	0.953395	3.413089	0.203242
H	1.619318	2.853752	-0.463880
H	0.190392	3.879860	-0.428417
C	1.749415	4.515439	0.925626
H	2.225983	5.170429	0.184313
H	1.053436	5.147929	1.497602
C	2.801556	3.931481	1.878003
H	3.563264	3.398566	1.292725
H	3.318733	4.738151	2.414172
C	2.161733	2.952458	2.871955
H	2.931852	2.498632	3.508966
H	1.486293	3.505283	3.542806
C	1.371733	1.846030	2.150937
H	2.062104	1.224985	1.568189
H	0.901325	1.191076	2.892861
C	3.537973	0.877285	-0.948693
H	3.284776	1.698406	-1.613264
C	2.728492	-0.269378	-0.906115
C	3.125759	-1.293424	-0.026688
H	2.548822	-2.213624	0.023033
C	4.248161	-1.160581	0.792370
H	4.511433	-1.969589	1.472983
C	5.051784	-0.012464	0.746987
C	6.298436	0.106219	1.593224
H	6.176181	-0.392930	2.561431
H	7.166577	-0.354631	1.101440
H	6.554980	1.153974	1.785237
C	4.674185	1.001276	-0.142389
H	5.277321	1.905993	-0.208195
C	2.181860	-0.965079	-2.891774
C	2.509479	0.217896	-3.789883
H	2.450146	-0.102320	-4.840653
H	1.820639	1.057083	-3.657855
H	3.525644	0.578253	-3.609280
C	3.264278	-2.036513	-2.938107
H	3.044305	-2.871265	-2.266667
H	3.313624	-2.438467	-3.962376

H	4.248405	-1.636896	-2.679135
C	0.832632	-1.526618	-3.019953
H	0.707850	-2.544154	-2.648212
C	-0.288085	-0.900182	-3.518536
H	-1.220830	-1.448950	-3.571388
H	-0.244700	0.048762	-4.042625

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.11180380 Predicted Change= -5.083163D-09
Zero-point correction (ZPE)= -2135.2223 0.88941
Internal Energy (U)= -2135.1754 0.93638
Enthalpy (H)= -2135.1744 0.93733
Gibbs Free Energy (G)= -2135.3024 0.80939

Frequencies -- -287.5205 13.7402 24.9558

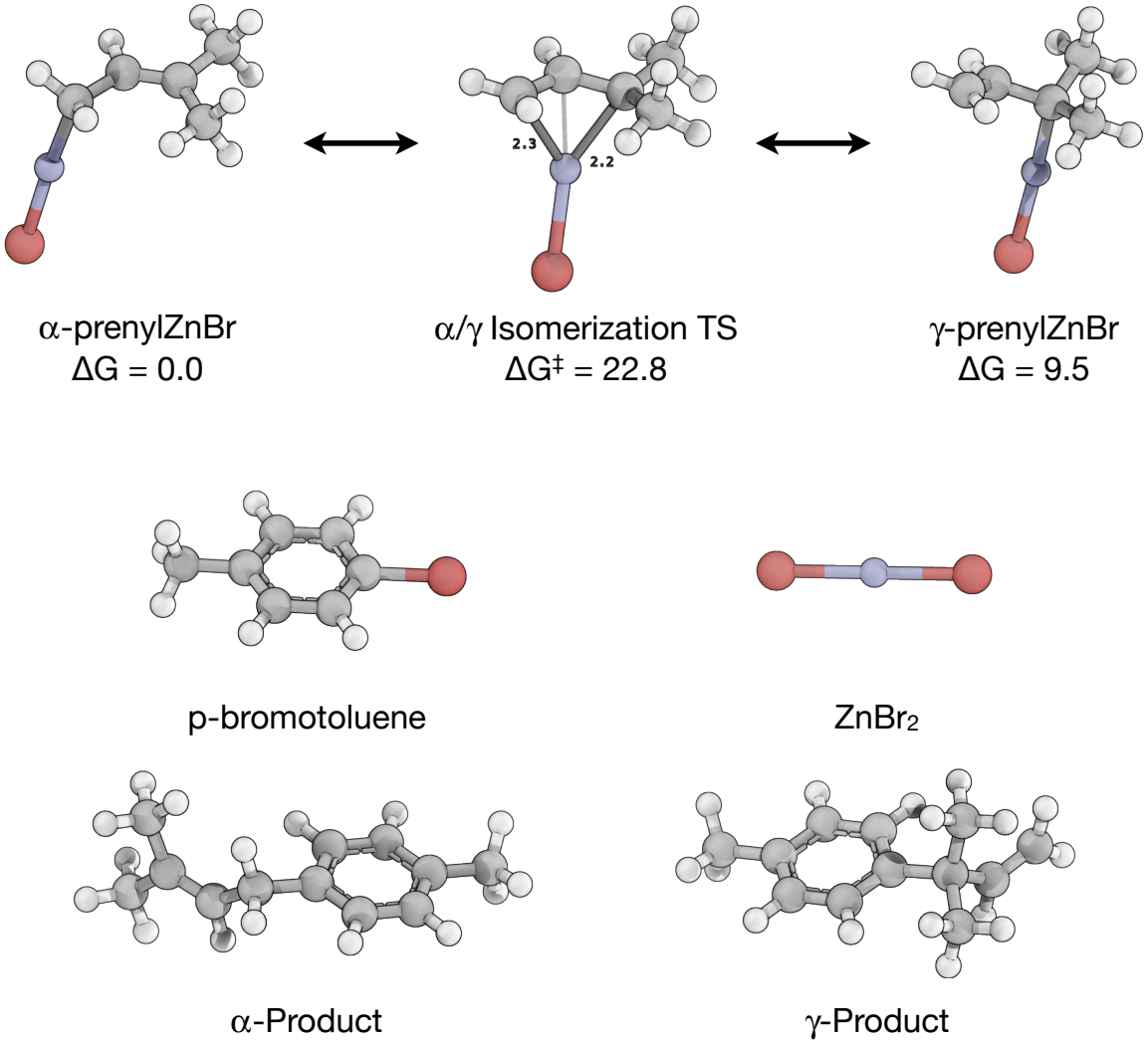


Figure A3.2. Structures for all relevant minor intermediates, starting materials, and products; including the interconversion of prenylZnBr.[1] Energies are displayed in kcal/mol and distances in Å. Computed structures are rendered in Pymol.[2]

a-prenylZnBr:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C5H9BrZn C1[X(C5H9BrZn)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -274.741185418 Predicted Change= -4.179115D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.02094 ll	0.00180	[NO]	0.02094 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.270521	1.511996	-0.037352
H	1.511769	1.792602	0.991438
H	1.171115	2.430130	-0.624438
C	2.247675	0.567028	-0.653786
H	2.265395	0.581095	-1.744980
C	3.080623	-0.296948	-0.041655
C	4.003082	-1.182749	-0.843001
H	3.893022	-1.020053	-1.920040
H	3.811053	-2.246371	-0.639658
H	5.055165	-1.003238	-0.579211
C	3.169857	-0.471564	1.453816
H	2.898708	-1.497276	1.743669
H	2.523243	0.213116	2.009323
H	4.199195	-0.315174	1.805332
Zn	-0.564866	0.642611	-0.000526
Br	-2.657521	-0.542278	-0.008394

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -274.741185418 Predicted Change= -4.179115D-07
Zero-point correction (ZPE)= -274.6140 0.12715

Internal Energy (U)=	-274.6038	0.13735
Enthalpy (H)=	-274.6028	0.13829
Gibbs Free Energy (G)=	-274.6531	0.08802

Frequencies -- 25.6209 41.5671 81.0463

$\Delta G_{Solvation}$ = -0.0342800329999591

a/g-prenylZnBr:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C5H9BrZn C1[X(C5H9BrZn)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -274.706185584 Predicted Change= -1.259105D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00034 II	0.00180	[YES]	0.00034 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.412138	2.042563	0.112499
H	1.429291	2.148402	1.195352
H	1.301640	2.960498	-0.452652
C	1.979163	0.917340	-0.515565
H	2.158515	1.009877	-1.591490
C	2.083705	-0.419332	-0.000677
C	2.807395	-1.456878	-0.836251
H	3.888154	-1.470557	-0.619343
H	2.692988	-1.266227	-1.910055
H	2.432104	-2.467367	-0.638489
C	2.205932	-0.613696	1.508628
H	3.215361	-0.348924	1.863236
H	2.024357	-1.657827	1.783638
H	1.508270	0.000346	2.097135
Zn	-0.033637	0.231208	-0.142269
Br	-2.359187	-0.247555	0.026541

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -274.706185584 Predicted Change= -1.259105D-09

Zero-point correction (ZPE)=	-274.5804	0.12574
Internal Energy (U)=	-274.5709	0.13523
Enthalpy (H)=	-274.5700	0.13618
Gibbs Free Energy (G)=	-274.6168	0.08929

Frequencies -- -223.1991 54.6105 76.0052

$\Delta G_{Solvation}$ = -0.0264277869999887

g-prenylZnBr:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C5H9BrZn C1[X(C5H9BrZn)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -274.727231796 Predicted Change= -1.076481D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.00864 ll	0.00180	[NO]	0.00864 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.869635	1.977353	-0.090616
H	3.051944	2.044971	0.978143
H	3.145044	2.845575	-0.681958
C	2.330649	0.893173	-0.668302
H	2.194840	0.910581	-1.752702
C	1.890703	-0.376113	-0.005726
C	2.302865	-1.603594	-0.838198
H	3.400252	-1.698878	-0.846755
H	1.976256	-1.526897	-1.882278
H	1.897087	-2.534507	-0.425979
C	2.366088	-0.516086	1.445721
H	3.467049	-0.510452	1.482224
H	2.025815	-1.459194	1.887916
H	2.018049	0.299075	2.090560
Zn	-0.158090	-0.193226	-0.007030
Br	-2.542665	0.147946	0.008699

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -274.727231796 Predicted Change= -1.076481D-07
Zero-point correction (ZPE)= -274.6001 0.12706

Internal Energy (U)= -274.5901 0.13712
Enthalpy (H)= -274.5891 0.13806
Gibbs Free Energy (G)= -274.6379 0.08924

Frequencies -- 35.1449 44.4986 104.6673

$\Delta G_{Solvation}$ = -0.03451731100000019

p-bromotoluene:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas
Freq

Pointgroup= C1 Stoichiometry= C7H7Br C1[X(C7H7Br)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -284.120087119 Predicted Change= -1.537413D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009 ll	0.00045	[YES]	0.00002 ll	0.00030	[YES]
Displ	0.00064 ll	0.00180	[YES]	0.00064 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.312390	0.000006	-0.000567
C	0.366574	1.214021	-0.004396
C	0.366566	-1.214020	-0.004399
C	1.762788	-1.201156	-0.010221
C	1.762795	1.201172	-0.010223
C	2.484003	0.000004	-0.010181
H	2.297508	-2.148246	-0.016771
C	3.994889	-0.000010	0.015526
H	-0.177564	2.152182	-0.006892
H	2.297524	2.148256	-0.016765
H	-0.177559	-2.152182	-0.006886
H	4.374545	-0.000391	1.046110
H	4.404203	0.886293	-0.480638
H	4.404203	-0.885961	-0.481274
Br	-2.284978	-0.000002	0.003140

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -284.120087119 Predicted Change= -1.537413D-07
Zero-point correction (ZPE)= -284.0020 0.11803
Internal Energy (U)= -283.9943 0.12572

Enthalpy (H)= -283.9934 0.12666
Gibbs Free Energy (G)= -284.0363 0.08373

Frequencies -- 29.5690 104.8033 206.9485

$\Delta G_{Solvation}$ = -0.00293244800002412

$ZnBr^2$:

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= Br2Zn C1[X(Br2Zn)] #Atoms= 3
Charge = 0 Multiplicity = 1

SCF Energy= -92.0235652765 Predicted Change= -2.393722D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ll	0.00045	[YES]	0.00001 ll	0.00030	[YES]
Displ	0.00034 ll	0.00180	[YES]	0.00034 ll	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Br	1.727500	-0.163127	-1.583811
Br	-1.727508	0.162957	1.583836
Zn	0.000009	0.000199	-0.000029

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -92.0235652765 Predicted Change= -2.393722D-09
Zero-point correction (ZPE)= -92.0222 0.00136
Internal Energy (U)= -92.0176 0.00594
Enthalpy (H)= -92.0166 0.00689
Gibbs Free Energy (G)= -92.0463 -0.02280

Frequencies -- 63.5376 187.9715 347.2022

$\Delta G_{Solvation}$ = -0.0497805409999899

a-Product:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16 C1[X(C12H16)] #Atoms= 28

Charge = 0 Multiplicity = 1

SCF Energy= -466.901455254 Predicted Change= -3.719157D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ll	0.00045	[YES]	0.00000 ll	0.00030	[YES]
Displ	0.01570 ll	0.00180	[NO]	0.01570 ll	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.418386	0.663281	0.141582
C	-1.496130	1.493665	-0.181332
C	-0.684904	-0.692577	0.381346
C	-1.982791	-1.192838	0.307898
C	-2.797304	0.991098	-0.255955
C	-3.065096	-0.360521	-0.014758
H	-2.160866	-2.248596	0.503500
C	-4.467473	-0.915020	-0.119429
H	-1.319144	2.550214	-0.372774
H	-3.616264	1.661822	-0.507621
C	0.996633	1.214692	0.252969
H	0.137698	-1.360841	0.624392
H	-4.610395	-1.469918	-1.056492
H	-5.216440	-0.116532	-0.095046
H	-4.687946	-1.608487	0.700576
C	2.005418	0.440906	-0.560044
H	1.292092	1.246422	1.308722
H	0.986865	2.260482	-0.086970
C	3.131954	-0.159748	-0.144143
C	3.633802	-0.176596	1.279905
C	4.023183	-0.885129	-1.125955
H	4.141506	-1.941982	-0.847443

H	5.034017	-0.452967	-1.137296
H	3.626211	-0.845345	-2.145210
H	3.790641	-1.208917	1.622461
H	2.957153	0.310774	1.985830
H	4.609542	0.324284	1.352113
H	1.761888	0.372312	-1.621252

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -466.901455254 Predicted Change= -3.719157D-08
Zero-point correction (ZPE)= -466.6551 0.24630
Internal Energy (U)= -466.6422 0.25924
Enthalpy (H)= -466.6412 0.26019
Gibbs Free Energy (G)= -466.6963 0.20510

Frequencies -- 21.3677 36.1636 48.3462

$\Delta G_{Solvation}$ = -0.00262043399999357

g-Product:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16 C1[X(C12H16)] #Atoms= 28

Charge = 0 Multiplicity = 1

SCF Energy= -466.888865594 Predicted Change= -4.168447D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 II	0.00045	[YES]	0.00000 II	0.00030	[YES]
Displ	0.00156 II	0.00180	[YES]	0.00156 II	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.125222	0.213696	0.013463
C	0.449791	-1.058129	0.176842
C	0.746934	1.293058	-0.167978
C	2.132914	1.109974	-0.181668
C	1.829773	-1.238675	0.164609
C	2.702147	-0.155532	-0.017607
H	2.780325	1.972802	-0.324337
C	4.199117	-0.359275	-0.055190
H	-0.198463	-1.920601	0.307251
H	2.238005	-2.239111	0.295220
C	-1.659255	0.368179	0.080653
H	0.357960	2.297261	-0.299838
H	4.536871	-1.008915	0.760996
H	4.734632	0.592072	0.028851
H	4.515627	-0.832983	-0.994084
C	-2.287568	-0.670488	-0.838331
C	-2.129412	1.754040	-0.420411
C	-2.110782	0.200701	1.548219
C	-3.161203	-1.624834	-0.512673
H	-1.973252	-0.584044	-1.879872
H	-1.798905	1.946903	-1.447345
H	-1.753379	2.561925	0.217304

H	-3.223358	1.798273	-0.403519
H	-3.517700	-1.773807	0.502726
H	-3.557558	-2.301604	-1.265176
H	-1.828854	-0.778868	1.947285
H	-3.197815	0.310056	1.640385
H	-1.637541	0.964357	2.174582

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -466.888865594 Predicted Change= -4.168447D-10
Zero-point correction (ZPE)= -466.6424 0.24643
Internal Energy (U)= -466.6299 0.25893
Enthalpy (H)= -466.6289 0.25988
Gibbs Free Energy (G)= -466.6814 0.20742

Frequencies -- 35.7079 41.2865 87.3352

$\Delta G_{Solvation}$ = -0.00246640799997522

Appendix IV.

Computational Data for Chapter 5

Predicting Amorphous Metal Oxide Band Gaps
Rapid Band Gap Prediction of Amorphous Metal Oxides

1. RANDOMIZED CUBE SCRIPT:

This script needs an input file such as this:
atoms= In Ga Zn O
stoic= 1 1 1 4
cube= 5 5 5

This denotes an InGaZnO4 stoiciometry in a 5x5x5 cell.

Start of script:

```
---------------------------------------------------------------------------------------------
#!/bin/zsh
echo "Thank you for using Random-Atoms"
echo "The correct way to set up a run is this:"
echo "Random-Amorphous 'txt file' 'the number of outputs you want'"
echo "ie: Random-Atoms ZnSnSbO.txt 5"
echo "would make random xyz files with the atoms, stoiciometry, and cube size
enclosed in the said txt file and make five outputs"

if test -f $1
then
basedir=`pwd`
base=`basename $1 .txt`
txt=$1
totiteration=$2

if test -d $base
then
        echo "$base exists"
else
        mkdir $base
fi

cubexyz=(`grep "cube=" $txtlcut -d '=' -f2`)
cubex=$cubexyz[1]
cubey=$cubexyz[2]
cubez=$cubexyz[3]

cubexmath=`echo "$cubex - 1"lbc`
cubeymath=`echo "$cubey - 1"lbc`
cubezmath=`echo "$cubez - 1"lbc`

cubemath=`echo "$cubex * $cubey * $cubez"lbc`
cubeiteration=1
```

```
xcube=0
ycube=0
zcube=0

rm $base-cube.tmp
echo "Making the cube! Please be patient."

while [[ $cubeiteration -le $cubemath ]]
do
	echo "$xcube$ycube$zcube " >> $base-cube.tmp

	if [[ $xcube -lt $cubexmath ]]
	then
		xcube=`echo "$xcube + 1"|bc`
	else
		xcube=0
		if [[ $ycube -lt $cubeymath ]]
		then
			ycube=`echo "$ycube + 1"|bc`
		else
			ycube=0
			if [[ $zcube -lt $cubezmath ]]
			then
				zcube=`echo "$zcube + 1"|bc`
			else
				echo "This should be the end."
			fi
		fi
	fi
	cubeiteration=`echo "$cubeiteration + 1"|bc`
done


iterations=1

atoms=`grep "atoms=" $txt|cut -d '=' -f2`
stoic=`grep "stoic=" $txt|cut -d '=' -f2`
declare -a atomsarray
atomsarray=(`echo ${atoms//  / }`)
declare -a stoicarray
stoicarray=(`echo ${stoic//  / }`)
numatoms=${#atomsarray[*]}
```

```
if [[ $stoicarray[1] = "" ]]
then
	stoicarray[1]=0
fi
if [[ $stoicarray[2] = "" ]]
then
	stoicarray[2]=0
fi
if [[ $stoicarray[3] = "" ]]
then
	stoicarray[3]=0
fi
if [[ $stoicarray[4] = "" ]]
then
	stoicarray[4]=0
fi
if [[ $stoicarray[5] = "" ]]
then
	stoicarray[5]=0
fi
if [[ $stoicarray[6] = "" ]]
then
	stoicarray[6]=0
fi
if [[ $stoicarray[7] = "" ]]
then
	stoicarray[7]=0
fi
if [[ $stoicarray[8] = "" ]]
then
	stoicarray[8]=0
fi

stoicsum=`echo "$stoicarray[1] + $stoicarray[2] + $stoicarray[3] + $stoicarray[4] +
$stoicarray[5] + $stoicarray[6] + $stoicarray[7] + $stoicarray[8]"lbc`

xyzmath=`echo "$cubemath / $stoicsum"lbclcut -d '.' -f1`
xyznum=`echo "$xyzmath * $stoicsum"lbc`

stoicsum1=`echo "$stoicarray[1] * $xyzmath"lbc`
stoicsum2=`echo "$stoicarray[2] * $xyzmath"lbc`
stoicsum3=`echo "$stoicarray[3] * $xyzmath"lbc`
stoicsum4=`echo "$stoicarray[4] * $xyzmath"lbc`
stoicsum5=`echo "$stoicarray[5] * $xyzmath"lbc`
```

```
stoicsum6=`echo "$stoicarray[6] * $xyzmath"lbc`
stoicsum7=`echo "$stoicarray[7] * $xyzmath"lbc`
stoicsum8=`echo "$stoicarray[8] * $xyzmath"lbc`

echo
"++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++"
echo "Running Randome-Amorphous $txt $totiteration $xyznum"
echo
"++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++"
echo "Atom to change to is: $atomsarray[@]"
echo "Stoichiometry is: $stoicarray[@]"
echo "Nuber of atoms is: $numatoms"
echo "Your job is running please be patient."

while [[ $iterations -le $totiteration ]]
do
echo "Running iteration $iterations."
var=(`cat $base-cube.tmp`)

        echo $xyznum > $base.xyz
        echo $base >> $base.xyz


        count=1
        while [[ $count -le $stoicsum1 ]]
        do
                numvar=${#var[*]}
                NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
                echo "$atomsarray[1] $var[$NUMBER1]" >> $base.xyz
                var[$NUMBER1]=()
                count=`echo "$count + 1"lbc`
        done

        count=1
        while [[ $count -le $stoicsum2 ]]
        do
                numvar=${#var[*]}
                NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
                echo "$atomsarray[2] $var[$NUMBER1]" >> $base.xyz
                var[$NUMBER1]=()
                count=`echo "$count + 1"lbc`
        done
```

```
count=1
while [[ $count -le $stoicsum3 ]]
do
	numvar=${#var[*]}
	NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
	echo "$atomsarray[3] $var[$NUMBER1]" >> $base.xyz
	var[$NUMBER1]=()
	count=`echo "$count + 1"|bc`
done

count=1
while [[ $count -le $stoicsum4 ]]
do
	numvar=${#var[*]}
	NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
	echo "$atomsarray[4] $var[$NUMBER1]" >> $base.xyz
	var[$NUMBER1]=()
	count=`echo "$count + 1"|bc`
done

count=1
while [[ $count -le $stoicsum5 ]]
do
	numvar=${#var[*]}
	NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
	echo "$atomsarray[5] $var[$NUMBER1]" >> $base.xyz
	var[$NUMBER1]=()
	count=`echo "$count + 1"|bc`
done

count=1
while [[ $count -le $stoicsum6 ]]
do
	numvar=${#var[*]}
	NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
	echo "$atomsarray[6] $var[$NUMBER1]" >> $base.xyz
	var[$NUMBER1]=()
	count=`echo "$count + 1"|bc`
done

count=1
while [[ $count -le $stoicsum7 ]]
do
```

```
        numvar=${#var[*]}
        NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
        echo "$atomsarray[7] $var[$NUMBER1]" >> $base.xyz
        var[$NUMBER1]=()
        count=`echo "$count + 1"|bc`
    done

    count=1
    while [[ $count -le $stoicsum8 ]]
    do
        numvar=${#var[*]}
        NUMBER1=$[ ( $RANDOM % $numvar )  + 1 ]
        echo "$atomsarray[8] $var[$NUMBER1]" >> $base.xyz
        var[$NUMBER1]=()
        count=`echo "$count + 1"|bc`
    done



    count=1
    while [[ $count -le $xyznum ]]
    do
        xyz=`tail -n$count $base.xyz|head -n1|cut -d ' ' -f2`
        xmath=`echo "$xyz[1] * 3"|bc`
        ymath=`echo "$xyz[2] * 3"|bc`
        zmath=`echo "$xyz[3] * 3"|bc`
        sed 's/ '$xyz'/ '$xmath'.0 '$ymath'.0 '$zmath'.0/' $base.xyz > $base.tmp
        mv $base.tmp $base.xyz
        count=`echo "$count + 1"|bc`
    done

mv $base.xyz $base/$base-$iterations.xyz
iterations=`echo "$iterations + 1"|bc`

done
rm $base-cube.tmp
else
    echo "Your txt file does not exist!"
    echo "One is being made for you and is named random.txt"
    echo "atoms= Zn Sn Sb O" > random.txt
    echo "stoic= 3 1 2 2" >> random.txt
    echo "cube= 5 5 5" >> random.txt

fi
```

2. FORCE FIELD PERAMETERS FOR GULP MD AND ANEALING

All of these parameters are based on a set created by Pedone et al.[1]

```
#Charges
species
zn 1.2
al 1.8
si 2.4
sn 2.4
o -1.2
sb 1.8
ga 1.8
in 1.8


#Morse potentials
morse
zn core o core 0.001221 2.347100 3.167030 0.0000  0.000 15.000 0 0 0
al core o core 0.361581 1.900442 2.164818 0.0000 0.000 15.000 0 0 0
si core o core 0.340554 2.006700 2.100000 0.0000 0.000 15.000 0 0 0
sn core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
o core o core 0.042395 1.379316 3.618701 0.0000 0.000 15.000 0 0 0
sb core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
ga core o core 0.038263 2.105200 2.668100 0.0000 0.000 15.000 0 0 0
in core o core .72974993E-01 1.9342 2.82499 0.0000 0.000 15.000 0 0 0


#lennard potentials
lennard 12 6
zn   core o     core 1.0  0.0  0.0  15.0 0 0
al   core o     core 0.9  0.0  0.0  15.0 0 0
si   core o     core 1.0  0.0  0.0  15.0 0 0
sn   core o     core 3.0  0.0  0.0  15.0 0 0
o   core o     core 22.0  0.0  0.0  15.0 0 0
sb   core o     core 3.0  0.0  0.0  15.0 0 0
ga   core o     core 0.9  0.0  0.0  15.0 0 0
in   core o     core 3.0  0.0  0.0  15.0 0 0
```

3. EXPLANATION OF HOW THE CEDAR BAND GAP METHOD IS COMPUTED:

Using this equation to calculate the fundamental gap energy (E_{FG}):

$$E_{FG} = E(N_0+n) + E(N_0-n) - 2E(N_0)$$

Where:

N_0 is the valence electrons
N the saturation parameter
$n = N_0/N$

For this study we used N = 63.

Example:
For ZnO in the 555 cell and N = 63.

$N_0 = 1116$
$n = 17.7143$

You must run three calculations where the charge is at 0, -17.7143, and +17.7143. Using the equation above:

$E_{FG} = E(N_0+n) + E(N_0-n) - 2E(N_0)$

$E(N_0) = -11084.04272342$ Ry

$E(N_0+n) = -11093.32117843$ Ry

$E(N_0-n) = -11069.48047842$ Ry

$E_{FG} = -11093.32117843$ Ry + -11069.48047842 Ry – 2(-11084.04272342 Ry)

$E_{FG} = 5.28378998999688$ Ry

13.605698066 Ry = 1eV

$E_{FG} = 4.06$eV

4. AN EXAMPLE MC INPUT FILE FOR GULP

```
montecarlo conv
cell
12.2 12.2 12.2 90 90 90
cartesian
##########GEOM DATA##########
#Charges
species
zn 1.2
al 1.8
si 2.4
sn 2.4
o -1.2
sb 1.8
ga 1.8
in 1.8
#Morse potentials
morse
zn core o core 0.001221 2.347100 3.167030 0.0000  0.000 15.000 0 0 0
al core o core 0.361581 1.900442 2.164818 0.0000 0.000 15.000 0 0 0
si core o core 0.340554 2.006700 2.100000 0.0000 0.000 15.000 0 0 0
sn core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
o core o core 0.042395 1.379316 3.618701 0.0000 0.000 15.000 0 0 0
sb core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
ga core o core 0.038263 2.105200 2.668100 0.0000 0.000 15.000 0 0 0
in core o core .72974993E-01 1.9342 2.82499 0.0000 0.000 15.000 0 0 0
#lennard potentials
lennard 12 6
zn   core o     core 1.0  0.0  0.0  15.0 0 0
al   core o     core 0.9  0.0  0.0  15.0 0 0
si   core o     core 1.0  0.0  0.0  15.0 0 0
sn   core o     core 3.0  0.0  0.0  15.0 0 0
o   core o     core 22.0  0.0  0.0  15.0 0 0
sb   core o     core 3.0  0.0  0.0  15.0 0 0
ga   core o     core 0.9  0.0  0.0  15.0 0 0
in   core o     core 3.0  0.0  0.0  15.0 0 0
temperature 4000
mcsample 10000 IGZO-XXX-X.gmc
mcmaxdisplacement 0.1 0.2 10
mctrial 4000000
output cif IGZO-XXX-X.cif
dump IGZO-XXX-X.frs
```

5. AN EXAMPLE MD ANEELING INPUT FILE FOR GULP

```
md conv conse
cell
12.2000 12.2000 12.2000 90.0000 90.0000 90.0000
fractional
##########GEOM DATA##########
#Charges
species
zn 1.2
al 1.8
si 2.4
sn 2.4
o -1.2
sb 1.8
ga 1.8
in 1.8
#Morse potentials
morse
zn core o core 0.001221 2.347100 3.167030 0.0000  0.000 15.000 0 0 0
al core o core 0.361581 1.900442 2.164818 0.0000 0.000 15.000 0 0 0
si core o core 0.340554 2.006700 2.100000 0.0000 0.000 15.000 0 0 0
sn core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
o core o core 0.042395 1.379316 3.618701 0.0000 0.000 15.000 0 0 0
sb core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
ga core o core 0.038263 2.105200 2.668100 0.0000 0.000 15.000 0 0 0
in core o core .72974993E-01 1.9342 2.82499 0.0000 0.000 15.000 0 0 0
#lennard potentials
lennard 12 6
zn   core o     core 1.0  0.0  0.0  15.0 0 0
al   core o     core 0.9  0.0  0.0  15.0 0 0
si   core o     core 1.0  0.0  0.0  15.0 0 0
sn   core o     core 3.0  0.0  0.0  15.0 0 0
o   core o     core 22.0  0.0  0.0  15.0 0 0
sb   core o     core 3.0  0.0  0.0  15.0 0 0
ga   core o     core 0.9  0.0  0.0  15.0 0 0
in   core o     core 3.0  0.0  0.0  15.0 0 0
temperature 4000 -0.01 1000 100
ensemble nvt
tau_thermostat  0.1 ps
tau_barostat  0.1 p
pressure 0.000000 GPa
write 100
sample 10
timestep 1 fs
```

```
equilibration 0.1 ps
production 1 ps
output cif IGZO-001-1.cif
dump IGZO-001-1.frs
```

6. AN EXAMPLE MD EQUILIBRATION INPUT FILE FOR GULP

```
md conv conse
cell
11.1166 11.1166 11.1166 90.0000 90.0000 90.0000
fractional
##########GEOM DATA##########
#Charges
species
zn 1.2
al 1.8
si 2.4
sn 2.4
o -1.2
sb 1.8
ga 1.8
in 1.8
#Morse potentials
morse
zn core o core 0.001221 2.347100 3.167030 0.0000  0.000 15.000 0 0 0
al core o core 0.361581 1.900442 2.164818 0.0000 0.000 15.000 0 0 0
si core o core 0.340554 2.006700 2.100000 0.0000 0.000 15.000 0 0 0
sn core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
o core o core 0.042395 1.379316 3.618701 0.0000 0.000 15.000 0 0 0
sb core o core 0.079400 2.156770 2.633076 0.0000 0.000 15.000 0 0 0
ga core o core 0.038263 2.105200 2.668100 0.0000 0.000 15.000 0 0 0
in core o core .72974993E-01 1.9342 2.82499 0.0000 0.000 15.000 0 0 0
#lennard potentials
lennard 12 6
zn   core o     core 1.0  0.0  0.0  15.0 0 0
al   core o     core 0.9  0.0  0.0  15.0 0 0
si   core o     core 1.0  0.0  0.0  15.0 0 0
sn   core o     core 3.0  0.0  0.0  15.0 0 0
o   core o     core 22.0  0.0  0.0  15.0 0 0
sb   core o     core 3.0  0.0  0.0  15.0 0 0
ga   core o     core 0.9  0.0  0.0  15.0 0 0
in   core o     core 3.0  0.0  0.0  15.0 0 0
temperature 300
ensemble nvt
tau_thermostat  0.1 ps
tau_barostat  0.1 p
pressure 0.000000 GPa
write 100
sample 10
timestep 1 fs
```

```
equilibration 0.1 ps
production 500 ps
output cif IGZO-001-1.cif
dump IGZO-001-1.frs
```

7. SINGLE POINT ENERGIES AND TEMPLATE INPUT FILE OF THE 555 CELLS FOR: ZNO, GA_2O_3, IN_2O_3, GA_2ZNO_4, $GA_2ZN_8O_{11}$, IN_2ZNO_4, $INGAZNO_4$, AND $INGAO_3$

IGZO-001-1-1

Analyzing GULP Output File for Supporting Information: IGZO-001-1-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.7143 SCF Energy = -11069.48047842 Ry
Charge = 0.0000 SCF Energy = -11084.04272342 Ry
Charge = 17.7143 SCF Energy = -11093.32117843 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-001-1-1"  ,
        title = "IGZO-001-1-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1166 ,
        B = 11.1166 ,
        C = 11.1166 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 124  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
```

```
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1166  0.  0.
  6.8069543E-16  11.1166  0.
  6.8069543E-16  6.8069543E-16  11.1166
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Zn 0.32775 0.20904 0.11361
Zn 0.06360 0.83180 0.85404
Zn 0.47841 0.18216 0.53247
Zn 0.57609 0.24073 0.26088
Zn 0.56127 0.65896 0.67955
Zn 0.91067 0.88888 0.02247
Zn 0.02081 0.61776 0.67391
Zn 0.33288 0.79633 0.69853
Zn 0.24026 0.46903 0.05322
Zn 0.00010 0.57999 0.95249
Zn 0.29850 0.74840 0.98092
Zn 0.56291 0.90981 0.61266
Zn 0.41850 0.48826 0.62368
Zn 0.08540 0.38548 0.73688
Zn 0.83282 0.18157 0.10750
Zn 0.74645 0.99492 0.89158
Zn 0.00970 0.44840 0.48312
Zn 0.24469 0.86447 0.42239
Zn 0.25905 0.54563 0.79900
Zn 0.07575 0.25386 0.26456
Zn 0.07171 0.52798 0.21716
Zn 0.58007 0.28021 0.00113
Zn 0.33056 0.41026 0.31934
Zn 0.75274 0.07900 0.64293
Zn 0.79256 0.34663 0.59856
Zn 0.57307 0.34832 0.75610
Zn 0.07139 0.90597 0.59747
Zn 0.48339 0.09175 0.79247
Zn 0.73443 0.58749 0.52310
Zn 0.51859 0.98855 0.35180
Zn 0.75139 0.93143 0.20261
```

Zn 0.52363 0.01903 0.06524
Zn 0.99101 0.71402 0.41634
Zn 0.24098 0.12502 0.37082
Zn 0.01212 0.16755 0.52682
Zn 0.55975 0.50972 0.19342
Zn 0.25397 0.32397 0.56375
Zn 0.07158 0.30562 0.00469
Zn 0.32134 0.27206 0.85505
Zn 0.24325 0.99584 0.91092
Zn 0.74472 0.44889 0.03525
Zn 0.81078 0.39713 0.29337
Zn 0.25041 0.06437 0.63987
Zn 0.56743 0.76967 0.12877
Zn 0.82822 0.81020 0.71794
Zn 0.51979 0.84477 0.89432
Zn 0.06505 0.05373 0.07527
Zn 0.49643 0.70625 0.39908
Zn 0.78715 0.52739 0.75684
Zn 0.30992 0.92394 0.16413
Zn 0.32476 0.66865 0.24418
Zn 0.83267 0.26987 0.86009
Zn 0.07161 0.77080 0.14432
Zn 0.82902 0.66133 0.24903
Zn 0.57370 0.43524 0.45517
Zn 0.75399 0.71403 0.96919
Zn 0.74249 0.86063 0.45115
Zn 0.98801 0.97026 0.32988
Zn 0.99351 0.11478 0.79222
Zn 0.50612 0.55983 0.92720
Zn 0.75836 0.14751 0.38874
Zn 0.24441 0.60805 0.51582
O 0.25230 0.82901 0.84764
O 0.24898 0.05951 0.06762
O 0.57902 0.00750 0.90326
O 0.00028 0.19859 0.10719
O 0.30807 0.62532 0.66465
O 0.58575 0.93450 0.20103
O 0.05931 0.46110 0.05472
O 0.99234 0.66366 0.25224
O 0.77284 0.77784 0.13613
O 0.75459 0.23705 0.24700
O 0.26432 0.37381 0.73556
O 0.73729 0.35652 0.75387
O 0.06360 0.86254 0.43522

O 0.31608 0.70681 0.40505
O 0.49839 0.80700 0.72495
O 0.24276 0.25126 0.25502
O 0.49461 0.65594 0.23836
O 0.07277 0.11404 0.37327
O 0.31333 0.17287 0.52073
O 0.55648 0.07311 0.64048
O 0.05614 0.99585 0.91548
O 0.07002 0.05769 0.64706
O 0.57390 0.13597 0.39211
O 0.01945 0.74601 0.98547
O 0.49697 0.39876 0.30357
O 0.33359 0.98262 0.32496
O 0.81468 0.70309 0.42265
O 0.74984 0.42885 0.45727
O 0.55305 0.59597 0.51193
O 0.42280 0.86272 0.02989
O 0.23273 0.77676 0.14646
O 0.49432 0.26009 0.85561
O 0.58524 0.69762 0.96968
O 0.72682 0.65828 0.68749
O 0.30376 0.09638 0.80239
O 0.82427 0.55408 0.92573
O 0.49277 0.18097 0.12116
O 0.53098 0.34085 0.58355
O 0.01544 0.27262 0.84633
O 0.00915 0.92515 0.16433
O 0.82103 0.10778 0.79175
O 0.75256 0.91857 0.61113
O 0.81162 0.84956 0.87967
O 0.09196 0.54664 0.80911
O 0.26283 0.90539 0.58140
O 0.25234 0.31117 0.00244
O 0.08282 0.31602 0.57224
O 0.91337 0.48258 0.64167
O 0.31704 0.44335 0.47866
O 0.79262 0.02607 0.06199
O 0.81327 0.98095 0.35606
O 0.56760 0.44246 0.04049
O 0.07579 0.60316 0.50842
O 0.56682 0.85332 0.44751
O 0.75010 0.51594 0.20044
O 0.51705 0.51105 0.76423
O 0.84169 0.18833 0.53969

O 0.00047 0.78654 0.69216
O 0.99115 0.39725 0.32209
O 0.75893 0.28360 0.99839
O 0.24875 0.51963 0.20669
O 0.32872 0.58015 0.95126
K_POINTS gamma

IGZO-001-1-2

Analyzing GULP Output File for Supporting Information: IGZO-001-1-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.7143 SCF Energy = -11069.28833268 Ry
Charge = 0.0000 SCF Energy = -11083.86669571 Ry
Charge = 17.7143 SCF Energy = -11093.17340604 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-001-1-2"  ,
        title = "IGZO-001-1-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1166 ,
        B = 11.1166 ,
        C = 11.1166 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 124  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1166  0.  0.
  6.8069543E-16  11.1166  0.
  6.8069543E-16  6.8069543E-16  11.1166
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Zn 0.83104 0.99715 0.18658
Zn 0.23071 0.57344 0.15713
Zn 0.71449 0.16936 0.56756
Zn 0.17339 0.24980 0.84282
Zn 0.74340 0.37923 0.35618
Zn 0.23313 0.76932 0.96425
Zn 0.66957 0.50784 0.87408
Zn 0.97716 0.27414 0.67515
Zn 0.91784 0.55581 0.73710
Zn 0.98497 0.62146 0.01192
Zn 0.64164 0.96745 0.75817
Zn 0.41315 0.74639 0.53958
Zn 0.74958 0.29801 0.08525
Zn 0.49240 0.41905 0.20990
Zn 0.43561 0.88461 0.08767
Zn 0.65702 0.64537 0.42368
Zn 0.74934 0.90392 0.47679
Zn 0.65770 0.03529 0.02276
Zn 0.73740 0.44711 0.61654
Zn 0.92497 0.22120 0.39307
Zn 0.40700 0.21963 0.41521
Zn 0.14752 0.51107 0.88916
Zn 0.71120 0.24095 0.80708
Zn 0.75181 0.55936 0.14486
Zn 0.97924 0.96417 0.35794
Zn 0.96668 0.03867 0.62272
Zn 0.39764 0.81183 0.79276
Zn 0.99829 0.47960 0.47200
Zn 0.48594 0.01594 0.58666
Zn 0.98780 0.89748 0.04367
Zn 0.43940 0.94661 0.31730
Zn 0.49521 0.48484 0.47444
Zn 0.42980 0.55923 0.74261
Zn 0.47046 0.08655 0.87458
```

Zn 0.41582 0.36554 0.93391
Zn 0.32918 0.14606 0.70965
Zn 0.19136 0.08689 0.27382
Zn 0.66816 0.72316 0.70003
Zn 0.16760 0.96017 0.77453
Zn 0.25556 0.43895 0.61626
Zn 0.65977 0.83105 0.21630
Zn 0.92170 0.10774 0.85592
Zn 0.23719 0.03048 0.03589
Zn 0.16308 0.70031 0.69439
Zn 0.49858 0.30524 0.66967
Zn 0.73676 0.78222 0.95582
Zn 0.41959 0.67593 0.27869
Zn 0.49112 0.62780 0.00037
Zn 0.23084 0.90187 0.50098
Zn 0.15930 0.65648 0.41932
Zn 0.99426 0.17447 0.12510
Zn 0.25360 0.30468 0.10110
Zn 0.18382 0.85708 0.21859
Zn 0.89684 0.70065 0.26615
Zn 0.00130 0.42595 0.21716
Zn 0.48922 0.15741 0.14708
Zn 0.92567 0.36183 0.94091
Zn 0.67635 0.10969 0.30386
Zn 0.24973 0.38100 0.35299
Zn 0.91579 0.75386 0.53695
Zn 0.18512 0.17166 0.53654
Zn 0.93271 0.81749 0.79338
O 0.69489 0.14935 0.14717
O 0.73214 0.74334 0.52951
O 0.65891 0.01217 0.58741
O 0.42785 0.37363 0.35563
O 0.72537 0.56065 0.74089
O 0.84310 0.15609 0.70289
O 0.92646 0.76919 0.95352
O 0.15926 0.88468 0.05578
O 0.23687 0.36872 0.93741
O 0.66453 0.47410 0.47101
O 0.44708 0.24317 0.81907
O 0.92354 0.32506 0.10009
O 0.98724 0.70886 0.68511
O 0.98590 0.66123 0.41777
O 0.49678 0.82482 0.22472
O 0.17874 0.47821 0.46584

O 0.68142 0.63221 0.00285
O 0.49521 0.11993 0.30833
O 0.71451 0.95115 0.32415
O 0.92718 0.58182 0.16001
O 0.74906 0.21779 0.40729
O 0.65873 0.08830 0.86757
O 0.24087 0.20913 0.38746
O 0.43993 0.17434 0.57823
O 0.42121 0.77568 0.96274
O 0.17524 0.42801 0.21017
O 0.67060 0.41700 0.20048
O 0.20762 0.27923 0.66306
O 0.21165 0.02554 0.62262
O 0.92652 0.43842 0.62041
O 0.46766 0.96995 0.75865
O 0.91727 0.92843 0.50542
O 0.48353 0.03916 0.02373
O 0.94780 0.85783 0.21862
O 0.92806 0.38815 0.36009
O 0.22733 0.55152 0.74044
O 0.49342 0.50334 0.88147
O 0.31435 0.98417 0.19107
O 0.00586 0.26062 0.85083
O 0.48479 0.64492 0.43198
O 0.22635 0.81258 0.80403
O 0.01715 0.17915 0.53759
O 0.24284 0.08598 0.87027
O 0.16632 0.62609 0.01344
O 0.65758 0.30485 0.65972
O 0.15864 0.16524 0.12316
O 0.24232 0.70476 0.27904
O 0.97555 0.51076 0.88142
O 0.94073 0.10568 0.27480
O 0.74899 0.35214 0.92471
O 0.91953 0.06005 0.01843
O 0.00343 0.96976 0.76992
O 0.41330 0.56827 0.14986
O 0.14132 0.94206 0.37087
O 0.23824 0.74648 0.54794
O 0.42292 0.90651 0.47965
O 0.42551 0.45552 0.61344
O 0.72820 0.67836 0.27410
O 0.73255 0.83518 0.79721
O 0.42207 0.29682 0.09320

O 0.48114 0.70862 0.69845
O 0.71377 0.89074 0.07876
K_POINTS gamma

IGZO-001-1-3

Analyzing GULP Output File for Supporting Information: IGZO-001-1-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.7143 SCF Energy = -11069.24962186 Ry
Charge = 0.0000 SCF Energy = -11083.82492689 Ry
Charge = 17.7143 SCF Energy = -11093.11763317 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-001-1-3"  ,
        title = "IGZO-001-1-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1166 ,
        B = 11.1166 ,
        C = 11.1166 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 124  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1166  0.  0.
  6.8069543E-16  11.1166  0.
  6.8069543E-16  6.8069543E-16  11.1166
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Zn 0.39796 0.69032 0.49318
Zn 0.81998 0.67905 0.49097
Zn 0.29656 0.56977 0.95474
Zn 0.89785 0.93981 0.57062
Zn 0.65608 0.92788 0.71369
Zn 0.88606 0.30532 0.90722
Zn 0.55523 0.57132 0.36454
Zn 0.13904 0.86330 0.44123
Zn 0.83045 0.75815 0.75585
Zn 0.13180 0.34018 0.32919
Zn 0.63877 0.26197 0.04855
Zn 0.39486 0.31060 0.89513
Zn 0.88366 0.87751 0.28253
Zn 0.08171 0.04571 0.26689
Zn 0.55549 0.69826 0.89716
Zn 0.64629 0.96314 0.96184
Zn 0.06898 0.18844 0.77761
Zn 0.37530 0.36999 0.15832
Zn 0.22482 0.53571 0.53097
Zn 0.06371 0.60327 0.37483
Zn 0.14008 0.78553 0.18115
Zn 0.80119 0.56840 0.96909
Zn 0.40131 0.83023 0.03469
Zn 0.57552 0.13979 0.50410
Zn 0.14623 0.98378 0.98304
Zn 0.64285 0.43685 0.83893
Zn 0.89100 0.36710 0.17193
Zn 0.64393 0.78776 0.18651
Zn 0.89701 0.17825 0.36061
Zn 0.56521 0.18600 0.77243
Zn 0.90321 0.02080 0.84311
Zn 0.62575 0.62507 0.63684
Zn 0.30885 0.75149 0.76196
Zn 0.82110 0.20951 0.63203
```

Zn 0.06417 0.71313 0.91643
Zn 0.13097 0.45008 0.84224
Zn 0.39935 0.96868 0.55887
Zn 0.32193 0.10910 0.09299
Zn 0.64239 0.40325 0.58290
Zn 0.05017 0.51212 0.10138
Zn 0.80576 0.09472 0.10173
Zn 0.08007 0.66179 0.64487
Zn 0.73254 0.00022 0.41132
Zn 0.80646 0.61282 0.22516
Zn 0.15272 0.93019 0.72113
Zn 0.11201 0.09085 0.50794
Zn 0.88702 0.82750 0.02295
Zn 0.38917 0.40425 0.43006
Zn 0.64126 0.31058 0.30617
Zn 0.13560 0.26013 0.05737
Zn 0.39732 0.02011 0.82054
Zn 0.31905 0.23428 0.63457
Zn 0.85427 0.43208 0.43017
Zn 0.57131 0.04856 0.22493
Zn 0.30478 0.61955 0.22602
Zn 0.87411 0.48526 0.67541
Zn 0.33343 0.15169 0.35345
Zn 0.38420 0.49072 0.70227
Zn 0.57919 0.84217 0.43861
Zn 0.55988 0.51914 0.10696
Zn 0.36466 0.91129 0.28996
Zn 0.08508 0.34848 0.57787
O 0.38039 0.56518 0.37488
O 0.31942 0.93109 0.70029
O 0.08081 0.48909 0.68444
O 0.64552 0.74400 0.75440
O 0.14893 0.69504 0.48836
O 0.91042 0.68332 0.63581
O 0.90345 0.34537 0.57274
O 0.14103 0.75409 0.77150
O 0.81052 0.84721 0.43980
O 0.07123 0.30500 0.90126
O 0.81472 0.77402 0.17517
O 0.22588 0.00837 0.38252
O 0.30270 0.31781 0.31188
O 0.38216 0.53678 0.10808
O 0.89283 0.59486 0.36806
O 0.81403 0.44421 0.83144

O 0.56718 0.29608 0.90496
O 0.60114 0.90803 0.29119
O 0.32712 0.97295 0.97075
O 0.40397 0.05443 0.23013
O 0.11846 0.56021 0.96726
O 0.37944 0.70536 0.89977
O 0.56944 0.40979 0.43314
O 0.12728 0.61951 0.22264
O 0.56927 0.00771 0.82165
O 0.82495 0.93160 0.71673
O 0.64239 0.60811 0.24333
O 0.07123 0.83476 0.04072
O 0.82090 0.32461 0.31398
O 0.63557 0.56056 0.96850
O 0.39990 0.18730 0.77185
O 0.64124 0.14772 0.35654
O 0.55868 0.35234 0.16205
O 0.64670 0.23678 0.63638
O 0.14378 0.20167 0.62804
O 0.08404 0.02846 0.83667
O 0.34527 0.63456 0.63440
O 0.40235 0.14666 0.51185
O 0.05900 0.18777 0.37416
O 0.14940 0.09610 0.11325
O 0.32434 0.26850 0.04678
O 0.04839 0.87376 0.29763
O 0.87692 0.51819 0.10383
O 0.32589 0.78814 0.18813
O 0.86955 0.04330 0.25126
O 0.81701 0.26369 0.05364
O 0.31205 0.39302 0.57616
O 0.88095 0.17768 0.78399
O 0.57283 0.68731 0.49530
O 0.10049 0.45311 0.43975
O 0.84878 0.09052 0.50507
O 0.63631 0.08683 0.08136
O 0.57468 0.81972 0.02824
O 0.74800 0.53481 0.56934
O 0.82490 0.97488 0.97545
O 0.06953 0.36229 0.16839
O 0.07421 0.94808 0.57263
O 0.31508 0.44500 0.84338
O 0.59640 0.97629 0.55301
O 0.40343 0.85026 0.44350

O 0.55213 0.47700 0.71292
O 0.88610 0.70588 0.91129
K_POINTS gamma

IGZO-001-1-4

Analyzing GULP Output File for Supporting Information: IGZO-001-1-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.7143 SCF Energy = -11069.43623104 Ry
Charge = 0.0000 SCF Energy = -11083.97527108 Ry
Charge = 17.7143 SCF Energy = -11093.25838719 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-001-1-4"  ,
        title = "IGZO-001-1-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1166 ,
        B = 11.1166 ,
        C = 11.1166 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 124  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1166  0.  0.
  6.8069543E-16  11.1166  0.
  6.8069543E-16  6.8069543E-16  11.1166
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Zn 0.90071 0.45275 0.30576
Zn 0.54851 0.69620 0.48153
Zn 0.84885 0.02156 0.39052
Zn 0.08120 0.80750 0.94757
Zn 0.92641 0.29908 0.95358
Zn 0.97661 0.13367 0.71446
Zn 0.94962 0.27632 0.46832
Zn 0.50761 0.24745 0.22811
Zn 0.40289 0.16206 0.97024
Zn 0.20236 0.36462 0.91179
Zn 0.61457 0.95197 0.47474
Zn 0.24630 0.17155 0.22053
Zn 0.76333 0.31717 0.16044
Zn 0.31236 0.88620 0.89726
Zn 0.71250 0.06374 0.13253
Zn 0.71668 0.48788 0.45814
Zn 0.12493 0.09475 0.94966
Zn 0.20273 0.35867 0.37641
Zn 0.47781 0.43327 0.47645
Zn 0.90084 0.88378 0.14987
Zn 0.39953 0.15969 0.47926
Zn 0.30100 0.47360 0.64010
Zn 0.98941 0.53561 0.91062
Zn 0.66239 0.21988 0.90067
Zn 0.65626 0.80986 0.72983
Zn 0.48209 0.42635 0.97927
Zn 0.78975 0.34158 0.68769
Zn 0.72004 0.07741 0.65073
Zn 0.58722 0.53013 0.72552
Zn 0.97210 0.14811 0.23033
Zn 0.57304 0.52674 0.23638
Zn 0.84314 0.60780 0.63679
Zn 0.32114 0.46117 0.15072
Zn 0.29850 0.60679 0.39261
```

Zn 0.86175 0.01845 0.90361
Zn 0.17161 0.93789 0.71024
Zn 0.83912 0.60978 0.13898
Zn 0.44637 0.00453 0.72191
Zn 0.81145 0.76225 0.38586
Zn 0.22512 0.78070 0.54106
Zn 0.06293 0.41085 0.15323
Zn 0.50390 0.27557 0.72859
Zn 0.24389 0.19884 0.73714
Zn 0.16835 0.91865 0.15233
Zn 0.03232 0.40668 0.68213
Zn 0.05202 0.83641 0.40499
Zn 0.54697 0.68331 0.95834
Zn 0.24898 0.63481 0.95601
Zn 0.11160 0.65638 0.71399
Zn 0.92247 0.86820 0.63938
Zn 0.81160 0.76827 0.89406
Zn 0.58484 0.95858 0.97213
Zn 0.11978 0.67435 0.22503
Zn 0.39651 0.72734 0.72181
Zn 0.34389 0.89450 0.38736
Zn 0.36412 0.73512 0.15220
Zn 0.13144 0.08175 0.46863
Zn 0.63292 0.79359 0.21364
Zn 0.46034 0.99857 0.22208
Zn 0.67525 0.21778 0.39396
Zn 0.01776 0.56157 0.46707
Zn 0.76152 0.48005 0.92557
O 0.72798 0.48594 0.62597
O 0.60764 0.95616 0.65422
O 0.58900 0.94645 0.14125
O 0.74063 0.48775 0.20171
O 0.38137 0.74467 0.45086
O 0.40536 0.14365 0.15219
O 0.24415 0.19638 0.90541
O 0.32636 0.88230 0.69543
O 0.00013 0.56195 0.20030
O 0.19219 0.75619 0.06618
O 0.89459 0.87375 0.46829
O 0.04731 0.84193 0.23775
O 0.76393 0.31960 0.99386
O 0.29867 0.45756 0.46049
O 0.48409 0.41260 0.15114
O 0.13456 0.09554 0.65744

O 0.28725 0.60222 0.21645
O 0.85372 0.03203 0.20864
O 0.18968 0.37543 0.73017
O 0.24826 0.17679 0.39241
O 0.46346 0.43149 0.64814
O 0.66229 0.19872 0.22103
O 0.43629 0.01295 0.90297
O 0.16068 0.94058 0.88221
O 0.00533 0.56086 0.63291
O 0.53242 0.68874 0.13819
O 0.92346 0.88486 0.98094
O 0.93660 0.26844 0.63443
O 0.56582 0.54369 0.40022
O 0.08023 0.81786 0.64971
O 0.09942 0.64559 0.87474
O 0.79912 0.33820 0.40845
O 0.33795 0.88214 0.22219
O 0.41003 0.16335 0.65836
O 0.04639 0.40718 0.40692
O 0.32243 0.47658 0.97349
O 0.13086 0.07986 0.13295
O 0.38460 0.73528 0.91150
O 0.64889 0.80756 0.90907
O 0.18703 0.92669 0.45302
O 0.67066 0.22373 0.71987
O 0.84789 0.61546 0.96909
O 0.80427 0.76678 0.20698
O 0.71856 0.07783 0.47289
O 0.06118 0.40265 0.98660
O 0.13303 0.67328 0.41491
O 0.50647 0.28295 0.40713
O 0.86006 0.01490 0.72063
O 0.70682 0.06649 0.95976
O 0.19959 0.34129 0.20301
O 0.92611 0.30504 0.19900
O 0.59433 0.53303 0.89041
O 0.26944 0.63572 0.66749
O 0.97348 0.15282 0.89845
O 0.98133 0.12120 0.39803
O 0.50177 0.27601 0.89904
O 0.64295 0.79864 0.40334
O 0.55163 0.69461 0.67298
O 0.82397 0.74621 0.72312
O 0.85226 0.60299 0.44121

O 0.88835 0.42989 0.81599
O 0.46326 0.01882 0.40171
K_POINTS gamma

IGZO-001-1-5

Analyzing GULP Output File for Supporting Information: IGZO-001-1-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.7143 SCF Energy = -11069.28087171 Ry
Charge = 0.0000 SCF Energy = -11083.84356598 Ry
Charge = 17.7143 SCF Energy = -11093.14321538 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-001-1-5"  ,
        title = "IGZO-001-1-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1166 ,
        B = 11.1166 ,
        C = 11.1166 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 124  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1166  0.  0.
  6.8069543E-16  11.1166  0.
  6.8069543E-16  6.8069543E-16  11.1166
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Zn 0.97299 0.29488 0.12605
Zn 0.14244 0.99690 0.50682
Zn 0.02319 0.53547 0.98665
Zn 0.93273 0.57422 0.72484
Zn 0.62466 0.74126 0.79922
Zn 0.55454 0.08626 0.11744
Zn 0.52927 0.56922 0.12025
Zn 0.35038 0.80687 0.72419
Zn 0.80841 0.24710 0.59578
Zn 0.75819 0.55541 0.91575
Zn 0.54816 0.83237 0.52547
Zn 0.39741 0.57990 0.58611
Zn 0.80555 0.73971 0.59274
Zn 0.96613 0.07093 0.97312
Zn 0.67028 0.99043 0.63631
Zn 0.06223 0.07459 0.25125
Zn 0.27985 0.04580 0.04302
Zn 0.01727 0.30942 0.40048
Zn 0.29091 0.23560 0.45011
Zn 0.14123 0.48502 0.51082
Zn 0.75140 0.73419 0.32199
Zn 0.49145 0.83215 0.27032
Zn 0.42769 0.57225 0.84952
Zn 0.72033 0.25199 0.06747
Zn 0.86526 0.50589 0.45244
Zn 0.74730 0.24869 0.33767
Zn 0.58976 0.07810 0.37673
Zn 0.79128 0.49864 0.18680
Zn 0.13833 0.23810 0.93235
Zn 0.08625 0.24092 0.66409
Zn 0.24306 0.74739 0.20646
Zn 0.01713 0.83593 0.38624
Zn 0.53821 0.33819 0.51874
Zn 0.25200 0.49081 0.03820
```

Zn 0.90342 0.82683 0.85835
Zn 0.19296 0.97975 0.77235
Zn 0.19300 0.48879 0.77049
Zn 0.67800 0.77529 0.04353
Zn 0.08680 0.74865 0.66023
Zn 0.49062 0.34049 0.25752
Zn 0.41056 0.07718 0.59349
Zn 0.62409 0.25499 0.79113
Zn 0.80598 0.98595 0.16395
Zn 0.92820 0.06866 0.71334
Zn 0.35376 0.32922 0.73212
Zn 0.32225 0.99608 0.31585
Zn 0.89287 0.31860 0.86100
Zn 0.58414 0.42540 0.95090
Zn 0.12142 0.90655 0.10319
Zn 0.41589 0.25205 0.99768
Zn 0.59439 0.57121 0.39269
Zn 0.84578 0.99463 0.43007
Zn 0.20962 0.28556 0.18952
Zn 0.71120 0.01014 0.90861
Zn 0.93585 0.74171 0.13377
Zn 0.08385 0.53651 0.22898
Zn 0.47718 0.01834 0.84918
Zn 0.66189 0.48650 0.66457
Zn 0.43902 0.80700 0.99511
Zn 0.17098 0.74032 0.92592
Zn 0.33143 0.50447 0.31254
Zn 0.28618 0.74374 0.46210
O 0.81137 0.33150 0.19594
O 0.32629 0.33112 0.30174
O 0.02068 0.49532 0.38790
O 0.40285 0.75907 0.58310
O 0.62046 0.07603 0.77797
O 0.66166 0.31402 0.64354
O 0.72736 0.31198 0.91245
O 0.59078 0.75853 0.37978
O 0.40296 0.25031 0.58332
O 0.54132 0.27312 0.11364
O 0.41600 0.50432 0.00217
O 0.01257 0.77795 0.98753
O 0.49061 0.01243 0.25417
O 0.43539 0.06100 0.99647
O 0.33159 0.81705 0.32045
O 0.14590 0.04961 0.92650

O 0.81015 0.05334 0.58663
O 0.76675 0.71657 0.89994
O 0.54863 0.00084 0.52368
O 0.71832 0.07723 0.06176
O 0.52349 0.73539 0.12290
O 0.57199 0.25846 0.37746
O 0.92993 0.57401 0.13274
O 0.60388 0.88973 0.93917
O 0.07309 0.23183 0.25877
O 0.85977 0.80808 0.44517
O 0.34629 0.50349 0.72258
O 0.87770 0.99016 0.85642
O 0.28545 0.56302 0.46369
O 0.80710 0.56169 0.60941
O 0.74590 0.06570 0.31455
O 0.21881 0.02744 0.19540
O 0.14978 0.82504 0.51346
O 0.18725 0.80126 0.76992
O 0.67501 0.51889 0.05497
O 0.85902 0.30908 0.45116
O 0.66105 0.81648 0.65459
O 0.01103 0.00325 0.40034
O 0.09971 0.41086 0.09432
O 0.24106 0.57991 0.19684
O 0.10014 0.06513 0.66428
O 0.36621 0.98905 0.73775
O 0.19119 0.31988 0.78929
O 0.93529 0.76074 0.71428
O 0.91115 0.49683 0.87226
O 0.48135 0.30402 0.85805
O 0.26124 0.82816 0.03850
O 0.14014 0.30270 0.51474
O 0.29174 0.05964 0.46207
O 0.25863 0.25358 0.03635
O 0.98082 0.23084 0.97396
O 0.07712 0.78842 0.23577
O 0.44902 0.73617 0.83810
O 0.75289 0.56731 0.33736
O 0.54777 0.50515 0.53354
O 0.17167 0.57262 0.91945
O 0.50546 0.50647 0.27230
O 0.96807 0.00131 0.12524
O 0.08919 0.55973 0.65139
O 0.78689 0.81484 0.17380

O 0.60636 0.54039 0.81289
O 0.91878 0.25727 0.71479
K_POINTS gamma

IGZO-020-3-1

Analyzing GULP Output File for Supporting Information: IGZO-020-3-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -11151.12614720 Ry
Charge = 0.0000 SCF Energy = -11164.34269327 Ry
Charge = 17.4603 SCF Energy = -11171.41954745 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-020-3-1"  ,
        title = "IGZO-020-3-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.3797 ,
        B = 11.3797 ,
        C = 11.3797 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.3797  0.  0.
  6.96805659E-16  11.3797  0.
  6.96805659E-16  6.96805659E-16  11.3797
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.40600 0.88832 0.36376
Ga 0.43897 0.71451 0.12014
Ga 0.43454 0.50391 0.27486
Ga 0.67564 0.24772 0.88240
Ga 0.64143 0.40350 0.14416
Ga 0.50636 0.15595 0.49430
Ga 0.17298 0.57285 0.20993
Ga 0.97292 0.97284 0.52373
Ga 0.42070 0.65757 0.52555
Ga 0.67178 0.95684 0.46780
Ga 0.20594 0.76779 0.95567
Ga 0.32406 0.23220 0.32149
Ga 0.80458 0.20250 0.45783
Ga 0.50431 0.28827 0.69897
Ga 0.15771 0.45546 0.96618
Ga 0.66908 0.50807 0.72906
Ga 0.30789 0.52647 0.76204
Ga 0.48042 0.04348 0.90008
Ga 0.49671 0.94382 0.64841
Ga 0.25542 0.06648 0.58707
Ga 0.74197 0.66746 0.49088
Ga 0.32818 0.96772 0.11377
Ga 0.82750 0.46730 0.96693
Ga 0.99095 0.26206 0.91850
Ga 0.26215 0.81869 0.71368
Ga 0.82566 0.44735 0.31864
Ga 0.49146 0.71087 0.81057
Ga 0.61342 0.43616 0.46368
Ga 0.17582 0.06632 0.86489
Ga 0.31671 0.27600 0.86380
Ga 0.31219 0.37434 0.54558
Ga 0.98611 0.71014 0.66001
Ga 0.98128 0.47458 0.75397
Ga 0.49073 0.45869 0.95568
```

Ga 0.75264 0.82197 0.72610
Ga 0.74730 0.97559 0.97511
Ga 0.06386 0.46797 0.46526
Ga 0.17254 0.73480 0.44586
Ga 0.82428 0.23068 0.12307
Ga 0.67165 0.67997 0.99651
Ga 0.84564 0.00341 0.26140
Ga 0.07323 0.30951 0.20951
Ga 0.57239 0.10776 0.18525
Ga 0.02135 0.02210 0.06638
Ga 0.65663 0.81233 0.22895
Ga 0.05081 0.22495 0.63010
Ga 0.98518 0.89404 0.83782
Ga 0.93159 0.73031 0.29940
Ga 0.14345 0.04381 0.31957
Ga 0.98532 0.67803 0.01861
O 0.46374 0.04726 0.07050
O 0.82745 0.63381 0.02115
O 0.65856 0.99146 0.26244
O 0.32428 0.76784 0.43980
O 0.32540 0.45142 0.91221
O 0.98689 0.54553 0.59058
O 0.15493 0.62295 0.01588
O 0.28880 0.98752 0.27919
O 0.83987 0.60874 0.36948
O 0.51228 0.52236 0.77682
O 0.49427 0.97336 0.46818
O 0.65913 0.54828 0.57642
O 0.66147 0.92192 0.63473
O 0.61761 0.64934 0.17359
O 0.01516 0.65631 0.19118
O 0.14863 0.58660 0.37836
O 0.66290 0.32463 0.72744
O 0.82468 0.90245 0.85344
O 0.82432 0.72969 0.61500
O 0.83501 0.17921 0.28879
O 0.99216 0.72023 0.82377
O 0.15124 0.11464 0.69652
O 0.14276 0.49548 0.78254
O 0.99181 0.22182 0.09160
O 0.99134 0.40083 0.32816
O 0.66362 0.45401 0.97437
O 0.32759 0.54048 0.60014
O 0.15665 0.74076 0.60909

O 0.33198 0.38699 0.35824
O 0.01468 0.06354 0.90258
O 0.81480 0.39865 0.15213
O 0.78130 0.36042 0.46205
O 0.98030 0.90089 0.66659
O 0.49649 0.65496 0.97438
O 0.98105 0.30592 0.75155
O 0.02234 0.99932 0.23501
O 0.48053 0.42992 0.12893
O 0.82331 0.27623 0.94101
O 0.94670 0.15097 0.53710
O 0.16978 0.42680 0.13968
O 0.66464 0.12996 0.47688
O 0.33589 0.11816 0.86114
O 0.18676 0.89115 0.83444
O 0.48063 0.89865 0.82091
O 0.66591 0.70705 0.81063
O 0.33115 0.17150 0.48759
O 0.34538 0.32317 0.70225
O 0.31389 0.69570 0.81151
O 0.82356 0.50537 0.79199
O 0.33424 0.61322 0.21434
O 0.19804 0.03951 0.04125
O 0.66018 0.78621 0.41095
O 0.16187 0.27791 0.91303
O 0.64791 0.08768 0.89483
O 0.49366 0.29835 0.88481
O 0.02732 0.79891 0.40900
O 0.14139 0.34310 0.54277
O 0.13310 0.01229 0.47502
O 0.50998 0.32720 0.53227
O 0.82301 0.83183 0.21976
O 0.65189 0.23529 0.10951
O 0.63587 0.42692 0.30628
O 0.65488 0.85436 0.02924
O 0.49780 0.12049 0.66027
O 0.48435 0.83277 0.23253
O 0.47577 0.74977 0.63236
O 0.98981 0.45151 0.96207
O 0.48904 0.56404 0.41331
O 0.16852 0.20771 0.28932
O 0.32920 0.94195 0.63795
O 0.84030 0.96565 0.42864
O 0.03511 0.84792 0.00991

O 0.47339 0.18301 0.29695
O 0.31911 0.81813 0.05670
O 0.84212 0.04750 0.08203
K_POINTS gamma

IGZO-020-3-2

Analyzing GULP Output File for Supporting Information: IGZO-020-3-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -11151.11224691 Ry
Charge = 0.0000 SCF Energy = -11164.25897204 Ry
Charge = 17.4603 SCF Energy = -11171.47301323 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-020-3-2"  ,
        title = "IGZO-020-3-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.3797 ,
        B = 11.3797 ,
        C = 11.3797 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.3797  0.  0.
  6.96805659E-16  11.3797  0.
  6.96805659E-16  6.96805659E-16  11.3797
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.59573 0.89800 0.69456
Ga 0.76433 0.11388 0.77704
Ga 0.76946 0.54239 0.87879
Ga 0.62759 0.38890 0.43548
Ga 0.55155 0.58256 0.02927
Ga 0.93768 0.13687 0.55460
Ga 0.27215 0.58438 0.69385
Ga 0.67087 0.10397 0.49075
Ga 0.41940 0.94395 0.50292
Ga 0.09853 0.39235 0.63285
Ga 0.77802 0.85472 0.37926
Ga 0.92713 0.44997 0.43473
Ga 0.52936 0.93863 0.24935
Ga 0.18639 0.58706 0.98465
Ga 0.70406 0.36135 0.14715
Ga 0.93427 0.09474 0.99372
Ga 0.30157 0.88806 0.75487
Ga 0.36026 0.79483 0.03825
Ga 0.27368 0.61884 0.25070
Ga 0.36264 0.15068 0.30216
Ga 0.48785 0.64990 0.79295
Ga 0.01236 0.62663 0.78800
Ga 0.83549 0.84063 0.83808
Ga 0.76910 0.05645 0.20124
Ga 0.59627 0.34327 0.82739
Ga 0.61117 0.12922 0.01177
Ga 0.02532 0.75919 0.24035
Ga 0.42964 0.30880 0.05640
Ga 0.44513 0.12804 0.77977
Ga 0.43122 0.62310 0.47988
Ga 0.27396 0.33684 0.83416
Ga 0.93316 0.51018 0.10748
Ga 0.78107 0.74778 0.09428
Ga 0.10669 0.87353 0.95711
```

Ga 0.93465 0.79222 0.56809
Ga 0.11021 0.02471 0.22701
Ga 0.11939 0.94822 0.53375
Ga 0.26867 0.16688 0.58194
Ga 0.10988 0.32086 0.06097
Ga 0.17899 0.34314 0.35320
Ga 0.28277 0.08435 0.01296
Ga 0.10984 0.63163 0.49112
Ga 0.43560 0.37252 0.60291
Ga 0.43853 0.43253 0.26947
Ga 0.77042 0.39257 0.65838
Ga 0.69058 0.66087 0.60099
Ga 0.60292 0.64879 0.29960
Ga 0.10329 0.11144 0.79856
Ga 0.93685 0.24126 0.25132
Ga 0.94131 0.33306 0.85622
O 0.93746 0.36512 0.67034
O 0.94832 0.92236 0.94294
O 0.60533 0.04045 0.15104
O 0.94534 0.21888 0.41878
O 0.60623 0.37148 0.65215
O 0.95563 0.97683 0.56888
O 0.76480 0.55749 0.70758
O 0.77854 0.41689 0.49181
O 0.92411 0.75645 0.73008
O 0.26293 0.51252 0.86218
O 0.27108 0.59421 0.52006
O 0.43819 0.54987 0.66406
O 0.93548 0.13955 0.81666
O 0.60655 0.16213 0.81385
O 0.28363 0.91398 0.96290
O 0.09312 0.48326 0.06626
O 0.32350 0.72790 0.76391
O 0.45941 0.42975 0.44705
O 0.10080 0.71299 0.90475
O 0.91352 0.43202 0.25963
O 0.42254 0.20100 0.62002
O 0.28214 0.15745 0.80795
O 0.76959 0.79081 0.53516
O 0.77379 0.23155 0.21460
O 0.46865 0.70467 0.95102
O 0.77382 0.48069 0.04746
O 0.77025 0.33514 0.83173
O 0.57606 0.99066 0.56139

O 0.60433 0.74007 0.71381
O 0.12521 0.00059 0.38751
O 0.15142 0.94532 0.77575
O 0.28124 0.98711 0.58009
O 0.10362 0.87686 0.14740
O 0.74786 0.02338 0.37567
O 0.64205 0.65814 0.13566
O 0.43030 0.62315 0.30155
O 0.59780 0.29770 0.03225
O 0.26503 0.36364 0.64039
O 0.95213 0.60763 0.49878
O 0.08807 0.42012 0.46220
O 0.93615 0.51476 0.87871
O 0.26368 0.66707 0.09652
O 0.77105 0.71588 0.93064
O 0.61083 0.60778 0.46737
O 0.44997 0.47716 0.09808
O 0.93242 0.81267 0.36249
O 0.11431 0.09658 0.97046
O 0.43780 0.01501 0.36433
O 0.27017 0.22524 0.41984
O 0.94666 0.08656 0.17486
O 0.76647 0.09772 0.99146
O 0.60956 0.22800 0.42889
O 0.44255 0.12240 0.99241
O 0.11351 0.31866 0.82007
O 0.43194 0.27928 0.22560
O 0.10721 0.55373 0.68591
O 0.43445 0.32971 0.84182
O 0.26871 0.29790 0.01514
O 0.13352 0.66721 0.31839
O 0.78136 0.15461 0.61774
O 0.45345 0.96102 0.76163
O 0.73372 0.94657 0.76982
O 0.59308 0.52387 0.88257
O 0.63603 0.80860 0.32050
O 0.43259 0.85133 0.16508
O 0.79782 0.88792 0.17309
O 0.62576 0.45399 0.26996
O 0.95593 0.28694 0.01281
O 0.09481 0.27343 0.22441
O 0.25287 0.08673 0.17995
O 0.10028 0.16146 0.62304
O 0.43601 0.78421 0.52293

O 0.92848 0.67209 0.13934
O 0.10889 0.78498 0.55828
O 0.27207 0.45395 0.27497
K_POINTS gamma

IGZO-020-3-3

Analyzing GULP Output File for Supporting Information: IGZO-020-3-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -11150.98500130 Ry
Charge = 0.0000 SCF Energy = -11164.03640362 Ry
Charge = 17.4603 SCF Energy = -11171.19344458 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-020-3-3"  ,
        title = "IGZO-020-3-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.3797 ,
        B = 11.3797 ,
        C = 11.3797 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.3797  0.  0.
  6.96805659E-16  11.3797  0.
  6.96805659E-16  6.96805659E-16  11.3797
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.41651 0.58401 0.38602
Ga 0.56778 0.26110 0.10927
Ga 0.61797 0.73680 0.30814
Ga 0.42917 0.26637 0.33670
Ga 0.81157 0.25119 0.26405
Ga 0.47201 0.58478 0.73153
Ga 0.06008 0.43361 0.60063
Ga 0.18856 0.05327 0.42311
Ga 0.75359 0.42970 0.06580
Ga 0.97816 0.91098 0.00161
Ga 0.81852 0.15856 0.97434
Ga 0.96933 0.98285 0.71262
Ga 0.47526 0.10125 0.56562
Ga 0.18942 0.75631 0.40859
Ga 0.73232 0.91459 0.86661
Ga 0.19346 0.43414 0.37898
Ga 0.67974 0.59892 0.53698
Ga 0.26033 0.09192 0.73468
Ga 0.29919 0.24939 0.01574
Ga 0.68269 0.99047 0.20459
Ga 0.59497 0.33173 0.81652
Ga 0.95343 0.76962 0.23186
Ga 0.38448 0.84762 0.65040
Ga 0.65315 0.91153 0.51939
Ga 0.73424 0.75231 0.08256
Ga 0.37635 0.06579 0.16080
Ga 0.77598 0.32146 0.57023
Ga 0.18710 0.90240 0.17726
Ga 0.65130 0.43549 0.33678
Ga 0.12374 0.57472 0.84045
Ga 0.73785 0.60187 0.85938
Ga 0.07892 0.22433 0.86119
Ga 0.94870 0.59515 0.04048
Ga 0.87070 0.08226 0.45128
```

Ga 0.90751 0.77173 0.49914
Ga 0.23862 0.83512 0.89504
Ga 0.90018 0.40248 0.82300
Ga 0.29217 0.39670 0.79476
Ga 0.12164 0.74758 0.66504
Ga 0.42357 0.92129 0.36266
Ga 0.20540 0.58012 0.14357
Ga 0.91931 0.52344 0.35069
Ga 0.00330 0.07875 0.21327
Ga 0.05697 0.35212 0.12413
Ga 0.39947 0.39287 0.56309
Ga 0.72839 0.09971 0.68664
Ga 0.52049 0.76977 0.90851
Ga 0.45793 0.51054 0.02566
Ga 0.49161 0.08345 0.89275
Ga 0.40112 0.74975 0.15064
O 0.24655 0.77223 0.57504
O 0.88229 0.09187 0.62188
O 0.26035 0.08353 0.56575
O 0.72592 0.09075 0.86078
O 0.45115 0.24827 0.51223
O 0.69709 0.91375 0.69437
O 0.69796 0.75086 0.90232
O 0.19030 0.74145 0.18905
O 0.54200 0.23765 0.93221
O 0.74938 0.26179 0.09768
O 0.94453 0.07196 0.04246
O 0.81226 0.23885 0.43367
O 0.58283 0.30246 0.28170
O 0.57288 0.57807 0.31991
O 0.09339 0.40267 0.80014
O 0.77234 0.59037 0.04894
O 0.02501 0.76140 0.38957
O 0.28709 0.92755 0.76596
O 0.59905 0.92109 0.32310
O 0.16647 0.42868 0.21209
O 0.97564 0.59556 0.21507
O 0.63342 0.74115 0.47979
O 0.77720 0.75568 0.25352
O 0.18203 0.07539 0.21136
O 0.81076 0.91196 0.47804
O 0.72960 0.41396 0.88067
O 0.90867 0.56520 0.85813
O 0.84728 0.61801 0.47343

O 0.11526 0.56155 0.00366
O 0.92931 0.76270 0.05378
O 0.36015 0.76457 0.97677
O 0.92095 0.24047 0.87616
O 0.81373 0.07585 0.26993
O 0.26401 0.24110 0.80490
O 0.36212 0.90950 0.17673
O 0.92671 0.41930 0.04490
O 0.35340 0.09364 0.99217
O 0.29383 0.55469 0.77417
O 0.90019 0.92324 0.85389
O 0.45567 0.75196 0.75405
O 0.66974 0.43606 0.49898
O 0.22887 0.39223 0.57448
O 0.53280 0.58409 0.89819
O 0.97133 0.25394 0.22124
O 0.03886 0.44433 0.43471
O 0.45918 0.92977 0.53652
O 0.58572 0.43307 0.08442
O 0.90294 0.38820 0.65274
O 0.64053 0.08236 0.55099
O 0.54890 0.92814 0.91600
O 0.14253 0.90485 0.00496
O 0.00592 0.84776 0.61814
O 0.13722 0.73675 0.82033
O 0.03116 0.07862 0.40640
O 0.46156 0.39381 0.73123
O 0.79791 0.43272 0.28108
O 0.56580 0.75128 0.13261
O 0.45852 0.09525 0.73345
O 0.66476 0.59218 0.70157
O 0.01675 0.91679 0.21462
O 0.06129 0.59377 0.65048
O 0.23891 0.60146 0.38638
O 0.39127 0.08854 0.33490
O 0.68651 0.26191 0.69721
O 0.44504 0.56033 0.55766
O 0.56831 0.08992 0.13697
O 0.75230 0.91505 0.07222
O 0.13853 0.26363 0.00989
O 0.37738 0.57889 0.14245
O 0.09440 0.08322 0.77902
O 0.37647 0.41315 0.37532
O 0.42881 0.75322 0.33852

```
O 0.24253 0.90651 0.37643
O 0.34332 0.40826 0.96074
O 0.38735 0.24321 0.16478
K_POINTS  gamma
```

IGZO-020-3-4

Analyzing GULP Output File for Supporting Information: IGZO-020-3-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -11151.09206260 Ry
Charge = 0.0000 SCF Energy = -11164.28815873 Ry
Charge = 17.4603 SCF Energy = -11171.42156223 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-020-3-4"  ,
        title = "IGZO-020-3-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.3797 ,
        B = 11.3797 ,
        C = 11.3797 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.3797  0.  0.
  6.96805659E-16  11.3797  0.
  6.96805659E-16  6.96805659E-16  11.3797
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.63699 0.12344 0.98317
Ga 0.45545 0.15030 0.47156
Ga 0.25117 0.31329 0.41927
Ga 0.05384 0.06049 0.86580
Ga 0.81423 0.35214 0.33387
Ga 0.85250 0.24698 0.82596
Ga 0.60235 0.65184 0.48864
Ga 0.08513 0.73644 0.66263
Ga 0.40046 0.03604 0.96539
Ga 0.88639 0.18769 0.09295
Ga 0.03345 0.79109 0.92659
Ga 0.74031 0.90226 0.43764
Ga 0.23473 0.99334 0.41262
Ga 0.96868 0.49502 0.79639
Ga 0.34060 0.14468 0.21340
Ga 0.57111 0.82564 0.71552
Ga 0.73029 0.84605 0.94360
Ga 0.87152 0.48835 0.09797
Ga 0.36709 0.76975 0.15394
Ga 0.56483 0.14902 0.70733
Ga 0.69525 0.41908 0.62223
Ga 0.03306 0.81991 0.38379
Ga 0.00421 0.14695 0.34874
Ga 0.19289 0.48898 0.64000
Ga 0.66031 0.15757 0.28719
Ga 0.58398 0.58818 0.18243
Ga 0.08310 0.64522 0.16844
Ga 0.80803 0.66952 0.68284
Ga 0.34217 0.98063 0.65228
Ga 0.24899 0.65589 0.40130
Ga 0.52382 0.39991 0.38119
Ga 0.27799 0.46834 0.20874
Ga 0.29273 0.82440 0.87057
Ga 0.59682 0.92799 0.18922
```

Ga 0.05794 0.48341 0.37864
Ga 0.49271 0.64089 0.91566
Ga 0.63802 0.39718 0.98403
Ga 0.37993 0.65583 0.63452
Ga 0.10275 0.97694 0.14270
Ga 0.00382 0.32347 0.57953
Ga 0.85561 0.79905 0.16253
Ga 0.36646 0.30771 0.99916
Ga 0.82517 0.64071 0.37008
Ga 0.26484 0.22907 0.72887
Ga 0.02464 0.99631 0.58649
Ga 0.78193 0.16357 0.54129
Ga 0.45359 0.84528 0.41681
Ga 0.21416 0.55334 0.91967
Ga 0.46110 0.40418 0.75585
Ga 0.79068 0.98161 0.73493
O 0.60319 0.82650 0.48361
O 0.52027 0.30611 0.04989
O 0.41712 0.31614 0.46148
O 0.25499 0.14880 0.41509
O 0.14470 0.81413 0.79413
O 0.66442 0.64379 0.31582
O 0.11509 0.66887 0.00134
O 0.33908 0.66180 0.86480
O 0.32289 0.15806 0.04859
O 0.04905 0.30428 0.39211
O 0.69321 0.50262 0.08633
O 0.09427 0.48888 0.19698
O 0.47279 0.84542 0.26016
O 0.46562 0.50072 0.25933
O 0.19148 0.97834 0.58746
O 0.98044 0.15765 0.55868
O 0.80366 0.98456 0.55362
O 0.54708 0.65513 0.66075
O 0.06560 0.65589 0.36053
O 0.60934 0.16161 0.51412
O 0.57761 0.98389 0.69076
O 0.21561 0.65340 0.60311
O 0.39102 0.82283 0.67972
O 0.01346 0.82491 0.54760
O 0.51740 0.14474 0.87151
O 0.75276 0.81563 0.72979
O 0.82709 0.18176 0.36844
O 0.67901 0.98884 0.31692

O 0.78616 0.66420 0.52305
O 0.60301 0.49325 0.50286
O 0.81112 0.33501 0.54026
O 0.23980 0.01116 0.23411
O 0.99882 0.10282 0.18628
O 0.73093 0.14014 0.12004
O 0.34512 0.32561 0.83708
O 0.48745 0.14070 0.29330
O 0.73490 0.99789 0.90099
O 0.95956 0.33918 0.73302
O 0.36331 0.49165 0.66360
O 0.96072 0.65736 0.74727
O 0.39163 0.14950 0.64938
O 0.32812 0.98382 0.83374
O 0.92451 0.48688 0.94586
O 0.95947 0.98357 0.74350
O 0.13903 0.50900 0.78755
O 0.74184 0.28679 0.93322
O 0.05267 0.99085 0.39387
O 0.88120 0.49002 0.35806
O 0.32743 0.85347 0.02715
O 0.26201 0.65701 0.21401
O 0.76639 0.51505 0.72801
O 0.88331 0.80065 0.97132
O 0.90040 0.64261 0.16272
O 0.22921 0.48814 0.39340
O 0.48929 0.66741 0.08140
O 0.08770 0.94964 0.98319
O 0.71015 0.84878 0.11833
O 0.58642 0.78568 0.88243
O 0.04544 0.83225 0.19491
O 0.86365 0.34085 0.16457
O 0.15047 0.15331 0.80047
O 0.41896 0.68252 0.45089
O 0.94325 0.16477 0.93825
O 0.04368 0.48895 0.55473
O 0.65740 0.33142 0.31703
O 0.29287 0.46179 0.03780
O 0.29859 0.30685 0.23884
O 0.85847 0.81246 0.33854
O 0.19392 0.32260 0.59954
O 0.58717 0.32458 0.70091
O 0.76401 0.15392 0.71465
O 0.52757 0.48995 0.88220

O 0.52679 0.01068 0.06542
O 0.24253 0.82729 0.39463
O 0.40292 0.98322 0.47544
K_POINTS gamma

IGZO-020-3-5

Analyzing GULP Output File for Supporting Information: IGZO-020-3-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -11151.13912176 Ry
Charge = 0.0000 SCF Energy = -11164.24406809 Ry
Charge = 17.4603 SCF Energy = -11171.35890990 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-020-3-5"  ,
        title = "IGZO-020-3-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.3797 ,
        B = 11.3797 ,
        C = 11.3797 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.3797  0.  0.
  6.96805659E-16  11.3797  0.
  6.96805659E-16  6.96805659E-16  11.3797
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.66866 0.63805 0.76812
Ga 0.88801 0.61967 0.27050
Ga 0.31108 0.19510 0.99220
Ga 0.68030 0.61744 0.09610
Ga 0.94626 0.98489 0.90339
Ga 0.04029 0.33819 0.26249
Ga 0.91841 0.74440 0.77273
Ga 0.85603 0.42645 0.79199
Ga 0.95749 0.48314 0.04475
Ga 0.48869 0.29736 0.52696
Ga 0.31992 0.41021 0.30045
Ga 0.32154 0.70260 0.41555
Ga 0.47756 0.41152 0.07597
Ga 0.49403 0.19881 0.25286
Ga 0.44922 0.95783 0.19182
Ga 0.16357 0.93964 0.44278
Ga 0.85341 0.24947 0.59261
Ga 0.57420 0.54715 0.49394
Ga 0.08503 0.21390 0.78238
Ga 0.22824 0.17029 0.57159
Ga 0.69612 0.84600 0.92985
Ga 0.84779 0.59286 0.57385
Ga 0.72697 0.06679 0.41565
Ga 0.95143 0.00277 0.28033
Ga 0.16315 0.94656 0.07364
Ga 0.39358 0.58327 0.85063
Ga 0.05227 0.38318 0.58874
Ga 0.12650 0.75276 0.24345
Ga 0.14639 0.70823 0.93433
Ga 0.15897 0.44195 0.86256
Ga 0.73342 0.03271 0.11376
Ga 0.74512 0.34425 0.34383
Ga 0.90413 0.79154 0.08756
Ga 0.28833 0.50017 0.59404
```

Ga 0.58367 0.73553 0.29748
Ga 0.56126 0.36827 0.82026
Ga 0.17085 0.93960 0.74288
Ga 0.70552 0.14581 0.85053
Ga 0.65954 0.92550 0.66264
Ga 0.20599 0.13324 0.26782
Ga 0.98237 0.18744 0.06629
Ga 0.08405 0.55354 0.40299
Ga 0.10765 0.71839 0.59783
Ga 0.42015 0.77810 0.66768
Ga 0.92360 0.92227 0.57895
Ga 0.46656 0.97651 0.45923
Ga 0.37385 0.67335 0.12242
Ga 0.45249 0.12182 0.73324
Ga 0.72818 0.31537 0.06291
Ga 0.39303 0.93185 0.90718
O 0.18308 0.10427 0.71954
O 0.96749 0.95356 0.73106
O 0.84558 0.38918 0.96177
O 0.33179 0.87994 0.75897
O 0.86530 0.59598 0.77632
O 0.79560 0.23360 0.75067
O 0.74648 0.85029 0.09234
O 0.22719 0.33989 0.58940
O 0.52560 0.88274 0.59234
O 0.03830 0.38007 0.77457
O 0.41409 0.26568 0.09908
O 0.64124 0.27105 0.23101
O 0.93815 0.75424 0.60473
O 0.79302 0.22119 0.45516
O 0.56963 0.04818 0.13038
O 0.54356 0.88105 0.90127
O 0.07565 0.57357 0.23838
O 0.86027 0.40486 0.24771
O 0.77252 0.00896 0.91691
O 0.81248 0.17710 0.08212
O 0.33329 0.88393 0.44668
O 0.63987 0.46269 0.08460
O 0.67752 0.47055 0.76127
O 0.19062 0.10277 0.43680
O 0.96298 0.97612 0.08088
O 0.76453 0.97011 0.55201
O 0.39247 0.09626 0.88370
O 0.11547 0.77479 0.08019

O 0.49369 0.65787 0.39892
O 0.38967 0.11752 0.58035
O 0.25997 0.52240 0.40781
O 0.99692 0.14666 0.90594
O 0.20620 0.30549 0.26262
O 0.46540 0.45475 0.91575
O 0.64333 0.40942 0.44496
O 0.31002 0.68560 0.59066
O 0.71673 0.64280 0.27405
O 0.01961 0.16078 0.24800
O 0.68609 0.67756 0.93985
O 0.53258 0.69373 0.14155
O 0.08714 0.55211 0.95368
O 0.10767 0.55271 0.58246
O 0.37321 0.49437 0.16615
O 0.62124 0.25763 0.93257
O 0.37155 0.07671 0.26983
O 0.96594 0.97203 0.43487
O 0.94064 0.78408 0.24715
O 0.44499 0.45967 0.55701
O 0.14645 0.92585 0.91039
O 0.73296 0.80693 0.75281
O 0.35587 0.89713 0.07038
O 0.04584 0.39074 0.42007
O 0.42890 0.30310 0.36934
O 0.88295 0.41811 0.60687
O 0.29617 0.72709 0.25210
O 0.20240 0.10667 0.08581
O 0.13928 0.93937 0.25894
O 0.13762 0.89613 0.59325
O 0.27886 0.50569 0.77097
O 0.10558 0.72741 0.77396
O 0.03243 0.34898 0.09148
O 0.91552 0.59076 0.42547
O 0.60843 0.05498 0.74337
O 0.54062 0.89176 0.32050
O 0.87526 0.61331 0.09216
O 0.78450 0.02363 0.27441
O 0.50170 0.27574 0.70278
O 0.13222 0.74056 0.41971
O 0.01435 0.21303 0.61125
O 0.21573 0.28760 0.90474
O 0.49820 0.66457 0.75543
O 0.92046 0.81668 0.91827

```
O 0.69036 0.62564 0.58115
O 0.31880 0.66042 0.96814
O 0.56927 0.11026 0.42999
K_POINTS  gamma
```

IGZO-021-4-1

Analyzing GULP Output File for Supporting Information: IGZO-021-4-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10617.60255163 Ry
Charge = 0.0000 SCF Energy = -10630.37514927 Ry
Charge = 16.7302 SCF Energy = -10637.80854820 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-021-4-1"  ,
        title = "IGZO-021-4-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1461 ,
        B = 11.1461 ,
        C = 11.1461 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1461  0.  0.
  6.82501784E-16  11.1461  0.
  6.82501784E-16  6.82501784E-16  11.1461
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.53156 0.14325 0.92434
Ga 0.41421 0.87251 0.99645
Ga 0.93897 0.13447 0.50036
Ga 0.17511 0.50566 0.65270
Ga 0.28709 0.44078 0.38991
Ga 0.21906 0.50281 0.12147
Ga 0.38745 0.19422 0.27737
Ga 0.45071 0.27001 0.56677
Ga 0.62569 0.39302 0.79890
Ga 0.15838 0.72646 0.05221
Ga 0.63376 0.75633 0.12435
Ga 0.89696 0.65396 0.63869
Ga 0.99537 0.40454 0.51219
Ga 0.74487 0.99914 0.07960
Ga 0.09727 0.27175 0.23126
Ga 0.75889 0.46953 0.09064
Ga 0.79128 0.89499 0.58588
Ga 0.80706 0.34700 0.33280
Ga 0.19628 0.19617 0.56172
Ga 0.28139 0.72338 0.49707
Ga 0.52010 0.78685 0.65974
Ga 0.64714 0.86766 0.87177
Ga 0.29306 0.12901 0.03208
Ga 0.07488 0.28223 0.92750
Ga 0.87740 0.32282 0.76400
Ga 0.04870 0.98436 0.13021
Ga 0.67066 0.51974 0.54378
Ga 0.49324 0.55178 0.99057
Ga 0.08932 0.90166 0.64918
Ga 0.67326 0.12750 0.66067
Ga 0.41767 0.66758 0.23956
Ga 0.03444 0.85888 0.40170
Ga 0.38506 0.00500 0.73745
```

Ga 0.30207 0.93094 0.28904
Zn 0.51867 0.98453 0.46603
Zn 0.44183 0.55250 0.69691
Zn 0.77979 0.94542 0.31676
Zn 0.60761 0.20482 0.14946
Zn 0.64571 0.74211 0.41837
Zn 0.17620 0.95251 0.88311
Zn 0.90533 0.03987 0.81186
Zn 0.89968 0.74284 0.15630
Zn 0.55762 0.43951 0.27575
Zn 0.28246 0.74451 0.78548
Zn 0.34233 0.36222 0.87966
Zn 0.03471 0.56999 0.86609
Zn 0.75050 0.59560 0.84392
Zn 0.84896 0.20739 0.04824
Zn 0.93081 0.82330 0.89673
Zn 0.64581 0.15645 0.37377
Zn 0.88759 0.59312 0.33242
O 0.93505 0.81414 0.61062
O 0.01084 0.40713 0.83903
O 0.57085 0.14669 0.52966
O 0.47698 0.82385 0.82119
O 0.24807 0.65927 0.18034
O 0.24133 0.18568 0.19923
O 0.79984 0.93972 0.90817
O 0.40302 0.04973 0.34997
O 0.18563 0.41576 0.25242
O 0.34087 0.93184 0.13039
O 0.08134 0.07156 0.58154
O 0.91283 0.97726 0.41599
O 0.09838 0.57112 0.02307
O 0.97916 0.73080 0.31075
O 0.34961 0.47079 0.01889
O 0.02064 0.81713 0.05776
O 0.02839 0.92981 0.81532
O 0.37832 0.03697 0.90994
O 0.78148 0.85814 0.17918
O 0.36214 0.79286 0.37212
O 0.36936 0.69625 0.65139
O 0.69556 0.81727 0.71107
O 0.34511 0.16525 0.65229
O 0.13166 0.92889 0.26938
O 0.91581 0.29775 0.60259
O 0.93352 0.43870 0.36073

O 0.72053 0.26813 0.73619
O 0.24589 0.56141 0.48935
O 0.65501 0.05838 0.23875
O 0.74772 0.43667 0.91637
O 0.68541 0.15110 0.01151
O 0.53373 0.39882 0.61301
O 0.41417 0.51397 0.31168
O 0.04730 0.21993 0.38529
O 0.58017 0.71452 0.27016
O 0.01137 0.54290 0.59671
O 0.67283 0.90320 0.46465
O 0.54085 0.26868 0.29753
O 0.93118 0.19496 0.86777
O 0.90764 0.66892 0.82675
O 0.24070 0.91588 0.73187
O 0.69863 0.70965 0.96799
O 0.46735 0.70349 0.06944
O 0.76378 0.52043 0.67948
O 0.57304 0.65816 0.56045
O 0.81886 0.04661 0.64474
O 0.58981 0.91978 0.02934
O 0.30948 0.45641 0.73709
O 0.59299 0.48680 0.12015
O 0.14350 0.04337 0.01867
O 0.58660 0.05165 0.78507
O 0.23361 0.25176 0.92526
O 0.02614 0.28240 0.08261
O 0.15180 0.64372 0.76414
O 0.15535 0.82859 0.50848
O 0.14391 0.35140 0.58195
O 0.82347 0.59342 0.16364
O 0.45813 0.92728 0.60307
O 0.68466 0.45249 0.39131
O 0.77742 0.32265 0.17394
O 0.26082 0.79631 0.94322
O 0.44706 0.17378 0.08471
O 0.54446 0.54346 0.83140
O 0.89797 0.05582 0.12705
O 0.33530 0.28632 0.44161
O 0.78823 0.20473 0.40974
O 0.49682 0.29867 0.86244
O 0.79144 0.65324 0.47546
K_POINTS gamma

IGZO-021-4-2

Analyzing GULP Output File for Supporting Information: IGZO-021-4-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10617.74301922 Ry
Charge = 0.0000 SCF Energy = -10630.44999366 Ry
Charge = 16.7302 SCF Energy = -10637.88142098 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-021-4-2"  ,
        title = "IGZO-021-4-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1461 ,
        B = 11.1461 ,
        C = 11.1461 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1461  0.  0.
  6.82501784E-16  11.1461  0.
  6.82501784E-16  6.82501784E-16  11.1461
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.32481 0.84573 0.15088
Ga 0.71511 0.65882 0.44965
Ga 0.47626 0.01326 0.34790
Ga 0.05921 0.79802 0.26377
Ga 0.10691 0.44294 0.69102
Ga 0.40296 0.51840 0.61691
Ga 0.58224 0.05684 0.61925
Ga 0.10137 0.91145 0.54517
Ga 0.80400 0.21611 0.68157
Ga 0.31771 0.03623 0.70043
Ga 0.26682 0.15742 0.07499
Ga 0.66724 0.07306 0.12202
Ga 0.43892 0.51027 0.32332
Ga 0.46464 0.89182 0.89915
Ga 0.82980 0.89077 0.29602
Ga 0.59722 0.72693 0.68558
Ga 0.82671 0.32337 0.20620
Ga 0.07142 0.21198 0.53084
Ga 0.18045 0.04951 0.32168
Ga 0.53727 0.14764 0.87632
Ga 0.86441 0.54862 0.78276
Ga 0.08145 0.18548 0.85152
Ga 0.82709 0.90376 0.57619
Ga 0.60185 0.35996 0.49296
Ga 0.66191 0.49061 0.06431
Ga 0.64211 0.41472 0.79149
Ga 0.02452 0.70804 0.01867
Ga 0.77660 0.16042 0.40107
Ga 0.96803 0.10208 0.12152
Ga 0.00077 0.64099 0.51467
Ga 0.52603 0.28365 0.22042
Ga 0.85002 0.01927 0.86573
Ga 0.17827 0.92754 0.92341
```

Ga 0.22998 0.57138 0.15927
Zn 0.34354 0.23677 0.44534
Zn 0.44090 0.61128 0.98021
Zn 0.73417 0.72973 0.91219
Zn 0.90703 0.39754 0.44970
Zn 0.79641 0.26302 0.93880
Zn 0.96528 0.79017 0.77345
Zn 0.40001 0.38119 0.96798
Zn 0.91731 0.45679 0.00399
Zn 0.29255 0.77974 0.67092
Zn 0.18413 0.45629 0.41710
Zn 0.59035 0.80478 0.15279
Zn 0.12398 0.30554 0.25718
Zn 0.97049 0.54847 0.23664
Zn 0.77827 0.65619 0.17981
Zn 0.14181 0.43591 0.95923
Zn 0.31655 0.29107 0.73178
Zn 0.25482 0.69543 0.40756
O 0.10518 0.61879 0.33316
O 0.28910 0.51594 0.00670
O 0.81076 0.39116 0.68363
O 0.72509 0.74386 0.31070
O 0.54288 0.03270 0.99754
O 0.18101 0.27233 0.96578
O 0.16654 0.71939 0.55391
O 0.17751 0.28797 0.43029
O 0.32545 0.52850 0.46307
O 0.69244 0.59475 0.75446
O 0.33623 0.10397 0.34205
O 0.41625 0.26237 0.85603
O 0.13458 0.14149 0.19797
O 0.97157 0.81875 0.42906
O 0.93993 0.71248 0.17119
O 0.88613 0.63660 0.92395
O 0.86040 0.15598 0.23945
O 0.35012 0.64578 0.26016
O 0.58081 0.54735 0.44670
O 0.91451 0.16699 0.79983
O 0.53869 0.40667 0.64911
O 0.73212 0.32398 0.36232
O 0.83554 0.85305 0.86522
O 0.04833 0.46733 0.54028
O 0.05610 0.53788 0.08188
O 0.66797 0.27510 0.10831

O 0.40387 0.25068 0.11051
O 0.90457 0.22652 0.51331
O 0.72283 0.92628 0.17138
O 0.24107 0.42101 0.24466
O 0.66996 0.23452 0.81626
O 0.74811 0.02557 0.67308
O 0.58865 0.80331 0.83119
O 0.11360 0.26456 0.68829
O 0.35063 0.17660 0.60814
O 0.48396 0.03185 0.75288
O 0.27174 0.98382 0.05076
O 0.52531 0.97541 0.49701
O 0.42984 0.77202 0.02233
O 0.09318 0.05734 0.47554
O 0.71494 0.77392 0.57231
O 0.97614 0.93718 0.21857
O 0.85466 0.56767 0.43655
O 0.08608 0.79105 0.88918
O 0.02681 0.46585 0.83386
O 0.32331 0.87062 0.81474
O 0.94213 0.29837 0.04384
O 0.66200 0.66131 0.06735
O 0.97400 0.37894 0.28770
O 0.80996 0.48493 0.15907
O 0.97602 0.91694 0.65762
O 0.53288 0.48083 0.93130
O 0.79429 0.09051 0.99991
O 0.20027 0.06954 0.81123
O 0.45832 0.89570 0.23154
O 0.43836 0.67772 0.66167
O 0.18104 0.74471 0.11338
O 0.76627 0.42560 0.92439
O 0.26121 0.92634 0.58950
O 0.94431 0.65255 0.67780
O 0.20490 0.88046 0.31166
O 0.53610 0.47097 0.19116
O 0.58168 0.12676 0.27093
O 0.47154 0.33234 0.38248
O 0.79450 0.99198 0.43637
O 0.64667 0.20704 0.55810
O 0.27620 0.44896 0.69725
O 0.03335 0.03891 0.97531
K_POINTS gamma

IGZO-021-4-3

Analyzing GULP Output File for Supporting Information: IGZO-021-4-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10618.04736872 Ry
Charge = 0.0000 SCF Energy = -10630.80100466 Ry
Charge = 16.7302 SCF Energy = -10638.15711562 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-021-4-3"  ,
        title = "IGZO-021-4-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1461 ,
        B = 11.1461 ,
        C = 11.1461 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1461  0.  0.
  6.82501784E-16  11.1461  0.
  6.82501784E-16  6.82501784E-16  11.1461
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.47711 0.69621 0.52012
Ga 0.21660 0.87266 0.60310
Ga 0.42345 0.42631 0.59177
Ga 0.68580 0.76143 0.39537
Ga 0.23240 0.57940 0.20318
Ga 0.99017 0.42722 0.62929
Ga 0.99092 0.13721 0.76316
Ga 0.94459 0.31927 0.98555
Ga 0.13356 0.11952 0.52334
Ga 0.60019 0.57668 0.78835
Ga 0.45154 0.18639 0.66711
Ga 0.73665 0.78569 0.68169
Ga 0.71125 0.47115 0.52132
Ga 0.78732 0.39662 0.24072
Ga 0.73684 0.13424 0.10906
Ga 0.89779 0.87641 0.26217
Ga 0.72448 0.65211 0.11669
Ga 0.43776 0.66213 0.01336
Ga 0.94599 0.62194 0.36885
Ga 0.57058 0.24884 0.38904
Ga 0.20683 0.57944 0.50248
Ga 0.47047 0.18641 0.15953
Ga 0.17200 0.84234 0.32094
Ga 0.01545 0.13779 0.27745
Ga 0.29463 0.32767 0.32308
Ga 0.00955 0.71728 0.72114
Ga 0.22146 0.79846 0.92069
Ga 0.23908 0.03119 0.82305
Ga 0.16796 0.50184 0.88636
Ga 0.21943 0.28962 0.72069
Ga 0.67639 0.07576 0.63701
Ga 0.49378 0.87247 0.16772
Ga 0.99203 0.70489 0.03692
```

Ga 0.03167 0.99424 0.03747
Zn 0.77773 0.00675 0.86160
Zn 0.31130 0.98871 0.09030
Zn 0.85732 0.21112 0.49781
Zn 0.44567 0.97081 0.44474
Zn 0.28234 0.06919 0.29803
Zn 0.84303 0.55780 0.85580
Zn 0.71723 0.02970 0.35225
Zn 0.75886 0.30674 0.74854
Zn 0.53976 0.12144 0.92453
Zn 0.04151 0.40244 0.30794
Zn 0.20321 0.23808 0.02400
Zn 0.51124 0.51444 0.24167
Zn 0.91471 0.96124 0.55328
Zn 0.49909 0.88997 0.71502
Zn 0.66244 0.39725 0.00254
Zn 0.34265 0.67458 0.73445
Zn 0.42554 0.38223 0.92254
O 0.83467 0.36407 0.59360
O 0.49156 0.02063 0.08592
O 0.18966 0.42224 0.23651
O 0.17687 0.20166 0.36000
O 0.58644 0.74057 0.08960
O 0.18645 0.95203 0.45587
O 0.01026 0.77198 0.33965
O 0.70427 0.13249 0.47608
O 0.80925 0.90499 0.41708
O 0.53248 0.63371 0.37903
O 0.42359 0.12216 0.36344
O 0.17833 0.45204 0.72214
O 0.11428 0.00986 0.68650
O 0.45253 0.34068 0.26680
O 0.63028 0.77406 0.55109
O 0.03623 0.20143 0.08716
O 0.57908 0.89552 0.32422
O 0.84514 0.04462 0.21788
O 0.78240 0.74490 0.25203
O 0.23091 0.66186 0.35399
O 0.18504 0.95845 0.97061
O 0.38898 0.58126 0.14606
O 0.85017 0.09246 0.66673
O 0.72272 0.44172 0.85582
O 0.94876 0.56050 0.72255
O 0.92050 0.29009 0.32075

O 0.49334 0.73014 0.75341
O 0.74226 0.67864 0.79687
O 0.06086 0.25586 0.62206
O 0.68593 0.37705 0.37966
O 0.62934 0.16891 0.23058
O 0.39247 0.09801 0.83200
O 0.79942 0.29973 0.07726
O 0.33659 0.90862 0.24932
O 0.02541 0.45425 0.95534
O 0.15715 0.18896 0.84202
O 0.26579 0.63539 0.88162
O 0.39249 0.34493 0.74314
O 0.79929 0.60595 0.46474
O 0.52706 0.26593 0.01680
O 0.28454 0.86672 0.77012
O 0.69594 0.07879 0.96992
O 0.51411 0.03038 0.61211
O 0.97813 0.08588 0.45122
O 0.28176 0.17032 0.60284
O 0.09983 0.99074 0.22360
O 0.05161 0.51318 0.47385
O 0.13793 0.71753 0.60462
O 0.13761 0.67944 0.11366
O 0.36032 0.81292 0.02114
O 0.84536 0.63710 0.01584
O 0.37985 0.83262 0.53793
O 0.51167 0.53942 0.92424
O 0.05675 0.74157 0.88251
O 0.90516 0.26604 0.83665
O 0.31045 0.42073 0.46194
O 0.91343 0.51821 0.24531
O 0.26852 0.37952 0.96699
O 0.62279 0.19550 0.74661
O 0.68053 0.92973 0.75379
O 0.36065 0.59081 0.59580
O 0.89840 0.82621 0.65643
O 0.51153 0.29554 0.54194
O 0.66210 0.49632 0.16028
O 0.94663 0.03144 0.89724
O 0.58793 0.52045 0.62673
O 0.30412 0.15271 0.13839
O 0.95519 0.86050 0.09315
K_POINTS gamma

IGZO-021-4-4

Analyzing GULP Output File for Supporting Information: IGZO-021-4-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10617.70818924 Ry
Charge = 0.0000 SCF Energy = -10630.45340922 Ry
Charge = 16.7302 SCF Energy = -10637.87919137 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-021-4-4"  ,
        title = "IGZO-021-4-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1461 ,
        B = 11.1461 ,
        C = 11.1461 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1461  0.  0.
  6.82501784E-16  11.1461  0.
  6.82501784E-16  6.82501784E-16  11.1461
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.68766 0.69942 0.82662
Ga 0.33404 0.79439 0.49198
Ga 0.34773 0.26287 0.77975
Ga 0.96722 0.06099 0.60286
Ga 0.14911 0.91775 0.24717
Ga 0.28611 0.17925 0.05611
Ga 0.61486 0.91024 0.39882
Ga 0.69024 0.44772 0.47806
Ga 0.42092 0.32821 0.43706
Ga 0.66849 0.40181 0.01804
Ga 0.38282 0.07225 0.28759
Ga 0.27661 0.80277 0.97986
Ga 0.33951 0.52147 0.60883
Ga 0.55812 0.10929 0.89342
Ga 0.27131 0.54315 0.30938
Ga 0.76253 0.72561 0.10696
Ga 0.70031 0.16859 0.46942
Ga 0.87730 0.94591 0.32204
Ga 0.02950 0.13381 0.12271
Ga 0.54918 0.58357 0.19213
Ga 0.05427 0.54717 0.57604
Ga 0.43559 0.81123 0.23923
Ga 0.07656 0.16395 0.83339
Ga 0.46861 0.83737 0.74641
Ga 0.96464 0.87707 0.78785
Ga 0.89423 0.30616 0.62120
Ga 0.21987 0.72042 0.73615
Ga 0.57644 0.37399 0.74778
Ga 0.99462 0.37353 0.33877
Ga 0.44408 0.08160 0.60086
Ga 0.77195 0.98209 0.98602
Ga 0.81714 0.75566 0.56149
Ga 0.57265 0.66212 0.56190
```

Ga 0.44811 0.56622 0.91030
Zn 0.92750 0.49400 0.05500
Zn 0.55066 0.85225 0.01855
Zn 0.99786 0.65974 0.91786
Zn 0.82893 0.48063 0.78730
Zn 0.22335 0.97058 0.69207
Zn 0.06538 0.81113 0.48022
Zn 0.81554 0.23101 0.89410
Zn 0.59668 0.13335 0.17624
Zn 0.97330 0.85652 0.08625
Zn 0.41251 0.35812 0.15318
Zn 0.01555 0.63790 0.22948
Zn 0.19724 0.23610 0.56328
Zn 0.11446 0.44504 0.79786
Zn 0.76649 0.45240 0.24753
Zn 0.82657 0.20591 0.19396
Zn 0.71567 0.00650 0.69005
Zn 0.20324 0.50924 0.03622
O 0.29903 0.87907 0.34167
O 0.59645 0.29409 0.45286
O 0.30107 0.35598 0.55212
O 0.50883 0.50871 0.55730
O 0.40647 0.91669 0.58779
O 0.12668 0.13604 0.98953
O 0.96703 0.44770 0.67142
O 0.92073 0.91063 0.93636
O 0.99328 0.25069 0.23115
O 0.29269 0.86291 0.81746
O 0.87210 0.14652 0.04693
O 0.39018 0.68927 0.67334
O 0.24400 0.07922 0.20250
O 0.08424 0.47789 0.42278
O 0.14316 0.84895 0.07690
O 0.85244 0.90076 0.66742
O 0.70089 0.30854 0.16142
O 0.28877 0.63487 0.94410
O 0.73680 0.07730 0.83864
O 0.49215 0.22960 0.69726
O 0.77004 0.85620 0.43347
O 0.27466 0.35053 0.05714
O 0.62805 0.77333 0.68117
O 0.00522 0.99632 0.20754
O 0.59327 0.75477 0.18529
O 0.51299 0.96905 0.27615

O 0.62040 0.53403 0.82717
O 0.99199 0.96627 0.46375
O 0.37926 0.15423 0.43769
O 0.04119 0.22024 0.55072
O 0.81958 0.87808 0.17678
O 0.81971 0.40251 0.95154
O 0.97091 0.68867 0.55351
O 0.53128 0.99423 0.78032
O 0.28461 0.12398 0.66198
O 0.62037 0.03988 0.04447
O 0.50160 0.47686 0.05354
O 0.51268 0.73074 0.89263
O 0.52221 0.76367 0.43598
O 0.91848 0.48652 0.22446
O 0.76657 0.09810 0.31589
O 0.62143 0.27972 0.90541
O 0.06309 0.01260 0.73763
O 0.60692 0.03510 0.51887
O 0.06112 0.77639 0.31781
O 0.36138 0.40430 0.30726
O 0.63286 0.51400 0.32688
O 0.05048 0.50463 0.94086
O 0.72969 0.61470 0.53721
O 0.83450 0.36522 0.42654
O 0.71086 0.56702 0.09773
O 0.93550 0.22931 0.77972
O 0.40290 0.44172 0.79488
O 0.92325 0.68767 0.08064
O 0.73320 0.37646 0.66012
O 0.44307 0.19478 0.18217
O 0.17950 0.29395 0.79874
O 0.70607 0.81379 0.96217
O 0.38568 0.16797 0.91995
O 0.84266 0.64527 0.81473
O 0.18743 0.82291 0.59064
O 0.39789 0.85341 0.07359
O 0.39414 0.64551 0.23535
O 0.19209 0.54930 0.68757
O 0.07623 0.75189 0.81378
O 0.81722 0.13979 0.57421
O 0.15831 0.55724 0.18769
O 0.29656 0.62868 0.46320
K_POINTS gamma

IGZO-021-4-5

Analyzing GULP Output File for Supporting Information: IGZO-021-4-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10617.70530257 Ry
Charge = 0.0000 SCF Energy = -10630.45865322 Ry
Charge = 16.7302 SCF Energy = -10637.78411630 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-021-4-5"  ,
        title = "IGZO-021-4-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.1461 ,
        B = 11.1461 ,
        C = 11.1461 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.1461  0.  0.
  6.82501784E-16  11.1461  0.
  6.82501784E-16  6.82501784E-16  11.1461
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.20562 0.94800 0.56149
Ga 0.95485 0.89636 0.61961
Ga 0.67515 0.45069 0.35696
Ga 0.41116 0.97214 0.80366
Ga 0.78118 0.30652 0.86915
Ga 0.02697 0.23183 0.96755
Ga 0.13556 0.87928 0.88009
Ga 0.58175 0.16512 0.25492
Ga 0.58626 0.78566 0.85454
Ga 0.39502 0.52540 0.51415
Ga 0.18676 0.49695 0.26156
Ga 0.27736 0.37227 0.02901
Ga 0.85896 0.63309 0.49873
Ga 0.76139 0.17454 0.51438
Ga 0.12225 0.67905 0.66919
Ga 0.68489 0.75907 0.12050
Ga 0.76586 0.94243 0.34013
Ga 0.20274 0.42340 0.65505
Ga 0.43405 0.57027 0.24192
Ga 0.46032 0.00688 0.50704
Ga 0.69442 0.91028 0.61800
Ga 0.06511 0.16882 0.67279
Ga 0.27494 0.04659 0.27111
Ga 0.78618 0.34400 0.15477
Ga 0.30871 0.63735 0.90324
Ga 0.61985 0.52505 0.99216
Ga 0.46796 0.40699 0.78820
Ga 0.86792 0.02318 0.83020
Ga 0.04750 0.52037 0.88933
Ga 0.01074 0.34724 0.44430
Ga 0.29331 0.75869 0.38860
Ga 0.91424 0.60778 0.23153
Ga 0.68470 0.40908 0.64742
```

Ga 0.40691 0.82887 0.11036
Zn 0.66534 0.00912 0.99828
Zn 0.28385 0.17948 0.84006
Zn 0.37060 0.75873 0.64293
Zn 0.81022 0.67796 0.78588
Zn 0.90023 0.75416 0.98920
Zn 0.02111 0.83976 0.34440
Zn 0.94717 0.97064 0.09807
Zn 0.06525 0.24730 0.21070
Zn 0.41717 0.12728 0.08132
Zn 0.40116 0.29667 0.39804
Zn 0.94399 0.43641 0.65694
Zn 0.61641 0.64658 0.59302
Zn 0.35478 0.21810 0.62435
Zn 0.00155 0.06743 0.37177
Zn 0.56970 0.76517 0.38278
Zn 0.14911 0.73718 0.12275
Zn 0.59339 0.14069 0.77544
O 0.69307 0.33556 0.49424
O 0.45738 0.68804 0.50560
O 0.08320 0.90474 0.72244
O 0.12673 0.10824 0.27564
O 0.54857 0.81554 0.02907
O 0.58229 0.08920 0.10540
O 0.04731 0.82947 0.02249
O 0.56863 0.96146 0.84125
O 0.58639 0.59225 0.14431
O 0.91574 0.20608 0.43963
O 0.17207 0.81374 0.28295
O 0.79956 0.90725 0.00907
O 0.31502 0.37977 0.52052
O 0.52544 0.49199 0.64334
O 0.83324 0.46754 0.25794
O 0.77529 0.55612 0.67644
O 0.61211 0.32992 0.79526
O 0.37705 0.24939 0.98424
O 0.98433 0.06869 0.95350
O 0.06850 0.58930 0.17952
O 0.12050 0.21115 0.82478
O 0.35134 0.98245 0.14657
O 0.82166 0.91288 0.51178
O 0.68304 0.08137 0.63598
O 0.27653 0.59128 0.35843
O 0.21203 0.77726 0.54345

O 0.28614 0.57599 0.64420
O 0.67332 0.83552 0.27013
O 0.37893 0.92808 0.63829
O 0.69328 0.09982 0.35560
O 0.93350 0.70508 0.36019
O 0.27593 0.97769 0.89407
O 0.64316 0.31780 0.23934
O 0.93482 0.63855 0.88620
O 0.10673 0.37147 0.32012
O 0.14575 0.28543 0.07450
O 0.20487 0.49510 0.93176
O 0.06006 0.95014 0.47929
O 0.45455 0.51304 0.91976
O 0.17149 0.71901 0.82927
O 0.49685 0.48046 0.37792
O 0.91403 0.95915 0.26275
O 0.43117 0.75662 0.27013
O 0.96832 0.71836 0.60725
O 0.07915 0.32056 0.58908
O 0.42734 0.13887 0.76424
O 0.39861 0.18697 0.26213
O 0.72915 0.40549 0.00384
O 0.42353 0.74696 0.80825
O 0.58269 0.90687 0.47996
O 0.93179 0.47769 0.49499
O 0.06836 0.51522 0.71424
O 0.70165 0.61502 0.44569
O 0.75420 0.13716 0.89176
O 0.32945 0.97015 0.41446
O 0.83443 0.87754 0.75815
O 0.46447 0.17302 0.50225
O 0.63261 0.77277 0.68711
O 0.93239 0.08053 0.68732
O 0.68525 0.66837 0.90877
O 0.21074 0.11120 0.61012
O 0.90440 0.23540 0.13121
O 0.31867 0.47021 0.16433
O 0.82675 0.68689 0.12600
O 0.96029 0.37783 0.91675
O 0.29879 0.71737 0.05390
O 0.82782 0.31801 0.69953
O 0.32208 0.35202 0.75001
K_POINTS gamma

IGZO-028-11-1

Analyzing GULP Output File for Supporting Information: IGZO-028-11-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -14.9206 SCF Energy = -9371.64497313 Ry
Charge = 0.0000 SCF Energy = -9383.42724514 Ry
Charge = 14.9206 SCF Energy = -9390.81018922 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-028-11-1"  ,
        title = "IGZO-028-11-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 10.5889 ,
        B = 10.5889 ,
        C = 10.5889 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 105  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  10.5889  0.  0.
  6.48383125E-16  10.5889  0.
  6.48383125E-16  6.48383125E-16  10.5889
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.49123 0.37279 0.87911
Ga 0.61697 0.39178 0.41087
Ga 0.08313 0.21224 0.67100
Ga 0.59588 0.70415 0.34723
Ga 0.97508 0.47920 0.63138
Ga 0.89327 0.33929 0.21850
Ga 0.99296 0.35742 0.92569
Ga 0.43023 0.89183 0.53122
Ga 0.70740 0.93619 0.55691
Ga 0.84497 0.19957 0.48644
Zn 0.00157 0.95864 0.55661
Zn 0.22610 0.18941 0.17046
Zn 0.90968 0.81013 0.34652
Zn 0.01134 0.04634 0.28308
Zn 0.09483 0.12081 0.98081
Zn 0.70920 0.71206 0.11744
Zn 0.72170 0.00445 0.27133
Zn 0.93160 0.61852 0.94028
Zn 0.54211 0.59188 0.68164
Zn 0.37484 0.07504 0.93487
Zn 0.36142 0.32266 0.38381
Zn 0.64123 0.48524 0.12189
Zn 0.42223 0.97280 0.24378
Zn 0.11591 0.36046 0.41067
Zn 0.86839 0.56780 0.34569
Zn 0.38885 0.68698 0.11720
Zn 0.19664 0.82372 0.34971
Zn 0.72129 0.32384 0.71568
Zn 0.61919 0.97105 0.05554
Zn 0.24356 0.50913 0.76132
Zn 0.22326 0.96152 0.73415
Zn 0.53442 0.14234 0.47772
Zn 0.23577 0.73020 0.64200
```

Zn 0.98501 0.85291 0.84181
Zn 0.23252 0.43988 0.02626
Zn 0.44110 0.80870 0.84924
Zn 0.58247 0.05935 0.78142
Zn 0.15703 0.57399 0.29037
Zn 0.23208 0.09290 0.44030
Zn 0.73859 0.22548 0.00292
Zn 0.74109 0.56282 0.84349
Zn 0.21510 0.90060 0.04436
Zn 0.52993 0.22887 0.14930
Zn 0.71254 0.81925 0.84553
Zn 0.86185 0.08577 0.78319
Zn 0.17194 0.66290 0.01380
Zn 0.36105 0.23406 0.67370
Zn 0.93230 0.71532 0.62168
Zn 0.36778 0.57617 0.48873
Zn 0.90428 0.91526 0.06523
O 0.88554 0.43179 0.78637
O 0.93029 0.10365 0.61439
O 0.60945 0.45133 0.78180
O 0.53714 0.54800 0.42410
O 0.00592 0.32795 0.55014
O 0.31914 0.76799 0.45868
O 0.39025 0.02845 0.41026
O 0.53326 0.03489 0.60934
O 0.75087 0.41602 0.28369
O 0.30999 0.84598 0.19624
O 0.35917 0.85642 0.69593
O 0.93519 0.00222 0.92226
O 0.87771 0.93411 0.23631
O 0.59303 0.70806 0.79917
O 0.15076 0.29295 0.06176
O 0.38978 0.11732 0.11783
O 0.52306 0.27889 0.30994
O 0.87973 0.30815 0.04447
O 0.74009 0.95239 0.72511
O 0.55375 0.63254 0.16594
O 0.08022 0.87620 0.69235
O 0.76085 0.69845 0.29466
O 0.05709 0.71206 0.32367
O 0.00844 0.45366 0.28957
O 0.87414 0.57574 0.52639
O 0.21836 0.01272 0.90236
O 0.31650 0.76020 0.96057

O 0.73950 0.84496 0.01588
O 0.72043 0.31871 0.54186
O 0.86958 0.70678 0.80034
O 0.08426 0.51665 0.94479
O 0.10069 0.59180 0.66187
O 0.44699 0.21066 0.82379
O 0.58315 0.34925 0.03688
O 0.59022 0.80600 0.49165
O 0.57439 0.90225 0.23226
O 0.86782 0.84931 0.51387
O 0.71562 0.19440 0.82406
O 0.02541 0.21373 0.83117
O 0.34874 0.46197 0.91102
O 0.92251 0.19936 0.33199
O 0.25385 0.57607 0.13836
O 0.21326 0.23471 0.34009
O 0.37002 0.60052 0.65843
O 0.71430 0.07692 0.44195
O 0.77613 0.57635 0.01747
O 0.03397 0.77470 0.99481
O 0.26510 0.47860 0.40051
O 0.51650 0.95833 0.91668
O 0.67938 0.11923 0.13576
O 0.11429 0.03514 0.13248
O 0.22021 0.10828 0.61824
O 0.44318 0.30453 0.53964
O 0.10775 0.97863 0.41378
O 0.20882 0.33465 0.71617
K_POINTS gamma

IGZO-028-11-2

Analyzing GULP Output File for Supporting Information: IGZO-028-11-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -14.9206 SCF Energy = -9372.26485597 Ry
Charge = 0.0000 SCF Energy = -9384.07297538 Ry
Charge = 14.9206 SCF Energy = -9391.37122276 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-028-11-2"  ,
        title = "IGZO-028-11-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 10.5889 ,
        B = 10.5889 ,
        C = 10.5889 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 105  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  10.5889  0.  0.
  6.48383125E-16  10.5889  0.
  6.48383125E-16  6.48383125E-16  10.5889
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.60150 0.41295 0.66158
Ga 0.40481 0.29769 0.48119
Ga 0.89453 0.49160 0.33617
Ga 0.13832 0.99535 0.86123
Ga 0.02190 0.25861 0.13698
Ga 0.83738 0.75274 0.24894
Ga 0.76560 0.59182 0.82963
Ga 0.55352 0.40867 0.02527
Ga 0.79168 0.67983 0.55193
Ga 0.53162 0.74818 0.66151
Zn 0.80426 0.32310 0.87791
Zn 0.41765 0.93996 0.81725
Zn 0.98651 0.93864 0.41240
Zn 0.15014 0.12075 0.57763
Zn 0.43788 0.60606 0.20844
Zn 0.48104 0.67056 0.93924
Zn 0.79552 0.03133 0.26130
Zn 0.25707 0.77395 0.63638
Zn 0.13711 0.60365 0.85024
Zn 0.05847 0.66968 0.46492
Zn 0.67278 0.23441 0.42372
Zn 0.55252 0.81691 0.36814
Zn 0.25571 0.87318 0.36620
Zn 0.26849 0.46416 0.03982
Zn 0.64616 0.83693 0.09801
Zn 0.35570 0.20362 0.76616
Zn 0.75292 0.27424 0.17398
Zn 0.94825 0.76413 0.96579
Zn 0.14865 0.67386 0.15990
Zn 0.60720 0.50934 0.35192
Zn 0.20799 0.14511 0.30497
Zn 0.97537 0.82159 0.68387
Zn 0.04087 0.42971 0.62319
```

Zn 0.34400 0.88997 0.07724
Zn 0.85687 0.06031 0.99311
Zn 0.41585 0.02848 0.53641
Zn 0.96938 0.50249 0.04256
Zn 0.33576 0.60478 0.47769
Zn 0.48821 0.08251 0.26928
Zn 0.95892 0.23993 0.43466
Zn 0.18294 0.44214 0.34306
Zn 0.08735 0.30460 0.86255
Zn 0.56988 0.11216 0.99538
Zn 0.07772 0.94838 0.14618
Zn 0.71987 0.99255 0.54363
Zn 0.63426 0.14010 0.71491
Zn 0.29752 0.19196 0.04750
Zn 0.92447 0.12379 0.71800
Zn 0.71407 0.89964 0.82317
Zn 0.33694 0.49281 0.75766
O 0.81234 0.33842 0.39191
O 0.14381 0.02151 0.41871
O 0.57640 0.11495 0.53938
O 0.33387 0.56897 0.91860
O 0.12014 0.72604 0.72881
O 0.88227 0.14814 0.14530
O 0.57749 0.47643 0.18442
O 0.39893 0.89092 0.64678
O 0.88220 0.47386 0.89810
O 0.83415 0.76163 0.81086
O 0.68911 0.86946 0.27328
O 0.99140 0.64479 0.26084
O 0.43652 0.04759 0.09112
O 0.92423 0.79530 0.51035
O 0.56417 0.37828 0.48528
O 0.99543 0.93292 0.97351
O 0.79751 0.71531 0.07974
O 0.48807 0.74450 0.09130
O 0.26514 0.54817 0.21147
O 0.01337 0.23913 0.60044
O 0.90611 0.56630 0.64618
O 0.65650 0.82161 0.55711
O 0.38753 0.63436 0.64867
O 0.38988 0.33193 0.02836
O 0.11576 0.36548 0.02790
O 0.31764 0.16903 0.58987
O 0.65619 0.15296 0.27390

O 0.85625 0.06414 0.43909
O 0.78165 0.02883 0.71482
O 0.48322 0.65854 0.37266
O 0.21188 0.15730 0.85880
O 0.71636 0.30053 0.72372
O 0.42660 0.93825 0.37430
O 0.70194 0.98437 0.00277
O 0.50006 0.09360 0.81619
O 0.37112 0.20380 0.33222
O 0.30204 0.43472 0.46189
O 0.06050 0.99339 0.70145
O 0.94572 0.90047 0.24451
O 0.55808 0.79714 0.82904
O 0.08783 0.28729 0.30591
O 0.65347 0.58911 0.66421
O 0.20609 0.74433 0.46047
O 0.93351 0.19526 0.88184
O 0.07383 0.64794 0.99933
O 0.66558 0.27239 0.01124
O 0.04478 0.49455 0.44666
O 0.77299 0.61396 0.39075
O 0.89209 0.40289 0.17103
O 0.27303 0.90332 0.91375
O 0.44665 0.36035 0.72268
O 0.16232 0.43478 0.75201
O 0.21173 0.84537 0.19066
O 0.61341 0.52850 0.91388
O 0.15197 0.11570 0.12915
K_POINTS gamma

IGZO-028-11-3

Analyzing GULP Output File for Supporting Information: IGZO-028-11-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -14.9206 SCF Energy = -9372.14380666 Ry
Charge = 0.0000 SCF Energy = -9383.94598216 Ry
Charge = 14.9206 SCF Energy = -9391.25215933 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-028-11-3"  ,
        title = "IGZO-028-11-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 10.5889 ,
        B = 10.5889 ,
        C = 10.5889 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 105  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  10.5889  0.  0.
  6.48383125E-16  10.5889  0.
  6.48383125E-16  6.48383125E-16  10.5889
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.14284 0.61127 0.74605
Ga 0.54765 0.37792 0.42774
Ga 0.12661 0.04480 0.41619
Ga 0.54251 0.94315 0.48016
Ga 0.27086 0.48719 0.25428
Ga 0.82166 0.46437 0.15907
Ga 0.05156 0.65360 0.04509
Ga 0.31256 0.43027 0.95431
Ga 0.09660 0.35837 0.64323
Ga 0.75709 0.69068 0.36105
Zn 0.62652 0.18702 0.61231
Zn 0.93217 0.77638 0.56422
Zn 0.82075 0.26636 0.79758
Zn 0.58280 0.49043 0.84676
Zn 0.40560 0.12885 0.28775
Zn 0.01163 0.37147 0.94543
Zn 0.61232 0.92343 0.19408
Zn 0.58764 0.64994 0.12057
Zn 0.05380 0.77020 0.31398
Zn 0.53378 0.21409 0.88555
Zn 0.39286 0.42729 0.65535
Zn 0.33630 0.18245 0.56940
Zn 0.70153 0.19596 0.20382
Zn 0.64073 0.70880 0.61084
Zn 0.22980 0.16326 0.84030
Zn 0.45273 0.96294 0.75372
Zn 0.98986 0.22119 0.24341
Zn 0.35317 0.69544 0.05631
Zn 0.84885 0.87774 0.13064
Zn 0.18930 0.97473 0.15304
Zn 0.80214 0.46778 0.50185
Zn 0.88096 0.23859 0.49902
Zn 0.23807 0.61457 0.49396
```

Zn 0.73691 0.97522 0.69544
Zn 0.41634 0.69186 0.80058
Zn 0.86236 0.54289 0.83905
Zn 0.39672 0.99535 0.02004
Zn 0.53320 0.34457 0.14148
Zn 0.21124 0.24518 0.11570
Zn 0.24050 0.84651 0.59688
Zn 0.82301 0.00760 0.38910
Zn 0.19356 0.85704 0.87541
Zn 0.98381 0.06496 0.97934
Zn 0.47977 0.63275 0.38253
Zn 0.35177 0.83942 0.31264
Zn 0.02677 0.47906 0.34520
Zn 0.64328 0.78841 0.89693
Zn 0.03576 0.03596 0.69694
Zn 0.90945 0.82446 0.84000
Zn 0.68898 0.05152 0.97204
O 0.51130 0.66469 0.95441
O 0.14452 0.98527 0.57177
O 0.59598 0.85488 0.72887
O 0.72868 0.42023 0.80744
O 0.37131 0.39543 0.12068
O 0.14760 0.61072 0.34503
O 0.96054 0.11795 0.38888
O 0.62176 0.79210 0.45357
O 0.99337 0.39279 0.50022
O 0.99718 0.78317 0.14988
O 0.83834 0.30230 0.22944
O 0.71454 0.76669 0.19697
O 0.65814 0.48112 0.10922
O 0.58015 0.92757 0.01333
O 0.35193 0.75302 0.46290
O 0.91127 0.22159 0.94925
O 0.22193 0.24380 0.68712
O 0.11050 0.02787 0.85827
O 0.21196 0.58963 0.09866
O 0.47357 0.30762 0.57370
O 0.80751 0.64021 0.55333
O 0.06210 0.09598 0.14002
O 0.11839 0.36497 0.23582
O 0.07056 0.72412 0.88717
O 0.78780 0.69817 0.86414
O 0.44736 0.36917 0.85897
O 0.75178 0.02092 0.22197

O 0.23052 0.49070 0.61953
O 0.71463 0.31822 0.50742
O 0.31783 0.10690 0.13178
O 0.85002 0.94681 0.96685
O 0.26756 0.15585 0.40261
O 0.47421 0.97156 0.30893
O 0.93496 0.20304 0.66696
O 0.28511 0.85410 0.04403
O 0.69755 0.03907 0.51687
O 0.44229 0.69620 0.21785
O 0.18003 0.91148 0.31733
O 0.62350 0.53914 0.38845
O 0.02969 0.46575 0.77306
O 0.38944 0.47376 0.38468
O 0.28466 0.56794 0.85115
O 0.31690 0.83406 0.76364
O 0.54565 0.24252 0.29543
O 0.67776 0.12070 0.78692
O 0.91586 0.83989 0.40947
O 0.51097 0.59617 0.68491
O 0.38794 0.08020 0.86401
O 0.44609 0.03545 0.59285
O 0.61742 0.19969 0.03866
O 0.18100 0.31700 0.95766
O 0.93723 0.51323 0.02752
O 0.89605 0.90654 0.68554
O 0.10235 0.72001 0.60699
O 0.87660 0.56329 0.30091
K_POINTS gamma

IGZO-028-11-4

Analyzing GULP Output File for Supporting Information: IGZO-028-11-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -14.9206 SCF Energy = -9372.02033798 Ry
Charge = 0.0000 SCF Energy = -9383.82454029 Ry
Charge = 14.9206 SCF Energy = -9391.10922512 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-028-11-4"  ,
        title = "IGZO-028-11-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 10.5889 ,
        B = 10.5889 ,
        C = 10.5889 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 105  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  10.5889  0.  0.
  6.48383125E-16  10.5889  0.
  6.48383125E-16  6.48383125E-16  10.5889
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.35292 0.43296 0.39863
Ga 0.88890 0.40274 0.23698
Ga 0.67191 0.43283 0.46921
Ga 0.62788 0.21365 0.78139
Ga 0.00693 0.70801 0.75780
Ga 0.59531 0.13000 0.51072
Ga 0.87024 0.79162 0.00436
Ga 0.90192 0.22043 0.86290
Ga 0.14266 0.58903 0.27264
Ga 0.45673 0.71016 0.46455
Zn 0.72838 0.65954 0.69009
Zn 0.61129 0.97242 0.98948
Zn 0.17545 0.24856 0.90663
Zn 0.02803 0.10448 0.34156
Zn 0.43291 0.25342 0.99382
Zn 0.71878 0.83343 0.48355
Zn 0.42206 0.80986 0.16144
Zn 0.36430 0.52327 0.07120
Zn 0.09082 0.51346 0.99194
Zn 0.34362 0.96203 0.90547
Zn 0.15781 0.80913 0.07274
Zn 0.21509 0.32055 0.15899
Zn 0.50059 0.06578 0.24996
Zn 0.86338 0.19997 0.58377
Zn 0.76422 0.07244 0.27900
Zn 0.19453 0.63386 0.55448
Zn 0.51692 0.29028 0.23287
Zn 0.69888 0.25224 0.05881
Zn 0.54500 0.91218 0.71449
Zn 0.91800 0.82329 0.27112
Zn 0.05534 0.36615 0.45798
Zn 0.25950 0.07195 0.16655
Zn 0.99029 0.06448 0.08555
```

Zn 0.10565 0.18111 0.65839
Zn 0.27537 0.90273 0.62632
Zn 0.99401 0.89703 0.56094
Zn 0.28655 0.69601 0.83486
Zn 0.64104 0.51768 0.05851
Zn 0.65142 0.73721 0.22220
Zn 0.28360 0.12676 0.44421
Zn 0.81095 0.94476 0.76518
Zn 0.36160 0.17480 0.71507
Zn 0.54629 0.71113 0.92183
Zn 0.90613 0.60608 0.47597
Zn 0.09127 0.96242 0.83112
Zn 0.06659 0.44128 0.71323
Zn 0.58051 0.48879 0.77286
Zn 0.83588 0.49225 0.91024
Zn 0.32642 0.43671 0.80020
Zn 0.20089 0.85667 0.35460
O 0.45269 0.10719 0.40536
O 0.52997 0.66860 0.09172
O 0.99874 0.06850 0.53280
O 0.95706 0.26182 0.32150
O 0.78497 0.43047 0.10509
O 0.32957 0.13315 0.88216
O 0.29548 0.92185 0.08484
O 0.63595 0.53430 0.60350
O 0.90080 0.61244 0.65720
O 0.13409 0.16470 0.09317
O 0.81443 0.48236 0.38971
O 0.61277 0.71460 0.38845
O 0.92206 0.00325 0.24261
O 0.79520 0.11488 0.73309
O 0.81161 0.74552 0.15748
O 0.89221 0.78630 0.44389
O 0.51961 0.39166 0.38081
O 0.52901 0.07673 0.67993
O 0.74543 0.33485 0.84071
O 0.52529 0.39613 0.07413
O 0.75689 0.89714 0.92310
O 0.56360 0.92204 0.17177
O 0.42428 0.81548 0.59986
O 0.23239 0.30310 0.42318
O 0.95379 0.65806 0.92199
O 0.48598 0.33008 0.76565
O 0.23046 0.86691 0.80479

O 0.02038 0.90420 0.00337
O 0.99886 0.39714 0.88589
O 0.96657 0.87456 0.73519
O 0.15709 0.80273 0.53913
O 0.10072 0.75516 0.23862
O 0.34676 0.57857 0.50342
O 0.21673 0.33038 0.72578
O 0.22198 0.65477 0.00849
O 0.65222 0.18842 0.21500
O 0.26662 0.38822 0.98890
O 0.35564 0.77258 0.32122
O 0.49731 0.87102 0.88663
O 0.04858 0.47750 0.17111
O 0.70442 0.00903 0.42960
O 0.15227 0.60434 0.72773
O 0.29337 0.48344 0.24112
O 0.38611 0.19963 0.16811
O 0.85895 0.16340 0.02016
O 0.69339 0.26403 0.52481
O 0.19333 0.03042 0.33343
O 0.43446 0.58745 0.83984
O 0.70193 0.83029 0.66239
O 0.98641 0.32143 0.62104
O 0.04981 0.13413 0.81658
O 0.25336 0.08372 0.61083
O 0.08157 0.53882 0.42898
O 0.68775 0.59578 0.88320
O 0.59326 0.15503 0.95254
K_POINTS gamma

IGZO-028-11-5

Analyzing GULP Output File for Supporting Information: IGZO-028-11-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -14.9206 SCF Energy = -9371.55961936 Ry
Charge = 0.0000 SCF Energy = -9383.32941410 Ry
Charge = 14.9206 SCF Energy = -9390.66001066 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-028-11-5"  ,
        title = "IGZO-028-11-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 10.5889 ,
        B = 10.5889 ,
        C = 10.5889 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 105  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  10.5889  0.  0.
  6.48383125E-16  10.5889  0.
  6.48383125E-16  6.48383125E-16  10.5889
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
Ga 0.37209 0.39915 0.51666
Ga 0.71256 0.46620 0.34459
Ga 0.21101 0.94025 0.94057
Ga 0.83884 0.91010 0.26131
Ga 0.58530 0.47187 0.04590
Ga 0.56737 0.20364 0.37296
Ga 0.69113 0.74335 0.46136
Ga 0.67120 0.18603 0.04674
Ga 0.08775 0.70809 0.38907
Ga 0.61850 0.95292 0.91990
Zn 0.08114 0.09534 0.76661
Zn 0.95580 0.66454 0.62787
Zn 0.76975 0.50771 0.83130
Zn 0.89036 0.00423 0.99148
Zn 0.82806 0.19908 0.48772
Zn 0.72514 0.20319 0.75992
Zn 0.85901 0.46440 0.10816
Zn 0.70011 0.77364 0.73290
Zn 0.59798 0.04583 0.63105
Zn 0.29495 0.82330 0.23748
Zn 0.35612 0.17440 0.96065
Zn 0.05293 0.53787 0.89817
Zn 0.18205 0.90448 0.58164
Zn 0.45207 0.08461 0.16387
Zn 0.07136 0.76152 0.10366
Zn 0.50488 0.31842 0.80340
Zn 0.87623 0.16363 0.20467
Zn 0.55528 0.82429 0.22270
Zn 0.88951 0.95988 0.62600
Zn 0.00294 0.26999 0.98934
Zn 0.99410 0.42846 0.40511
Zn 0.31045 0.46898 0.95746
Zn 0.48460 0.58317 0.76176
```

Zn 0.12876 0.48349 0.19184
Zn 0.93183 0.37897 0.69144
Zn 0.29679 0.29491 0.26281
Zn 0.98040 0.80328 0.86284
Zn 0.34144 0.14406 0.68215
Zn 0.14136 0.24150 0.47116
Zn 0.20638 0.34530 0.75673
Zn 0.40844 0.86747 0.72286
Zn 0.43698 0.94320 0.44572
Zn 0.20626 0.68899 0.77011
Zn 0.43549 0.73140 0.00063
Zn 0.64665 0.47056 0.61665
Zn 0.40368 0.54851 0.24419
Zn 0.02253 0.03105 0.42999
Zn 0.37237 0.70118 0.50088
Zn 0.76261 0.73752 0.02231
Zn 0.16835 0.08024 0.18966
O 0.65766 0.61216 0.74506
O 0.02188 0.13210 0.10312
O 0.90456 0.80510 0.11657
O 0.76714 0.02805 0.14137
O 0.98765 0.85594 0.38312
O 0.02710 0.96399 0.88930
O 0.74987 0.55091 0.00192
O 0.80743 0.79703 0.59003
O 0.24338 0.79542 0.42331
O 0.35056 0.83449 0.89445
O 0.24620 0.07546 0.82490
O 0.36630 0.70148 0.68509
O 0.03504 0.43564 0.04131
O 0.47930 0.42907 0.65459
O 0.09246 0.78173 0.67753
O 0.60091 0.81619 0.03488
O 0.40525 0.28053 0.38651
O 0.50606 0.06437 0.98927
O 0.81490 0.28774 0.10235
O 0.80520 0.81750 0.87093
O 0.13579 0.36845 0.33526
O 0.58512 0.91127 0.74735
O 0.33896 0.97893 0.60401
O 0.24684 0.28015 0.60315
O 0.42130 0.70413 0.18806
O 0.35091 0.31926 0.87251
O 0.96782 0.30888 0.54127

O 0.03004 0.58040 0.49100
O 0.69983 0.81263 0.30531
O 0.42510 0.94518 0.25879
O 0.03681 0.25598 0.80965
O 0.04477 0.02452 0.60369
O 0.20477 0.50852 0.81440
O 0.59034 0.48110 0.21969
O 0.60255 0.32967 0.95540
O 0.36303 0.54491 0.42463
O 0.87191 0.47647 0.27764
O 0.77430 0.09509 0.62937
O 0.10481 0.70604 0.93076
O 0.12306 0.65646 0.22668
O 0.55639 0.06759 0.46575
O 0.87412 0.08798 0.36333
O 0.75155 0.10106 0.90393
O 0.51134 0.16949 0.70879
O 0.52512 0.78939 0.48335
O 0.94083 0.54602 0.76761
O 0.30173 0.16082 0.12164
O 0.18636 0.90567 0.11033
O 0.15522 0.10641 0.35739
O 0.69512 0.31495 0.43657
O 0.75202 0.37022 0.72498
O 0.57504 0.19972 0.20278
O 0.30214 0.44688 0.14153
O 0.47283 0.56618 0.94295
O 0.69660 0.57219 0.47800
K_POINTS gamma

IGZO-110-3-1

Analyzing GULP Output File for Supporting Information: IGZO-110-3-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -10452.68822187 Ry
Charge = 0.0000 SCF Energy = -10466.67840981 Ry
Charge = 17.4603 SCF Energy = -10475.72553135 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-110-3-1"  ,
        title = "IGZO-110-3-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.5264 ,
        B = 11.5264 ,
        C = 11.5264 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.5264  0.  0.
  7.05788443E-16  11.5264  0.
  7.05788443E-16  7.05788443E-16  11.5264
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.16649 0.55529 0.41952
In 0.30636 0.02229 0.32120
In 0.89039 0.25118 0.82452
In 0.53001 0.31530 0.15474
In 0.60936 0.65864 0.51088
In 0.67338 0.38935 0.65911
In 0.06873 0.12640 0.02208
In 0.80753 0.16438 0.14131
In 0.62965 0.09634 0.68848
In 0.29504 0.10051 0.68994
In 0.10145 0.40082 0.99012
In 0.14472 0.36423 0.73308
In 0.47726 0.83603 0.79580
In 0.23500 0.62255 0.84709
In 0.02175 0.11124 0.30537
In 0.58237 0.92297 0.27144
In 0.65153 0.89657 0.98189
In 0.81189 0.51423 0.06587
In 0.84025 0.87174 0.17924
In 0.35848 0.09119 0.02409
In 0.92761 0.46475 0.53581
In 0.16855 0.27001 0.47958
In 0.12982 0.87748 0.14822
In 0.30401 0.71607 0.59010
In 0.46824 0.20704 0.44484
Ga 0.57018 0.55834 0.87515
Ga 0.03128 0.07027 0.63367
Ga 0.60792 0.64096 0.16511
Ga 0.97518 0.39016 0.25325
Ga 0.00539 0.77122 0.65989
Ga 0.70942 0.42875 0.36162
Ga 0.79924 0.91881 0.50399
Ga 0.39393 0.33637 0.87001
```

Ga 0.37778 0.51817 0.07648
Ga 0.39873 0.79469 0.06390
Ga 0.85858 0.65936 0.34141
Ga 0.36111 0.74194 0.31020
Ga 0.96554 0.77208 0.93124
Ga 0.40883 0.42545 0.63507
Ga 0.44936 0.46844 0.37120
Ga 0.88775 0.98169 0.87053
Ga 0.18494 0.90899 0.84193
Ga 0.46899 0.89623 0.51638
Ga 0.06907 0.83552 0.42430
Ga 0.63726 0.18339 0.92036
Ga 0.75758 0.72309 0.74252
Ga 0.10528 0.62007 0.15291
Ga 0.82978 0.18168 0.47246
Ga 0.90237 0.51671 0.80049
Ga 0.25950 0.30331 0.22004
O 0.13664 0.94883 0.33069
O 0.77795 0.66844 0.19954
O 0.01445 0.75064 0.08338
O 0.48196 0.75147 0.61591
O 0.55206 0.23650 0.60383
O 0.86444 0.39533 0.93831
O 0.42101 0.65120 0.16300
O 0.30539 0.79850 0.77346
O 0.33123 0.28889 0.70722
O 0.23399 0.27777 0.06127
O 0.04219 0.95359 0.92291
O 0.98553 0.55959 0.36671
O 0.47547 0.19027 0.91404
O 0.73918 0.87973 0.36136
O 0.13913 0.95608 0.67820
O 0.50310 0.43214 0.77777
O 0.24374 0.81137 0.01487
O 0.77368 0.32994 0.49639
O 0.95116 0.86973 0.53218
O 0.99236 0.50738 0.12046
O 0.69637 0.55296 0.74823
O 0.46096 0.40281 0.00714
O 0.12861 0.71408 0.53089
O 0.81528 0.14924 0.32519
O 0.97215 0.00466 0.16470
O 0.34478 0.36006 0.45727
O 0.19532 0.19519 0.31000

O 0.45906 0.92519 0.97732
O 0.51627 0.78057 0.38450
O 0.58812 0.79484 0.12584
O 0.97251 0.09236 0.48982
O 0.91579 0.62923 0.65694
O 0.31004 0.11719 0.49852
O 0.66681 0.25447 0.06019
O 0.26140 0.43466 0.86788
O 0.63365 0.76313 0.84513
O 0.98586 0.30971 0.40518
O 0.81653 0.40878 0.23670
O 0.89033 0.38450 0.69912
O 0.71738 0.78972 0.58868
O 0.31298 0.85525 0.46282
O 0.20656 0.04243 0.11769
O 0.88173 0.83492 0.77801
O 0.11501 0.43754 0.57098
O 0.41867 0.17249 0.20324
O 0.30566 0.54683 0.66375
O 0.66700 0.03126 0.85407
O 0.26817 0.04579 0.86785
O 0.86558 0.62952 0.91029
O 0.70344 0.24821 0.78653
O 0.15451 0.41915 0.28135
O 0.90928 0.07731 0.73421
O 0.21632 0.55680 0.05835
O 0.12158 0.19600 0.64471
O 0.35485 0.60425 0.41341
O 0.37581 0.88173 0.21251
O 0.49950 0.02232 0.40878
O 0.76868 0.56534 0.44815
O 0.82994 0.87139 0.99420
O 0.99533 0.25584 0.14979
O 0.68959 0.00295 0.13537
O 0.59191 0.53516 0.29280
O 0.38462 0.41273 0.22692
O 0.95001 0.78665 0.32433
O 0.53664 0.48029 0.53188
O 0.05866 0.49797 0.83133
O 0.63532 0.55148 0.02896
O 0.08598 0.74331 0.81574
O 0.42133 0.63628 0.93424
O 0.57375 0.32019 0.33968
O 0.73434 0.05538 0.54691

O 0.07228 0.24726 0.87950
O 0.86647 0.12794 0.96647
O 0.19330 0.70787 0.26954
O 0.47604 0.98612 0.66387
K_POINTS gamma

IGZO-110-3-2

Analyzing GULP Output File for Supporting Information: IGZO-110-3-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -10452.47780064 Ry
Charge = 0.0000 SCF Energy = -10466.45164716 Ry
Charge = 17.4603 SCF Energy = -10475.46091504 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-110-3-2"  ,
        title = "IGZO-110-3-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.5264 ,
        B = 11.5264 ,
        C = 11.5264 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.5264  0.  0.
  7.05788443E-16  11.5264  0.
  7.05788443E-16  7.05788443E-16  11.5264
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.84275 0.12488 0.35600
In 0.12826 0.98875 0.24521
In 0.33917 0.76021 0.75773
In 0.24700 0.23055 0.15548
In 0.27753 0.70423 0.26314
In 0.97075 0.03727 0.56404
In 0.14824 0.79642 0.01277
In 0.15115 0.80228 0.50145
In 0.75709 0.57253 0.10356
In 0.92097 0.18369 0.09869
In 0.40289 0.95445 0.25991
In 0.67797 0.61557 0.60489
In 0.62828 0.82836 0.81178
In 0.79829 0.27886 0.67181
In 0.55847 0.35793 0.56361
In 0.61144 0.07623 0.48272
In 0.30232 0.09015 0.46284
In 0.44333 0.44675 0.09865
In 0.83523 0.90232 0.09642
In 0.96179 0.70609 0.22798
In 0.37907 0.57522 0.56496
In 0.60857 0.49850 0.87174
In 0.49618 0.72787 0.05563
In 0.37049 0.98707 0.95418
In 0.77977 0.41795 0.37661
Ga 0.51927 0.58664 0.31268
Ga 0.11672 0.61821 0.77804
Ga 0.62611 0.05275 0.12474
Ga 0.82755 0.69832 0.89695
Ga 0.28544 0.30723 0.63520
Ga 0.65525 0.28014 0.01720
Ga 0.11344 0.11517 0.95227
Ga 0.97589 0.59515 0.49291
```

Ga 0.49366 0.80482 0.51476
Ga 0.27822 0.39407 0.35818
Ga 0.96340 0.77852 0.69538
Ga 0.64633 0.81778 0.28873
Ga 0.05433 0.31121 0.48911
Ga 0.81674 0.83133 0.46222
Ga 0.87669 0.00119 0.84609
Ga 0.13529 0.50981 0.04154
Ga 0.15450 0.97790 0.73620
Ga 0.08217 0.31292 0.78486
Ga 0.64898 0.13354 0.80682
Ga 0.54459 0.27959 0.30315
Ga 0.90616 0.40002 0.92797
Ga 0.30424 0.49652 0.86845
Ga 0.98838 0.42087 0.23340
Ga 0.38227 0.24331 0.89055
Ga 0.43931 0.03932 0.68676
O 0.11577 0.13714 0.77198
O 0.80620 0.05682 0.18749
O 0.13350 0.35404 0.63016
O 0.33401 0.75652 0.54553
O 0.03617 0.26178 0.95061
O 0.02978 0.62133 0.63988
O 0.45873 0.04094 0.11120
O 0.27617 0.57793 0.71324
O 0.28149 0.08374 0.27619
O 0.44825 0.96895 0.52544
O 0.01138 0.05729 0.36911
O 0.78521 0.72317 0.72156
O 0.14639 0.37570 0.24292
O 0.79821 0.99849 0.49506
O 0.67722 0.10996 0.97547
O 0.14955 0.79831 0.71644
O 0.34844 0.16811 0.62618
O 0.14782 0.63871 0.13969
O 0.92781 0.21432 0.53263
O 0.51773 0.74476 0.67405
O 0.16546 0.95826 0.92952
O 0.37934 0.34141 0.24079
O 0.97701 0.43856 0.43001
O 0.64336 0.87318 0.12076
O 0.97110 0.94728 0.73832
O 0.53329 0.61165 0.47067
O 0.65231 0.67651 0.94055

O 0.30243 0.55527 0.38380
O 0.73171 0.43970 0.56642
O 0.78800 0.88004 0.90170
O 0.94560 0.04915 0.97397
O 0.26971 0.41916 0.03396
O 0.58937 0.43169 0.33416
O 0.96050 0.82835 0.54271
O 0.80931 0.31453 0.02460
O 0.61884 0.20124 0.62861
O 0.21842 0.87112 0.34725
O 0.82225 0.82912 0.29159
O 0.92953 0.35478 0.77241
O 0.62006 0.22231 0.17134
O 0.46371 0.18811 0.41056
O 0.98738 0.47049 0.06793
O 0.86987 0.71570 0.06193
O 0.42795 0.60372 0.18653
O 0.81546 0.65921 0.47860
O 0.66474 0.31451 0.83031
O 0.06194 0.67893 0.38914
O 0.37886 0.39953 0.53140
O 0.98896 0.70731 0.85130
O 0.46619 0.79258 0.31957
O 0.15513 0.99017 0.56761
O 0.03929 0.86356 0.14300
O 0.59799 0.99507 0.31006
O 0.44003 0.55938 0.93817
O 0.45309 0.82277 0.90772
O 0.20013 0.27384 0.43621
O 0.10083 0.12816 0.12618
O 0.28030 0.16393 0.96810
O 0.64661 0.66276 0.23593
O 0.48613 0.30833 0.98787
O 0.32266 0.95237 0.76004
O 0.31858 0.34922 0.79427
O 0.86453 0.53751 0.24811
O 0.47668 0.12171 0.83265
O 0.65269 0.82485 0.47094
O 0.90434 0.28305 0.25484
O 0.70093 0.24066 0.41147
O 0.23125 0.66549 0.90779
O 0.30921 0.83293 0.12926
O 0.12613 0.47982 0.86172
O 0.53571 0.49928 0.69565

O 0.59449 0.98054 0.72557
O 0.62383 0.46074 0.07216
O 0.80809 0.52878 0.91049
O 0.80159 0.11147 0.75697
K_POINTS gamma

IGZO-110-3-3

Analyzing GULP Output File for Supporting Information: IGZO-110-3-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -10452.41897588 Ry
Charge = 0.0000 SCF Energy = -10466.41521826 Ry
Charge = 17.4603 SCF Energy = -10475.43084302 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-110-3-3"  ,
        title = "IGZO-110-3-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.5264 ,
        B = 11.5264 ,
        C = 11.5264 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.5264  0.  0.
  7.05788443E-16  11.5264  0.
  7.05788443E-16  7.05788443E-16  11.5264
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.58789 0.54979 0.47793
In 0.03414 0.30559 0.11139
In 0.62378 0.83813 0.55242
In 0.66653 0.95645 0.79557
In 0.85155 0.74876 0.79342
In 0.15461 0.92387 0.48507
In 0.85272 0.72872 0.50124
In 0.17403 0.96335 0.75358
In 0.69186 0.47082 0.74007
In 0.43941 0.83925 0.21345
In 0.59618 0.68705 0.90158
In 0.14627 0.68301 0.72052
In 0.19433 0.15443 0.31502
In 0.43818 0.97498 0.96222
In 0.32802 0.65932 0.43951
In 0.89417 0.00268 0.58246
In 0.58462 0.41093 0.18478
In 0.73697 0.94821 0.05920
In 0.78159 0.22078 0.75288
In 0.28872 0.25364 0.81952
In 0.68179 0.21133 0.50020
In 0.01182 0.35995 0.81079
In 0.81022 0.52990 0.03380
In 0.41729 0.80169 0.68040
In 0.32511 0.28059 0.08871
Ga 0.12370 0.52235 0.95329
Ga 0.39677 0.51039 0.85055
Ga 0.96149 0.28927 0.48022
Ga 0.64255 0.67365 0.22226
Ga 0.18598 0.43489 0.61425
Ga 0.90923 0.51737 0.59036
Ga 0.46184 0.08490 0.68169
Ga 0.31041 0.73810 0.96025
```

Ga 0.52793 0.13547 0.21388
Ga 0.83841 0.47352 0.30626
Ga 0.04880 0.80740 0.96793
Ga 0.17424 0.82259 0.22929
Ga 0.10876 0.53927 0.25128
Ga 0.92536 0.74320 0.19539
Ga 0.69244 0.94201 0.31217
Ga 0.20402 0.01537 0.03593
Ga 0.95310 0.07638 0.90761
Ga 0.18443 0.17006 0.57064
Ga 0.54410 0.25651 0.92486
Ga 0.42867 0.06547 0.43028
Ga 0.34237 0.58043 0.15458
Ga 0.31144 0.39170 0.35187
Ga 0.43676 0.33908 0.58265
Ga 0.97656 0.01584 0.19391
Ga 0.77829 0.22668 0.24415
O 0.29176 0.74001 0.13207
O 0.41382 0.36998 0.93469
O 0.07675 0.03598 0.61856
O 0.82830 0.31908 0.38449
O 0.89197 0.56547 0.42426
O 0.69260 0.77775 0.39195
O 0.70075 0.08353 0.20155
O 0.52459 0.98586 0.31757
O 0.77697 0.59837 0.85939
O 0.92921 0.17108 0.21364
O 0.61063 0.37087 0.59940
O 0.33316 0.68014 0.79573
O 0.03129 0.41812 0.54220
O 0.10372 0.88290 0.09264
O 0.09339 0.97889 0.30026
O 0.21468 0.58743 0.56487
O 0.64840 0.09440 0.67427
O 0.42972 0.45387 0.46228
O 0.47552 0.95606 0.55562
O 0.86716 0.40713 0.70871
O 0.06983 0.70205 0.26236
O 0.33503 0.97596 0.13226
O 0.27335 0.05925 0.44650
O 0.59430 0.78814 0.72344
O 0.06771 0.18571 0.44709
O 0.67429 0.33111 0.87098
O 0.81163 0.63641 0.20560

O 0.47969 0.80351 0.98831
O 0.37743 0.58806 0.99340
O 0.98005 0.45933 0.97724
O 0.92815 0.71635 0.02674
O 0.95664 0.65788 0.65931
O 0.85924 0.20494 0.58826
O 0.63217 0.83823 0.17666
O 0.39907 0.42373 0.20000
O 0.02238 0.85037 0.81462
O 0.19071 0.32757 0.25325
O 0.76617 0.36937 0.14953
O 0.53893 0.55227 0.79324
O 0.66645 0.51223 0.32071
O 0.46203 0.95927 0.78407
O 0.29010 0.10254 0.68782
O 0.14340 0.27895 0.69439
O 0.72842 0.83247 0.91344
O 0.23627 0.83887 0.64003
O 0.74280 0.01728 0.44567
O 0.98170 0.44694 0.22071
O 0.90747 0.00788 0.03988
O 0.17034 0.33340 0.95550
O 0.48225 0.21504 0.78066
O 0.62093 0.24704 0.31704
O 0.91440 0.22619 0.90130
O 0.25341 0.54741 0.32299
O 0.26288 0.30927 0.49203
O 0.47292 0.19081 0.52532
O 0.34786 0.13997 0.96704
O 0.47846 0.70142 0.53166
O 0.98064 0.85522 0.49149
O 0.38185 0.17916 0.27579
O 0.26550 0.89657 0.91690
O 0.14636 0.13574 0.12990
O 0.34243 0.40799 0.69743
O 0.10967 0.07021 0.89786
O 0.78972 0.85631 0.63958
O 0.62125 0.57973 0.07242
O 0.28203 0.82133 0.35567
O 0.14677 0.68580 0.91851
O 0.53746 0.24070 0.09282
O 0.84474 0.04005 0.79217
O 0.17739 0.53090 0.10391
O 0.86386 0.88968 0.23136

```
O 0.12525 0.49840 0.78756
O 0.61484 0.04928 0.95614
O 0.73876 0.59718 0.58997
O 0.47784 0.65944 0.27192
K_POINTS  gamma
```

IGZO-110-3-4

Analyzing GULP Output File for Supporting Information: IGZO-110-3-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -10452.45019548 Ry
Charge = 0.0000 SCF Energy = -10466.49300101 Ry
Charge = 17.4603 SCF Energy = -10475.49900994 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-110-3-4"  ,
        title = "IGZO-110-3-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.5264 ,
        B = 11.5264 ,
        C = 11.5264 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.5264  0.  0.
  7.05788443E-16  11.5264  0.
  7.05788443E-16  7.05788443E-16  11.5264
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.82751 0.65197 0.92801
In 0.57339 0.14074 0.38756
In 0.49837 0.43196 0.25955
In 0.72414 0.02892 0.04308
In 0.77602 0.44208 0.71160
In 0.02055 0.24507 0.34624
In 0.46107 0.87824 0.23042
In 0.72811 0.70120 0.21286
In 0.81213 0.46295 0.36210
In 0.41053 0.02171 0.91983
In 0.63535 0.07948 0.74567
In 0.86868 0.01970 0.30958
In 0.17920 0.29250 0.90463
In 0.99889 0.13150 0.06170
In 0.67468 0.76371 0.70625
In 0.10104 0.54055 0.41905
In 0.33605 0.74183 0.77716
In 0.89167 0.92940 0.78807
In 0.30670 0.16011 0.69566
In 0.80669 0.19050 0.54666
In 0.08775 0.01796 0.54940
In 0.09389 0.61142 0.89157
In 0.59014 0.78737 0.97913
In 0.02917 0.35383 0.63961
In 0.21919 0.34843 0.18240
Ga 0.26132 0.07260 0.14950
Ga 0.48793 0.19449 0.11331
Ga 0.32011 0.13556 0.41569
Ga 0.26334 0.79698 0.03501
Ga 0.76514 0.91001 0.52286
Ga 0.82045 0.24434 0.87296
Ga 0.50743 0.32371 0.84592
Ga 0.27882 0.45830 0.70342
```

Ga 0.65630 0.45926 0.01489
Ga 0.16546 0.89261 0.29835
Ga 0.29683 0.62900 0.27681
Ga 0.00421 0.63194 0.15554
Ga 0.32125 0.38539 0.45626
Ga 0.54043 0.62332 0.43954
Ga 0.14961 0.96999 0.85692
Ga 0.21993 0.75299 0.55396
Ga 0.72641 0.27423 0.20871
Ga 0.54712 0.56373 0.73588
Ga 0.46283 0.88316 0.50712
Ga 0.37719 0.53727 0.99621
Ga 0.92097 0.38701 0.06262
Ga 0.94068 0.77955 0.39597
Ga 0.99208 0.86404 0.08240
Ga 0.58512 0.35277 0.53362
Ga 0.96883 0.69151 0.66729
O 0.45381 0.05646 0.74476
O 0.41858 0.56713 0.15377
O 0.02500 0.09767 0.24435
O 0.59460 0.34713 0.11445
O 0.01974 0.68957 0.50693
O 0.98687 0.53235 0.01942
O 0.81876 0.08342 0.88339
O 0.25036 0.02523 0.30769
O 0.15574 0.46254 0.80274
O 0.60834 0.88622 0.58128
O 0.74390 0.40781 0.53034
O 0.18900 0.19170 0.08023
O 0.78051 0.79742 0.37641
O 0.95872 0.72854 0.82768
O 0.39830 0.24239 0.23849
O 0.83405 0.23305 0.33065
O 0.88025 0.74604 0.08194
O 0.59344 0.64346 0.58712
O 0.66970 0.62032 0.05220
O 0.71013 0.59477 0.78612
O 0.91370 0.60968 0.29924
O 0.65779 0.24329 0.84675
O 0.29561 0.45997 0.31267
O 0.28064 0.87922 0.87357
O 0.21472 0.42209 0.56185
O 0.28925 0.63998 0.93197
O 0.63546 0.85084 0.15712

O 0.02965 0.34814 0.18452
O 0.10282 0.73666 0.03758
O 0.72748 0.04032 0.42010
O 0.15597 0.70169 0.70714
O 0.57307 0.41044 0.69533
O 0.47729 0.47204 0.45320
O 0.05800 0.96200 0.71944
O 0.41561 0.25720 0.48410
O 0.38173 0.57511 0.70682
O 0.01983 0.96869 0.94829
O 0.87575 0.97502 0.12967
O 0.47826 0.76165 0.38066
O 0.79534 0.43220 0.16974
O 0.62064 0.20112 0.56806
O 0.51208 0.48005 0.91702
O 0.98473 0.28052 0.94124
O 0.83602 0.78996 0.63180
O 0.98791 0.17741 0.51675
O 0.58922 0.97607 0.92684
O 0.93717 0.93773 0.45923
O 0.93680 0.52839 0.69291
O 0.13969 0.24035 0.71868
O 0.15493 0.86583 0.46315
O 0.85513 0.28160 0.71096
O 0.52330 0.72632 0.81867
O 0.20286 0.25622 0.38123
O 0.02877 0.82886 0.25882
O 0.13888 0.59480 0.22945
O 0.18644 0.94382 0.09463
O 0.97997 0.40911 0.45049
O 0.77820 0.42862 0.91842
O 0.28561 0.78298 0.23839
O 0.35181 0.82423 0.60382
O 0.78527 0.01577 0.65079
O 0.26301 0.08098 0.55228
O 0.62055 0.31429 0.34620
O 0.81244 0.22030 0.07590
O 0.64400 0.56968 0.32870
O 0.44961 0.21058 0.95750
O 0.41756 0.80580 0.04765
O 0.36136 0.32908 0.77070
O 0.62369 0.12145 0.18941
O 0.25695 0.64562 0.44596
O 0.27627 0.41389 0.02896

O 0.23888 0.10378 0.87667
O 0.75381 0.82926 0.87852
O 0.41213 0.03974 0.11951
O 0.45327 0.00572 0.40127
K_POINTS gamma

IGZO-110-3-5

Analyzing GULP Output File for Supporting Information: IGZO-110-3-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -10452.34030074 Ry
Charge = 0.0000 SCF Energy = -10466.39597963 Ry
Charge = 17.4603 SCF Energy = -10475.44779065 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-110-3-5"  ,
        title = "IGZO-110-3-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.5264 ,
        B = 11.5264 ,
        C = 11.5264 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.5264  0.  0.
  7.05788443E-16  11.5264  0.
  7.05788443E-16  7.05788443E-16  11.5264
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.33236 0.89386 0.03181
In 0.58874 0.77548 0.18098
In 0.33306 0.38388 0.34508
In 0.47196 0.94926 0.76400
In 0.30331 0.11427 0.36678
In 0.33127 0.86916 0.50633
In 0.82551 0.13365 0.89506
In 0.23816 0.60296 0.56599
In 0.51676 0.23367 0.78047
In 0.54167 0.29615 0.45596
In 0.87518 0.63891 0.22367
In 0.16393 0.46036 0.04906
In 0.82390 0.85096 0.00164
In 0.05171 0.77105 0.75790
In 0.79194 0.89234 0.34342
In 0.29485 0.69293 0.82000
In 0.00591 0.50118 0.68023
In 0.75170 0.37077 0.70815
In 0.75659 0.15444 0.17179
In 0.24148 0.69343 0.27320
In 0.66121 0.38306 0.98470
In 0.44623 0.28816 0.09481
In 0.06792 0.43321 0.40242
In 0.87607 0.93393 0.66010
In 0.02886 0.14693 0.37051
Ga 0.52448 0.63453 0.37906
Ga 0.81217 0.32195 0.40545
Ga 0.33222 0.43172 0.83911
Ga 0.92679 0.37506 0.13225
Ga 0.16541 0.02983 0.63713
Ga 0.25218 0.29323 0.62634
Ga 0.66324 0.46349 0.24253
Ga 0.55003 0.98858 0.35492
```

Ga 0.64329 0.80788 0.55055
Ga 0.01375 0.74996 0.44913
Ga 0.75882 0.64019 0.75811
Ga 0.43323 0.55665 0.09416
Ga 0.86739 0.58239 0.95051
Ga 0.68319 0.10527 0.57326
Ga 0.06974 0.92453 0.22598
Ga 0.16183 0.15448 0.07811
Ga 0.58919 0.03407 0.00576
Ga 0.51349 0.56350 0.63017
Ga 0.30678 0.13424 0.87147
Ga 0.57358 0.74803 0.89116
Ga 0.78868 0.60025 0.49201
Ga 0.07907 0.76155 0.06154
Ga 0.05815 0.97629 0.91090
Ga 0.03120 0.32212 0.88582
Ga 0.95685 0.20890 0.63221
O 0.37173 0.52646 0.70526
O 0.90053 0.25929 0.28341
O 0.69548 0.26025 0.84663
O 0.56705 0.11070 0.45294
O 0.02366 0.59302 0.50417
O 0.50657 0.46224 0.37319
O 0.50724 0.92666 0.10388
O 0.50282 0.87299 0.59217
O 0.41441 0.22802 0.27268
O 0.22172 0.02126 0.49962
O 0.30636 0.04152 0.73609
O 0.75874 0.03151 0.03112
O 0.32027 0.44019 0.14963
O 0.90934 0.90435 0.84858
O 0.73356 0.70799 0.92609
O 0.75446 0.77362 0.66589
O 0.36987 0.27568 0.50850
O 0.01412 0.15453 0.91473
O 0.15584 0.79831 0.92310
O 0.41135 0.65451 0.50508
O 0.62870 0.63199 0.51990
O 0.17826 0.64108 0.10821
O 0.17123 0.27385 0.36921
O 0.74786 0.49353 0.85827
O 0.97204 0.44812 0.97434
O 0.79988 0.48660 0.37758
O 0.39602 0.95137 0.35198

O 0.14878 0.61193 0.74029
O 0.57943 0.65150 0.75389
O 0.73353 0.25504 0.54501
O 0.95342 0.32550 0.50447
O 0.68395 0.01999 0.26905
O 0.42444 0.67770 0.25029
O 0.22502 0.52725 0.37674
O 0.82841 0.27097 0.04596
O 0.55288 0.44467 0.12405
O 0.74512 0.96319 0.52608
O 0.17297 0.38730 0.87243
O 0.93557 0.68811 0.05062
O 0.85238 0.72702 0.41781
O 0.34466 0.26721 0.76069
O 0.13525 0.19422 0.67057
O 0.07610 0.29162 0.10003
O 0.20156 0.03144 0.96791
O 0.21477 0.86129 0.17222
O 0.27200 0.79485 0.66830
O 0.08479 0.96350 0.74943
O 0.52080 0.68029 0.03607
O 0.47961 0.36766 0.91392
O 0.00767 0.92296 0.06697
O 0.33443 0.56243 0.94172
O 0.58276 0.09725 0.69635
O 0.77332 0.80525 0.17662
O 0.45732 0.07923 0.90738
O 0.59878 0.19294 0.06127
O 0.94140 0.99478 0.31268
O 0.61245 0.82564 0.38679
O 0.92887 0.64350 0.80832
O 0.64997 0.61988 0.26713
O 0.16572 0.41907 0.58443
O 0.00034 0.48264 0.22831
O 0.02691 0.76691 0.26407
O 0.78829 0.48433 0.12350
O 0.67985 0.31050 0.29991
O 0.62450 0.91118 0.89317
O 0.14906 0.08607 0.22500
O 0.57740 0.39244 0.63466
O 0.81231 0.52874 0.63207
O 0.84209 0.11845 0.70812
O 0.41336 0.81698 0.87634
O 0.98711 0.81412 0.58704

```
O 0.93712 0.33743 0.75009
O 0.29541 0.22467 0.01484
O 0.18687 0.76921 0.43464
O 0.98473 0.07800 0.53670
K_POINTS  gamma
```

IGZO-111-4-1

Analyzing GULP Output File for Supporting Information: IGZO-111-4-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10143.12161490 Ry
Charge = 0.0000 SCF Energy = -10156.27892625 Ry
Charge = 16.7302 SCF Energy = -10164.88520590 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-111-4-1"  ,
        title = "IGZO-111-4-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.2579 ,
        B = 11.2579 ,
        C = 11.2579 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  4 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.2579  0.  0.
  6.8934756E-16  11.2579  0.
  6.8934756E-16  6.8934756E-16  11.2579
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.85750 0.62439 0.91304
In 0.21235 0.09292 0.57652
In 0.48887 0.20744 0.66280
In 0.11865 0.78441 0.73215
In 0.60795 0.74860 0.72390
In 0.76288 0.33642 0.94860
In 0.08704 0.82437 0.42639
In 0.27185 0.26994 0.84001
In 0.62259 0.81157 0.01433
In 0.38579 0.92070 0.77971
In 0.10426 0.85079 0.06270
In 0.01788 0.48632 0.67144
In 0.61754 0.74034 0.35013
In 0.95853 0.18898 0.44713
In 0.11651 0.51483 0.94696
In 0.98084 0.21378 0.79383
In 0.86767 0.67816 0.19806
Ga 0.68937 0.04259 0.82935
Ga 0.69096 0.97851 0.54585
Ga 0.86246 0.69043 0.54489
Ga 0.73518 0.44183 0.69111
Ga 0.18179 0.31116 0.26566
Ga 0.20334 0.58720 0.47553
Ga 0.48202 0.47262 0.58338
Ga 0.39314 0.18405 0.15554
Ga 0.42615 0.93918 0.45700
Ga 0.63165 0.48875 0.13295
Ga 0.88038 0.89376 0.91555
Ga 0.43204 0.20834 0.39400
Ga 0.51323 0.50371 0.86722
Ga 0.96859 0.44473 0.38651
Ga 0.63369 0.02501 0.25939
```

Ga 0.21097 0.03902 0.30251
Ga 0.33036 0.73400 0.23670
Zn 0.84512 0.10057 0.07369
Zn 0.33663 0.69739 0.97927
Zn 0.35412 0.42559 0.08183
Zn 0.16199 0.55619 0.21368
Zn 0.31150 0.58607 0.74341
Zn 0.94813 0.37998 0.13172
Zn 0.93435 0.99440 0.63139
Zn 0.16594 0.00180 0.86529
Zn 0.38160 0.71828 0.57389
Zn 0.21073 0.34762 0.53716
Zn 0.69744 0.48005 0.40450
Zn 0.41392 0.48546 0.31841
Zn 0.08115 0.14502 0.06314
Zn 0.73981 0.26011 0.27903
Zn 0.38286 0.94080 0.09335
Zn 0.92097 0.98364 0.27407
Zn 0.49115 0.15256 0.94490
O 0.83538 0.33188 0.74819
O 0.72390 0.61748 0.08703
O 0.12917 0.15097 0.89941
O 0.66491 0.85509 0.20764
O 0.77642 0.63682 0.38945
O 0.21473 0.49408 0.63254
O 0.18737 0.69008 0.32838
O 0.56885 0.92067 0.86088
O 0.52244 0.44319 0.02403
O 0.24388 0.94387 0.44845
O 0.85713 0.02588 0.78677
O 0.64428 0.48269 0.56512
O 0.73783 0.35868 0.14370
O 0.92867 0.46595 0.99232
O 0.46184 0.32903 0.50159
O 0.94949 0.82149 0.29941
O 0.99722 0.01085 0.10736
O 0.42367 0.77845 0.10412
O 0.21825 0.20811 0.41966
O 0.27756 0.25168 0.65470
O 0.63929 0.06653 0.67365
O 0.28790 0.94397 0.96403
O 0.20190 0.15795 0.18191
O 0.76505 0.98725 0.99843
O 0.64448 0.19037 0.89705

O 0.81225 0.35594 0.40547
O 0.38561 0.07167 0.29244
O 0.05621 0.03238 0.36743
O 0.60044 0.95732 0.40631
O 0.42134 0.09310 0.52917
O 0.23024 0.89772 0.19770
O 0.92882 0.76212 0.03258
O 0.04218 0.62578 0.81234
O 0.43220 0.79390 0.36117
O 0.47171 0.61893 0.67099
O 0.83072 0.05110 0.51130
O 0.78114 0.77706 0.83536
O 0.84658 0.57356 0.66773
O 0.37472 0.25732 0.01090
O 0.45916 0.84967 0.60502
O 0.04840 0.88424 0.88282
O 0.29814 0.73911 0.81560
O 0.91386 0.22922 0.99979
O 0.72021 0.80581 0.56059
O 0.20275 0.95320 0.71520
O 0.01403 0.35999 0.53147
O 0.79168 0.09979 0.23448
O 0.40423 0.11108 0.80614
O 0.32384 0.50368 0.90073
O 0.37950 0.56001 0.46889
O 0.00258 0.29414 0.27743
O 0.97067 0.53223 0.24274
O 0.03614 0.13049 0.62132
O 0.49305 0.38551 0.73884
O 0.69579 0.49191 0.84950
O 0.01252 0.60273 0.48802
O 0.09456 0.37176 0.81234
O 0.50149 0.05980 0.09659
O 0.54353 0.67607 0.88976
O 0.97790 0.82811 0.60032
O 0.21911 0.72285 0.57321
O 0.17950 0.44610 0.37374
O 0.37106 0.32106 0.25515
O 0.34265 0.56458 0.18775
O 0.16211 0.41252 0.10803
O 0.17763 0.67742 0.04914
O 0.58536 0.19381 0.31203
O 0.58737 0.53660 0.29328
K_POINTS gamma

IGZO-111-4-2

Analyzing GULP Output File for Supporting Information: IGZO-111-4-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10143.11216091 Ry
Charge = 0.0000 SCF Energy = -10156.48400275 Ry
Charge = 16.7302 SCF Energy = -10165.03682349 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-111-4-2"  ,
        title = "IGZO-111-4-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.2579 ,
        B = 11.2579 ,
        C = 11.2579 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  4 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.2579  0.  0.
  6.8934756E-16  11.2579  0.
  6.8934756E-16  6.8934756E-16  11.2579
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.90263 0.79144 0.86853
In 0.43789 0.76610 0.39137
In 0.81380 0.24005 0.49530
In 0.46688 0.20167 0.15114
In 0.57413 0.97110 0.54695
In 0.31068 0.95553 0.60050
In 0.74046 0.51553 0.39339
In 0.18948 0.16061 0.21025
In 0.75632 0.06936 0.06608
In 0.45058 0.45261 0.43301
In 0.12355 0.09876 0.78590
In 0.63592 0.67693 0.61933
In 0.14067 0.43821 0.50738
In 0.18201 0.80863 0.83375
In 0.10544 0.77966 0.48823
In 0.34513 0.65503 0.65352
In 0.50289 0.90698 0.17248
Ga 0.26880 0.59100 0.26713
Ga 0.56185 0.59566 0.17959
Ga 0.80464 0.81964 0.38665
Ga 0.82270 0.12350 0.76418
Ga 0.05618 0.13665 0.50265
Ga 0.05251 0.96512 0.04686
Ga 0.13141 0.42491 0.15158
Ga 0.46312 0.74394 0.93611
Ga 0.63980 0.90500 0.83003
Ga 0.09780 0.50351 0.82471
Ga 0.98213 0.26097 0.99673
Ga 0.27598 0.27384 0.94043
Ga 0.90731 0.60616 0.64163
Ga 0.53331 0.15607 0.83081
Ga 0.22155 0.86178 0.23856
```

Ga 0.34399 0.37271 0.71107
Ga 0.31876 0.00090 0.97754
Zn 0.87634 0.91715 0.61837
Zn 0.95917 0.97957 0.29428
Zn 0.06504 0.67786 0.08084
Zn 0.32985 0.54983 0.98335
Zn 0.32624 0.21001 0.46320
Zn 0.69364 0.07093 0.30161
Zn 0.54038 0.20745 0.47558
Zn 0.77358 0.78300 0.10720
Zn 0.63217 0.40270 0.66742
Zn 0.70183 0.33539 0.13719
Zn 0.84342 0.51585 0.09264
Zn 0.71672 0.60826 0.87272
Zn 0.52401 0.44067 0.93150
Zn 0.93094 0.32814 0.69770
Zn 0.73642 0.32678 0.87785
Zn 0.91685 0.25771 0.26099
Zn 0.98296 0.60511 0.31772
O 0.78928 0.92951 0.25323
O 0.86380 0.37976 0.36644
O 0.78656 0.94433 0.75574
O 0.21316 0.78667 0.63880
O 0.42311 0.10784 0.54262
O 0.34321 0.03798 0.15988
O 0.72284 0.84070 0.53109
O 0.98907 0.53899 0.15392
O 0.03609 0.93924 0.87029
O 0.83686 0.67200 0.33392
O 0.21791 0.50545 0.69778
O 0.02078 0.29516 0.55851
O 0.79280 0.68574 0.75679
O 0.10271 0.97921 0.21587
O 0.83644 0.35442 0.01191
O 0.18410 0.18346 0.39484
O 0.49105 0.52876 0.64740
O 0.76988 0.54022 0.57833
O 0.78921 0.63969 0.00359
O 0.24006 0.25177 0.76886
O 0.31492 0.62627 0.45446
O 0.14146 0.04455 0.60347
O 0.61882 0.36583 0.46743
O 0.61202 0.75024 0.17685
O 0.49200 0.58342 0.02022

O 0.32172 0.36062 0.54245
O 0.68513 0.48553 0.20669
O 0.17760 0.45476 0.31860
O 0.40810 0.14533 0.94429
O 0.21923 0.55674 0.09620
O 0.65699 0.46147 0.83163
O 0.28468 0.29237 0.11013
O 0.70893 0.14054 0.88303
O 0.93583 0.12890 0.37519
O 0.95844 0.81467 0.07503
O 0.36281 0.76521 0.22070
O 0.96594 0.48191 0.73009
O 0.20821 0.87420 0.02729
O 0.55735 0.02139 0.73941
O 0.28548 0.97113 0.80560
O 0.06704 0.65835 0.89381
O 0.51035 0.29311 0.74106
O 0.46323 0.80788 0.58624
O 0.26658 0.88075 0.40729
O 0.33304 0.68608 0.85728
O 0.58327 0.31065 0.03172
O 0.13300 0.71443 0.28245
O 0.10538 0.38252 0.94636
O 0.97070 0.78094 0.66184
O 0.02636 0.60517 0.49556
O 0.67447 0.11302 0.46706
O 0.36012 0.41459 0.89072
O 0.53642 0.92310 0.36209
O 0.76133 0.19759 0.21196
O 0.44868 0.25844 0.33629
O 0.96647 0.20145 0.83426
O 0.57412 0.63997 0.42880
O 0.42923 0.53282 0.25839
O 0.16433 0.12364 0.98759
O 0.03741 0.28706 0.16048
O 0.95308 0.87619 0.43730
O 0.93829 0.09190 0.05947
O 0.57414 0.75519 0.81164
O 0.90331 0.10026 0.61381
O 0.59300 0.06507 0.16019
O 0.76694 0.28477 0.69774
O 0.71734 0.90268 0.98280
O 0.45521 0.88825 0.99447
K_POINTS gamma

IGZO-111-4-3

Analyzing GULP Output File for Supporting Information: IGZO-111-4-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10142.98565069 Ry
Charge = 0.0000 SCF Energy = -10156.41073091 Ry
Charge = 16.7302 SCF Energy = -10164.99842047 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-111-4-3"  ,
        title = "IGZO-111-4-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.2579 ,
        B = 11.2579 ,
        C = 11.2579 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  4 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.2579  0.  0.
  6.8934756E-16  11.2579  0.
  6.8934756E-16  6.8934756E-16  11.2579
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.60411 0.36860 0.51530
In 0.90692 0.33579 0.49238
In 0.96423 0.68656 0.55012
In 0.53763 0.02956 0.18305
In 0.52594 0.63892 0.41973
In 0.58816 0.40635 0.22696
In 0.09197 0.64971 0.01672
In 0.38969 0.27735 0.99451
In 0.12033 0.32499 0.11091
In 0.42609 0.18621 0.66321
In 0.76211 0.64792 0.08868
In 0.89277 0.43361 0.85912
In 0.04802 0.54140 0.32945
In 0.38584 0.21369 0.32606
In 0.30491 0.50861 0.26178
In 0.88124 0.72481 0.81213
In 0.25117 0.00147 0.52190
Ga 0.37601 0.84538 0.31945
Ga 0.71567 0.18113 0.33329
Ga 0.13977 0.26260 0.66396
Ga 0.06794 0.85591 0.27076
Ga 0.97797 0.97107 0.69178
Ga 0.78798 0.88413 0.31894
Ga 0.57178 0.46298 0.95866
Ga 0.25226 0.66478 0.52088
Ga 0.74010 0.12693 0.61334
Ga 0.21803 0.06009 0.17421
Ga 0.55705 0.99039 0.46267
Ga 0.77785 0.59181 0.36743
Ga 0.85227 0.38261 0.17977
Ga 0.93306 0.15297 0.86409
Ga 0.23759 0.03449 0.84590
```

Ga 0.58482 0.73765 0.85956
Ga 0.56341 0.05332 0.87160
Zn 0.76329 0.91956 0.02050
Zn 0.31142 0.41462 0.53365
Zn 0.30164 0.86037 0.05939
Zn 0.05516 0.92616 0.97228
Zn 0.72645 0.82944 0.59587
Zn 0.98286 0.06175 0.42550
Zn 0.12402 0.25203 0.36592
Zn 0.46480 0.69897 0.11432
Zn 0.92611 0.09314 0.15120
Zn 0.42534 0.87101 0.71235
Zn 0.71891 0.56099 0.68459
Zn 0.16937 0.73522 0.77015
Zn 0.68184 0.30394 0.78871
Zn 0.34972 0.60793 0.90540
Zn 0.43855 0.50820 0.72185
Zn 0.70834 0.22121 0.03051
Zn 0.21381 0.41729 0.83629
O 0.03734 0.79747 0.12016
O 0.06169 0.26446 0.52745
O 0.67800 0.71654 0.71154
O 0.57065 0.62945 0.99973
O 0.69195 0.97533 0.55169
O 0.53551 0.89648 0.84037
O 0.75892 0.82140 0.16922
O 0.32733 0.24218 0.49961
O 0.47135 0.42743 0.37567
O 0.39549 0.58364 0.55179
O 0.80080 0.20806 0.18233
O 0.57627 0.29034 0.96374
O 0.13271 0.68275 0.62276
O 0.23144 0.39793 0.67820
O 0.41334 0.45245 0.88540
O 0.44009 0.67830 0.78789
O 0.95879 0.37617 0.05088
O 0.94172 0.96531 0.30000
O 0.05785 0.72637 0.38209
O 0.90760 0.01825 0.99875
O 0.72480 0.36773 0.35371
O 0.64388 0.04771 0.02011
O 0.86942 0.08943 0.70339
O 0.84348 0.15614 0.44360
O 0.07698 0.14058 0.14711

O 0.22090 0.90115 0.23822
O 0.88680 0.56373 0.70753
O 0.55089 0.81908 0.42194
O 0.61882 0.14186 0.73572
O 0.67730 0.47169 0.81719
O 0.21307 0.31162 0.95143
O 0.91644 0.51966 0.45859
O 0.80681 0.75797 0.42265
O 0.23481 0.13000 0.69592
O 0.35876 0.15326 0.14052
O 0.40543 0.12160 0.86518
O 0.26535 0.88244 0.77038
O 0.18548 0.58011 0.86172
O 0.22203 0.98247 0.00392
O 0.76405 0.31784 0.62726
O 0.15075 0.53195 0.16180
O 0.20772 0.53320 0.42230
O 0.67305 0.00989 0.31950
O 0.38502 0.67665 0.27953
O 0.56413 0.21897 0.24175
O 0.86774 0.55472 0.23017
O 0.73733 0.79053 0.92162
O 0.30398 0.70719 0.02633
O 0.01550 0.29637 0.77989
O 0.80143 0.24297 0.89353
O 0.23956 0.33052 0.26744
O 0.29888 0.81916 0.47000
O 0.58498 0.18081 0.47882
O 0.17972 0.10627 0.34630
O 0.05699 0.03677 0.82675
O 0.99598 0.34533 0.29936
O 0.42122 0.01484 0.34857
O 0.89110 0.83567 0.66019
O 0.04706 0.79181 0.86804
O 0.42898 0.43388 0.12690
O 0.70874 0.43995 0.08870
O 0.49190 0.36535 0.66061
O 0.66972 0.55837 0.51632
O 0.45437 0.86446 0.14432
O 0.90995 0.59761 0.95694
O 0.43055 0.99747 0.59362
O 0.06493 0.98548 0.54514
O 0.63602 0.59596 0.26845
K_POINTS gamma

IGZO-111-4-4

Analyzing GULP Output File for Supporting Information: IGZO-111-4-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10142.99630563 Ry
Charge = 0.0000 SCF Energy = -10156.40818334 Ry
Charge = 16.7302 SCF Energy = -10164.93586022 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-111-4-4"  ,
        title = "IGZO-111-4-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.2579 ,
        B = 11.2579 ,
        C = 11.2579 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  4 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.2579  0.  0.
  6.8934756E-16  11.2579  0.
  6.8934756E-16  6.8934756E-16  11.2579
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.99407 0.98201 0.48884
In 0.43905 0.42838 0.98752
In 0.04283 0.35682 0.67269
In 0.29406 0.52206 0.58894
In 0.38340 0.73548 0.78227
In 0.66312 0.96472 0.84967
In 0.64799 0.03410 0.34017
In 0.08112 0.48047 0.31163
In 0.32698 0.27246 0.72992
In 0.46629 0.72301 0.05522
In 0.15824 0.55212 0.88858
In 0.77834 0.11270 0.61885
In 0.96255 0.37487 0.04953
In 0.43975 0.78229 0.43184
In 0.37325 0.47378 0.28617
In 0.88106 0.23063 0.38220
In 0.31760 0.00318 0.52344
Ga 0.37423 0.03548 0.85202
Ga 0.57794 0.49529 0.74236
Ga 0.07317 0.07386 0.72684
Ga 0.31044 0.93138 0.18658
Ga 0.87497 0.76926 0.32822
Ga 0.80606 0.49938 0.28164
Ga 0.24192 0.25137 0.01805
Ga 0.58391 0.56973 0.46059
Ga 0.72511 0.78573 0.60681
Ga 0.96573 0.82563 0.85456
Ga 0.86514 0.57002 0.78512
Ga 0.97562 0.66445 0.56892
Ga 0.21230 0.26433 0.46940
Ga 0.77719 0.39209 0.58176
Ga 0.79868 0.11400 0.11273
```

Ga 0.36426 0.19312 0.25754
Ga 0.77456 0.85396 0.08413
Zn 0.67321 0.69320 0.89033
Zn 0.59004 0.23517 0.88790
Zn 0.01498 0.10420 0.97088
Zn 0.54484 0.04740 0.58645
Zn 0.08894 0.16309 0.22559
Zn 0.19341 0.65073 0.12513
Zn 0.84297 0.25649 0.83691
Zn 0.20010 0.82500 0.96096
Zn 0.16564 0.76038 0.35461
Zn 0.52031 0.02851 0.06628
Zn 0.93590 0.63682 0.04521
Zn 0.03798 0.90478 0.17749
Zn 0.58898 0.28183 0.19557
Zn 0.69849 0.48397 0.01271
Zn 0.19280 0.78153 0.62512
Zn 0.62623 0.73071 0.23598
Zn 0.52712 0.31647 0.49739
O 0.23796 0.34285 0.29136
O 0.21731 0.61328 0.27882
O 0.32082 0.15275 0.41395
O 0.47446 0.77500 0.24159
O 0.81891 0.87101 0.91945
O 0.40812 0.08042 0.67638
O 0.72179 0.14737 0.80131
O 0.16514 0.19135 0.62947
O 0.67340 0.93917 0.65435
O 0.01885 0.86933 0.33928
O 0.28510 0.88312 0.36300
O 0.78844 0.39988 0.41309
O 0.61623 0.45760 0.57588
O 0.89403 0.77068 0.14735
O 0.44634 0.57520 0.69968
O 0.41185 0.58329 0.43922
O 0.43394 0.54205 0.13117
O 0.36826 0.34421 0.55286
O 0.06419 0.53468 0.10076
O 0.13063 0.68066 0.50089
O 0.86314 0.76862 0.50778
O 0.51660 0.08682 0.91136
O 0.98736 0.45896 0.85989
O 0.93728 0.02889 0.12899
O 0.81966 0.05111 0.43906

O 0.05749 0.14938 0.40231
O 0.62428 0.19411 0.54960
O 0.49165 0.34347 0.81338
O 0.20633 0.65602 0.73815
O 0.73352 0.18664 0.24667
O 0.72799 0.86401 0.27364
O 0.05351 0.97310 0.87269
O 0.88773 0.26494 0.58199
O 0.66875 0.58629 0.30788
O 0.12360 0.40970 0.49319
O 0.08378 0.22608 0.06764
O 0.29335 0.67666 0.97475
O 0.39292 0.27406 0.10485
O 0.40408 0.91804 0.05592
O 0.50367 0.33285 0.32893
O 0.69246 0.00368 0.05967
O 0.71640 0.65818 0.72142
O 0.75491 0.40360 0.76209
O 0.92661 0.01256 0.66474
O 0.56164 0.55538 0.91085
O 0.60851 0.71714 0.50370
O 0.23852 0.08710 0.18082
O 0.14487 0.94416 0.60320
O 0.92396 0.60738 0.33459
O 0.82069 0.47570 0.12384
O 0.35321 0.80514 0.59788
O 0.00376 0.20715 0.81050
O 0.05970 0.72738 0.94485
O 0.27749 0.16264 0.88630
O 0.54907 0.81424 0.85306
O 0.61620 0.33577 0.04519
O 0.85002 0.22801 0.00559
O 0.25365 0.40695 0.96875
O 0.94810 0.72391 0.72760
O 0.49873 0.08806 0.22573
O 0.51982 0.96626 0.44957
O 0.18217 0.83472 0.13534
O 0.81314 0.61632 0.92895
O 0.96357 0.34569 0.25987
O 0.29095 0.89688 0.83944
O 0.64847 0.74132 0.06521
O 0.91328 0.51073 0.62099
O 0.20531 0.41557 0.73285
K_POINTS gamma

IGZO-111-4-5

Analyzing GULP Output File for Supporting Information: IGZO-111-4-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -10143.23153437 Ry
Charge = 0.0000 SCF Energy = -10156.72139184 Ry
Charge = 16.7302 SCF Energy = -10165.27008955 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-111-4-5"  ,
        title = "IGZO-111-4-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.2579 ,
        B = 11.2579 ,
        C = 11.2579 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  4 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.2579  0.  0.
  6.8934756E-16  11.2579  0.
  6.8934756E-16  6.8934756E-16  11.2579
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
Ga      69.723          Ga.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.10293 0.57652 0.54120
In 0.33982 0.80201 0.79276
In 0.72773 0.13630 0.59873
In 0.00928 0.07617 0.38225
In 0.71246 0.19606 0.31204
In 0.69129 0.66892 0.20346
In 0.15548 0.27551 0.56904
In 0.82983 0.60785 0.93529
In 0.55348 0.85435 0.54363
In 0.75180 0.92068 0.32061
In 0.45567 0.23437 0.60917
In 0.52365 0.58180 0.97594
In 0.97982 0.15243 0.74728
In 0.92726 0.13864 0.08721
In 0.53279 0.40539 0.40868
In 0.85690 0.86403 0.60229
In 0.89945 0.45796 0.70558
Ga 0.02911 0.76008 0.77258
Ga 0.17960 0.92997 0.23689
Ga 0.36922 0.03324 0.04268
Ga 0.64200 0.70090 0.75940
Ga 0.35403 0.76082 0.10059
Ga 0.86818 0.35482 0.46837
Ga 0.46781 0.66192 0.33253
Ga 0.76628 0.62236 0.48353
Ga 0.93035 0.82255 0.11441
Ga 0.26366 0.39745 0.35907
Ga 0.48054 0.94637 0.27931
Ga 0.29358 0.82785 0.47436
Ga 0.27116 0.15227 0.83279
Ga 0.39165 0.56229 0.61076
Ga 0.16604 0.99058 0.63305
```

Ga 0.48995 0.30099 0.91738
Ga 0.19271 0.21295 0.17259
Zn 0.64209 0.10288 0.06323
Zn 0.19166 0.63531 0.28276
Zn 0.05811 0.37038 0.96114
Zn 0.32572 0.10035 0.42153
Zn 0.72842 0.38319 0.14766
Zn 0.63374 0.86001 0.03608
Zn 0.54686 0.00609 0.81829
Zn 0.78750 0.28642 0.88753
Zn 0.61459 0.46581 0.71683
Zn 0.83473 0.93540 0.87534
Zn 0.44766 0.26688 0.17092
Zn 0.13087 0.94887 0.95022
Zn 0.98998 0.76164 0.39044
Zn 0.13261 0.64951 0.99816
Zn 0.00596 0.39534 0.23737
Zn 0.29014 0.46946 0.07828
Zn 0.17089 0.51330 0.78653
O 0.49462 0.43072 0.59748
O 0.18995 0.96450 0.41009
O 0.91768 0.18341 0.90914
O 0.14692 0.25862 0.36595
O 0.59189 0.32763 0.23734
O 0.62622 0.35581 0.84844
O 0.74467 0.57064 0.76340
O 0.28591 0.13281 0.60179
O 0.82221 0.70704 0.32746
O 0.29335 0.34018 0.19435
O 0.85075 0.36390 0.29824
O 0.23923 0.63660 0.13106
O 0.24078 0.91452 0.08159
O 0.61501 0.24509 0.48277
O 0.71574 0.53266 0.08308
O 0.11163 0.49800 0.32137
O 0.49748 0.18174 0.03341
O 0.34353 0.07836 0.22222
O 0.57335 0.11575 0.70260
O 0.58218 0.81757 0.33556
O 0.42183 0.70266 0.50809
O 0.27115 0.62331 0.69832
O 0.11442 0.30717 0.76471
O 0.16635 0.71966 0.43431
O 0.50717 0.58746 0.76322

```
O 0.83631 0.28062 0.69523
O 0.84609 0.06734 0.24046
O 0.75664 0.23937 0.06916
O 0.38016 0.27297 0.41593
O 0.24498 0.44627 0.54465
O 0.85397 0.18871 0.45248
O 0.38918 0.71666 0.94716
O 0.86937 0.78429 0.80914
O 0.37674 0.52392 0.34884
O 0.66255 0.71689 0.95121
O 0.02773 0.59112 0.73803
O 0.24711 0.16882 0.00328
O 0.68406 0.97485 0.50007
O 0.54239 0.83826 0.73930
O 0.38856 0.25749 0.79429
O 0.91211 0.91009 0.42684
O 0.43529 0.42830 0.00981
O 0.70335 0.73843 0.59309
O 0.43003 0.96411 0.44449
O 0.34361 0.79380 0.28963
O 0.91323 0.43857 0.90271
O 0.92933 0.66131 0.52462
O 0.47987 0.91389 0.09787
O 0.67419 0.99338 0.94031
O 0.29741 0.87774 0.63383
O 0.49980 0.66500 0.16084
O 0.04404 0.82557 0.22598
O 0.09274 0.07418 0.19614
O 0.84089 0.01849 0.72119
O 0.76298 0.84063 0.13320
O 0.13999 0.04239 0.80397
O 0.05396 0.10953 0.57267
O 0.60856 0.05561 0.24584
O 0.62524 0.58019 0.37682
O 0.76317 0.46272 0.53413
O 0.17358 0.48942 0.94801
O 0.05019 0.29927 0.12044
O 0.05381 0.86791 0.65111
O 0.37952 0.00553 0.87325
O 0.97074 0.68036 0.03616
O 0.96585 0.94966 0.00133
O 0.15080 0.78351 0.88093
O 0.00160 0.39825 0.54352
K_POINTS  gamma
```

IGZO-200-3-1

Analyzing GULP Output File for Supporting Information: IGZO-200-3-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -9754.06732018 Ry
Charge = 0.0000 SCF Energy = -9768.30042008 Ry
Charge = 17.4603 SCF Energy = -9778.11386609 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-200-3-1"  ,
        title = "IGZO-200-3-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.8325 ,
        B = 11.8325 ,
        C = 11.8325 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.8325  0.  0.
  7.24531663E-16  11.8325  0.
  7.24531663E-16  7.24531663E-16  11.8325
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.40446 0.16854 0.14653
In 0.68505 0.11508 0.11531
In 0.88498 0.60656 0.94334
In 0.64074 0.68532 0.67076
In 0.92059 0.64712 0.28760
In 0.72911 0.44537 0.76143
In 0.13788 0.18674 0.18213
In 0.58014 0.61278 0.25078
In 0.53323 0.92523 0.21518
In 0.44659 0.21306 0.87243
In 0.52072 0.96134 0.92385
In 0.92535 0.64799 0.64499
In 0.44963 0.48158 0.81773
In 0.24821 0.61725 0.63119
In 0.59709 0.66726 0.98420
In 0.35327 0.43246 0.08452
In 0.26672 0.30190 0.61193
In 0.65199 0.36499 0.03448
In 0.47279 0.51249 0.49726
In 0.97629 0.01060 0.00829
In 0.00562 0.32192 0.66530
In 0.17782 0.51632 0.86407
In 0.87764 0.28192 0.29399
In 0.37972 0.77212 0.77195
In 0.76885 0.12755 0.52032
In 0.91319 0.30247 0.98727
In 0.96911 0.03471 0.71170
In 0.25046 0.97620 0.99286
In 0.54340 0.27257 0.61857
In 0.09755 0.48074 0.44424
In 0.36003 0.69669 0.05649
In 0.59120 0.31340 0.30556
In 0.09032 0.80959 0.82143
In 0.95285 0.97369 0.29595
```

In 0.42293 0.11944 0.41504
In 0.80481 0.83850 0.83676
In 0.77111 0.82864 0.14283
In 0.09156 0.82870 0.51599
In 0.59001 0.97313 0.65341
In 0.16004 0.23282 0.90459
In 0.76929 0.81503 0.44721
In 0.27750 0.04342 0.69209
In 0.08882 0.47009 0.13066
In 0.75820 0.47411 0.48011
In 0.76097 0.15678 0.80405
In 0.08489 0.76238 0.10128
In 0.10417 0.12975 0.46847
In 0.25209 0.94030 0.26595
In 0.28167 0.64902 0.32862
In 0.42878 0.81143 0.49700
O 0.12391 0.97885 0.13078
O 0.48917 0.33243 0.13787
O 0.16179 0.19923 0.73144
O 0.66664 0.53612 0.10335
O 0.35465 0.00259 0.86240
O 0.74518 0.69059 0.28482
O 0.57631 0.10728 0.52951
O 0.57352 0.34834 0.86413
O 0.75794 0.74099 0.99186
O 0.94146 0.82809 0.69659
O 0.11034 0.59195 0.28519
O 0.47563 0.66981 0.39108
O 0.21438 0.78412 0.69826
O 0.10992 0.95842 0.37113
O 0.41310 0.93338 0.36585
O 0.84610 0.03179 0.14503
O 0.28098 0.15722 0.01758
O 0.03129 0.63099 0.82551
O 0.28262 0.52363 0.46725
O 0.91790 0.47529 0.38404
O 0.32146 0.36174 0.90091
O 0.45982 0.78416 0.92379
O 0.38339 0.55141 0.21875
O 0.68671 0.90790 0.30014
O 0.52509 0.13279 0.01943
O 0.61388 0.83407 0.54449
O 0.94416 0.81607 0.20604
O 0.75389 0.28282 0.42501

O 0.85222 0.98072 0.44418
O 0.11047 0.98945 0.61225
O 0.31399 0.60929 0.80663
O 0.96167 0.34692 0.15970
O 0.21199 0.35234 0.17175
O 0.96850 0.61323 0.09871
O 0.94310 0.75527 0.43382
O 0.00062 0.15429 0.31362
O 0.86574 0.01258 0.86593
O 0.70888 0.27182 0.68330
O 0.11292 0.99269 0.85710
O 0.95176 0.17130 0.58026
O 0.44170 0.67329 0.62330
O 0.21736 0.80061 0.96305
O 0.39891 0.19252 0.69951
O 0.41015 0.92284 0.64884
O 0.76722 0.02658 0.66287
O 0.28650 0.13447 0.27547
O 0.54147 0.13862 0.26458
O 0.03788 0.16869 0.02802
O 0.60890 0.47713 0.36717
O 0.52122 0.75313 0.13699
O 0.46458 0.31057 0.45830
O 0.12538 0.31324 0.49674
O 0.75272 0.21433 0.97424
O 0.64138 0.93937 0.06339
O 0.27057 0.12772 0.51900
O 0.59954 0.58190 0.80958
O 0.62280 0.47349 0.60715
O 0.21925 0.56913 0.04369
O 0.93426 0.23711 0.81321
O 0.97943 0.83370 0.96156
O 0.06741 0.39995 0.95218
O 0.15107 0.43722 0.69438
O 0.07752 0.62050 0.56754
O 0.58826 0.07995 0.80448
O 0.80241 0.43618 0.92190
O 0.80050 0.65228 0.77435
O 0.25465 0.77011 0.46180
O 0.40505 0.41915 0.65681
O 0.88556 0.45635 0.64509
O 0.72621 0.27535 0.18781
O 0.63238 0.84005 0.77895
O 0.77206 0.64946 0.54058

O 0.37844 0.96526 0.12392
O 0.24693 0.77549 0.19177
O 0.45279 0.55244 0.98992
K_POINTS gamma

IGZO-200-3-2

Analyzing GULP Output File for Supporting Information: IGZO-200-3-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -9753.93892264 Ry
Charge = 0.0000 SCF Energy = -9768.15468102 Ry
Charge = 17.4603 SCF Energy = -9777.94926036 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-200-3-2"  ,
        title = "IGZO-200-3-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.8325 ,
        B = 11.8325 ,
        C = 11.8325 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.8325  0.  0.
  7.24531663E-16  11.8325  0.
  7.24531663E-16  7.24531663E-16  11.8325
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.73044 0.77500 0.82336
In 0.41412 0.39602 0.86493
In 0.92327 0.49858 0.08464
In 0.71388 0.75743 0.16295
In 0.02107 0.08954 0.19322
In 0.51381 0.92561 0.99284
In 0.06148 0.47508 0.48626
In 0.01414 0.76970 0.51050
In 0.39699 0.39770 0.14593
In 0.52048 0.33364 0.63449
In 0.61987 0.39485 0.38390
In 0.66306 0.13048 0.46281
In 0.32938 0.81474 0.84669
In 0.48629 0.97025 0.31674
In 0.17776 0.91791 0.31145
In 0.42615 0.66544 0.18577
In 0.83459 0.00183 0.64635
In 0.87847 0.23501 0.02164
In 0.78461 0.60095 0.61423
In 0.65937 0.13882 0.18061
In 0.70178 0.44007 0.83570
In 0.34426 0.12928 0.13339
In 0.83877 0.28792 0.60616
In 0.15016 0.00068 0.98602
In 0.34946 0.48736 0.44251
In 0.49304 0.63359 0.66385
In 0.88146 0.28528 0.30611
In 0.21727 0.31928 0.64074
In 0.60827 0.72574 0.42562
In 0.17298 0.28054 0.97127
In 0.01572 0.44105 0.79251
In 0.01598 0.14300 0.78981
In 0.15377 0.36092 0.24960
In 0.82461 0.96482 0.99558
```

In 0.99170 0.78335 0.13711
In 0.51316 0.64335 0.94458
In 0.32666 0.76570 0.47706
In 0.03952 0.13414 0.49425
In 0.37228 0.11473 0.81922
In 0.03231 0.73357 0.83687
In 0.15731 0.63725 0.28226
In 0.65066 0.44357 0.11820
In 0.20378 0.55589 0.98653
In 0.52189 0.90971 0.66895
In 0.67736 0.12170 0.81080
In 0.23025 0.60826 0.68605
In 0.84032 0.92606 0.35071
In 0.85985 0.58242 0.33939
In 0.32059 0.18669 0.41237
In 0.18506 0.94268 0.66354
O 0.18509 0.13342 0.84440
O 0.45721 0.35035 0.45896
O 0.85534 0.12987 0.49901
O 0.93821 0.60834 0.50454
O 0.33184 0.00572 0.98190
O 0.54011 0.27888 0.14266
O 0.35464 0.25814 0.98686
O 0.48894 0.13074 0.41512
O 0.55911 0.43699 0.95527
O 0.30901 0.26962 0.25004
O 0.28377 0.51376 0.26480
O 0.35397 0.97024 0.70968
O 0.67823 0.85294 0.00572
O 0.85454 0.90493 0.16559
O 0.86379 0.64369 0.14944
O 0.90626 0.36966 0.46570
O 0.60651 0.62540 0.09387
O 0.94440 0.81474 0.96322
O 0.30888 0.03358 0.28567
O 0.37452 0.55661 0.04744
O 0.19886 0.40940 0.08234
O 0.86202 0.87315 0.52493
O 0.28399 0.76058 0.29488
O 0.63658 0.74460 0.62349
O 0.97960 0.07366 0.97139
O 0.02934 0.76851 0.32047
O 0.03384 0.26594 0.64847
O 0.78661 0.94786 0.81081

O 0.84969 0.14882 0.19150
O 0.52398 0.79055 0.81700
O 0.00538 0.29521 0.89508
O 0.97884 0.33299 0.13822
O 0.51498 0.03332 0.14217
O 0.21284 0.14285 0.55283
O 0.09903 0.92714 0.14778
O 0.68198 0.61587 0.86746
O 0.52341 0.49446 0.25931
O 0.20911 0.36659 0.45569
O 0.35160 0.47816 0.62542
O 0.52896 0.03317 0.84058
O 0.11758 0.65594 0.11277
O 0.67692 0.00173 0.33661
O 0.47910 0.87605 0.48543
O 0.22057 0.41302 0.84500
O 0.67041 0.29259 0.54316
O 0.35104 0.74647 0.66263
O 0.01672 0.54230 0.92921
O 0.76362 0.75592 0.33359
O 0.87883 0.69773 0.73637
O 0.84788 0.43739 0.71492
O 0.70036 0.24623 0.31997
O 0.03388 0.50412 0.30406
O 0.45944 0.63641 0.47810
O 0.05526 0.21956 0.32649
O 0.10995 0.75743 0.66182
O 0.53270 0.79018 0.26304
O 0.01196 0.01352 0.65915
O 0.42162 0.56858 0.80865
O 0.70006 0.56043 0.44203
O 0.20334 0.67102 0.86114
O 0.41097 0.78181 0.01932
O 0.65956 0.03758 0.63524
O 0.72800 0.12434 0.99360
O 0.58846 0.27622 0.79219
O 0.01747 0.00506 0.36140
O 0.79531 0.39705 0.98667
O 0.84621 0.17325 0.75235
O 0.11238 0.48281 0.65092
O 0.16595 0.15409 0.09518
O 0.61379 0.49336 0.66961
O 0.37303 0.26038 0.71616
O 0.78827 0.44278 0.24277

```
O 0.19715 0.61632 0.47600
O 0.19791 0.88722 0.48708
O 0.16657 0.89127 0.84354
K_POINTS  gamma
```

IGZO-200-3-3

Analyzing GULP Output File for Supporting Information: IGZO-200-3-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -9754.06822625 Ry
Charge = 0.0000 SCF Energy = -9768.29534099 Ry
Charge = 17.4603 SCF Energy = -9778.05687634 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-200-3-3"  ,
        title = "IGZO-200-3-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.8325 ,
        B = 11.8325 ,
        C = 11.8325 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.8325  0.  0.
  7.24531663E-16  11.8325  0.
  7.24531663E-16  7.24531663E-16  11.8325
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.30796 0.47305 0.67446
In 0.85519 0.62839 0.56117
In 0.36514 0.14682 0.69069
In 0.74830 0.24606 0.96577
In 0.17622 0.69019 0.56397
In 0.20108 0.01051 0.22805
In 0.67871 0.84210 0.68409
In 0.16703 0.36197 0.20819
In 0.97570 0.87536 0.73470
In 0.83409 0.70901 0.88157
In 0.65949 0.78815 0.11104
In 0.18693 0.65377 0.22430
In 0.48884 0.01393 0.19325
In 0.02759 0.86946 0.39154
In 0.54097 0.57869 0.59221
In 0.59667 0.26933 0.24850
In 0.35274 0.80510 0.04834
In 0.72111 0.43851 0.77222
In 0.17496 0.67891 0.88293
In 0.65712 0.52139 0.33721
In 0.66979 0.12078 0.72142
In 0.51504 0.65758 0.86087
In 0.55116 0.29419 0.52633
In 0.88044 0.64137 0.24367
In 0.69417 0.51098 0.04976
In 0.04760 0.22411 0.42851
In 0.85664 0.32501 0.28353
In 0.69315 0.79554 0.39444
In 0.39728 0.83761 0.68573
In 0.94520 0.16169 0.77123
In 0.36347 0.47011 0.38069
In 0.21697 0.00635 0.87583
In 0.14234 0.00875 0.57609
In 0.42454 0.54396 0.10715
```

In 0.39180 0.77147 0.35682
In 0.34790 0.18194 0.05194
In 0.80343 0.98149 0.93691
In 0.81242 0.32290 0.55316
In 0.97975 0.51331 0.04100
In 0.07633 0.50617 0.42620
In 0.46727 0.33815 0.85722
In 0.52264 0.97743 0.90205
In 0.31832 0.19255 0.39469
In 0.83393 0.04168 0.50456
In 0.03767 0.83334 0.07316
In 0.80629 0.05315 0.23859
In 0.20174 0.33809 0.89382
In 0.52711 0.99378 0.44950
In 0.02490 0.18236 0.06402
In 0.02904 0.47804 0.74357
O 0.07019 0.02625 0.76450
O 0.65630 0.08952 0.90430
O 0.97776 0.59483 0.85879
O 0.00460 0.68918 0.49073
O 0.65542 0.43005 0.59878
O 0.25408 0.19928 0.21706
O 0.09326 0.36588 0.04559
O 0.55116 0.97957 0.71567
O 0.84427 0.75649 0.69886
O 0.57248 0.64137 0.03980
O 0.51053 0.17517 0.11603
O 0.51867 0.89294 0.06424
O 0.19838 0.35619 0.39102
O 0.35347 0.35767 0.00000
O 0.48081 0.49326 0.77491
O 0.53873 0.24341 0.72176
O 0.01914 0.26300 0.23279
O 0.54780 0.72489 0.70006
O 0.17832 0.85378 0.96006
O 0.18170 0.16807 0.97167
O 0.32759 0.00407 0.08271
O 0.86567 0.48202 0.65081
O 0.61298 0.37516 0.94612
O 0.19475 0.50530 0.82030
O 0.84252 0.40978 0.95372
O 0.39343 0.10815 0.87932
O 0.69495 0.59960 0.85389
O 0.70331 0.68399 0.25354

O 0.83611 0.55839 0.39256
O 0.44909 0.84353 0.51610
O 0.83595 0.90538 0.35628
O 0.13756 0.49889 0.59708
O 0.34213 0.63808 0.96609
O 0.82134 0.00336 0.73960
O 0.82978 0.66867 0.05285
O 0.10273 0.64375 0.05253
O 0.95571 0.37182 0.44335
O 0.95015 0.18666 0.58495
O 0.31445 0.31045 0.75629
O 0.23726 0.61787 0.39586
O 0.76816 0.94032 0.10991
O 0.49672 0.59534 0.40056
O 0.69862 0.16784 0.55391
O 0.42239 0.42661 0.55112
O 0.21864 0.16670 0.55425
O 0.99725 0.77375 0.24007
O 0.05400 0.30505 0.79143
O 0.76884 0.21853 0.15348
O 0.44726 0.14101 0.52372
O 0.10103 0.05213 0.37841
O 0.03202 0.01753 0.13598
O 0.45800 0.30660 0.35545
O 0.36795 0.02511 0.32819
O 0.19476 0.85009 0.48813
O 0.78988 0.26904 0.76247
O 0.69676 0.34467 0.37753
O 0.37666 0.69879 0.20074
O 0.62063 0.09053 0.30848
O 0.97991 0.94059 0.55409
O 0.81509 0.47239 0.17553
O 0.68052 0.67914 0.52295
O 0.89703 0.13377 0.94955
O 0.21358 0.83278 0.21826
O 0.54869 0.86328 0.30413
O 0.57027 0.45177 0.18825
O 0.04935 0.53486 0.25142
O 0.93440 0.85476 0.91480
O 0.28360 0.97622 0.70070
O 0.69267 0.92378 0.52184
O 0.40356 0.84038 0.86833
O 0.86754 0.15678 0.37042
O 0.11540 0.74963 0.72794

```
O 0.68681 0.84778 0.88276
O 0.33539 0.66282 0.64502
O 0.29318 0.48396 0.21382
K_POINTS  gamma
```

IGZO-200-3-4

Analyzing GULP Output File for Supporting Information: IGZO-200-3-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -9754.02216491 Ry
Charge = 0.0000 SCF Energy = -9768.23968834 Ry
Charge = 17.4603 SCF Energy = -9778.03103643 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-200-3-4"  ,
        title = "IGZO-200-3-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.8325 ,
        B = 11.8325 ,
        C = 11.8325 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.8325  0.  0.
  7.24531663E-16  11.8325  0.
  7.24531663E-16  7.24531663E-16  11.8325
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.44200 0.03840 0.22870
In 0.84885 0.30719 0.00529
In 0.86561 0.57606 0.13410
In 0.55163 0.25116 0.05682
In 0.93968 0.27792 0.67754
In 0.99656 0.51990 0.45234
In 0.19056 0.26980 0.45363
In 0.09140 0.79168 0.56495
In 0.94548 0.08664 0.42498
In 0.96187 0.49777 0.81708
In 0.14725 0.05006 0.67133
In 0.36282 0.74827 0.49934
In 0.58826 0.48939 0.13964
In 0.20123 0.98136 0.37373
In 0.61860 0.19404 0.76907
In 0.11636 0.71801 0.26012
In 0.66364 0.77236 0.17621
In 0.83434 0.94568 0.69240
In 0.00172 0.76775 0.82943
In 0.90224 0.84153 0.37242
In 0.14710 0.28342 0.88952
In 0.99106 0.12675 0.15766
In 0.29516 0.80283 0.76725
In 0.66487 0.11005 0.50794
In 0.24496 0.20778 0.19919
In 0.39154 0.30328 0.65888
In 0.43511 0.77438 0.00107
In 0.16786 0.52871 0.66430
In 0.73486 0.04431 0.23696
In 0.34220 0.07789 0.88575
In 0.66572 0.44965 0.87762
In 0.18992 0.90639 0.05397
In 0.91066 0.85525 0.07604
In 0.71684 0.39643 0.59366
```

In 0.37207 0.45134 0.89408
In 0.40473 0.74415 0.25694
In 0.17719 0.62078 0.00158
In 0.71858 0.73592 0.88132
In 0.39410 0.05512 0.53492
In 0.31273 0.48550 0.38770
In 0.50766 0.29214 0.33920
In 0.65468 0.82672 0.48611
In 0.80493 0.35120 0.31541
In 0.49374 0.58217 0.67676
In 0.65994 0.01718 0.97079
In 0.54880 0.91000 0.72941
In 0.81820 0.66313 0.63939
In 0.96993 0.07561 0.90058
In 0.06401 0.40495 0.15076
In 0.59488 0.55970 0.41000
O 0.68667 0.27044 0.92036
O 0.08569 0.37503 0.73214
O 0.03413 0.20171 0.52994
O 0.14050 0.89209 0.23532
O 0.59385 0.09251 0.13092
O 0.56746 0.37907 0.72979
O 0.51298 0.41537 0.98741
O 0.93289 0.80704 0.65263
O 0.12007 0.23219 0.07308
O 0.53565 0.72510 0.38716
O 0.50857 0.12803 0.91346
O 0.93195 0.74053 0.22468
O 0.32842 0.26669 0.84090
O 0.04264 0.70072 0.42629
O 0.94413 0.47478 0.28684
O 0.68347 0.03071 0.77784
O 0.46336 0.47660 0.29046
O 0.21291 0.43688 0.98286
O 0.57896 0.85476 0.90642
O 0.25383 0.92215 0.55089
O 0.20654 0.36115 0.27880
O 0.84078 0.11820 0.02981
O 0.04436 0.93898 0.46971
O 0.49611 0.87839 0.16039
O 0.69666 0.81071 0.67266
O 0.59535 0.60855 0.83187
O 0.28223 0.73365 0.11872
O 0.27940 0.67152 0.35868

O 0.81479 0.41730 0.75339
O 0.74293 0.92047 0.09581
O 0.23052 0.69347 0.62351
O 0.51541 0.18130 0.61266
O 0.15547 0.10489 0.84852
O 0.36751 0.89626 0.36023
O 0.10376 0.57515 0.16011
O 0.64838 0.33329 0.19411
O 0.80215 0.71347 0.47032
O 0.06370 0.76902 0.99632
O 0.96100 0.07433 0.71133
O 0.74741 0.21173 0.63407
O 0.54819 0.11905 0.36668
O 0.80767 0.98251 0.51271
O 0.52945 0.66288 0.11589
O 0.43642 0.56869 0.51120
O 0.34240 0.64387 0.90443
O 0.31494 0.12479 0.36849
O 0.95909 0.25797 0.87017
O 0.66543 0.57269 0.58946
O 0.91639 0.00103 0.25884
O 0.10363 0.14569 0.30053
O 0.54191 0.95243 0.54761
O 0.31581 0.88969 0.92166
O 0.38671 0.99170 0.73849
O 0.03352 0.99593 0.04393
O 0.65107 0.37977 0.43027
O 0.12733 0.87142 0.75795
O 0.30304 0.04968 0.10664
O 0.26236 0.16859 0.61025
O 0.86272 0.65086 0.81561
O 0.70470 0.57994 0.24757
O 0.11193 0.62198 0.82580
O 0.44795 0.76246 0.66980
O 0.71039 0.88789 0.31418
O 0.34198 0.47594 0.71515
O 0.42268 0.24214 0.17835
O 0.75283 0.47817 0.02891
O 0.78366 0.16919 0.36356
O 0.98116 0.56848 0.63324
O 0.36759 0.32480 0.46601
O 0.90850 0.28920 0.17088
O 0.86882 0.89166 0.87613
O 0.78974 0.70869 0.04319

```
O 0.86726 0.39622 0.50213
O 0.96742 0.45516 0.99485
O 0.15932 0.45052 0.49704
K_POINTS  gamma
```

IGZO-200-3-5

Analyzing GULP Output File for Supporting Information: IGZO-200-3-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -17.4603 SCF Energy = -9754.07657734 Ry
Charge = 0.0000 SCF Energy = -9768.33948741 Ry
Charge = 17.4603 SCF Energy = -9778.09402805 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-200-3-5"  ,
        title = "IGZO-200-3-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.8325 ,
        B = 11.8325 ,
        C = 11.8325 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 125  ,
        ntyp  =  2 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.8325  0.  0.
  7.24531663E-16  11.8325  0.
  7.24531663E-16  7.24531663E-16  11.8325
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.85149 0.82940 0.24051
In 0.06058 0.33642 0.13826
In 0.93209 0.13569 0.27292
In 0.04893 0.61438 0.46749
In 0.91986 0.82323 0.94411
In 0.54780 0.47227 0.89506
In 0.37448 0.27393 0.68131
In 0.25932 0.82660 0.60985
In 0.63514 0.91866 0.01680
In 0.57858 0.51447 0.31604
In 0.71369 0.35359 0.10846
In 0.26437 0.47825 0.93885
In 0.07909 0.96343 0.09339
In 0.03965 0.66087 0.76157
In 0.57958 0.47342 0.60119
In 0.70893 0.00675 0.43261
In 0.42800 0.02176 0.43295
In 0.60050 0.10312 0.19986
In 0.68608 0.25027 0.75055
In 0.88829 0.51733 0.26643
In 0.75648 0.69143 0.76435
In 0.73981 0.99317 0.78356
In 0.10843 0.34527 0.71717
In 0.30817 0.57223 0.35440
In 0.12499 0.86541 0.34486
In 0.24042 0.77795 0.90355
In 0.91237 0.86463 0.59044
In 0.18138 0.08005 0.55278
In 0.21950 0.14028 0.25326
In 0.14412 0.65544 0.12784
In 0.86321 0.15887 0.98013
In 0.07052 0.00784 0.80514
In 0.36548 0.35298 0.16058
In 0.41734 0.01501 0.76516
```

In 0.77683 0.67106 0.47245
In 0.55402 0.82135 0.27575
In 0.50200 0.73020 0.55311
In 0.49925 0.20998 0.95137
In 0.89069 0.15885 0.59489
In 0.21424 0.18427 0.94632
In 0.29687 0.54547 0.64265
In 0.45260 0.28162 0.43458
In 0.49785 0.74195 0.82160
In 0.87834 0.45454 0.63769
In 0.78382 0.32517 0.41560
In 0.42638 0.65270 0.09981
In 0.11519 0.31339 0.42613
In 0.94558 0.49328 0.96737
In 0.68995 0.65292 0.06944
In 0.35576 0.95191 0.08220
O 0.95651 0.32954 0.30474
O 0.42229 0.11556 0.59401
O 0.02548 0.50864 0.14781
O 0.43313 0.85044 0.67178
O 0.78798 0.80593 0.06131
O 0.15494 0.34858 0.99302
O 0.89693 0.65670 0.87857
O 0.48292 0.60312 0.69291
O 0.42585 0.42355 0.32006
O 0.23443 0.98920 0.70469
O 0.97181 0.96142 0.25127
O 0.51027 0.04576 0.03970
O 0.40040 0.40800 0.55759
O 0.57784 0.12308 0.38369
O 0.40198 0.87893 0.90280
O 0.76352 0.02119 0.60547
O 0.69277 0.95006 0.23797
O 0.20542 0.99776 0.97283
O 0.77494 0.18127 0.17284
O 0.13233 0.60413 0.94547
O 0.60178 0.59847 0.47478
O 0.71026 0.68679 0.27384
O 0.33485 0.66868 0.52019
O 0.90229 0.67401 0.62130
O 0.73486 0.43039 0.27324
O 0.29449 0.52541 0.13293
O 0.21307 0.25539 0.59564
O 0.80332 0.52668 0.07818

O 0.08796 0.13286 0.39033
O 0.76136 0.30929 0.60547
O 0.54461 0.26920 0.15567
O 0.36376 0.17361 0.83610
O 0.82497 0.85574 0.43346
O 0.18410 0.70268 0.30829
O 0.86257 0.50174 0.46100
O 0.01424 0.02186 0.61109
O 0.90708 0.32278 0.03013
O 0.10414 0.18100 0.80485
O 0.30790 0.17787 0.09990
O 0.45196 0.67053 0.28356
O 0.82972 0.15469 0.42054
O 0.73391 0.04746 0.95926
O 0.59098 0.10906 0.78870
O 0.54550 0.88737 0.44590
O 0.20834 0.96396 0.22160
O 0.32996 0.16734 0.39324
O 0.87998 0.87141 0.77591
O 0.64693 0.85429 0.83847
O 0.54820 0.78871 0.09681
O 0.60617 0.36932 0.45299
O 0.84806 0.16628 0.78227
O 0.53621 0.36164 0.74367
O 0.41432 0.37343 0.97039
O 0.02222 0.79158 0.09801
O 0.23398 0.69553 0.73747
O 0.27451 0.41749 0.76934
O 0.66307 0.32671 0.93330
O 0.44410 0.96409 0.24641
O 0.99008 0.30662 0.57031
O 0.08499 0.82737 0.84280
O 0.08951 0.53252 0.63352
O 0.63215 0.63330 0.90534
O 0.68956 0.76439 0.60888
O 0.28451 0.77616 0.07601
O 0.26139 0.93684 0.46830
O 0.96612 0.44325 0.80050
O 0.39198 0.62078 0.92327
O 0.93595 0.67294 0.33831
O 0.55822 0.52791 0.10326
O 0.96619 0.01028 0.95818
O 0.20059 0.32440 0.25630
O 0.06377 0.14635 0.13914

```
O 0.17213 0.48786 0.42348
O 0.07969 0.79140 0.52284
O 0.72837 0.52054 0.69733
K_POINTS  gamma
```

IGZO-201-4-1

Analyzing GULP Output File for Supporting Information: IGZO-201-4-1
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -9667.49466373 Ry
Charge = 0.0000 SCF Energy = -9681.23110068 Ry
Charge = 16.7302 SCF Energy = -9690.55494254 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-201-4-1"  ,
        title = "IGZO-201-4-1" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.4274 ,
        B = 11.4274 ,
        C = 11.4274 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.4274  0.  0.
  6.99726442E-16  11.4274  0.
  6.99726442E-16  6.99726442E-16  11.4274
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.85099 0.00950 0.03264
In 0.68719 0.87352 0.17238
In 0.18404 0.44770 0.03975
In 0.17136 0.30847 0.72857
In 0.85724 0.34248 0.66335
In 0.96359 0.52777 0.84586
In 0.17532 0.77532 0.49056
In 0.39707 0.50362 0.87101
In 0.93855 0.71473 0.02564
In 0.53543 0.71024 0.39236
In 0.52708 0.31736 0.66117
In 0.48349 0.01575 0.07570
In 0.29646 0.50847 0.31407
In 0.67046 0.48642 0.90489
In 0.03611 0.13444 0.17979
In 0.40303 0.97813 0.57016
In 0.85879 0.03046 0.37945
In 0.38087 0.19380 0.85508
In 0.22116 0.71750 0.12595
In 0.69392 0.16504 0.52194
In 0.86411 0.75087 0.42964
In 0.18589 0.97430 0.02877
In 0.88135 0.26860 0.94336
In 0.67903 0.22811 0.17804
In 0.35356 0.23334 0.50091
In 0.47452 0.70362 0.07574
In 0.30431 0.23259 0.20366
In 0.33206 0.91777 0.29484
In 0.05280 0.04706 0.57198
In 0.62038 0.44071 0.42771
In 0.19727 0.68937 0.80711
In 0.06553 0.54571 0.57125
In 0.72468 0.62933 0.63751
```

In 0.76111 0.56637 0.21539
Zn 0.36397 0.52654 0.56951
Zn 0.04121 0.09598 0.82418
Zn 0.53385 0.06252 0.34903
Zn 0.02567 0.85384 0.24433
Zn 0.73732 0.79098 0.86672
Zn 0.65008 0.19287 0.87184
Zn 0.95164 0.81430 0.70694
Zn 0.24432 0.95958 0.75465
Zn 0.81417 0.03089 0.74008
Zn 0.01008 0.58226 0.28555
Zn 0.98066 0.36815 0.14956
Zn 0.90783 0.35002 0.40814
Zn 0.48517 0.73387 0.71740
Zn 0.67005 0.88513 0.59377
Zn 0.54696 0.93025 0.84301
Zn 0.11217 0.28071 0.43984
Zn 0.51186 0.42911 0.12448
O 0.89923 0.72206 0.83225
O 0.20296 0.05025 0.22659
O 0.80407 0.10790 0.88562
O 0.52914 0.54038 0.00941
O 0.12419 0.49650 0.75367
O 0.35676 0.41330 0.14474
O 0.42348 0.88729 0.72970
O 0.68663 0.29855 0.99597
O 0.77222 0.33353 0.49124
O 0.90937 0.70554 0.22280
O 0.62491 0.69566 0.20466
O 0.34948 0.37357 0.62847
O 0.13593 0.29193 0.14678
O 0.70763 0.13776 0.33865
O 0.88953 0.53791 0.64767
O 0.98718 0.25312 0.75984
O 0.54444 0.85289 0.98175
O 0.23279 0.56738 0.48788
O 0.32784 0.87810 0.10545
O 0.25541 0.33521 0.36623
O 0.58224 0.75078 0.56946
O 0.20687 0.12367 0.80051
O 0.67715 0.04245 0.09888
O 0.41739 0.14897 0.66168
O 0.92044 0.98838 0.21189
O 0.63805 0.41158 0.23251

O 0.37120 0.81553 0.45732
O 0.82178 0.79959 0.59916
O 0.59120 0.00617 0.51639
O 0.37735 0.67059 0.22896
O 0.52119 0.09101 0.89245
O 0.53328 0.27699 0.48394
O 0.68520 0.22088 0.70098
O 0.50547 0.35661 0.84012
O 0.07071 0.83746 0.08724
O 0.87616 0.22665 0.12628
O 0.99605 0.40865 0.99536
O 0.09459 0.72407 0.65765
O 0.01982 0.37649 0.52767
O 0.16502 0.79457 0.30030
O 0.86377 0.09186 0.55810
O 0.69188 0.91992 0.75812
O 0.37647 0.06495 0.40961
O 0.02890 0.08318 0.98768
O 0.46263 0.53292 0.42495
O 0.80024 0.83841 0.01852
O 0.62070 0.46977 0.62296
O 0.63476 0.65549 0.80858
O 0.00543 0.64819 0.43194
O 0.21002 0.94818 0.59016
O 0.08418 0.62961 0.97168
O 0.32047 0.11706 0.03021
O 0.79305 0.56688 0.02400
O 0.75116 0.87721 0.34998
O 0.14023 0.55660 0.19908
O 0.99472 0.19160 0.36022
O 0.27213 0.35962 0.89074
O 0.91347 0.45087 0.27308
O 0.16851 0.20183 0.56292
O 0.49495 0.17645 0.21514
O 0.72316 0.60375 0.40426
O 0.21353 0.86463 0.87065
O 0.36493 0.62743 0.72247
O 0.51659 0.92166 0.24993
O 0.00016 0.91194 0.44424
O 0.31596 0.63183 0.98089
O 0.81556 0.41098 0.82955
O 0.97831 0.97318 0.73777
K_POINTS gamma

IGZO-201-4-2

Analyzing GULP Output File for Supporting Information: IGZO-201-4-2
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -9667.52375369 Ry
Charge = 0.0000 SCF Energy = -9681.24642482 Ry
Charge = 16.7302 SCF Energy = -9690.62714962 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-201-4-2"  ,
        title = "IGZO-201-4-2" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.4274 ,
        B = 11.4274 ,
        C = 11.4274 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.4274  0.  0.
  6.99726442E-16  11.4274  0.
  6.99726442E-16  6.99726442E-16  11.4274
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.09352 0.88197 0.79413
In 0.10180 0.03963 0.53229
In 0.77876 0.37189 0.97073
In 0.52442 0.28964 0.08079
In 0.55305 0.51510 0.83408
In 0.01657 0.98086 0.11658
In 0.74691 0.35495 0.25841
In 0.64746 0.85054 0.28792
In 0.31709 0.53839 0.07045
In 0.61387 0.86051 0.82686
In 0.27137 0.84358 0.25809
In 0.97315 0.28995 0.67213
In 0.56478 0.55281 0.30347
In 0.39235 0.21146 0.61289
In 0.75441 0.04426 0.08012
In 0.85846 0.69331 0.84162
In 0.92939 0.80794 0.32913
In 0.27494 0.17690 0.00334
In 0.63082 0.66137 0.59014
In 0.60950 0.01911 0.58868
In 0.87763 0.57296 0.43153
In 0.84426 0.10963 0.43493
In 0.23464 0.38582 0.79899
In 0.55654 0.12184 0.32706
In 0.34526 0.48740 0.56218
In 0.08779 0.35068 0.43649
In 0.86074 0.07266 0.79566
In 0.87712 0.83613 0.58890
In 0.35191 0.35212 0.30288
In 0.78066 0.66405 0.10534
In 0.54625 0.16481 0.83846
In 0.64172 0.35057 0.54495
In 0.29046 0.86309 0.97740
```

In 0.08222 0.69140 0.09557
Zn 0.99717 0.21708 0.97373
Zn 0.18806 0.64355 0.80511
Zn 0.40595 0.73940 0.43531
Zn 0.37467 0.72037 0.70183
Zn 0.20013 0.14320 0.76400
Zn 0.01351 0.47762 0.92827
Zn 0.45706 0.99345 0.09759
Zn 0.24448 0.11174 0.24099
Zn 0.23341 0.58434 0.31611
Zn 0.79212 0.48254 0.69342
Zn 0.34304 0.97461 0.48643
Zn 0.98956 0.47754 0.16644
Zn 0.14509 0.73850 0.52367
Zn 0.01980 0.22346 0.22370
Zn 0.03867 0.57468 0.65410
Zn 0.53648 0.71186 0.04917
Zn 0.33998 0.94006 0.72912
O 0.20890 0.31887 0.62225
O 0.18786 0.53992 0.93077
O 0.35590 0.23527 0.80061
O 0.04167 0.44991 0.77103
O 0.27647 0.05879 0.63025
O 0.94544 0.36894 0.28974
O 0.21933 0.61844 0.63307
O 0.48366 0.85518 0.99585
O 0.44993 0.84096 0.32023
O 0.99294 0.71761 0.47233
O 0.18448 0.24717 0.31012
O 0.68523 0.85229 0.64771
O 0.44412 0.34306 0.48465
O 0.69529 0.03653 0.88868
O 0.68028 0.98266 0.41100
O 0.57301 0.20838 0.65942
O 0.11391 0.14585 0.11673
O 0.82387 0.64438 0.64477
O 0.11136 0.87310 0.61492
O 0.24819 0.71981 0.39511
O 0.27458 0.77727 0.81566
O 0.96685 0.36599 0.04529
O 0.94201 0.61767 0.99591
O 0.09457 0.85657 0.99007
O 0.54888 0.37218 0.24843
O 0.69631 0.23123 0.39746

O 0.14360 0.25216 0.88706
O 0.60130 0.00075 0.17875
O 0.70772 0.48828 0.40674
O 0.70865 0.23666 0.10651
O 0.34495 0.34989 0.07582
O 0.46069 0.07617 0.47722
O 0.38002 0.48722 0.74791
O 0.39040 0.83339 0.57876
O 0.78151 0.08066 0.62417
O 0.81726 0.35153 0.61132
O 0.41209 0.17931 0.23609
O 0.71909 0.76511 0.95562
O 0.14608 0.52582 0.18320
O 0.58840 0.33965 0.91072
O 0.22336 0.00063 0.38618
O 0.63013 0.49683 0.66029
O 0.86328 0.26130 0.84600
O 0.00546 0.19763 0.49774
O 0.48074 0.57527 0.99537
O 0.03813 0.09447 0.71300
O 0.46042 0.13112 0.01132
O 0.49878 0.99098 0.75016
O 0.89643 0.88050 0.77349
O 0.38821 0.55704 0.25490
O 0.53251 0.69936 0.76037
O 0.29980 0.98632 0.13434
O 0.76262 0.73576 0.42638
O 0.94226 0.95286 0.44645
O 0.83467 0.87071 0.18624
O 0.99258 0.47475 0.54007
O 0.74540 0.48471 0.12445
O 0.48725 0.60854 0.47977
O 0.76341 0.52494 0.85472
O 0.23285 0.46069 0.41568
O 0.91576 0.62507 0.24416
O 0.89640 0.10813 0.24148
O 0.24849 0.01259 0.86948
O 0.07810 0.83622 0.23426
O 0.03339 0.68922 0.77867
O 0.92296 0.05722 0.97488
O 0.62067 0.69336 0.19158
O 0.27094 0.72285 0.10002
K_POINTS gamma

IGZO-201-4-3

Analyzing GULP Output File for Supporting Information: IGZO-201-4-3
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -9667.47769287 Ry
Charge = 0.0000 SCF Energy = -9681.21395705 Ry
Charge = 16.7302 SCF Energy = -9690.58772676 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-201-4-3"  ,
        title = "IGZO-201-4-3" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.4274 ,
        B = 11.4274 ,
        C = 11.4274 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.4274  0.  0.
  6.99726442E-16  11.4274  0.
  6.99726442E-16  6.99726442E-16  11.4274
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.77111 0.21052 0.36436
In 0.88356 0.24426 0.08507
In 0.60951 0.50417 0.40579
In 0.31504 0.43424 0.46043
In 0.68299 0.75749 0.83516
In 0.96053 0.12876 0.58241
In 0.41352 0.65316 0.59766
In 0.92056 0.88365 0.44108
In 0.15647 0.57618 0.65700
In 0.73883 0.42713 0.86107
In 0.69034 0.14708 0.81398
In 0.39451 0.42445 0.11531
In 0.57530 0.62257 0.04867
In 0.52367 0.27853 0.59501
In 0.65514 0.75796 0.53748
In 0.38562 0.76789 0.83611
In 0.04706 0.26774 0.33314
In 0.60234 0.24762 0.08284
In 0.27395 0.76700 0.13102
In 0.02428 0.47567 0.00624
In 0.04924 0.10862 0.86705
In 0.79763 0.48470 0.19765
In 0.52352 0.97701 0.99387
In 0.81451 0.95176 0.01390
In 0.82544 0.42352 0.55791
In 0.24897 0.20272 0.59752
In 0.46900 0.44923 0.78587
In 0.07487 0.79397 0.90733
In 0.43855 0.95489 0.65656
In 0.17906 0.74594 0.39449
In 0.04095 0.36517 0.73847
In 0.02713 0.00803 0.20003
In 0.47247 0.92652 0.33915
```

In 0.90355 0.66959 0.65817
Zn 0.21622 0.02686 0.42287
Zn 0.86350 0.64935 0.97089
Zn 0.00806 0.72712 0.15924
Zn 0.37159 0.21505 0.87326
Zn 0.73034 0.75759 0.21510
Zn 0.31334 0.11453 0.17383
Zn 0.18657 0.26596 0.05516
Zn 0.25713 0.54130 0.90437
Zn 0.87246 0.93176 0.73382
Zn 0.45244 0.19601 0.33391
Zn 0.45395 0.63893 0.29265
Zn 0.11913 0.49588 0.23309
Zn 0.87568 0.63875 0.38048
Zn 0.27374 0.00727 0.93287
Zn 0.70346 0.98972 0.23624
Zn 0.15487 0.88544 0.66934
Zn 0.65818 0.03839 0.51601
O 0.26380 0.61138 0.49304
O 0.15038 0.94989 0.83621
O 0.88189 0.66142 0.22174
O 0.55498 0.91361 0.50913
O 0.42621 0.24667 0.17663
O 0.20203 0.42936 0.09541
O 0.57891 0.43564 0.05281
O 0.83729 0.48199 0.01365
O 0.11877 0.49800 0.84098
O 0.75040 0.24862 0.96186
O 0.51404 0.16399 0.93547
O 0.15774 0.16664 0.18775
O 0.99592 0.71109 0.46828
O 0.28158 0.01796 0.57935
O 0.90954 0.27561 0.48090
O 0.00933 0.66017 0.00881
O 0.60472 0.33371 0.75798
O 0.77592 0.82494 0.66132
O 0.97900 0.39956 0.19548
O 0.35997 0.40786 0.92785
O 0.47489 0.47028 0.57069
O 0.38365 0.25409 0.72393
O 0.13420 0.65401 0.23056
O 0.51954 0.67095 0.44590
O 0.09730 0.92067 0.36258
O 0.77008 0.78899 0.40214

O 0.11949 0.15835 0.46586
O 0.82562 0.62311 0.81449
O 0.50710 0.78903 0.96640
O 0.10023 0.86884 0.09498
O 0.64021 0.59838 0.23799
O 0.09810 0.18494 0.70493
O 0.58854 0.09918 0.64657
O 0.38294 0.26063 0.47084
O 0.85445 0.92597 0.20349
O 0.30471 0.80463 0.65347
O 0.01448 0.30121 0.94644
O 0.66750 0.06611 0.10303
O 0.44209 0.46451 0.32245
O 0.81833 0.04804 0.48171
O 0.34207 0.58648 0.76068
O 0.89945 0.85247 0.88198
O 0.39883 0.96331 0.83289
O 0.60017 0.10623 0.35659
O 0.98438 0.50390 0.61195
O 0.66318 0.32882 0.48404
O 0.08129 0.72762 0.72461
O 0.72911 0.30142 0.20565
O 0.59867 0.86778 0.22149
O 0.23401 0.15579 0.94503
O 0.82157 0.48885 0.37992
O 0.73832 0.59263 0.57719
O 0.59191 0.57111 0.85428
O 0.16709 0.40934 0.35682
O 0.34897 0.06119 0.32216
O 0.92161 0.15305 0.25828
O 0.95017 0.07036 0.02335
O 0.34508 0.96410 0.07680
O 0.25062 0.70681 0.94508
O 0.85537 0.34793 0.73614
O 0.33595 0.79265 0.30602
O 0.73296 0.73000 0.02152
O 0.87565 0.09265 0.76092
O 0.54324 0.76927 0.70156
O 0.00114 0.93729 0.60721
O 0.67676 0.95111 0.87396
O 0.20466 0.40251 0.62295
O 0.40304 0.62634 0.12943
K_POINTS gamma

IGZO-201-4-4

Analyzing GULP Output File for Supporting Information: IGZO-201-4-4
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -9667.35809211 Ry
Charge = 0.0000 SCF Energy = -9681.00829617 Ry
Charge = 16.7302 SCF Energy = -9690.43469357 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-201-4-4"  ,
        title = "IGZO-201-4-4" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.4274 ,
        B = 11.4274 ,
        C = 11.4274 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.4274  0.  0.
  6.99726442E-16  11.4274  0.
  6.99726442E-16  6.99726442E-16  11.4274
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.92761 0.53356 0.80899
In 0.82507 0.97480 0.05889
In 0.93155 0.49430 0.20058
In 0.58157 0.17327 0.09854
In 0.64726 0.33238 0.78910
In 0.64872 0.54128 0.04618
In 0.77925 0.51658 0.53152
In 0.13157 0.38975 0.93442
In 0.12335 0.21618 0.16551
In 0.65669 0.41139 0.29096
In 0.02307 0.71755 0.56827
In 0.65056 0.06109 0.83312
In 0.91788 0.25443 0.69014
In 0.40360 0.09083 0.63733
In 0.36317 0.37914 0.22408
In 0.14256 0.73652 0.82897
In 0.26312 0.86439 0.49096
In 0.91167 0.90951 0.78543
In 0.03174 0.78108 0.26441
In 0.74876 0.01262 0.56170
In 0.74215 0.72153 0.32481
In 0.68779 0.74240 0.83524
In 0.56501 0.86050 0.11539
In 0.24832 0.17814 0.41307
In 0.06317 0.40119 0.46576
In 0.47670 0.62193 0.33884
In 0.54602 0.57560 0.63315
In 0.19684 0.59393 0.09908
In 0.51741 0.92698 0.42137
In 0.84077 0.27094 0.99786
In 0.01501 0.02544 0.48576
In 0.08096 0.10373 0.87732
In 0.87600 0.22715 0.33199
```

In 0.14927 0.88960 0.04696
Zn 0.41479 0.70179 0.90979
Zn 0.36720 0.99355 0.90205
Zn 0.40175 0.46230 0.89921
Zn 0.61936 0.25695 0.55423
Zn 0.15029 0.16360 0.66145
Zn 0.21477 0.57866 0.36215
Zn 0.33226 0.08160 0.11621
Zn 0.42037 0.84226 0.72907
Zn 0.27356 0.63477 0.57990
Zn 0.19936 0.41389 0.70195
Zn 0.35887 0.37886 0.51085
Zn 0.73625 0.01016 0.28663
Zn 0.78550 0.78226 0.57375
Zn 0.36921 0.21294 0.84789
Zn 0.90408 0.69677 0.02611
Zn 0.34647 0.85858 0.23709
Zn 0.52582 0.17506 0.38147
O 0.50251 0.80208 0.27831
O 0.24031 0.38447 0.37242
O 0.76815 0.40418 0.12270
O 0.74070 0.17760 0.67081
O 0.09009 0.11056 0.32791
O 0.64336 0.98838 0.00907
O 0.34481 0.56424 0.21814
O 0.57307 0.06291 0.26658
O 0.31462 0.58707 0.95357
O 0.42800 0.14034 0.98498
O 0.47588 0.98380 0.78590
O 0.23004 0.37973 0.09111
O 0.86691 0.08516 0.89008
O 0.00809 0.07110 0.69335
O 0.79880 0.15001 0.16623
O 0.31439 0.19242 0.23416
O 0.19756 0.76164 0.65193
O 0.02068 0.24491 0.01406
O 0.25861 0.10715 0.79363
O 0.41867 0.89524 0.57523
O 0.09125 0.59568 0.26143
O 0.98826 0.91724 0.14497
O 0.11630 0.53252 0.78246
O 0.56393 0.71747 0.99533
O 0.67091 0.25529 0.40142
O 0.20894 0.05345 0.54829

O 0.73595 0.87679 0.20930
O 0.07885 0.28057 0.78781
O 0.61790 0.62249 0.46419
O 0.96420 0.71449 0.75254
O 0.33102 0.68673 0.44119
O 0.20820 0.78564 0.19524
O 0.34045 0.97547 0.36273
O 0.89989 0.89424 0.58821
O 0.57029 0.06989 0.52173
O 0.68620 0.85954 0.45774
O 0.50240 0.70898 0.75676
O 0.18590 0.07748 0.03943
O 0.08805 0.84664 0.42937
O 0.83586 0.04898 0.40448
O 0.83656 0.36109 0.82685
O 0.93789 0.44705 0.61769
O 0.40783 0.21989 0.49782
O 0.13547 0.56974 0.50361
O 0.97176 0.22752 0.50374
O 0.00308 0.49313 0.00841
O 0.36363 0.50612 0.62008
O 0.82571 0.82863 0.94461
O 0.66900 0.22661 0.94255
O 0.64582 0.40972 0.61930
O 0.72154 0.90934 0.73112
O 0.06937 0.71740 0.99922
O 0.37835 0.92421 0.09107
O 0.31037 0.82835 0.87751
O 0.63513 0.59265 0.22399
O 0.19885 0.30133 0.58255
O 0.53081 0.33255 0.16706
O 0.00209 0.33987 0.26737
O 0.30280 0.35656 0.84167
O 0.87599 0.67385 0.18532
O 0.87193 0.67556 0.45850
O 0.73613 0.64956 0.66761
O 0.07409 0.91874 0.87575
O 0.48513 0.43572 0.38791
O 0.82387 0.45111 0.36837
O 0.77966 0.59740 0.92251
O 0.49938 0.21947 0.74177
O 0.55125 0.46061 0.89746
K_POINTS gamma

IGZO-201-4-5

Analyzing GULP Output File for Supporting Information: IGZO-201-4-5
Using PWSCF v.5.0.1 on #Procs=4
Charge = -16.7302 SCF Energy = -9667.48990594 Ry
Charge = 0.0000 SCF Energy = -9681.12889770 Ry
Charge = 16.7302 SCF Energy = -9690.54372863 Ry

Input File:

==========

```
&CONTROL
        calculation =  "scf"  ,
        pseudo_dir = "/share/apps/QuantumEspresso/PSEUDO"  ,
        prefix = "IGZO-201-4-5"  ,
        title = "IGZO-201-4-5" ,
        outdir = "./" ,
        disk_io = "low" ,
        /
&SYSTEM
        ibrav = 0 ,
        A = 11.4274 ,
        B = 11.4274 ,
        C = 11.4274 ,
        cosAB = 1.32679e-06 ,
        cosAC = 1.32679e-06 ,
        cosBC = 1.32679e-06 ,
        tot_charge  = 0 ,
        nat  = 119  ,
        ntyp  =  3 ,
        input_dft = "PBE" ,
        ecutwfc  =  25.0 ,
        occupations  =  "smearing" ,
        smearing  =  "mp" ,
        degauss  =  0.005
        lda_plus_u=.true. ,
        Hubbard_U(1)=3.0 ,
        Hubbard_U(2)=3.0 ,
        Hubbard_U(3)=3.0 ,
        Hubbard_U(4)=3.0 ,
/
&ELECTRONS
        electron_maxstep = 100 ,
        conv_thr = 1.D-6 ,
        mixing_beta = 0.3 ,
        mixing_mode = "local-TF" ,
```

```
        mixing_ndim = 8  ,
/
CELL_PARAMETERS angstrom
  11.4274  0.  0.
  6.99726442E-16  11.4274  0.
  6.99726442E-16  6.99726442E-16  11.4274
ATOMIC_SPECIES
O       15.999          O.pbe-n-rrkjus.UPF
Zn      65.41   Zn.pbe-dn-rrkjus.UPF
In      114.82          In.pbe-dn-rrkjus.UPF
ATOMIC_POSITIONS crystal
In 0.47276 0.05999 0.59656
In 0.16731 0.82061 0.08651
In 0.90795 0.09967 0.72604
In 0.46851 0.52819 0.28408
In 0.83447 0.79976 0.03732
In 0.34623 0.81887 0.30610
In 0.59050 0.19833 0.83936
In 0.11563 0.44912 0.45435
In 0.96803 0.28785 0.25754
In 0.27871 0.25788 0.97335
In 0.20909 0.09985 0.69717
In 0.19206 0.62259 0.80754
In 0.83997 0.31122 0.93638
In 0.95790 0.97497 0.26720
In 0.04722 0.09793 0.01767
In 0.76627 0.51616 0.12439
In 0.08770 0.33994 0.76072
In 0.35594 0.93396 0.90154
In 0.52972 0.77463 0.08990
In 0.34819 0.61423 0.55413
In 0.82283 0.51896 0.46963
In 0.20307 0.10044 0.39623
In 0.73882 0.77259 0.28932
In 0.68679 0.22109 0.58156
In 0.08613 0.78183 0.47718
In 0.96954 0.85694 0.80876
In 0.39644 0.38661 0.75783
In 0.05834 0.46272 0.04803
In 0.55505 0.01585 0.33583
In 0.99336 0.64729 0.25205
In 0.62126 0.30112 0.32054
In 0.66848 0.88364 0.80420
In 0.78416 0.92247 0.51151
```

In 0.53125 0.64297 0.81747
Zn 0.24025 0.57119 0.23950
Zn 0.75148 0.10795 0.21537
Zn 0.95780 0.20656 0.49939
Zn 0.31880 0.55745 0.03152
Zn 0.35694 0.30196 0.47166
Zn 0.30380 0.04028 0.16028
Zn 0.55876 0.76366 0.51411
Zn 0.51056 0.16090 0.07057
Zn 0.76516 0.71277 0.63581
Zn 0.76777 0.05159 0.00565
Zn 0.27740 0.85977 0.60005
Zn 0.88111 0.60065 0.88843
Zn 0.55543 0.44920 0.01168
Zn 0.54712 0.46163 0.54654
Zn 0.31220 0.31237 0.24035
Zn 0.99966 0.58880 0.64644
Zn 0.73242 0.45226 0.76127
O 0.35011 0.89252 0.10354
O 0.11493 0.26908 0.07503
O 0.14794 0.76082 0.28651
O 0.06584 0.98401 0.71477
O 0.25840 0.55839 0.39593
O 0.57541 0.15763 0.45554
O 0.76181 0.28958 0.74560
O 0.82899 0.85686 0.68099
O 0.99061 0.20729 0.87108
O 0.21702 0.06621 0.93766
O 0.68719 0.68957 0.12878
O 0.88678 0.37254 0.10189
O 0.37708 0.42638 0.57313
O 0.79458 0.23051 0.30994
O 0.17338 0.62757 0.08779
O 0.74646 0.72572 0.47285
O 0.35383 0.18803 0.13619
O 0.90538 0.80498 0.20514
O 0.12228 0.47912 0.64871
O 0.94292 0.87580 0.43510
O 0.71854 0.47937 0.93823
O 0.47177 0.59092 0.98415
O 0.58995 0.15080 0.20353
O 0.70354 0.19812 0.97903
O 0.63276 0.05399 0.72054
O 0.58385 0.48436 0.71577

O 0.39168 0.66602 0.20891
O 0.13398 0.99478 0.18549
O 0.36420 0.01370 0.31535
O 0.60352 0.43891 0.17712
O 0.04785 0.20671 0.63553
O 0.91525 0.61445 0.04886
O 0.23382 0.78549 0.90835
O 0.21040 0.29049 0.36834
O 0.81368 0.57490 0.29233
O 0.51289 0.82218 0.89623
O 0.88323 0.08669 0.11738
O 0.36153 0.58442 0.74866
O 0.99695 0.61101 0.47863
O 0.82784 0.54933 0.66360
O 0.22715 0.45129 0.91732
O 0.30912 0.15177 0.54067
O 0.06440 0.46691 0.25223
O 0.30915 0.43991 0.15438
O 0.47186 0.08394 0.92613
O 0.02344 0.12814 0.36201
O 0.54962 0.82628 0.29490
O 0.48042 0.32984 0.93141
O 0.97014 0.44572 0.87010
O 0.19363 0.93686 0.48576
O 0.67432 0.39640 0.48187
O 0.00330 0.67267 0.79176
O 0.83426 0.10852 0.55880
O 0.76229 0.72445 0.87812
O 0.44339 0.35256 0.34227
O 0.19319 0.71853 0.62269
O 0.34074 0.96660 0.70599
O 0.51793 0.59831 0.45033
O 0.00862 0.87916 0.99460
O 0.58968 0.92963 0.51231
O 0.25607 0.25822 0.78225
O 0.84622 0.00010 0.87863
O 0.95038 0.36205 0.44944
O 0.50817 0.24120 0.67994
O 0.60931 0.74665 0.67971
O 0.68279 0.92635 0.04790
O 0.39281 0.79445 0.49404
O 0.74558 0.96879 0.31134
K_POINTS gamma

8. SINGLE POINT ENERGIES AND TEMPLATE INPUT FILE OF THE 777 CELLS FOR: ZNO, GA_2O_3, IN_2O_3, GA_2ZNO_4, $GA_2ZN_8O_{11}$, IN_2ZNO_4, INGAZNO$_4$, AND INGAO$_3$

IGZO-001-1 (ZnO)

File	Energy (Ry)
IGZO-001-1-1_0	-30572.46763
IGZO-001-1-1_-48.8571	-30532.79638
IGZO-001-1-1_48.8571	-30597.85747
IGZO-001-1-2_0	-30569.97805
IGZO-001-1-2_-48.8571	-30530.48397
IGZO-001-1-2_48.8571	-30595.38047
IGZO-001-1-3_0	-30569.76448
IGZO-001-1-3_-48.8571	-30530.26301
IGZO-001-1-3_48.8571	-30595.17958
IGZO-001-1-4_0	-30570.07493
IGZO-001-1-4_-48.8571	-30530.52578
IGZO-001-1-4_48.8571	-30595.53493
IGZO-001-1-5_0	-30571.10387
IGZO-001-1-5_-48.8571	-30531.58386
IGZO-001-1-5_48.8571	-30596.68588
Average Band Gap	**3.93 eV**

IGZO-020-3 (Ga_2O_3)

File	Energy (Ry)
IGZO-020-3-1_0	-30368.41681
IGZO-020-3-1_-47.4921	-30333.22237
IGZO-020-3-1_47.4921	-30388.03035
IGZO-020-3-2_0	-30368.55823
IGZO-020-3-2_-47.4921	-30333.39614
IGZO-020-3-2_47.4921	-30388.2009
IGZO-020-3-3_0	-30368.56691
IGZO-020-3-3_-47.4921	-30333.43241
IGZO-020-3-3_47.4921	-30388.24802
IGZO-020-3-4_0	-30368.25114
IGZO-020-3-4_-47.4921	-30333.06585
IGZO-020-3-4_47.4921	-30387.85539
IGZO-020-3-5_0	-30368.20681
IGZO-020-3-5_-47.4921	-30332.91907
IGZO-020-3-5_47.4921	-30387.88559
Average Band Gap	**4.45 eV**

IGZO-021-4 (Ga_2ZnO_4)

File	Energy (Ry)
IGZO-021-4-1_0	-30643.5566
IGZO-021-4-1_-48.2222	-30606.95535
IGZO-021-4-1_48.2222	-30664.67858
IGZO-021-4-2_0	-30643.78132
IGZO-021-4-2_-48.2222	-30607.2151
IGZO-021-4-2_48.2222	-30665.03476
IGZO-021-4-3_0	-30643.33577
IGZO-021-4-3_-48.2222	-30606.75975
IGZO-021-4-3_48.2222	-30664.50527
IGZO-021-4-4_0	-30643.0296
IGZO-021-4-4_-48.2222	-30606.50843
IGZO-021-4-4_48.2222	-30664.1615
IGZO-021-4-5_0	-30643.38801
IGZO-021-4-5_-48.2222	-30606.90291
IGZO-021-4-5_48.2222	-30664.61681
Average Band Gap	**4.34 eV**

IGZO-028-11 ($Ga_2Zn_8O_{11}$)

File	Energy (Ry)
IGZO-028-11-1_0	-30028.86001
IGZO-028-11-1_-47.746	-29991.09958
IGZO-028-11-1_47.746	-30052.12225
IGZO-028-11-2_0	-30029.25767
IGZO-028-11-2_-47.746	-29991.60881
IGZO-028-11-2_47.746	-30052.54589
IGZO-028-11-3_0	-30028.83881
IGZO-028-11-3_-47.746	-29991.201
IGZO-028-11-3_47.746	-30052.07974
IGZO-028-11-4_0	-30028.67692
IGZO-028-11-4_-47.746	-29991.08628
IGZO-028-11-4_47.746	-30052.0229
IGZO-028-11-5_0	-30028.63143
IGZO-028-11-5_-47.746	-29990.9933
IGZO-028-11-5_47.746	-30051.98578
Average Band Gap	**4.09 eV**

IGZO-110-3 ($InGaO_3$)

File	Energy (Ry)
IGZO-110-3-1_0	-28468.39599
IGZO-110-3-1_-47.4921	-28430.40963
IGZO-110-3-1_47.4921	-28492.99193
IGZO-110-3-2_0	-28468.23176
IGZO-110-3-2_-47.4921	-28430.42992
IGZO-110-3-2_47.4921	-28492.84058
IGZO-110-3-3_0	-28468.60638
IGZO-110-3-3_-47.4921	-28430.5609
IGZO-110-3-3_47.4921	-28493.07081
IGZO-110-3-4_0	-28468.65304
IGZO-110-3-4_-47.4921	-28430.64929
IGZO-110-3-4_47.4921	-28493.26411
IGZO-110-3-5_0	-28468.69917
IGZO-110-3-5_-47.4921	-28430.7511
IGZO-110-3-5_47.4921	-28493.35137
Average Band Gap	**3.83 eV**

IGZO-111-4 ($InGaZnO_4$)

File	Energy (Ry)
IGZO-111-4-1_0	-29272.91464
IGZO-111-4-1_-48.2222	-29234.83644
IGZO-111-4-1_48.2222	-29297.80797
IGZO-111-4-2_0	-29273.04842
IGZO-111-4-2_-48.2222	-29234.7415
IGZO-111-4-2_48.2222	-29297.69464
IGZO-111-4-3_0	-29273.0147
IGZO-111-4-3_-48.2222	-29234.67453
IGZO-111-4-3_48.2222	-29297.72246
IGZO-111-4-4_0	-29273.05765
IGZO-111-4-4_-48.2222	-29234.747
IGZO-111-4-4_48.2222	-29297.78988
IGZO-111-4-5_0	-29272.88175
IGZO-111-4-5_-48.2222	-29234.57157
IGZO-111-4-5_48.2222	-29297.45287
Average Band Gap	**3.83 eV**

IGZO-200-3 (In_2O_3)

File	Energy (Ry)
IGZO-200-3-1_0	-26569.12583
IGZO-200-3-1_-47.4921	-26530.74193
IGZO-200-3-1_47.4921	-26595.73706
IGZO-200-3-2_0	-26568.94407
IGZO-200-3-2_-47.4921	-26530.47927
IGZO-200-3-2_47.4921	-26595.55075
IGZO-200-3-3_0	-26570.87413
IGZO-200-3-3_-47.4921	-26532.45522
IGZO-200-3-3_47.4921	-26597.41473
IGZO-200-3-4_0	-26569.11242
IGZO-200-3-4_-47.4921	-26530.79624
IGZO-200-3-4_47.4921	-26595.75526
IGZO-200-3-5_0	-26570.1019
IGZO-200-3-5_-47.4921	-26531.71238
IGZO-200-3-5_47.4921	-26596.57548
Average Band Gap	**3.39 eV**

IGZO-201-4 (In_2ZnO_4)

File	Energy (Ry)
IGZO-201-4-1_0	-27905.78946
IGZO-201-4-1_-48.2222	-27866.40375
IGZO-201-4-1_48.2222	-27932.88139
IGZO-201-4-2_0	-27905.57763
IGZO-201-4-2_-48.2222	-27866.27312
IGZO-201-4-2_48.2222	-27932.64929
IGZO-201-4-3_0	-27905.38601
IGZO-201-4-3_-48.2222	-27866.08239
IGZO-201-4-3_48.2222	-27932.41174
IGZO-201-4-4_0	-27905.64497
IGZO-201-4-4_-48.2222	-27866.25213
IGZO-201-4-4_48.2222	-27932.71548
IGZO-201-4-5_0	-27905.89061
IGZO-201-4-5_-48.2222	-27866.68221
IGZO-201-4-5_48.2222	-27933.00969
Average Band Gap	**3.45 eV**

9. SINGLE POINT ENERGIES OF THE 999 CELLS FOR: ZNO, GA_2O_3, IN_2O_3, GA_2ZNO_4, $GA_2ZN_8O_{11}$, IN_2ZNO_4, INGAZNO4, AND $INGAO_3$

IGZO-001-1 (ZnO)

File	Energy (Ry)
IGZO-001-1-1_0	-65071.1709
IGZO-001-1-1_-104	-64986.42876
IGZO-001-1-1_104	-65125.23799
IGZO-001-1-2_0	-65077.87174
IGZO-001-1-2_-104	-64992.76941
IGZO-001-1-2_104	-65131.90265
IGZO-001-1-3_0	-65071.22675
IGZO-001-1-3_-104	-64986.53209
IGZO-001-1-3_104	-65125.35819
IGZO-001-1-4_0	-65071.0771
IGZO-001-1-4_-104	-64986.52005
IGZO-001-1-4_104	-65125.22981
IGZO-001-1-5_0	-65071.6481
IGZO-001-1-5_-104	-64986.92063
IGZO-001-1-5_104	-65125.75688
Average Band Gap	**4.01 eV**

IGZO-020-3 (Ga_2O_3)

File	Energy (Ry)
IGZO-020-3-1_0	-64755.59832
IGZO-020-3-1_-101.27	-64680.07317
IGZO-020-3-1_101.27	-64797.4085
IGZO-020-3-2_0	-64755.31087
IGZO-020-3-2_-101.27	-64679.5715
IGZO-020-3-2_101.27	-64797.02779
IGZO-020-3-3_0	-64755.3083
IGZO-020-3-3_-101.27	-64679.67625
IGZO-020-3-3_101.27	-64797.13607
IGZO-020-3-4_0	-64755.07287
IGZO-020-3-4_-101.27	-64679.42068
IGZO-020-3-4_101.27	-64796.90598
IGZO-020-3-5_0	-64755.21679
IGZO-020-3-5_-101.27	-64679.83549
IGZO-020-3-5_101.27	-64797.26696
Average Band Gap	**4.53 eV**

IGZO-021-4 (Ga_2ZnO_4)

File	Energy (Ry)
IGZO-021-4-1_0	-65037.46126
IGZO-021-4-1_-102.349	-64959.34793
IGZO-021-4-1_102.349	-65082.09343
IGZO-021-4-2_0	-65037.44357
IGZO-021-4-2_-102.349	-64959.47243
IGZO-021-4-2_102.349	-65082.1878
IGZO-021-4-3_0	-65037.35218
IGZO-021-4-3_-102.349	-64959.58666
IGZO-021-4-3_102.349	-65082.33074
IGZO-021-4-4_0	-65037.32416
IGZO-021-4-4_-102.349	-64959.19201
IGZO-021-4-4_102.349	-65082.28695
IGZO-021-4-5_0	-65037.67956
IGZO-021-4-5_-102.349	-64959.60902
IGZO-021-4-5_102.349	-65082.50172
Average Band Gap	**4.41 eV**

IGZO-028-11 ($Ga_2Zn_8O_{11}$)

File	Energy (Ry)
IGZO-028-11-1_0	-63810.60062
IGZO-028-11-1_-101.46	-63730.17151
IGZO-028-11-1_101.46	-63860.17181
IGZO-028-11-2_0	-63810.67524
IGZO-028-11-2_-101.46	-63730.27126
IGZO-028-11-2_101.46	-63860.06526
IGZO-028-11-3_0	-63810.38657
IGZO-028-11-3_-101.46	-63730.08014
IGZO-028-11-3_101.46	-63859.86953
IGZO-028-11-4_0	-63810.81792
IGZO-028-11-4_-101.46	-63730.41337
IGZO-028-11-4_101.46	-63860.27651
IGZO-028-11-5_0	-63810.338
IGZO-028-11-5_-101.46	-63730.05244
IGZO-028-11-5_101.46	-63859.79891
Average Band Gap	**4.14 eV**

IGZO-110-3 ($InGaO_3$)

File	Energy (Ry)
IGZO-110-3-1_0	-60704.67506
IGZO-110-3-1_-101.27	-60623.30241
IGZO-110-3-1_101.27	-60757.02125
IGZO-110-3-2_0	-60704.68725
IGZO-110-3-2_-101.27	-60623.13181
IGZO-110-3-2_101.27	-60757.05527
IGZO-110-3-3_0	-60704.33076
IGZO-110-3-3_-101.27	-60623.04965
IGZO-110-3-3_101.27	-60756.75117
IGZO-110-3-4_0	-60704.37644
IGZO-110-3-4_-101.27	-60623.21806
IGZO-110-3-4_101.27	-60756.73385
IGZO-110-3-5_0	-60704.92808
IGZO-110-3-5_-101.27	-60623.71148
IGZO-110-3-5_101.27	-60757.32603
Average Band Gap	**3.89 eV**

IGZO-111-4 ($InGaZnO_4$)

File	Energy (Ry)
IGZO-111-4-1_0	-62131.8762
IGZO-111-4-1_-102.349	-62050.60855
IGZO-111-4-1_102.349	-62184.47511
IGZO-111-4-2_0	-62132.28402
IGZO-111-4-2_-102.349	-62050.5026
IGZO-111-4-2_102.349	-62184.60156
IGZO-111-4-3_0	-62131.76121
IGZO-111-4-3_-102.349	-62050.17774
IGZO-111-4-3_102.349	-62184.19248
IGZO-111-4-4_0	-62132.1996
IGZO-111-4-4_-102.349	-62050.81668
IGZO-111-4-4_102.349	-62184.64509
IGZO-111-4-5_0	-62132.20874
IGZO-111-4-5_-102.349	-62050.78688
IGZO-111-4-5_102.349	-62184.62712
Average Band Gap	**3.86 eV**

IGZO-200-3 (In_2O_3)

File	Energy (Ry)
IGZO-200-3-1_0	-56655.23345
IGZO-200-3-1_-101.27	-56573.87038
IGZO-200-3-1_101.27	-56711.40318
IGZO-200-3-2_0	-56654.67342
IGZO-200-3-2_-101.27	-56573.27278
IGZO-200-3-2_101.27	-56710.72082
IGZO-200-3-3_0	-56655.36364
IGZO-200-3-3_-101.27	-56573.81268
IGZO-200-3-3_101.27	-56711.38646
IGZO-200-3-4_0	-56655.26388
IGZO-200-3-4_-101.27	-56573.6085
IGZO-200-3-4_101.27	-56711.32598
IGZO-200-3-5_0	-56655.66342
IGZO-200-3-5_-101.27	-56574.25019
IGZO-200-3-5_101.27	-56711.69825
Average Band Gap	**3.41 eV**

IGZO-201-4 (In_2ZnO_4)

File	Energy (Ry)
IGZO-201-4-1_0	-59227.22665
IGZO-201-4-1_-102.349	-59143.48784
IGZO-201-4-1_102.349	-59284.71185
IGZO-201-4-2_0	-59227.34797
IGZO-201-4-2_-102.349	-59143.47738
IGZO-201-4-2_102.349	-59284.72377
IGZO-201-4-3_0	-59227.05352
IGZO-201-4-3_-102.349	-59143.47203
IGZO-201-4-3_102.349	-59284.49335
IGZO-201-4-4_0	-59227.00678
IGZO-201-4-4_-102.349	-59143.40128
IGZO-201-4-4_102.349	-59284.56148
IGZO-201-4-5_0	-59227.1731
IGZO-201-4-5_-102.349	-59143.36189
IGZO-201-4-5_102.349	-59284.42951
Average Band Gap	**3.50 eV**

REFERENCES:

(1) Pedone, A.; Malavasi, G.; Menziani, M. C.; Cormack, A. N.; Segre, U. *J. Phys. Chem. B* **2006**, *110* (24), 11780–11795.

Appendix V.

ηScripts for Chapter 6

Accelerating and Automating Computational Chemistry through GPU Acceleration and ηScripts, a Toolkit of Scripts and Programs

1. ETA LIBRARIES:

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#
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1.1 EtaLibAtom.py:

```
#! /usr/bin/env python2.7

# Copyright (c) 2014, Thomas J. L. Mustard, O. Maduka Ogba, Paul Ha-Yeon Cheong
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#   OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN
ANY WAY OUT OF THE USE
#   OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF
SUCH DAMAGE.

import os
from sys import *

###============================================================
============================================================#
##
### --- Atom class --- ###
class Atom(object):
  def __init__(self):
    #Hold the string for the element
    self.e = ''
    #Hold the int for the element
    self.en = int(0)
    #Hold the float for the x coordinate
    self.x = float(0)
    #Hold the float for the y coordinate
    self.y = float(0)
    #Hold the float for the z coordinate
    self.z = float(0)
```

```
    #Hold a list of the neighbors
    self.neighbors = []
    #Hold a list of the distances for the neighbors
    self.neighborsdist = []
    #Hold the int for the atom nearest to this one
    self.nearest = int(0)
    #Hold the int for the atom nearest to this one
    self.nearestdist = float(100000000)
    #Hold a string for hybridization for this atom
    self.hybridization = ''
    #Hold an int/float for the charge of this atom
    self.charge = float(0)
    #Hold an int
    self.int = 0
    #Hold a string
    self.string = ''
    #Hold a string for the atomtype of this atom
    self.atomtype = ''

class ZMAT_Atom(object):
  def __init__(self):
    #Hold the string for the element
    self.e = ''
    #Hold the int for the element
    self.en = int(0)
    #Hold the float for the distance
    self.dist = float(0)
    #Hold the float for the angle
    self.angle = float(0)
    #Hold the float for the dihedral
    self.dihedral = float(0)
    #Hold the float for the distance
    self.atomdist = int(0)
    #Hold the float for the angle
    self.atomangle = int(0)
    #Hold the float for the dihedral
    self.atomdihedral = int(0)

### --- Input Arguments class --- ###
class InputArguments(object):
  def __init__(self):
    #ifile, config, charge, multi, writemod, modred, writeecp, ecplines,
writeclose, closelines
    #Hold the string for the input file
```

```
    self.ifile = ''
    #Hold the int for the charge
    self.charge = 0
    #Hold the int for the multiplicity
    self.multi = 1
    #Hold the list of config lines
    self.config = []
    #Hold the int/logic for the modredundant
    self.writemod = 0
    #Hold the list of modredundant lines
    self.modred = []
    #Hold the ecp string
    self.ecp = ""
    #Hold the int/logic for the ecp lines
    self.writeecp = 0
    #Hold the list of ecp lines
    self.ecplines = []
    #Hold the int/logic for the close lines
    self.writeclose = 0
    #Hold the list of closing lines
    self.closelines = []
    #Hold the close ecp string
    self.closeecp = ""
    #Hold the int/logic for the close ecp lines
    self.writecloseecp = 0
    #Hold the list of closing ecp lines
    self.closeecplines = []

### --- Reset Input Arguments class --- ###
def Eta_resetInputVariables(G0XInput):
  #Hold the string for the input file
  G0XInput.ifile = ''
  #Hold the int for the charge
  G0XInput.charge = 0
  #Hold the int for the multiplicity
  G0XInput.multi = 1
  #Hold the list of config lines
  G0XInput.config = []
  #Hold the int/logic for the modredundant
  G0XInput.writemod = 0
  #Hold the list of modredundant lines
  G0XInput.modred = []
  #Hold the ecp string
  G0XInput.ecp = ""
```

```
  #Hold the int/logic for the ecp lines
  G0XInput.writeecp = 0
  #Hold the list of ecp lines
  G0XInput.ecplines = []
  #Hold the int/logic for the close lines
  G0XInput.writeclose = 0
  #Hold the list of closing lines
  G0XInput.closelines = []
  #Hold the close ecp string
  G0XInput.closeecp = ""
  #Hold the int/logic for the close ecp lines
  G0XInput.writecloseecp = 0
  #Hold the list of closing ecp lines
  G0XInput.closeecplines = []
  return G0XInput

#Constants
auToAngstrom = 1.889725988579
hartreeTokcalmol = 627.509469
hartreeToeV = 27.21138386
kcalmolTokjoulemol = 4.184


###=============================================================
============================================================#
##

### --- Functions for Submission --- ###
###=============================================================
============================================================#
##
### --- Modify the text and return it --- ###
def Eta_returnModified(basename, program, queue, nproc, memory, file):
  #Setup some variables for snippets
  try:
    EtaDir = os.environ["ETADIR"]
  except os.error:
    EtaDir = "$ETADIR"
  try:
    AppDir = os.environ["APPDIR"]
  except os.error:
    AppDir = "$APPDIR"
  try:
    ScriptDir = os.environ["SCRIPTDIR"]
```

```
  except os.error:
    ScriptDir = "$SCRIPTDIR"
  #Start building up the modified text
  printLines = []
  f = open(file, 'r')
  for line in f:
    if "BASENAME!" in line:
      line = line.replace("BASENAME!", str(basename))
    if "PROGRAM!" in line:
      line = line.replace("PROGRAM!", str(program))
    if "QUE!" in line:
      line = line.replace("QUE!", str(queue))
    if "PROCS!" in line:
      line = line.replace("PROCS!", str(nproc))
    if "MEM!" in line:
      line = line.replace("MEM!", str(memory))
    if "ETADIR!" in line:
      line = line.replace("ETADIR!", str(EtaDir))
    if "SCRIPTDIR!" in line:
      line = line.replace("SCRIPTDIR!", str(ScriptDir))
    if "APPDIR!" in line:
      line = line.replace("APPDIR!", str(AppDir))
    printLines.append(line)
  f.close()
  return printLines

###============================================================
============================================================#
##

### --- Functions for files and directories --- ###
###============================================================
============================================================#
##
### --- Make directories if they do not exist --- ###
def Eta_makeDir(directory):
  if not os.path.exists(directory): os.makedirs(directory)
  return

### --- Delete file if it exists --- ###
def Eta_delFile(file):
  if os.path.isfile(file): os.remove(file)
  return
```

```
### --- Make directories if they do not exist --- ###
def Eta_basename(name, extension):
  basename = name[::-1].replace(extension[::-1], "")[::-1]
  return basename

###=========================================================
==========================================================#
##

### --- Functions to get and give element numbers and names --- ###
###=========================================================
==========================================================#
##
#A lowercase list of the elements
elementList = ["h", "he", "li", "be", "b", "c", "n", "o", "f", "ne", "na", "mg", "al",
"si", "p", "s", "cl", "ar", "k",
             "ca", "sc", "ti", "v", "cr", "mn", "fe", "co", "ni", "cu", "zn", "ga", "ge",
"as", "se", "br", "kr",
             "rb", "sr", "y", "zr", "nb", "mo", "tc", "ru", "rh", "pd", "ag", "cd", "in",
"sn", "sb", "te", "i", "xe",
             "cs", "ba", "la", "ce", "pr", "nd", "pm", "sm", "eu", "gd", "tb", "dy", "ho",
"er", "tm", "yb", "lu",
             "hf", "ta", "w", "re", "os", "ir", "pt", "au", "hg", "tl", "pb", "bi", "po", "at",
"rn", "fr", "ra",
             "ac", "th", "pa", "u", "np", "pu", "am", "cm", "bk", "cf", "es", "fm", "md",
"no", "lr", "rf", "db",
             "sg", "bh", "hs", "mt", "ds", "rg", "cn", "uut", "fl", "uup", "lv", "uus",
"uuo"]
#A list of the elements with there standard capitalization.
elementNames = ["H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne", "Na", "Mg",
"Al", "Si", "P", "S", "Cl", "Ar", "K",
              "Ca", "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Ga",
"Ge", "As", "Se", "Br", "Kr",
             "Rb", "Sr", "Y", "Zr", "Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd",
"In", "Sn", "Sb", "Te", "I",
             "Xe", "Cs", "Ba", "La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb",
"Dy", "Ho", "Er", "Tm", "Yb",
             "Lu", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg", "Tl", "Pb", "Bi",
"Po", "At", "Rn", "Fr",
             "Ra", "Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk", "Cf", "Es",
"Fm", "Md", "No", "Lr", "Rf",
             "Db", "Sg", "Bh", "Hs", "Mt", "Ds", "Rg", "Cn", "Uut", "Fl", "Uup", "Lv",
"Uus", "Uuo"]
```

```
#A list of the masses for each element (NOTE: I cannot attest to the scientific
accuracy for these masses)
elementMass = [1.0079, 4.0026, 6.941, 9.0122, 10.811, 12.0107, 14.0067,
15.9994, 18.9984, 20.1797, 22.9897, 24.305,
        26.9815, 28.0855, 30.9738, 32.065, 35.453, 39.0983, 39.948,
40.078, 44.9559, 47.867, 50.9415, 51.9961,
        54.938, 55.845, 58.6934, 58.9332, 63.546, 65.39, 69.723, 72.64,
74.9216, 78.96, 79.904, 83.8, 85.4678,
        87.62, 88.9059, 91.224, 92.9064, 95.94, 98, 101.07, 102.9055,
106.42, 107.8682, 112.411, 114.818, 118.71,
        121.76, 126.9045, 127.6, 131.293, 132.9055, 137.327, 138.9055,
140.116, 140.9077, 144.24, 145, 150.36,
        151.964, 157.25, 158.9253, 162.5, 164.9303, 167.259, 168.9342,
173.04, 174.967, 178.49, 180.9479, 183.84,
        186.207, 190.23, 192.217, 195.078, 196.9665, 200.59, 204.3833,
207.2, 208.9804, 209, 210, 222, 223, 226,
        227, 231.0359, 232.0381, 237, 238.0289, 243, 244, 247, 247, 251,
252, 257, 258, 259, 261, 262, 262, 264,
        266, 268, 272, 277]

#A list of the atoms that are 3rd row or below (aka large)
elementLarge = ["na", "mg", "al", "si", "p", "s", "cl", "ar", "k", "ca", "sc", "ti", "v",
"cr", "mn", "fe", "co", "ni",
         "cu", "zn", "ga", "ge", "as", "se", "br", "kr", "rb", "sr", "y", "zr", "nb",
"mo", "tc", "ru", "rh",
         "pd", "ag", "cd", "in", "sn", "sb", "te", "i", "xe", "cs", "ba", "la", "ce",
"pr", "nd", "pm", "sm",
         "eu", "gd", "tb", "dy", "ho", "er", "tm", "yb", "lu", "hf", "ta", "w", "re",
"os", "ir", "pt", "au",
         "hg", "tl", "pb", "bi", "po", "at", "rn", "fr", "ra", "ac", "th", "pa", "u", "np",
"pu", "am", "cm",
         "bk", "cf", "es", "fm", "md", "no", "lr", "rf", "db", "sg", "bh", "hs", "mt",
"ds", "rg", "cn", "uut",
         "fl", "uup", "lv", "uus", "uuo"]

#Check the elementList for the lowercase string and return the index for that
number + 1 (the atomic number)
def Eta_getElementNum(at1):
  element = elementList.index(at1.lower())
  return element + 1

#Check the elementName list for index (at1 - 1) and return the standard
capitalization
def Eta_getElementName(at1):
```

```
  element = elementNames[at1 - 1]
  return element

#Check the elementMass list for index (at1 - 1) and return the mass
def Eta_getElementMass(at1):
  atomicMass = elementMass[at1 - 1]
  return float(atomicMass)

###=========================================================
==========================================================#
##


### --- Lists and function to get ECP data and molecular charge --- ###
###=========================================================
==========================================================#
##
#A list of the element in the LANL2DZ ECP basis set
elementLANL2DZ_K = ["k", "ca", "sc", "ti", "v", "cr", "mn", "fe", "co", "ni", "cu",
"zn", "ga", "ge", "as", "se", "br",
                    "kr", "rb", "sr", "y", "zr", "nb", "mo", "tc", "ru", "rh", "pd", "ag", "cd",
"in", "sn", "sb", "te",
                    "i", "xe", "cs", "ba", "la", "hf", "ta", "w", "re", "os", "ir", "pt", "au",
"hg", "tl", "pb", "bi",
                    "u", "np", "pu"]
#A list of the element in the LANL08 ECP basis set
elementLANL08 = ["sc", "ti", "v", "cr", "mn", "fe", "co", "ni", "cu", "zn", "rb", "sr",
"y", "zr", "nb", "mo", "tc",
                    "ru", "rh", "pd", "ag", "cd", "in", "sn", "sb", "te", "i", "xe", "cs", "ba",
"la", "hf", "ta", "w",
                    "re", "os", "ir", "pt", "au", "hg", "tl", "pb", "bi"]

#A custom charge list for automatic charge calculation for ionic systems.
(Update as needed)
ionicReg = [1, 0, 1, 2, 3, -4, -3, -2, -1, 0, 1, 2, 3, "si", 3, "s", -1, "ar", 1, 2, "sc",
"ti", "v", "cr", "mn",
            "fe", "co", "0", "1", "0", 3, "ge", "as", "se", -1, "kr", "rb", "sr", "y", "zr", 5,
"mo", "tc", "ru",
            "rh", 0, 1, "cd", 3, "sn", "sb", "te", "i", "xe", "cs", "ba", "la", "ce", "pr",
"nd", "pm", "sm",
            "eu", "gd", "tb", "dy", "ho", "er", "tm", "yb", "lu", 3, "ta", "w", "re", "os",
"ir", 0, 1, "hg",
            "tl", "pb", "bi", "po", "at", "rn", "fr", "ra", "ac", "th", "pa", "u", "np", "pu",
"am", "cm", "bk", "cf",
```

```
          "es", "fm", "md", "no", "lr", "rf", "db", "sg", "bh", "hs", "mt", "ds", "rg",
"cn", "uut", "fl", "uup",
          "lv", "uus", "uuo"]

#Check the chargeList for the element at1 and return the charge associated
with it.
def Eta_getElementCharge(at1, chargeList):
  element = chargeList[at1]
  return element

### --- Calculate charge from file --- ###
def Eta_ionic(ionicswitch, ionicCM, ifilelol):
  #Start with charge zero
  charge = 0
  #Logic to use the ionicReg charge list
  if ionicCM.lower() == "reg":
    #Iterate through the list of atoms (skipping the number of atoms and the
second informational line) in the ifilelol
    for i in range(2, len(ifilelol)):
      #Sum the charge returned from the Eta_getElementCharge function, but
first cleaning the input with Eta_getElementNum
      charge += int(Eta_getElementCharge(Eta_getElementNum(ifilelol[i].e) - 1,
ionicReg))
  return charge



### --- General structure functions --- ###
###=====================================================
=====================================================#
##
### --- Parse the input XYZ file and convert it into a Atom Class list of lists ---
###
def Eta_XYZ_LOL(ifile):
  ### --- Open parent file, read it in and close it --- ###
  f = open(ifile, "r")
  ifileList = f.readlines()
  f.close()
  ### --- Create some variables needed for parsing the input file --- ###
  # ifilelength is used to gauge what line we are on and also allows us to
determine the number of lines in the file
  # ifilelol is a list of lists (lol) that will hold all the data of the input file
  # a_list is a temp list that will be appended to the ifilelol
  ################################
```

```
  #Find out the final length of the ifilelol
  ifileLength = len(ifileList)
  #Fill the ifilelol with 0's so that there is a place to put the atomic data
  ifilelol = [0] * ifileLength
  #### --- Input/parse the input file into a list of lists called ifilelol --- ###
  for i in range(ifileLength):
    #If i == 0 then put the number of atoms in as an int
    if i == 0:
      ifilelol[i] = int(ifileList[i].rstrip())
    #if i == 1 then put some information in as a string (here it is the second line
of the XYZ file)
    elif i == 1:
      ifilelol[i] = str(ifileList[i].rstrip())
    #if i >= 2 then make the instance of ifilelol an Atom class then fill it with
element data, and coordinate data
    elif i >= 2:
      line = ifileList[i].rstrip().split()
      ifilelol[i] = Atom()
      ifilelol[i].e = line[0]
      ifilelol[i].en = Eta_getElementNum(line[0])
      ifilelol[i].x = float(line[1])
      ifilelol[i].y = float(line[2])
      ifilelol[i].z = float(line[3])
  #If the XYZ file is longer or shorter than the list of data should be, warn the
user.
  if int(ifilelol[0]) + 2 != ifileLength:
    print "Your file is the wrong length!"
    print "Make sure you have the right number of atoms."
    exit(0)
  return ifilelol

### --- Output the structural data in an XYZ format
def Eta_outputXYZ(ofile, ifilelol):
  #Open the file for writing
  f = open(ofile, "w+")
  #iterate through the whole ifilelol and write each line in XYZ format to the file
  for i in range(len(ifilelol)):
    #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
    if isinstance(ifilelol[i], Atom):
      line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
    #else print the string (number of atoms or comment line)
    else:
```

```
      line = str(ifilelol[i])
    f.write(line + "\n")
  f.close
  return

### --- Output the trajectory data in an XYZ format and append it to the file
def Eta_outputXYZ_Traj(ofile, ifilelol):
  #Open the file for writing
  f = open(ofile, "a")
  #iterate through the whole ifilelol and write each line in XYZ format to the file
  for i in range(len(ifilelol)):
    #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
    if isinstance(ifilelol[i], Atom):
      line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
    #else print the string (number of atoms or comment line)
    else:
      line = str(ifilelol[i])
    f.write(line + "\n")
  f.close
  return

### --- Renumber atoms to put the atoms of interest at the front in the correct
order --- ###
def Eta_renumberbasic(ifilelol, badlist):
  #Create the real ifilelol and add the first two lines
  ifilelol_renumbered = ["0"] * len(ifilelol)
  ifilelol_renumbered[0] = ifilelol[0]
  ifilelol_renumbered[1] = ifilelol[1]
  #Iterate through the bond_angle_dihedral list and put them at the top of the
list
  for i, atom in enumerate(badlist):
    ifilelol_renumbered[i+2] = ifilelol[atom + 1]
  #Iterate throught the ifilelol and add the rest of the file to the renumbered
  usedBAD = 0
  for i in range(2, len(ifilelol)):
    if i-1 not in badlist:
      ifilelol_renumbered[i + len(badlist) - usedBAD] = ifilelol[i]
    else:
      usedBAD = usedBAD + 1
  return ifilelol_renumbered

### --- Import a large trajectory and export only the Xth geometry --- ###
```

```
def Eta_getGeomXX(trajectory, geometry):
  numAtoms = int(trajectory[0])
  geometryLength = numAtoms + 2
  startLine = (geometryLength * (geometry-1))
  endLine = startLine + geometryLength
  ifilelol = [0] * geometryLength
  count = 0
  for i in range(startLine, endLine):
    if isinstance(trajectory[i], Atom):
      ifilelol[count] = Atom()
      ifilelol[count] = trajectory[i]
    else:
      ifilelol[count] = trajectory[i]
    count += 1
  return ifilelol

### --- Snippet functions --- ###
###============================================================
============================================================#
##
### --- Open and parse the snippet file --- ###
def Eta_parseSnippet(snippet):
  #open the file for reading
  f = open(snippet)
  snipList = f.readlines()
  f.close()
  #set up some blank/zeroed variables
  configswitch = 0
  config = []
  ecpswitch = 0
  ecp = ""
  closeswitch = 0
  closelines = []
  writeecp = 0
  writeclose = 0
  #iterate through the length of the snippet file line by line
  for i, var in enumerate(snipList):
    #create a split line
    line = var.strip()
    #if the end of a section is set stop recording
    if line == "#END":
      ecpswitch = 0
      closeswitch = 0
      configswitch = 0
```

```
    #For the config section start collecting the lines
    elif configswitch == 1:
      config.append(line)
    #For the ecp section start collecting the lines
    elif ecpswitch == 1:
      ecp = line
    #For the close section start collecting the lines
    elif closeswitch == 1:
      closelines.append(line)
    #use the # lines to turn on collection of sections
    elif line == "#CONFIG":
      configswitch = 1
    elif line == "#ECP":
      writeecp = 1
      ecpswitch = 1
    elif line == "#CLOSE":
      writeclose = 1
      closeswitch = 1
  return (config, ecp, closelines, writeecp, writeclose)

### --- Interactive mode for CONFIG --- ###
def Eta_interactiveConfig(SOMETHIGN):
  #set up some blank/zeroed variables
  configswitch = 0
  config = []
  ecpswitch = 0
  ecp = ""
  closeswitch = 0
  closelines = []
  writeecp = 0
  writeclose = 0

  #Figure out the method
  var = input("Method:")
  if var == 1:
    config.append("#B3LYP/")
  elif var == 2:
    config.append("#M06/")
  elif var == 3:
    config.append("#M06-2X/")
  elif var == 4:
    config.append("#M06-2X/")
  #Figure out the basis set
  var = input("Will there be ECPs? (y/n)")
```

```
if var.lower() == "y":
  var = input("ECPs Type:")
  if var == 1:
    config.append("gen ")
    ecp.append("LANL2DZ")
  elif var == 2:
    config.append("gen ")
    ecp.append("SOMETHINGELSE")
var = input("Basis set:")
if var == 1:
  config.append("6-31G* ")
elif var == 2:
  config.append("6-311++G** ")
elif var == 2:
  config.append("6-311++G** ")
var = input("Job Type:")
var = input("Solvation:")
var = input("Extras:")

if SOMETHIGN == 1:
  #if the end of a section is set stop recording
  if line == "#END":
    ecpswitch = 0
    closeswitch = 0
    configswitch = 0
  #For the config section start collecting the lines
  elif configswitch == 1:
    config.append(line)
  #For the ecp section start collecting the lines
  elif ecpswitch == 1:
    ecp = line
  #For the close section start collecting the lines
  elif closeswitch == 1:
    closelines.append(line)
  #use the # lines to turn on collection of sections
  elif line == "#CONFIG":
    configswitch = 1
  elif line == "#ECP":
    writeecp = 1
    ecpswitch = 1
  elif line == "#CLOSE":
    writeclose = 1
    closeswitch = 1
return (config, ecp, closelines, writeecp, writeclose)
```

```
### --- Gaussian Specific functions --- ###
###============================================================
============================================================#
##
### --- Open and parse the snippet file --- ###
def Eta_parseSnippetG0X(snippet, G0XInput):
  #open the file for reading
  f = open(snippet)
  snipList = f.readlines()
  f.close()
  #set up some blank/zeroed variables
  configswitch = 0
  ecpswitch = 0
  closeswitch = 0
  closeecpswitch = 0
  #G0XInput.config = []
  #G0XInput.ecp = ""
  #G0XInput.closeecp = ""
  #G0XInput.closelines = []
  #G0XInput.writeecp = 0
  #G0XInput.writeclose = 0
  #G0XInput.writecloseecp = 0
  #Iterate through the length of the snippet file line by line
  for i, var in enumerate(snipList):
    #create a split line
    line = var.strip()
    #if the end of a section is set stop recording
    if line == "#END":
      ecpswitch = 0
      closeswitch = 0
      configswitch = 0
      closeecpswitch = 0
    #For the config section start collecting the lines
    elif configswitch == 1:
      G0XInput.config.append(line)
    #For the ecp section start collecting the lines
    elif ecpswitch == 1:
      G0XInput.ecp = line
    #For the close section start collecting the lines
    elif closeswitch == 1:
      G0XInput.closelines.append(line)
    #For the close ecp section start collecting the lines
```

```
    elif closeecpswitch == 1:
      G0XInput.closeecp = line
    #use the # lines to turn on collection of sections
    elif line == "#CONFIG":
      configswitch = 1
    elif line == "#ECP":
      G0XInput.writeecp = 1
      ecpswitch = 1
    elif line == "#ECPCLOSE":
      G0XInput.writecloseecp = 1
      closeecpswitch = 1
    elif line == "#CLOSE":
      G0XInput.writeclose = 1
      closeswitch = 1
  return G0XInput

### --- Parses the input G0X file --- ###
def Eta_parseInputG0X(ifile):
  config = []
  comment = ""
  charge = 0
  multi = 1
  initialgeom = []
  endlines = []
  inputNumAtoms = 0
  emptyline = 0
  endline = "no"
  the_file = open(ifile, 'r')
  for line in the_file:
    if line.strip() == "" and endline == "no":
      emptyline += 1
    if line.strip() != '' and emptyline == 0:
      config.append(line.strip())
    if line.strip() != '' and emptyline == 1:
      comment = line.strip()
    if line.strip() != '' and emptyline == 3:
      initialgeom.append(line.strip())
      inputNumAtoms += 1
    if line.strip() != '' and emptyline == 2:
      charge = int(line.split()[0])
      multi = int(line.split()[1])
      emptyline += 1
    if line.strip() != '' and emptyline == 4:
      endline = "yes"
```

```
      emptyline += 1
    if emptyline >= 5:
      endlines.append(line.strip())
  ifilelol = [0] * (inputNumAtoms + 2)
  ifilelol[0] = inputNumAtoms
  ifilelol[1] = comment
  for i, var in enumerate(initialgeom):
    line = var.split()
    ifilelol[i+2] = Atom()
    ifilelol[i+2].e = line[0]
    ifilelol[i+2].en = Eta_getElementNum(line[0])
    ifilelol[i+2].x = float(line[1])
    ifilelol[i+2].y = float(line[2])
    ifilelol[i+2].z = float(line[3])
  return config, endlines, charge, multi, ifilelol

### --- Parses the geometry and energy created by G0X and gives back the
last geometry in a list of lists --- ###
def Eta_parseOutputG0X(ifile):
  a_list = []
  geom = 0
  numAtoms = 0
  charge = 0
  multi = 1
  finalenergy = 0.0
  the_file = open(ifile, 'r')
  for idx, line in enumerate(the_file):
    if line.strip() != '':
      if line.split()[0] == 'SCF':
        finalenergy = float(line.split()[4])
      if line.split()[0] == 'NAtoms=':
        numAtoms = int(line.split()[1])
      if "---------------------------------------------" in line and geom >= 6:
        geom = 0
      if geom >= 1:
        geom += 1
      if line.strip() == "Standard orientation:":
        geom = 1
      if geom >= 5:
        a_list.append(line)
      #Get charge and multiplicity
      elif 'Multiplicity' in line:
        chargeMulti = line.split()
        charge = chargeMulti[2]
```

```
        multi = chargeMulti[-1]
  the_file.close()
  a_listDd = [x for x in a_list if x != " ----------------------------------------------------
-------------\n"]
  finalgeom =  [0] * (numAtoms + 2)
  finalgeom[0] = str(numAtoms)
  finalgeom[1] = "Energy: " + str(finalenergy)
  #print a_listDd
  for i in range(len(a_listDd) - numAtoms, len(a_listDd)):
    line = a_listDd[i].split()
    j = i - len(a_listDd) + numAtoms + 2
    finalgeom[j] = Atom()
    finalgeom[j].e = Eta_getElementName(int(line[1]))
    finalgeom[j].en = int(line[0])
    finalgeom[j].x = float(line[3])
    finalgeom[j].y = float(line[4])
    finalgeom[j].z = float(line[5])
  return (finalgeom, charge, multi)

### --- Parses the geometry and energy created by G0X and gives back the
trajectory in a list of lists --- ###
def Eta_parseOutputG0X_Traj(ifile):
  a_list = []
  geom = 0
  numAtoms = 0
  allEnergy = []
  trajectorygeom = []
  the_file = open(ifile, 'r')
  for idx, line in enumerate(the_file):
    if line.strip() != '':
      if line.split()[0] == 'SCF':
        allEnergy.append(float(line.split()[4]))
      if line.split()[0] == 'NAtoms=':
        numAtoms = int(line.split()[1])
      if "---------------------------------------------" in line and geom >= 6:
        geom = 0
      if geom >= 1:
        geom += 1
      if line.strip() == "Standard orientation:":
        geom = 1
      if geom >= 5:
        a_list.append(line)
      #Get charge and multiplicity
      elif 'Multiplicity' in line:
```

```
        chargeMulti = line.split()
        charge = chargeMulti[2]
        multi = chargeMulti[-1]
  the_file.close()
  a_listDd = [x for x in a_list if "---------------------------------------------------" not in
x]
  trajectorygeom = [0] * (len(a_listDd)/numAtoms * (numAtoms + 2))
  skip = 0
  for i in range(len(a_listDd)):
    if i % numAtoms == 0 and i/numAtoms != len(allEnergy):
      trajectorygeom[i+skip] = int(numAtoms)
      trajectorygeom[i+skip+1] = "Energy: " + str(allEnergy[i/numAtoms])
      skip = skip + 2
    elif i % numAtoms == 0 and i/numAtoms >= len(allEnergy):
      trajectorygeom[i+skip] = int(numAtoms)
      trajectorygeom[i+skip+1] = "Energy: " + str(allEnergy[-1])
      skip = skip + 2
    line = a_listDd[i].split()
    trajectorygeom[i+skip] = Atom()
    trajectorygeom[i+skip].e = Eta_getElementName(int(line[1]))
    trajectorygeom[i+skip].en = int(line[0])
    trajectorygeom[i+skip].x = float(line[3])
    trajectorygeom[i+skip].y = float(line[4])
    trajectorygeom[i+skip].z = float(line[5])
  return (trajectorygeom, charge, multi)

### --- Logic for the ECP data for G0X --- ###
def Eta_G0XECP(ecp, config, ifilelol):
  ecplines = []
  ecplist = []
  genlist = []
  if "LANL2DZ" in ecp:
    for i in range(2, len(ifilelol)):
      if ifilelol[i].e.lower() in elementLANL2DZ_K and ifilelol[i].e not in ecplist:
        ecplist.append(ifilelol[i].e)
      if ifilelol[i].e.lower() not in elementLANL2DZ_K and ifilelol[i].e not in
genlist:
        genlist.append(ifilelol[i].e)
    ecplines.append(' '.join(str(e) for e in genlist) + " 0")
    ecplines.append(ecp.split("/")[0])
    ecplines.append("****")
    if len(ecplist) > 0:
      ecplines.append(' '.join(str(e) for e in ecplist) + " 0")
      ecplines.append("LANL2DZ")
```

```
      ecplines.append("****")
      ecplines.append("")
      ecplines.append(' '.join(str(e) for e in ecplist) + " 0")
      ecplines.append("LANL2DZ")
    elif len(ecplist) == 0:
      for i in range(len(config)):
        config[i] = config[i].replace("pseudo=read ", "")
  elif "LANL08" in ecp:
    for i in range(2, len(ifilelol)):
      if ifilelol[i].e.lower() in elementLANL08 and ifilelol[i].e not in ecplist:
        ecplist.append(ifilelol[i].e)
      if ifilelol[i].e.lower() not in elementLANL08 and ifilelol[i].e not in genlist:
        genlist.append(ifilelol[i].e)
    ecplines.append(' '.join(str(e) for e in genlist) + " 0")
    ecplines.append(ecp.split("/")[0])
    ecplines.append("****")
    if len(ecplist) > 0:
      #ecplines.append(' '.join(str(e) for e in ecplist) + " 0")
      ecplines.append("@/share/apps/g09/basis/lanl08-bs.gbs")
      #ecplines.append("****")
      ecplines.append("")
      #ecplines.append(' '.join(str(e) for e in ecplist) + " 0")
      ecplines.append("@/share/apps/g09/basis/lanl08-ecp.gbs")
    elif len(ecplist) == 0:
      for i in range(len(config)):
        config[i] = config[i].replace("pseudo=read ", "")
  else:
    for i in range(2,len(ifilelol)):
      if ifilelol[i].e.lower() in elementLANL2DZ_K and ifilelol[i].e not in ecplist:
        ecplist.append(ifilelol[i].e)
      if ifilelol[i].e.lower() not in elementLANL2DZ_K and ifilelol[i].e not in
genlist:
        genlist.append(ifilelol[i].e)
    ecplines.append(' '.join(str(e) for e in genlist) + " 0")
    ecplines.append(ecp.split("/")[0])
    ecplines.append("****")
    if len(ecplist) > 0:
      ecplines.append(" ")
      ecplines.append(' '.join(str(e) for e in ecplist) + " 0")
      ecplines.append(ecp.split("/")[1])
      ecplines.append("****")
      ecplines.append("")
      ecplines.append(' '.join(str(e) for e in ecplist) + " 0")
      ecplines.append(ecp.split("/")[1])
```

```
    elif len(ecplist) == 0:
      for i in range(len(config)):
        config[i] = config[i].replace("pseudo=read ", "")
  return (config, ecplines)

### --- Out put the G0X input files --- ###
def Eta_outputG0X(ifile, G0XInput, ifilelol):
  #config, charge, multi, writemod, modred, writeecp, ecplines, writeclose,
closelines
  ofiletmp = ifile.split(".")
  ofile = ""
  for i in range(len(ofiletmp)):
    if i != len(ofiletmp) - 1:
      ofile += ofiletmp[i] + "."
    elif i == len(ofiletmp) - 1:
      ofile += "com"
  #print ofile
  f = open("NEWJOBS.G0X/" + ofile, "w+")
  for i, var in enumerate(G0XInput.config):
    f.write(var + "\n")
  f.write("\n")
  f.write(ifile + "\n")
  f.write("\n")
  f.write(str(G0XInput.charge) + "  " + str(G0XInput.multi) + "\n")
  for i in range(2, len(ifilelol)):
    line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
    f.write(line + "\n")
  f.write("\n")
  if G0XInput.writemod == 1:
    if len(G0XInput.modred) > 0 and G0XInput.modred[0] != "":
      for i, var in enumerate(G0XInput.modred):
        f.write(var + "\n")
    else:
      f.write("MODRED!\n")
    f.write("\n")
  if G0XInput.writeecp == 1:
    for i, var in enumerate(G0XInput.ecplines):
      f.write(var + "\n")
    f.write("\n")
  if G0XInput.writeclose == 1:
    for i, var in enumerate(G0XInput.closelines):
      f.write(var + "\n")
    f.write("\n")
```

```
  if G0XInput.writecloseecp == 1:
    for i, var in enumerate(G0XInput.closeecplines):
      f.write(var + "\n")
    f.write("\n")
  f.close()
  return

#Parse the Gaussian output file and print data to the screen
def Eta_TranslateG0XOutput(logfile, trans, printType):
  initLines = ['\033[1;34mPython Gaussian 0X Output File Parsing Script:
nGT.py\033[1;0m',
            '\033[1;34mScripted by Thomas J. L. Mustard, O. Maduka Ogba, Paul
Ha-Yeon Cheong\033[1;0m',
            '--------------------------------------------------------------------------------']
  if trans == "translate":
    for line in initLines:
      print line

  #Global Variables
  config = ''
  configSwitch = 0
  printLines = []
  programVersion = ''
  chk = ''
  nproc = ''
  mem = ''
  configLines = []
  configLinesAll = ''
  modSwitch = 0
  modLines = []
  pointStoic = ''
  point = ''
  stoic = ''
  chargeMulti = ''
  charge = ''
  multi = ''
  basisFunc = ''
  scfEnergy = ''
  predEChange = ''
  optSwitch = 0
  optComplete = 0
  optStep = 0
  if printType == "long" or printType == "extra":
    maxForce = []
```

```
  rmsDisp = []
  rmsForce = []
  maxDisp = []
else:
  maxForce = ''
  rmsForce = ''
  maxDisp = ''
  rmsDisp = ''
freqSwitch = 0
freqTemp = ''
if trans == "list":
  frequencies = ["0.00", "0.00", "0.00", "0.00", "0.00", "0.00"]
  negfreq = 0
  zeroPointE = '0.000000'
  thermE = '0.000000'
  enthalpyE = '0.000000'
  gibbsE = '0.000000'
  zeroPointESUM = '0.000000'
  thermESUM = '0.000000'
  enthalpyESUM = '0.000000'
  gibbsESUM = '0.000000'
  totalS = '0.000000'
  elecS = '0.000000'
  rotS = '0.000000'
  transS = '0.000000'
  vibS = '0.000000'
else:
  frequencies = ["0.00", "0.00", "0.00", "0.00", "0.00", "0.00"]
  negfreq = 0
  zeroPointE = ''
  thermE = ''
  enthalpyE = ''
  gibbsE = ''
  zeroPointESUM = ''
  thermESUM = ''
  enthalpyESUM = ''
  gibbsESUM = ''
  totalS = ''
  elecS = ''
  rotS = ''
  transS = ''
  vibS = ''
jobDone = 0
memSwitch = 0
```

```
f = open(logfile)
fileList = f.readlines()
f.close()
for i, var in enumerate(fileList):
  if i == 0 and 'Entering Gaussian System' not in var:
    print "Error! Not a Gaussian log file."
    exit(0)
  #Find the Gaussian Version
  elif 'Cite this work as:' in var:
    programVersion = fileList[i+1].rstrip().rstrip(',')
  #Find the chk file
  elif '%chk=' in var:
    chk = var.split('=')[1].rstrip()
  #Find the nproc used
  elif '%nproc=' in var:
    nproc = var.split('=')[1].rstrip()
  #Find the mem used
  elif '%mem' in var:
    mem = var.split('=')[1].rstrip()
    memSwitch = 1
  #Find the job configuration used
  elif memSwitch == 1 and "----------" in var:
    for j in range(1,5):
      if "-------" not in fileList[i+j]:
        configLines.append(fileList[i+j].strip())
        configLinesAll += fileList[i+j].strip()
      else:
        memSwitch = 0
        break
    #print configLinesAll
    if ' opt=' in configLinesAll:
      optSwitch = 1
    if 'modredundant' in configLinesAll:
      modSwitch = 1
    if 'freq' in configLinesAll:
      freqSwitch = 1
  #Check to see if modredundant is in the config
  elif modSwitch == 1:
    if 'The following ModRedundant input section has been read:' in var:
      for j in range(1,20):
        if len(fileList[i+j]) > 2:
          modLines.append(fileList[i+j].strip())
        else:
          break
```

```
#Get pointgroup and stoic
if 'Framework group' in var:
  pointStoic  = var.split()[-1]
  point = pointStoic.split('[')[0]
elif 'Stoichiometry' in var:
  stoic = var.split()[-1]
#Get charge and multiplicity
elif 'Multiplicity' in var:
  chargeMulti = var.split()
  charge = chargeMulti[2]
  multi = chargeMulti[-1]
#Find basis functions
#elif 'Two-electron integral symmetry is turned on.' in var:
#  basisFunc = fileList[i+1].strip().split()[0]
elif 'basis functions,' in var:
  basisFunc = var.strip().split()[0]
#Get SCF Energy and predicted change
elif 'SCF Done:' in var:
  scfEnergy = var.strip().split()[4]
elif 'Predicted change in Energy=' in var:
  predEChange = var.strip().split('=')[-1]
#Optimization parse
elif optSwitch == 1:
  if 'Optimization completed.' in var:
    optComplete = 1
  elif 'Optimization completed on the basis of negligible forces.' in var:
    optComplete = 2
  if printType == "none":
    if 'Maximum Force' in var:
      maxForce = var.rstrip().split()
      if maxForce[-1] == "NO":
        maxForce[-1] = '\033[1;31mNO!\033[1;0m'
      elif maxForce[-1] == "YES":
        maxForce[-1] = '\033[1;32mYES\033[1;0m'
    elif 'RMS     Force' in var:
      rmsForce = var.rstrip().split()
      if rmsForce[-1] == "NO":
        rmsForce[-1] = '\033[1;31mNO!\033[1;0m'
      elif rmsForce[-1] == "YES":
        rmsForce[-1] = '\033[1;32mYES\033[1;0m'
    elif 'Maximum Displacement' in var:
      maxDisp = var.rstrip().split()
      if maxDisp[-1] == "NO":
        maxDisp[-1] = '\033[1;31mNO!\033[1;0m'
```

```
      elif maxDisp[-1] == "YES":
        maxDisp[-1] = '\033[1;32mYES\033[1;0m'
    elif 'RMS     Displacement' in var:
      rmsDisp = var.rstrip().split()
      if rmsDisp[-1] == "NO":
        rmsDisp[-1] = '\033[1;31mNO!\033[1;0m'
      elif rmsDisp[-1] == "YES":
        rmsDisp[-1] = '\033[1;32mYES\033[1;0m'
    elif 'Step number' in var and 'out of a maximum' in var:
      optStep = var.split()[2].strip()
  elif printType == "long" or printType == "extra":
    if 'Step number' in var and 'out of a maximum' in var:
      optStep = var.split()[2].strip()
    elif 'Maximum Force' in var:
      maxForce.append(list(var.rstrip().split()))
      if maxForce[-1][-1] == "NO":
        maxForce[-1][-1] = '\033[1;31mNO!\033[1;0m'
      elif maxForce[-1][-1] == "YES":
        maxForce[-1][-1] = '\033[1;32mYES\033[1;0m'
    elif 'RMS     Force' in var:
      rmsForce.append(list(var.rstrip().split()))
      if rmsForce[-1][-1] == "NO":
        rmsForce[-1][-1] = '\033[1;31mNO!\033[1;0m'
      elif rmsForce[-1][-1] == "YES":
        rmsForce[-1][-1] = '\033[1;32mYES\033[1;0m'
    elif 'Maximum Displacement' in var:
      maxDisp.append(list(var.rstrip().split()))
      if maxDisp[-1][-1] == "NO":
        maxDisp[-1][-1] = '\033[1;31mNO!\033[1;0m'
      elif maxDisp[-1][-1] == "YES":
        maxDisp[-1][-1] = '\033[1;32mYES\033[1;0m'
    elif 'RMS     Displacement' in var:
      rmsDisp.append(list(var.rstrip().split()))
      if rmsDisp[-1][-1] == "NO":
        rmsDisp[-1][-1] = '\033[1;31mNO!\033[1;0m'
      elif rmsDisp[-1][-1] == "YES":
        rmsDisp[-1][-1] = '\033[1;32mYES\033[1;0m'


#Frequency and
if freqSwitch == 1:
  if 'Temperature' in var:
    freqTemp = var.strip()
  #elif 'Vibrational temperatures:' in var:
```

```
#  frequencies = var.strip().split(':')[-1].strip()
elif "Frequencies --" in var:
  if frequencies[0] == "0.00":
    frequencies = []
  if "---" in var:
    frequencies.append(var.split()[1].strip().replace('---', '-'))
    frequencies.append(var.split()[2].strip())
    frequencies.append(var.split()[3].strip())
  elif len(var.split()) == 3:
    frequencies.append(var.split()[2].strip())
    frequencies.append("0.000")
    frequencies.append("0.000")
    frequencies.append("0.000")
    frequencies.append("0.000")
    frequencies.append("0.000")
  elif len(var.split()) == 4:
    frequencies.append(var.split()[2].strip())
    frequencies.append(var.split()[3].strip())
    frequencies.append("0.000")
    frequencies.append("0.000")
    frequencies.append("0.000")
    frequencies.append("0.000")
  else:
    frequencies.append(var.split()[2].strip())
    frequencies.append(var.split()[3].strip())
    frequencies.append(var.split()[4].strip())
elif 'imaginary frequencies' in var:
  if var.strip().split()[0] == "******":
    negfreq = int(var.strip().split()[1])
  else:
    negfreq = int(var.strip().split()[0])
elif 'Zero-point correction' in var:
  zeroPointE = str(var.strip().split()[-2])
elif 'Thermal correction to Energy' in var:
  thermE = str(var.strip().split()[-1])
elif 'Thermal correction to Enthalpy' in var:
  enthalpyE = str(var.strip().split()[-1])
elif 'Thermal correction to Gibbs Free Energy' in var:
  gibbsE = str(var.strip().split()[-1])
elif 'Sum of electronic and zero-point Energies' in var:
  zeroPointESUM = str(var.strip().split()[-1])
elif 'Sum of electronic and thermal Energies' in var:
  thermESUM = str(var.strip().split()[-1])
elif 'Sum of electronic and thermal Enthalpies' in var:
```

```
        enthalpyESUM = str(var.strip().split()[-1])
      elif 'Sum of electronic and thermal Free Energies' in var:
        gibbsESUM = str(var.strip().split()[-1])
        totalS = str(fileList[i+4].strip().split()[-1])
        elecS = str(fileList[i+5].strip().split()[-1])
        transS = str(fileList[i+6].strip().split()[-1])
        rotS = str(fileList[i+7].strip().split()[-1])
        vibS = str(fileList[i+8].strip().split()[-1])
    if 'Normal termination of Gaussian' in var and len(fileList) - i < 10:
      jobDone = 1
    elif 'Error termination' in var and i - len(fileList) < 10:
      jobDone = 2

  if trans == "translate":
    #Printed output list
    #printLines = ['\033[1;44m
\033[1;0m']
    printLines = ['Analyzing Gaussian Output File: ' + logfile]
    printLines.append('Using ' + str(programVersion))
    printLines.append('[#Processors=' + nproc + '  Memory=' + mem + '
CheckPoint=' + chk + ']')

printLines.append('==========================================
==================================')

  elif trans == "archive":
    #Initial information
    printLines.append("Supporting Information: " + logfile)
    printLines.append("------------------------------------------------------------------------
----")
    printLines.append("Using: " + programVersion)

printLines.append("==========================================
==================================")

  if trans == "archive" or trans == "translate":
    #Print config
    for line in configLines:
      printLines.append(line)

    #Modredundant output
    if modSwitch == 1:
      for line in modLines:
        printLines.append(line)
```

```
    #Print pointgroup and stoichiometry
    printLines.append('-------------------------------------------------------------------------------
----')
    printLines.append('Pointgroup=' + point + '\tStoichiometry=' + stoic + '\t' +
pointStoic)

    #Print Charge Multi and BasisFunc
    printLines.append('Charge = ' + charge + '\tMultiplicity = ' + multi + '\tBasis
= ' + basisFunc)
    printLines.append('-------------------------------------------------------------------------------
----')

    #Print Energy
    printLines.append('SCF Energy = ' + scfEnergy + '\tPredicted Change = ' +
predEChange)
    printLines.append('-------------------------------------------------------------------------------
----')


    #Optimization output
    if optSwitch == 1:
      if optComplete >= 1 and optStep != 0:
        printLines.append('\033[1;32mOptimization completed.\033[0;0m  ---------
------------------  Optimization step: ' + optStep)
      elif optComplete >= 1 and optStep == 0:
        printLines.append('\033[1;32mOptimization completed.\033[0;0m')
      elif optComplete == 0 and optStep != 0:
        printLines.append('\033[1;31mOptimization incomplete.\033[0;0m  --------
------------------  Optimization step: ' + optStep)
      elif optComplete == 0 and optStep == 0:
        printLines.append('\033[1;31mOptimization incomplete.\033[0;0m')
      if optComplete == 2:
        printLines.append('\033[1;33mOptimization completed on the basis of
negligible forces.\033[0;0m')
      if len(maxForce) > 0 and printType == "none":
        printLines.append('Item      Max Val.    Criteria    Pass?      RMS Val.
Criteria    Pass?')
        printLines.append('Force     ' + maxForce[-3] + ' ll ' + maxForce[-2] + '    '
+ maxForce[-1] + '        ' + rmsForce[-3] + ' ll ' + rmsForce[-2] + '    ' +
rmsForce[-1])
        printLines.append('Disp      ' + maxDisp[-3] + ' ll ' + maxDisp[-2] + '    ' +
maxDisp[-1] + '        ' + rmsDisp[-3] + ' ll ' + rmsDisp[-2] + '    ' + rmsDisp[-1])
```

```
        printLines.append('-------------------------------------------------------------------------------')
      elif len(maxForce) > 0 and printType == "long":
        printLines.append('Opt Step:      Force [Max ll RMS]     Displacement [Max ll RMS]')
        for i in range(len(maxForce)):
          printLines.append(" " + str(i+1) + "  [" + maxForce[i][-3] + " (" + maxForce[i][-1] + ") ll " + rmsForce[i][-3] + " (" + rmsForce[i][-1] + ")]  [" + maxDisp[i][-3] + " (" + maxDisp[i][-1] + ") ll " + rmsDisp[i][-3] + " (" + rmsDisp[i][-1] + ")]")
          #printLines.append('Force     ' + maxForce[i][-3] + ' ll ' + maxForce[i][-2] + '    ' + maxForce[i][-1] + '        ' + rmsForce[i][-3] + ' ll ' + rmsForce[i][-2] + '    ' + rmsForce[i][-1])
          #printLines.append('Disp      ' + maxDisp[i][-3] + ' ll ' + maxDisp[i][-2] + ' ' + maxDisp[i][-1] + '        ' + rmsDisp[i][-3] + ' ll ' + rmsDisp[i][-2] + '    ' + rmsDisp[i][-1])
        printLines.append('-------------------------------------------------------------------------------')
      elif len(maxForce) > 0 and printType == "extra":
        printLines.append('Opt Step:      Force [Max ll RMS]     Displacement [Max ll RMS]')
        if len(maxForce) > 5:
          lastLines = len(maxForce) - 5
        else:
          lastLines = 0
        for i in range(lastLines,len(maxForce)):
          printLines.append(" " + str(i+1) + "  [" + maxForce[i][-3] + " (" + maxForce[i][-1] + ") ll " + rmsForce[i][-3] + " (" + rmsForce[i][-1] + ")]  [" + maxDisp[i][-3] + " (" + maxDisp[i][-1] + ") ll " + rmsDisp[i][-3] + " (" + rmsDisp[i][-1] + ")]")
          #printLines.append('Force     ' + maxForce[i][-3] + ' ll ' + maxForce[i][-2] + '    ' + maxForce[i][-1] + '        ' + rmsForce[i][-3] + ' ll ' + rmsForce[i][-2] + '    ' + rmsForce[i][-1])
          #printLines.append('Disp      ' + maxDisp[i][-3] + ' ll ' + maxDisp[i][-2] + ' ' + maxDisp[i][-1] + '        ' + rmsDisp[i][-3] + ' ll ' + rmsDisp[i][-2] + '    ' + rmsDisp[i][-1])
        printLines.append('-------------------------------------------------------------------------------')

    if trans == "archive":

      printLines.append("    Atomic        Coordinates (Angstroms)")
      printLines.append("    Type:           X       Y       Z")
```

```
    printLines.append('-------------------------------------------------------------------------
----')
    printLines.append("GEOM DATA!")

  if trans == "translate" or trans == "archive":
    #Frequency output
    if freqSwitch == 1 and len(enthalpyE) > 0:
      printLines.append('Statistical Thermodynamic Analysis for ' + logfile)
      printLines.append(freqTemp)

printLines.append('=========================================
==================================')
      printLines.append('SCF Energy=                                    ' +
scfEnergy)
      printLines.append('Zero-point correction (ZPE)=           ' + zeroPointE + '
' + zeroPointESUM)
      printLines.append('Internal Energy (U)=                ' + thermE + '       ' +
thermESUM)
      printLines.append('Enthalpy (H)=                       ' + enthalpyE + '       ' +
enthalpyESUM)
      printLines.append('Gibbs Free Energy (G)=              ' + gibbsE + '       '
+ gibbsESUM)
      printLines.append('Entropy (S) [Cal/Mol-Kelvin]=          ' + totalS)
      printLines.append('Entropy (S): electronic=            ' + elecS)
      printLines.append('Entropy (S): translational=         ' + transS)
      printLines.append('Entropy (S): rotational=            ' + rotS)
      printLines.append('Entropy (S): vibrational=           ' + vibS)
      printLines.append('Frequencies: ' + frequencies[0] + "  " + frequencies[1] +
"  " + frequencies[2] + "  " + frequencies[3] + "  " + frequencies[4] )
      if negfreq == 1:
        printLines.append('\033[1;33m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')
      elif negfreq >= 2:
        printLines.append('\033[1;31m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')
      printLines.append('-------------------------------------------------------------------------
-----')

  if trans == "translate":
    #Print end of file for long and extra
    if printType == "extra" or printType == "long":
      for i in range((len(fileList)-10), len(fileList)):
        printLines.append(fileList[i].strip())
    #Completed job
```

```
    if jobDone == 1:

printLines.append('=========================================
==================================')
      printLines.append('\033[1;32m################## JOB
COMPLETED ##################\033[0;0m')

printLines.append('=========================================
==================================')
    elif jobDone == 2:

printLines.append('=========================================
==================================')
      printLines.append('\033[1;31m!!!!!!!!!!!!!!!!!! !!!JOB FAILED!!!
!!!!!!!!!!!!!!!!!!\033[0;0m')

printLines.append('=========================================
==================================')



  elif trans == "list":
    line = scfEnergy + "  "
    line += zeroPointESUM + "  " + thermESUM + "  " + enthalpyESUM + "  " +
gibbsESUM + "  "
    if int(negfreq) == 0:
      line += '\033[1;32m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    elif int(negfreq) == 1:
      line += '\033[1;33m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    elif int(negfreq) >= 2:
      line += '\033[1;31m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    line += basisFunc + "  " + pointStoic + "  " + stoic + "  "
    if jobDone == 0:
      line += logfile.split("/")[-1]
    elif jobDone == 1:
      filename  = logfile.split("/")[-1]
      line += '\033[1;32m' + filename + '\033[0;0m'
    elif jobDone == 2:
      filename  = logfile.split("/")[-1]
      line += '\033[1;31m' + filename + '\033[0;0m'
    printLines.append(line)
```

```
  if trans != "archive":
    return printLines
  if trans == "archive":
    tableLines = []
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," + zeroPointE +
",=" + thermE  + "+RC[-2],=" + enthalpyE + "+RC[-3],=" + gibbsE + "+RC[-
4],=RC[-1]-MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," + zeroPointE +
"," + thermESUM + "," + enthalpyESUM + "," + gibbsESUM + ",=RC[-1]-
MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy)
    return printLines, tableLines



### --- Jaguar Specific Functions --- ###
###=========================================================
=========================================================#
##
### --- Parse the Jaguar OUT file for geometry information --- ###
def Eta_parseOutputJaguar(ifile):
  ### --- Open parent file --- ###
  f = open(ifile, "r")
  ifileList = f.readlines()
  f.close()
  ### --- Create some variables needed for parsing the input file --- ###
  # ifilelength is used to gauge what line we are on and also
  # allows us to determine the number of lines in the file
  # ifilelol is a list of lists (lol) that will hold all the data of the input file
  # a_list is a temp list that will be appended to the ifilelol
  ################################
  ifileLength = 0
  ifilelol = []
  a_list = []
  #### --- Input/parse the input file into a list of lists called ifilelol --- ###
  collectgeom = 0
  for i, var in enumerate(ifileList):
    #Grab charge and multiplicity
    if 'net molecular charge:' in var:
      charge = var.rstrip().split()[-1]
    elif 'multiplicity' in var:
      multi = var.rstrip().split()[-1]
    elif 'SCFE:' in var:
```

```
      finalenergy = var.strip().split("hartrees")[0].split()[-1]
    elif 'new geometry:' in var or 'final geometry:' in var:
      collectgeom = 1
      numAtoms = 0
      ifilelol = []
      #a_list = []
    elif len(var.strip()) == 0:
      collectgeom = 0
    elif collectgeom == 1 and 'angstroms' not in var and 'atom' not in var:
      a_list.append(var)
      numAtoms = numAtoms + 1
  finalgeom =  [0] * (numAtoms + 2)
  finalgeom[0] = str(numAtoms)
  finalgeom[1] = "Energy : " + str(finalenergy)
  for i in range(len(a_list) - numAtoms, len(a_list)):
    line = a_list[i].split()
    j = i - len(a_list) + numAtoms + 2
    finalgeom[j] = Atom()
    finalgeom[j].e = ''.join([k for k in line[0] if not k.isdigit()])
    finalgeom[j].en = Eta_getElementNum(finalgeom[j].e)
    finalgeom[j].x = float(line[1])
    finalgeom[j].y = float(line[2])
    finalgeom[j].z = float(line[3])
  return (finalgeom, charge, multi)

### --- Parse the Jaguar OUT file for geometry information --- ###
def Eta_parseOutputJaguar_Traj(ifile):
  ### --- Open parent file --- ###
  f = open(ifile, "r")
  ifileList = f.readlines()
  f.close()
  ### --- Create some variables needed for parsing the input file --- ###
  # ifilelength is used to gauge what line we are on and also
  # allows us to determine the number of lines in the file
  # ifilelol is a list of lists (lol) that will hold all the data of the input file
  # a_list is a temp list that will be appended to the ifilelol
  ################################
  a_list = []
  #### --- Input/parse the input file into a list of lists called ifilelol --- ###
  collectgeom = 0
  allEnergy = []
  for i, var in enumerate(ifileList):
    #Grab charge and multiplicity
    if 'net molecular charge:' in var:
```

```
      charge = var.rstrip().split()[-1]
    elif 'multiplicity' in var:
      multi = var.rstrip().split()[-1]
    elif 'SCFE:' in var:
      allEnergy.append(var.strip().split("hartrees")[0].split()[-1])
    elif 'new geometry:' in var or 'final geometry:' in var:
      collectgeom = 1
      numAtoms = 0
      ifilelol = []
      #a_list = []
    elif len(var.strip()) == 0:
      collectgeom = 0
    elif collectgeom == 1 and 'angstroms' not in var and 'atom' not in var:
      a_list.append(var)
      numAtoms = numAtoms + 1
  trajectorygeom = [0] * (len(a_list)/numAtoms * (numAtoms + 2))
  skip = 0
  for i in range(len(a_list)):
    if i % numAtoms == 0 and i/numAtoms != len(allEnergy):
      trajectorygeom[i+skip] = str(numAtoms)
      trajectorygeom[i+skip+1] = "Energy: " + str(allEnergy[i/numAtoms])
      skip = skip + 2
    elif i % numAtoms == 0 and i/numAtoms >= len(allEnergy):
      trajectorygeom[i+skip] = str(numAtoms)
      trajectorygeom[i+skip+1] = "Energy: " + str(allEnergy[-1])
      skip = skip + 2
    line = a_list[i].split()
    trajectorygeom[i+skip] = Atom()
    trajectorygeom[i+skip].e = ''.join([j for j in line[0] if not j.isdigit()])
    trajectorygeom[i+skip].en = Eta_getElementNum(trajectorygeom[i+skip].e)
    trajectorygeom[i+skip].x = float(line[1])
    trajectorygeom[i+skip].y = float(line[2])
    trajectorygeom[i+skip].z = float(line[3])
  return (trajectorygeom, charge, multi)

### --- Out put the Jaguar input files --- ###
def Eta_outputJaguar(ifile, config, charge, multi, writemod, modred, writeecp,
ecplines, writeclose, closelines, ifilelol):
  ofiletmp = ifile.split(".")
  ofile = ""
  for i in range(len(ofiletmp)):
    if i != len(ofiletmp) - 1:
      ofile += ofiletmp[i] + "."
    elif i == len(ofiletmp) - 1:
```

```
    ofile += "in"
  #print ofile
  f = open("NEWJOBS.JAG/" + ofile, "w+")
  f.write("&gen\n")
  for i, var in enumerate(config):
    f.write(var + "\n")
  f.write("molchg=" + str(charge) + "\n")
  f.write("multip=" + str(multi) + "\n")
  f.write("&\n")
  f.write("entry_name: " + ifile + "\n")
  f.write("&zmat\n")
  for i in range(2, len(ifilelol)):
    line = str(ifilelol[i].e) + str(i-1) + " " + str(ifilelol[i].x) + " " + str(ifilelol[i].y) + " "
+ str(ifilelol[i].z)
    f.write(line + "\n")
  f.write("&\n")
  if writemod == 1:
    f.write("&coord\n")
    if len(modred) > 0 and modred[0] != "":
      for i, var in enumerate(modred):
        f.write(var + "\n")
    else:
      f.write("MODRED!\n")
    f.write("&\n")
  f.close()
  return

#Parse the Jaguar output file and print data to the screen
def Eta_TranslateJaguarOutput(logfile, trans, printType):
  initLines = ['\033[1;34mPython Jaguar Output File Parsing Script:
nJT.py\033[1;0m',
            '\033[1;34mScripted by Thomas J. L. Mustard, O. Maduka Ogba, Paul
Ha-Yeon Cheong\033[1;0m',
            '--------------------------------------------------------------------------']
  if trans == "translate":
    for line in initLines:
      print line

  #Global Variables
  config = ''
  configSwitch = 0
  printLines = []
  programVersion = ''
  procs = ''
```

```
tmpFiles = ''
configLines = []
configLinesAll = ''
modSwitch = 0
modLines = []
pointStoic = ''
point = ''
stoic = ''
chargeMulti = ''
charge = ''
multi = ''
basisFunc = ''
scfEnergy = ''
predEChange = ''
optSwitch = 0
optComplete = 0
optStep = 0
if printType == "none":
  maxForce = ''
  rmsForce = ''
  maxDisp = ''
  rmsDisp = ''
  energyCon = ''
else:
  maxForce = []
  rmsForce = []
  maxDisp = []
  rmsDisp = []
  energyCon = []
freqSwitch = 0
freqTemp = ''
freqPres = ''
if trans == "list":
  frequencies = ["0.00", "0.00"]
  negfreq = 0
  zeroPointE = '0.000000'
  thermE = '0.000000'
  enthalpyE = '0.000000'
  gibbsE = '0.000000'
  zeroPointESUM = '0.000000'
  thermESUM = '0.000000'
  enthalpyESUM = '0.000000'
  gibbsESUM = '0.000000'
  totalS = '0.000000'
```

```
  elecS = '0.000000'
  rotS = '0.000000'
  transS = '0.000000'
  vibS = '0.000000'
else:
  frequencies = []
  negfreq = 0
  zeroPointE = ''
  thermE = ''
  enthalpyE = ''
  gibbsE = ''
  zeroPointESUM = ''
  thermESUM = ''
  enthalpyESUM = ''
  gibbsESUM = ''
  totalS = ''
  elecS = ''
  rotS = ''
  transS = ''
  vibS = ''
jobDone = 0
memSwitch = 0
f = open(logfile)
fileList = f.readlines()
f.close()
for i, var in enumerate(fileList):
  #if i < 30 and 'Jaguar version' not in var and jaguartext == 0:
  #  print "Error! Not a Jaguar out file."
  #exit(0)
  #Find the Gaussian Version
  if 'Jaguar version' in var:
    programVersion = var.rstrip().split(',')[0]
  #Find the tmp file
  elif 'Temporary files :' in var:
    tmpFiles = var.split(':')[1].rstrip()
  #Find the processors/threads used
  elif 'Using up to ' in var:
    procs = var.split('to')[1].rstrip()
  #Get pointgroup and stoic
  if 'Point Group used:' in var:
    point = var.split()[-1]
  elif 'Stoichiometry:' in var:
    stoic = var.split()[-1]
  #Get charge and multiplicity
```

```
elif 'net molecular charge:' in var:
  charge = var.rstrip().split()[-1]
elif 'multiplicity' in var:
  multi = var.rstrip().split()[-1]
#Find basis functions
elif 'basis set:' in var:
  basisFunc = var.strip().split()[-1]
#Find the job configuration used
if 'Non-default options chosen:' in var:
  for j in range(1,30):
    if 'Temporary integer options' not in fileList[i+j]:
      configLines.append(fileList[i+j].strip())
      if 'optimized' in fileList[i+j]:
        optSwitch = 1
      if 'modredundant' in fileList[i+j]:
        modSwitch = 1
      if "frequencies" in fileList[i+j]:
        freqSwitch = 1
    else:
      break
#Check to see if modredundant is in the config
elif modSwitch == 1:
  if 'The following ModRedundant input section has been read:' in var:
    for j in range(1,20):
      if len(fileList[i+j]) > 2:
        modLines.append(fileList[i+j].strip())
      else:
        break
#Get SCF Energy and predicted change
elif 'SCFE:' in var:
  scfEnergy = var.strip().split("hartrees")[0].split()[-1]
elif 'predicted energy change:' in var:
  predEChange = var.strip().split(':')[-1]
#Optimization parse
elif optSwitch == 1:
  if 'Geometry optimization was OK.' in var:
    optComplete = 1
  elif 'geometry optimization step' in var:
    optStep = var.split()[-1]
  if printType == "none":
    if 'gradient maximum:' in var:
      maxForce = var.rstrip().split(':')[-1].split()
      if maxForce[1] != ".":
        maxForce[1] = '\033[1;32mYES\033[0;m'
```

```
          else:
            maxForce[1] = '\033[1;31mNO!\033[0;m'
        elif 'gradient rms:' in var:
          rmsForce = var.rstrip().split(':')[-1].split()
          if rmsForce[1] != ".":
            rmsForce[1] = '\033[1;32mYES\033[0;m'
          else:
            rmsForce[1] = '\033[1;31mNO!\033[0;m'
        elif 'displacement maximum:' in var:
          maxDisp = var.rstrip().split(':')[-1].split()
          if maxDisp[1] != ".":
            maxDisp[1] = '\033[1;32mYES\033[0;m'
          else:
            maxDisp[1] = '\033[1;31mNO!\033[0;m'
        elif 'displacement rms:' in var:
          rmsDisp = var.rstrip().split(':')[-1].split()
          if rmsDisp[1] != ".":
            rmsDisp[1] = '\033[1;32mYES\033[0;m'
          else:
            rmsDisp[1] = '\033[1;31mNO!\033[0;m'
        elif 'energy change:' in var and 'predicted' not in var:
          energyCon = var.rstrip().split(':')[-1].split()
          if energyCon[1] != ".":
            energyCon[1] = '\033[1;32mYES\033[0;m'
          else:
            energyCon[1] = '\033[1;31mNO!\033[0;m'
      elif printType == "extra" or printType == "long":
        if 'gradient maximum:' in var:
          #Fix the fact that sometimes the energy convergence data is not printed
out for the first step
          if "energy change:" not in fileList[i-1]:
            energyCon.append([' ---N/A--- ', 'N/A', '(', '0.000000', ')'])
          maxForce.append(var.rstrip().split(':')[-1].split())
          if maxForce[-1][1] != ".":
            maxForce[-1][1] = '\033[1;32mYES\033[0;m'
          else:
            maxForce[-1][1] = '\033[1;31mNO!\033[0;m'
        elif 'gradient rms:' in var:
          rmsForce.append(var.rstrip().split(':')[-1].split())
          if rmsForce[-1][1] != ".":
            rmsForce[-1][1] = '\033[1;32mYES\033[0;m'
          else:
            rmsForce[-1][1] = '\033[1;31mNO!\033[0;m'
        elif 'displacement maximum:' in var:
```

```
      maxDisp.append(var.rstrip().split(':')[-1].split())
      if maxDisp[-1][1] != ".":
        maxDisp[-1][1] = '\033[1;32mYES\033[0;m'
      else:
        maxDisp[-1][1] = '\033[1;31mNO!\033[0;m'
    elif 'displacement rms:' in var:
      rmsDisp.append(var.rstrip().split(':')[-1].split())
      if rmsDisp[-1][1] != ".":
        rmsDisp[-1][1] = '\033[1;32mYES\033[0;m'
      else:
        rmsDisp[-1][1] = '\033[1;31mNO!\033[0;m'
    elif 'energy change:' in var and 'predicted' not in var:
      energyCon.append(var.rstrip().split(':')[-1].split())
      if energyCon[-1][1] != ".":
        energyCon[-1][1] = '\033[1;32mYES\033[0;m'
      else:
        energyCon[-1][1] = '\033[1;31mNO!\033[0;m'


#Frequency and
if freqSwitch == 1:
  if 'Thermochemical properties at' in var:
    freqPres = var.strip().split('s at')[-1].strip()
  elif 'T =' in var:
    freqTemp = var.strip().split('=')[-1].strip()
  elif 'frequencies' in var and 'frequencies' == var.split()[0]:
    if len(frequencies) != 0 and frequencies[0] == "0.00":
      frequencies = []
    if len(frequencies) < 5:
      frequencies.append(var.split()[1])
      frequencies.append(var.split()[2])
      frequencies.append(var.split()[3])
      frequencies.append(var.split()[4])
      frequencies.append(var.split()[5])
  #elif 'vibrational temperatures:' in var:
  #  frequencies = fileList[i+2].strip().split(':')[-1].strip()
  elif 'Number of imaginary frequencies:' in var:
    negfreq = int(var.strip().split(':')[-1])
  elif 'The zero point energy (ZPE):' in var:
    zeroPointE = str(var.strip().split(':')[-1])
  elif 'Total internal energy, Utot (SCFE + ZPE + U):' in var:
    thermESUM = str(var.strip().split(':')[-1])
    totalS = str(fileList[i-2].strip().split()[3])
    elecS = str(fileList[i-3].strip().split()[3])
```

```
        transS = str(fileList[i-6].strip().split()[3])
        rotS = str(fileList[i-5].strip().split()[3])
        vibS = str(fileList[i-4].strip().split()[3])
        thermE = str(fileList[i-2].strip().split()[1]).strip()
        enthalpyE = str(fileList[i-2].strip().split()[4]).strip()
        gibbsE = str(fileList[i-2].strip().split()[5]).strip()
      elif 'Total enthalpy, Htot (Utot + pV):' in var:
        enthalpyESUM = str(var.strip().split(':')[-1])
      elif 'Total Gibbs free energy, Gtot (Htot - T*S):' in var:
        gibbsESUM = str(var.strip().split(':')[-1])
    if 'Job' in var and 'completed on' in var and i - len(fileList) < 10:
      jobDone = 1

  if trans == "translate":
    #Printed output list
    printLines = ['Analyzing Jaguar Output File: ' + logfile]
    printLines.append('Using ' + str(programVersion))
    printLines.append('[#Processors=' + procs + '  Temp Files=' + tmpFiles + ']')

printLines.append('=========================================
==================================')

  elif trans == "archive":
    #Initial information
    printLines.append("Supporting Information: " + logfile)
    printLines.append("-----------------------------------------------------------------------
----")
    printLines.append("Using: " + programVersion)

printLines.append("=========================================
==================================")

  if trans == "translate" or trans == "archive":
    #Print config
    configLinestmp = ' '.join(str(e) for e in configLines)
    segments = list()
    while len(configLinestmp) > 0:
        segments.append( configLinestmp[:78] )
        configLinestmp = configLinestmp[78:]
    for line in segments:
      printLines.append(line)
    #printLines.append(' '.join(str(e) for e in configLines))

    #Modredundant output
```

```
    if modSwitch == 1:
      for line in modLines:
        printLines.append(line)

    #Print pointgroup and stoichiometry
    printLines.append('-------------------------------------------------------------------------------
----')
    printLines.append('Pointgroup = ' + point + '\tStoichiometry = ' + stoic )

    #Print Charge Multi and BasisFunc
    printLines.append('Charge = ' + charge + '\tMultiplicity = ' + multi + '\tBasis
= ' + basisFunc)
    printLines.append('-------------------------------------------------------------------------------
----')

    #Print Energy
    printLines.append('SCF Energy = ' + scfEnergy + '\tPredicted Change = ' +
predEChange)
    printLines.append('-------------------------------------------------------------------------------
----')


    #Optimization output
    if optSwitch == 1:
      if optComplete == 1:
        printLines.append('\033[1;32mOptimization completed.\033[0;m  ----------
----------  Optimization step: ' + str(optStep))
      else:
        printLines.append('\033[1;31mOptimization incomplete.\033[1;m  ----------
----------  Optimization step: ' + str(optStep))
      if len(maxForce) > 0 and printType == "none":
        printLines.append('Item      Max Val.    Criteria    Pass?      RMS Val.
Criteria    Pass?')
        printLines.append('Energy    ' + energyCon[-5] + ' ll ' + energyCon[-2] + '
' + energyCon[-4])
        printLines.append('Force     ' + maxForce[-5] + ' ll ' + maxForce[-2] + '   '
+ maxForce[-4] + '       ' + rmsForce[-5] + ' ll ' + rmsForce[-2] + '   ' +
rmsForce[-4])
        printLines.append('Disp      ' + maxDisp[-5] + ' ll ' + maxDisp[-2] + '   ' +
maxDisp[-4] + '       ' + rmsDisp[-5] + ' ll ' + rmsDisp[-2] + '   ' + rmsDisp[-4])
        printLines.append('-------------------------------------------------------------------------
-------')
      elif len(maxForce) > 0 and printType == "long":
```

```
        printLines.append('Opt Step:   Energy       Force [Max II RMS]
Displacement [Max II RMS]')
        for i in range(len(maxForce)):
          printLines.append(" " + str(i+1) + "  " + energyCon[i][-5] + " (" +
energyCon[i][-4] + ")  [" + maxForce[i][-5] + " (" + maxForce[i][-4] + ") II " +
rmsForce[i][-5] + " (" + rmsForce[i][-4] + ")]  [" + maxDisp[i][-5] + " (" +
maxDisp[i][-4] + ") II " + rmsDisp[i][-5] + " (" + rmsDisp[i][-4] + ")]")
        printLines.append('----------------------------------------------------------------------
-------')
      elif len(maxForce) > 0 and printType == "extra":
        printLines.append('Opt Step:   Energy       Force [Max II RMS]
Displacement [Max II RMS]')
        if len(maxForce) > 5:
          lastLines = len(maxForce) - 5
        else:
          lastLines = 0
        for i in range(lastLines,len(maxForce)):
          printLines.append(" " + str(i+1) + "  " + energyCon[i][-5] + " (" +
energyCon[i][-4] + ")  [" + maxForce[i][-5] + " (" + maxForce[i][-4] + ") II " +
rmsForce[i][-5] + " (" + rmsForce[i][-4] + ")]  [" + maxDisp[i][-5] + " (" +
maxDisp[i][-4] + ") II " + rmsDisp[i][-5] + " (" + rmsDisp[i][-4] + ")]")
        printLines.append('----------------------------------------------------------------------
-------')

  if trans == "archive":
    printLines.append("    Atomic        Coordinates (Angstroms)")
    printLines.append("    Type:           X       Y       Z")
    printLines.append('----------------------------------------------------------------------
----')
    printLines.append("GEOM DATA!")

  if trans == "translate" or trans == "archive":
    #Frequency output
    if freqSwitch == 1 and len(frequencies) > 0:
      printLines.append('Statistical Thermodynamic Analysis for ' + logfile)
      printLines.append('Computed at:  ' + freqTemp + '  and  ' + freqPres)

printLines.append('=========================================
==================================')
      printLines.append('SCF Energy=                                    ' +
scfEnergy)
      printLines.append('Zero-point correction (ZPE)=                    ' +
zeroPointE)
```

```
      printLines.append('Internal Energy (U)=                  ' + thermE + '       ' +
thermESUM)
      printLines.append('Enthalpy (H)=                         ' + enthalpyE + '       ' +
enthalpyESUM)
      printLines.append('Gibbs Free Energy (G)=                ' + gibbsE + '       '
+ gibbsESUM)
      printLines.append('Entropy (S) [Cal/Mol-Kelvin]=                         ' +
totalS)
      printLines.append('Entropy (S): electronic=                              ' + elecS)
      printLines.append('Entropy (S): translational=                           ' +
transS)
      printLines.append('Entropy (S): rotational=                              ' + rotS)
      printLines.append('Entropy (S): vibrational=                             ' + vibS)
      printLines.append('Frequencies:  ' + frequencies[0] + "   " + frequencies[1]
+ "   " + frequencies[2] + "   " + frequencies[3] + "   " + frequencies[4])
      if negfreq == 1:
        printLines.append('\033[1;33m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')
      elif negfreq >= 2:
        printLines.append('\033[1;31m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')

  if trans == "translate":
    #Print end of file for long and extra
    if printType == "extra" or printType == "long":
      printLines.append('----------------------------------------------------------------------------
-----')
      for i in range((len(fileList)-10), len(fileList)):
        printLines.append(fileList[i].strip())
    #Completed job
    if jobDone == 1:

printLines.append('=========================================
==================================')
      printLines.append('\033[1;32m##################            JOB
COMPLETED             ##################\033[0;m')

printLines.append('=========================================
==================================')

  if trans == "list":
    line = scfEnergy + "  "
    line += zeroPointE.split()[0] + "  " + thermESUM.split()[0] + "  " +
enthalpyESUM.split()[0] + "  " + gibbsESUM.split()[0] + "  "
```

```
    if negfreq == 0:
      line += '\033[1;32m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    elif negfreq == 1:
      line += '\033[1;33m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    elif negfreq >= 2:
      line += '\033[1;31m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    line += basisFunc + "  " + pointStoic + "  " + stoic + "  "
    if jobDone == 0:
      line += logfile.split("/")[-1]
    elif jobDone == 1:
      filename  = logfile.split("/")[-1]
      line += '\033[1;32m' + filename + '\033[0;0m'
    elif jobDone == 2:
      filename  = logfile.split("/")[-1]
      line += '\033[1;31m' + filename + '\033[0;0m'
    printLines.append(line)
    #if negfreq > 0 and trans != "archive":
    #    printLines.append('\033[1;31m              !!!Warning there were ' +
negfreq + ' negative frequencies!!!\033[0;m')

  if trans != "archive":
    return printLines
  if trans == "archive":
    tableLines = []
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," + zeroPointE +
",=" + thermE  + "+RC[-2],=" + enthalpyE + "+RC[-3],=" + gibbsE + "+RC[-
4],=RC[-1]-MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," + zeroPointE +
"," + thermESUM + "," + enthalpyESUM + "," + gibbsESUM + ",=RC[-1]-
MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy)
    return printLines, tableLines



### --- Turbomole Specific Functions --- ###
###=====================================================
=====================================================#
##
### --- Parse the Turbomole LOG file for geometry information --- ###
def Eta_parseOutputTM(ifile):
```

```
  ### --- Open parent file --- ###
  f = open(ifile, "r")
  ifileList = f.readlines()
  f.close()
  ### --- Create some variables needed for parsing the input file --- ###
  # ifilelength is used to gauge what line we are on and also
  # allows us to determine the number of lines in the file
  # ifilelol is a list of lists (lol) that will hold all the data of the input file
  # a_list is a temp list that will be appended to the ifilelol
  ################################
  charge = 0
  multi = -1
  a_list = []
  geom = 0
  numAtoms = 0
  finalenergy = 0
  finalgeom = []
  for i, line in enumerate(ifileList):
    if line.strip() != '':
      if line.split()[0] == 'l':
        if line.split()[1] == 'total':
          if line.split()[2] == 'energy':
            finalenergy = float(line.split()[4])
      if line.split()[0] == 'total:':
        numAtoms = int(line.split()[1])
      if line.split()[0] == "center":
        geom = 0
      if geom == 1:
        geom += 1
      if line.split()[0] == "atomic":
        if line.split()[1] == "coordinates":
          geom = 1
      if geom >= 2:
        a_list.append(line)
      elif 'charge' in line and '------------------------------------------------------------------
-----------' in ifileList[i+1]:
        charge = ifileList[i+2].strip().split()[-1]
      elif 'molecular charge' in line:
        charge = line.rstrip().split()[-1]
      elif 'real representations' in line:
        multi = line.strip().split()[2]
  a_listDd = [x for x in a_list if x != ""]
  finalgeom = [0] * (numAtoms + 2)
  finalgeom[0] = numAtoms
```

```
  finalgeom[1] = "Energy: " + str(finalenergy)
  for i in range(len(a_listDd)-numAtoms, len(a_listDd)):
    line = a_listDd[i].split()
    j = i - len(a_listDd) + numAtoms + 2
    finalgeom[j] = Atom()
    finalgeom[j].e = line[3]
    finalgeom[j].en = Eta_getElementNum(line[3])
    finalgeom[j].x = float(line[0])/auToAngstrom
    finalgeom[j].y = float(line[1])/auToAngstrom
    finalgeom[j].z = float(line[2])/auToAngstrom
  return (finalgeom, charge, multi)

### --- Parse the Turbomole LOG file for geometry information --- ###
def Eta_parseOutputTM_Traj(ifile):
  ### --- Open parent file --- ###
  f = open(ifile, "r")
  ifileList = f.readlines()
  f.close()
  ### --- Create some variables needed for parsing the input file --- ###
  # ifilelength is used to gauge what line we are on and also
  # allows us to determine the number of lines in the file
  # ifilelol is a list of lists (lol) that will hold all the data of the input file
  # a_list is a temp list that will be appended to the ifilelol
  ################################
  charge = 0
  multi = -1
  a_list = []
  geom = 0
  skipgeom = True
  numAtoms = 0
  allEnergy = []
  trajectorygeom = []
  for i, line in enumerate(ifileList):
    if line.strip() != '':
      if line.split()[0] == 'ENERGY' and line.split()[1] == '=':
        allEnergy.append(float(line.split()[2]))
      elif line.split()[0] == 'total:':
        numAtoms = int(line.split()[1])
      elif line.split()[0] == "center" or "*************" in line:
        geom = 0
      elif "S T A T P T" in  line:
        skipgeom = False
      elif line.split()[0] == "ATOM" and line.split()[1] == "CARTESIAN" and
line.split()[2] == "COORDINATES":
```

```
        #if line.split()[1] == "coordinates":
        if skipgeom == False:
          geom = 1
        skipgeom = True
      elif geom == 1:
        a_list.append(line)
      elif 'charge' in line and '----------------------------------------------------------------
-----------' in str(ifileList[i+1]):
        charge = ifileList[i+2].strip().split()[-1]
      elif 'molecular charge' in line:
        charge = line.rstrip().split()[-1]
      elif 'real representations' in line:
        multi = line.strip().split()[2]
  a_listDd = [x for x in a_list if x != ""]
  trajectorygeom = [0] * (len(a_listDd)/numAtoms * (numAtoms + 2))
  skip = 0
  for i in range(len(a_listDd)):
    if i % numAtoms == 0 and i/numAtoms != len(allEnergy):
      trajectorygeom[i+skip] = str(numAtoms)
      trajectorygeom[i+skip+1] = "Energy: " + str(allEnergy[i/numAtoms])
      skip = skip + 2
    elif i % numAtoms == 0 and i/numAtoms >= len(allEnergy):
      trajectorygeom[i+skip] = str(numAtoms)
      trajectorygeom[i+skip+1] = "Energy: " + str(allEnergy[-1])
      skip = skip + 2
    line = a_listDd[i].split()
    trajectorygeom[i+skip] = Atom()
    trajectorygeom[i+skip].en = Eta_getElementNum(line[1])
    trajectorygeom[i+skip].e =
Eta_getElementName(Eta_getElementNum(line[1]))
    trajectorygeom[i+skip].x = float(line[2])/auToAngstrom
    trajectorygeom[i+skip].y = float(line[3])/auToAngstrom
    trajectorygeom[i+skip].z = float(line[4])/auToAngstrom
  return (trajectorygeom, charge, multi)

### --- Out put the TM input files --- ###
def Eta_outputTM(ifile, config, charge, multi, writemod, modred, writeecp,
ecplines, writeclose, closelines, ifilelol):
  ofiletmp = ifile.split(".")
  ofile = ""
  currentdir = os.getcwd()
  for i in range(len(ofiletmp)):
    if i != len(ofiletmp) - 1:
      ofile += ofiletmp[i] + "."
```

```
      ifileBase = ofiletmp[i]
      outdir = currentdir + "/NEWJOBS.TM/" + ofiletmp[i] + ".Turbomole"
    elif i == len(ofiletmp) - 1:
      ofile += "tmol"
  if not os.path.exists(outdir): os.makedirs(outdir)
  f = open(outdir + "/" + ofile, "w+")
  f.write("$coord\n")
  for i in range(2, len(ifilelol)):
    if writemod == 1 and len(modred) > 0 and modred[0] != "":
      for var in modred:
        if var == i-1:
          line = str(ifilelol[i].x * auToAngstrom)[0:11]  + "   " + str(ifilelol[i].y *
auToAngstrom)[0:11] + "   " + str(ifilelol[i].z * auToAngstrom)[0:11] + "   " +
str(ifilelol[i].e).lower() + "  f"
    else:
      line = str(ifilelol[i].x * auToAngstrom)[0:11]  + "   " + str(ifilelol[i].y *
auToAngstrom)[0:11] + "   " + str(ifilelol[i].z * auToAngstrom)[0:11] + "   " +
str(ifilelol[i].e).lower()
    f.write(line + "\n")
  f.close()
  #Build define.in file for the define program
  f = open(outdir + '/define.in', "w+")
  for i, var in enumerate(config):
    if 'CHARGE!' in var:
      f.write(str(charge) + "\n")
    elif 'TMOL!' in var:
      f.write("a coord\n")
      #f.write("a " + ofile + "\n")
    elif 'TITLE!' in var:
      f.write(ifileBase + "\n")
    else:
      f.write(var + "\n")
  f.close()
  #Run the define program on define.in and output define.out
  os.chdir(outdir)
  os.system("ln -s " + ofile + " coord")
  os.system("define < define.in > define.out")
  f = open("control", "r")
  control = f.readlines()
  f.close()
  f = open("control", "w")
  for line in control:
    if '$end' in line:
      f.write("$statpt\n")
```

```
      f.write("   itrvec 0\n")
      f.write("   hssfreq 0\n")
      f.write("$maxcor    1000\n")
      f.write("$rpacor    1000\n")
      f.write(line)
    elif '$rij' in line:
      f.write("$ricore_slave    1\n")
      f.write(line)
    else:
      f.write(line)
  f.close()
  os.chdir(currentdir)
  return

#Parse the Turbomole output file and print data to the screen
def Eta_TranslateTMOutput(logfile, trans, printType):
  initLines = ['\033[1;34mPython Turbomole Output File Parsing Script:
nTMT.py\033[1;0m',
            '\033[1;34mScripted by Thomas J. L. Mustard, O. Maduka Ogba, Paul
Ha-Yeon Cheong\033[1;0m',
            '--------------------------------------------------------------------------------']
  if trans == "translate":
    for line in initLines:
      print line

  #Global Variables
  config = ''
  configSwitch = 0
  printLines = []
  programVersion = ''
  procs = ''
  tmpFiles = ''
  configLines = []
  configLinesAll = ''
  modSwitch = 0
  modLines = []
  pointStoic = ''
  point = ''
  stoic = ''
  numatoms = ''
  chargeMulti = ''
  charge = ''
  multi = ''
  basisFunc = ''
```

```
scfEnergy = ''
predEChange = ''
optSwitch = 0
optComplete = 0
optStep = 0
if printType == "none":
  energyCon = ''
  maxForce = ''
  rmsForce = ''
  maxDisp = ''
  rmsDisp = ''
else:
  energyCon = []
  maxForce = []
  rmsForce = []
  maxDisp = []
  rmsDisp = []
freqSwitch = 0
if trans == "list":
  frequencies = []
  zeroPointESUM = '0.00000'
  thermESUM = '0.00000'
  enthalpyESUM = '0.00000'
  gibbsESUM = '0.00000'
else:
  frequencies = []
  zeroPointESUM = ''
  thermESUM = ''
  enthalpyESUM = ''
  gibbsESUM = ''
freqTemp = ''
freqPres = ''
negfreq = 0
zeroPointE = ''
thermE = ''
enthalpyE = ''
gibbsE = ''
totalS = ''
entropyESUM = ''
elecS = ''
rotS = ''
transS = ''
vibS = ''
freehSwitch = 0
```

```
  jobDone = 0
  riccswitch = 0
  rhfenergy = ''
  correnergy = ''
  mp2energy = ''
  findbasis = 0
  findtheory = 0

  f = open(logfile)
  fileList = f.readlines()
  f.close()
  for i, var in enumerate(fileList):
    #if i < 30 and 'Jaguar version' not in var and jaguartext == 0:
    #  print "Error! Not a Jaguar out file."
    #exit(0)
    #Find the Gaussian Version
    if 'TURBOMOLE V' in var:
      programVersion = var.split(':')[1].split()[0] + " " + var.split(':')[1].split()[1]
    #Find the tmp file
    elif 'TURBOTMPDIR environment variable set to' in var:
      tmpFiles = var.split("'")[1].strip()
    #Find the processors/threads used
    elif 'PROCESSORS!' in var:
      procs = var.split('ON')[1].strip().split()[0]
    #Get pointgroup
    if 'symmetry group' in var:
      point = var.split()[-1]
    #Get stoic and number of atoms
    elif 'type   atoms' in var:
      stoic = ''
      for j in range(2,100):
        if '------------------------------------------------------------------------' not in
fileList[i+j]:
          stoic += fileList[i+j].split()[0].upper() + fileList[i+j].split()[1]

        else:
          break
      if 'total' in fileList[i+7]:
        numatoms = fileList[i+7].split()[1]
    #Get charge and multiplicity
    elif 'charge' in var and '----------------------------------------------------------------
---------' in fileList[i+1]:
      charge = fileList[i+2].strip().split()[-1]
    elif 'molecular charge' in var:
```

```
  charge = var.rstrip().split()[-1]
elif 'real representations' in var:
  multi = var.strip().split()[2]
#Find basis functions
elif 'number of basis functions' in var:
  basisFunc = var.strip().split(':')[-1].strip()
#Find the job configuration used
if 'Non-default options chosen:' in var:
  for j in range(1,30):
    if 'Temporary integer options' not in fileList[i+j]:
      configLines.append(fileList[i+j].strip())
      if 'modredundant' in fileList[i+j]:
        modSwitch = 1
    else:
      break
elif 'type   atoms  prim   cont   basis' in var and findbasis == 0:
  configLines.append("basis=" + fileList[i+2].split()[-2])
  findbasis += 1
elif 'density functional' in var and '--------' in fileList[i+1] and findtheory == 0:
  configLines.append("theory=" + fileList[i+2].split()[-1])
  findtheory += 1
elif 'jobex' in var and optSwitch == 0:
  optSwitch = 1
  configLines.append("optimization")
elif "a o f o r c e" in var or 'N u m F o r c e' in var:
  freqSwitch = 1
  configLines.append("freq:aoforce")
elif "f r e e   e n t h a l p y" in var or "freeh" in var:
  freehSwitch = 1
  configLines.append("freq:numforce")
#Check to see if modredundant is in the config
elif modSwitch == 1:
  if 'The following ModRedundant input section has been read:' in var:
    for j in range(1,20):
      if len(fileList[i+j]) > 2:
        modLines.append(fileList[i+j].strip())
      else:
        break
#Get SCF Energy and predicted change
elif 'total energy      =' in var:
  scfEnergy = var.strip().split("=")[1].split()[0]
#Check for ricc2 calculation
elif 'ricc2' in var:
  riccswitch = 1
```

```
  if 'RHF  energy' in var:
    rhfenergy = var.split(':')[1].split()[0].strip()
  elif 'Final MP2 energy' in var:
    mp2energy = var.split(':')[1].split()[0].strip()
  elif 'correlation energy' in var:
    correnergy = var.split(':')[1].split()[0].strip()
elif 'Predicted energy change:' in var:
  predEChange = var.strip().split(':')[-1].strip()
#Optimization parse
elif optSwitch == 1:
  if 'CONVERGENCY CRITERIA FULFILLED IN CYCLE' in var:
    optComplete = 1
  elif 'OPTIMIZATION CYCLE' in var:
    optStep = int(var.split()[-1])
  if printType == "none":
    if 'MAX gradient' in var:
      maxForce = var.strip().split()
      if maxForce[-3] == "yes":
        maxForce[-3] = '\033[1;32mYES\033[0;m'
      else:
        maxForce[-3] = '\033[1;31mNO!\033[0;m'
    elif 'RMS of gradient' in var:
      rmsForce = var.strip().split()
      if rmsForce[-3] == "yes":
        rmsForce[-3] = '\033[1;32mYES\033[0;m'
      else:
        rmsForce[-3] = '\033[1;31mNO!\033[0;m'
    elif 'MAX displacement' in var:
      maxDisp = var.strip().split()
      if maxDisp[-3] == "yes":
        maxDisp[-3] = '\033[1;32mYES\033[0;m'
      else:
        maxDisp[-3] = '\033[1;31mNO!\033[0;m'
    elif 'RMS of displacement' in var:
      rmsDisp = var.strip().split()
      if rmsDisp[-3] == "yes":
        rmsDisp[-3] = '\033[1;32mYES\033[0;m'
      else:
        rmsDisp[-3] = '\033[1;31mNO!\033[0;m'
    elif 'Energy change' in var:
      energyCon = var.strip().split()
      if energyCon[-3] == "yes":
        energyCon[-3] = '\033[1;32mYES\033[0;m'
      else:
```

```
            energyCon[-3] = '\033[1;31mNO!\033[0;m'
        if printType == "long" or printType == "extra":
          if 'MAX gradient' in var and 'Threshold' not in var:
            maxForce.append(var.strip().split())
            if maxForce[-1][-3] == "yes":
              maxForce[-1][-3] = '\033[1;32mYES\033[0;m'
            else:
              maxForce[-1][-3] = '\033[1;31mNO!\033[0;m'
          elif 'RMS of gradient' in var and 'Threshold' not in var:
            rmsForce.append(var.strip().split())
            if rmsForce[-1][-3] == "yes":
              rmsForce[-1][-3] = '\033[1;32mYES\033[0;m'
            else:
              rmsForce[-1][-3] = '\033[1;31mNO!\033[0;m'
          elif 'MAX displacement' in var and 'Threshold' not in var:
            maxDisp.append(var.strip().split())
            if maxDisp[-1][-3] == "yes":
              maxDisp[-1][-3] = '\033[1;32mYES\033[0;m'
            else:
              maxDisp[-1][-3] = '\033[1;31mNO!\033[0;m'
          elif 'RMS of displacement' in var and 'Threshold' not in var:
            rmsDisp.append(var.strip().split())
            if rmsDisp[-1][-3] == "yes":
              rmsDisp[-1][-3] = '\033[1;32mYES\033[0;m'
            else:
              rmsDisp[-1][-3] = '\033[1;31mNO!\033[0;m'
          elif 'Energy change' in var and 'ratio' not in var:
            energyCon.append(var.strip().split())
            if energyCon[-1][-3] == "yes":
              energyCon[-1][-3] = '\033[1;32mYES\033[0;m'
            else:
              energyCon[-1][-3] = '\033[1;31mNO!\033[0;m'

      #Frequency logic
      if freqSwitch == 1:
        if 'frequency' in var and not 'zero' in var:
          for i in range(1,len(var.split())):
            frequencies.append(var.split()[i])
        if 'zero point vibrational energy' in var:
          zeroPointE = str(float(fileList[i+2].split()[1]) / 4.184 / 2625.49962)
        elif 'T       p       ln(qtrans) ln(qrot) ln(qvib) chem.pot.   energy    entropy' in
var:
          freqTemp = fileList[i+3].split()[0]
          freqPres = fileList[i+3].split()[1]
```

```
        ###thermE = str((float(fileList[i+3].split()[1]) + (298.15 * 8.3144621 /
1000)) / 2625.49962)
        enthalpyE = str((float(fileList[i+7].split()[5]) + (298.15 * 8.3144621 /
1000)) / 2625.49962)
        gibbsE = str(float(fileList[i+3].split()[4]) / 2625.49962)
        totalS = str((float(fileList[i+3].split()[5]) * 298.15) / 2625.49962)
        thermESUM = str(float(thermE) + float(scfEnergy))
        enthalpyESUM = str(float(enthalpyE) + float(scfEnergy))
        gibbsESUM = str(float(gibbsE) + float(scfEnergy))
        entropyESUM = str(float(totalS) + float(scfEnergy))

    #Job complete logic
    if i - len(fileList) < 10 and 'total wall-time' in var: #i > len(fileList)-30 and
      jobDone = 1
    elif i - len(fileList) < 10 and ('next step' in var or 'OPTIMIZATION CYCLE' in
var or 'RUNNING PROGRAM' in var or 'STARTING ' in var): #i > len(fileList)-
30 and
      jobDone = 0

  if trans == "translate":
    #Printed output list
    printLines = ['Analyzing Turbomole Output File: ' + logfile]
    printLines.append('Using: ' + str(programVersion))
    printLines.append('[#Processors=' + procs + '  Temp Files=' + tmpFiles + ']')

printLines.append('==========================================
==================================')

  elif trans == "archive":
    #Initial information
    printLines.append("Supporting Information: " + logfile)
    printLines.append("------------------------------------------------------------------------
----")
    printLines.append("Using: " + programVersion)

printLines.append("==========================================
==================================")

  if trans == "translate" or trans == "archive":
        #Print config
    configLinestmp = ' '.join(str(e) for e in configLines)
    segments = list()
    while len(configLinestmp) > 0:
        segments.append( configLinestmp[:78] )
```

```
        configLinestmp = configLinestmp[78:]
    for line in segments:
      printLines.append(line)
    #printLines.append(' '.join(str(e) for e in configLines))

    #Modredundant output
    if modSwitch == 1:
      for line in modLines:
        printLines.append(line)

    #Print pointgroup and stoichiometry
    printLines.append('--------------------------------------------------------------------------------')
    printLines.append('Pointgroup = ' + point + '      Stoichiometry = ' + stoic + '  # of Atoms = ' + numatoms)

    #Print Charge Multi and BasisFunc
    printLines.append('Charge = ' + charge[0:5] + '       Multiplicity = ' + multi + '  Basis = ' + basisFunc)
    printLines.append('--------------------------------------------------------------------------------')

    #Print Energy
    printLines.append('SCF Energy = ' + scfEnergy + '\tPredicted Change = ' + predEChange)
    printLines.append('--------------------------------------------------------------------------------')

    #Print MP2 Energy
    if riccswitch == 1:
      printLines.append('RHF Energy: ' + rhfenergy + ' |  MP2 Energy: ' + mp2energy + ' | Correlation Energy: ' + correnergy)
      printLines.append('---------------------------------------------------------------------------------')

    #Optimization output
    if optSwitch == 1:
      if optComplete == 1 and optStep == 0:
        printLines.append('\033[1;32mOptimization completed.\033[0;m')
      elif optComplete == 1 and optStep >= 0:
        printLines.append('\033[1;32mOptimization completed.\033[0;m  ------------------------------  Optimization step: ' + str(optStep))
      elif optComplete == 0 and optStep == 0:
        printLines.append('\033[1;31mOptimization incomplete.\033[0;m')
```

```
    elif optComplete == 0 and optStep >= 0:
      printLines.append('\033[1;31mOptimization incomplete.\033[0;m  ----------
------------------  Optimization step: ' + str(optStep))
    if len(maxForce) > 0 and printType == "none":
      printLines.append('Item      Max Val.    Criteria    Pass?      RMS Val.
Criteria    Pass?')
      printLines.append('Energy    ' + energyCon[-2] + ' ll ' + energyCon[-1] + '
' + energyCon[-3])
      printLines.append('Force     ' + maxForce[-2] + ' ll ' + maxForce[-1] + '    '
+ maxForce[-3] + '        ' + rmsForce[-2] + ' ll ' + rmsForce[-1] + '    ' +
rmsForce[-3])
      printLines.append('Disp      ' + maxDisp[-2] + ' ll ' + maxDisp[-1] + '    ' +
maxDisp[-3] + '        ' + rmsDisp[-2] + ' ll ' + rmsDisp[-1] + '    ' + rmsDisp[-3])
      printLines.append('----------------------------------------------------------------------
-------')
    elif len(maxForce) > 0 and printType == "long":
      printLines.append('Opt Step:   Energy       Force [Max ll RMS]
Displacement [Max ll RMS]')
      for i in range(len(maxForce)):
        printLines.append(" " + str(i+1) + "  " + energyCon[i][-2] + " (" +
energyCon[i][-3] + ")  [" + maxForce[i][-2] + " (" + maxForce[i][-3] + ") ll " +
rmsForce[i][-2] + " (" + rmsForce[i][-3] + ")]  [" + maxDisp[i][-2] + " (" +
maxDisp[i][-3] + ") ll " + rmsDisp[i][-2] + " (" + rmsDisp[i][-3] + ")]")
      printLines.append('----------------------------------------------------------------------
-------')
    elif len(maxForce) > 0 and printType == "extra":
      printLines.append('Opt Step:   Energy       Force [Max ll RMS]
Displacement [Max ll RMS]')
      if len(maxForce) > 5:
        lastLines = len(maxForce) - 5
      else:
        lastLines = 0
      for i in range(lastLines,len(maxForce)):
        printLines.append(" " + str(i+1) + "  " + energyCon[i][-2] + " (" +
energyCon[i][-3] + ")  [" + maxForce[i][-2] + " (" + maxForce[i][-3] + ") ll " +
rmsForce[i][-2] + " (" + rmsForce[i][-3] + ")]  [" + maxDisp[i][-2] + " (" +
maxDisp[i][-3] + ") ll " + rmsDisp[i][-2] + " (" + rmsDisp[i][-3] + ")]")
      printLines.append('----------------------------------------------------------------------
-------')


  if trans == "archive":
    printLines.append('----------------------------------------------------------------------
----')
```

```
    printLines.append("    Atomic        Coordinates (Angstroms)")
    printLines.append("    Type:           X       Y       Z")
    printLines.append('--------------------------------------------------------------------------
----')
    printLines.append("GEOM DATA!")

  if trans == "translate" or trans == "archive":
    #Frequency output
    if freqSwitch == 1 and len(frequencies) > 0:
      printLines.append('Statistical Thermodynamic Analysis for ' + logfile)
    if freqSwitch == 1 and freehSwitch == 1:
       printLines.append('Computed at:  ' + freqTemp + '  and  ' + freqPres)

printLines.append('=========================================
==================================')
       printLines.append('SCF Energy=                                    ' +
scfEnergy)
       printLines.append('Zero-point correction (ZPE)=                    ' +
zeroPointE)
       printLines.append('Internal Energy (U)=                ' + thermE + '      ' +
thermESUM)
       printLines.append('Enthalpy (H)=                      ' + enthalpyE + '      ' +
enthalpyESUM)
       printLines.append('Gibbs Free Energy (G)=              ' + gibbsE + '      '
+ gibbsESUM)
       printLines.append('Entropy (S) [Cal/Mol-Kelvin]=                   ' +
totalS)
       printLines.append('Entropy (S): electronic=                        ' + elecS)
       printLines.append('Entropy (S): translational=                     ' +
transS)
       printLines.append('Entropy (S): rotational=                        ' + rotS)
       printLines.append('Entropy (S): vibrational=                       ' + vibS)
    if freqSwitch == 1 and len(frequencies) > 0:
      frequenciesNoZero = [x for x in frequencies if x != "0.00"]
      printLines.append('Frequencies: ' + frequenciesNoZero[0] + "  " +
frequenciesNoZero[1] + "  " + frequenciesNoZero[2] + "  " +
frequenciesNoZero[3] + "  " + frequenciesNoZero[4] + "  " +
frequenciesNoZero[5])
      for var in frequencies:
        if 'i' in var:
          negfreq = negfreq + 1
      if negfreq == 1:
        printLines.append('\033[1;33m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')
```

```
      elif negfreq >= 2:
        printLines.append('\033[1;31m              !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')

  if trans == "translate":
    #Print end of file for long and extra
    if printType == "extra" or printType == "long":
      for i in range((len(fileList)-10), len(fileList)):
        printLines.append(fileList[i].strip())
    #Completed job
    if jobDone == 1:

printLines.append('=============================================
==================================')
      printLines.append('\033[1;32m##################              JOB
COMPLETED              ##################\033[0;m')

printLines.append('=============================================
==================================')

  if trans == "list":
    if len(frequencies) == 2:
      frequenciesNoZero = frequencies
    else:
      frequenciesNoZero = [x for x in frequencies if x != "0.00"]
    line = scfEnergy + "  "
    line += zeroPointESUM + "  " + thermESUM + "  " + enthalpyESUM + "  " +
gibbsESUM + "  "
    frequenciesNoZero = [x for x in frequencies if x != "0.00"]
    if len(frequenciesNoZero) == 0:
      frequenciesNoZero = ["0.00000", "0.00000"]
    for var in frequencies:
        if 'i' in var:
          negfreq = negfreq + 1
    if negfreq == 0:
      line += '\033[1;32m' + frequenciesNoZero[0] + "  " + frequenciesNoZero[1]
+ '\033[1;0m' + "  "
    elif negfreq == 1:
      line += '\033[1;33m' + frequenciesNoZero[0] + "  " + frequenciesNoZero[1]
+ '\033[1;0m' + "  "
    elif negfreq >= 2:
      line += '\033[1;31m' + frequenciesNoZero[0] + "  " + frequenciesNoZero[1]
+ '\033[1;0m' + "  "
    line += basisFunc + "  " + pointStoic + "  " + stoic + "  "
```

```
    if jobDone == 0:
      line += logfile.split("/")[-1]
    elif jobDone == 1:
      filename  = logfile.split("/")[-1]
      line += '\033[1;32m' + filename + '\033[0;0m'
    elif jobDone == 2:
      filename  = logfile.split("/")[-1]
      line += '\033[1;31m' + filename + '\033[0;0m'
    printLines.append(line)

  if trans != "archive":
    return printLines
  if trans == "archive":
    tableLines = []
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," + zeroPointE +
",=" + thermE  + "+RC[-2],=" + enthalpyE + "+RC[-3],=" + gibbsE + "+RC[-
4],=RC[-1]-MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," + zeroPointE +
"," + thermESUM + "," + enthalpyESUM + "," + gibbsESUM + ",=RC[-1]-
MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy)
    return printLines, tableLines


### --- Terachem Specific Functions --- ###
###=========================================================
==========================================================#
##
### --- Parse the Terachem optim file for geometry information --- ###
def Eta_parseOptimTerachem(optimfile):
  f = open(optimfile)
  geomlist = f.readlines()
  f.close()
  numAtoms = int(geomlist[0])
  allEnergy = []
  for line in geomlist:
    if 'frame' in line:
      allEnergy.append(float(line.split()[0]))
  finalgeom = [0] * (numAtoms + 2)
  finalgeom[0] = str(numAtoms)
  for i in range(len(geomlist)-numAtoms-1, len(geomlist)):
    j = i - len(geomlist) + numAtoms + 2
    if i == len(geomlist)-numAtoms-1:
      line = geomlist[i].split()
```

```
      finalgeom[1] = "Energy: " + str(allEnergy[-1])
    if i > len(geomlist)-numAtoms-1:
      line = geomlist[i].split()
      finalgeom[j] = Atom()
      finalgeom[j].e = line[0]
      finalgeom[j].en = Eta_getElementNum(line[0])
      finalgeom[j].x = float(line[1])
      finalgeom[j].y = float(line[2])
      finalgeom[j].z = float(line[3])
  return finalgeom

def Eta_parseOptimTerachem_Traj(optimfile):
  f = open(optimfile)
  geomlist = f.readlines()
  f.close()
  numAtoms = int(geomlist[0])
  allEnergy = []
  for line in geomlist:
    if 'frame' in line:
      allEnergy.append(float(line.split()[0]))
  trajectorygeom = [0] * len(geomlist)
  skip = 0
  for i in range(len(geomlist)):
    if i % (numAtoms+2) == 0 and i/(numAtoms+2) != len(allEnergy):
      trajectorygeom[i] = geomlist[i].strip()
    elif 'frame' in geomlist[i]:
      trajectorygeom[i] = "Energy: " + str(float(geomlist[i].split()[0]))
    else:
      line = geomlist[i].split()
      trajectorygeom[i] = Atom()
      trajectorygeom[i].e = line[0]
      trajectorygeom[i].en = Eta_getElementNum(line[0])
      trajectorygeom[i].x = float(line[1])/auToAngstrom
      trajectorygeom[i].y = float(line[2])/auToAngstrom
      trajectorygeom[i].z = float(line[3])/auToAngstrom
  return trajectorygeom

### --- Out put the G0X input files --- ###
def Eta_outputTC(ifile, config, charge, multi, writemod, modred, writeecp,
ecplines, writeclose, closelines, ifilelol):
  ofiletmp = ifile.split(".")
  ofile = ""
  for i in range(len(ofiletmp)):
    if i != len(ofiletmp) - 1:
```

```
      ofile += ofiletmp[i] + "."
    elif i == len(ofiletmp) - 1:
      ofile += "tc"
  os.system("cp " + ifile + " NEWJOBS.TC/")
  f = open("NEWJOBS.TC/" + ofile , "w+")
  for i, var in enumerate(config):
    if 'BASE!' in var:
      linetmp = var.replace("BASE!", ifile)
      f.write(linetmp + "\n")
    elif 'SCRDIR!' in var:
      linetmp = var.replace("SCRDIR!", "./scr-" + ifile.lower())
      f.write(linetmp + "\n")
    elif 'CHARGE!' in var:
      linetmp = var.replace("CHARGE!", str(charge))
      f.write(linetmp + "\n")
    elif 'MULTI!' in var:
      linetmp = var.replace("MULTI!", str(multi))
      f.write(linetmp + "\n")
    else:
      f.write(var + "\n")
  if writemod == 1:
    f.write("$constraints\n")
    if len(modred) > 0 and modred[0] != "":
      for i, var in enumerate(modred):
        f.write(var + "\n")
    else:
      f.write("MODRED!\n")
    f.write("$end\n")
  if writeclose == 1:
    for i, var in enumerate(closelines):
      f.write(var + "\n")
    f.write("\n")
  f.close()
  return

#Parse the Gaussian output file and print data to the screen
def Eta_TranslateTCOutput(logfile, trans, printType):
  initLines = ['\033[1;34mPython Terachem Output File Parsing Script:
nTCT.py\033[1;0m',
            '\033[1;34mScripted by Thomas J. L. Mustard, O. Maduka Ogba, Paul
Ha-Yeon Cheong\033[1;0m',
            '--------------------------------------------------------------------------']
  if trans == "translate":
    for line in initLines:
```

```
    print line

#Global Variables
config = ''
configSwitch = 0
printLines = []
programVersion = ''
chk = ''
nproc = ''
mem = ''
configLines = []
configLinesAll = ''
modSwitch = 0
modLines = []
pointStoic = ''
point = ''
stoic = ''
chargeMulti = ''
charge = ''
multi = ''
basisFunc = ''
scfEnergy = ''
predEChange = ''
optSwitch = 0
optComplete = 0
optStep = 0
if printType == "long" or printType == "extra":
  maxForce = []
  rmsDisp = []
  rmsForce = []
  maxDisp = []
  energyCon = []
else:
  maxForce = ''
  rmsForce = ''
  maxDisp = ''
  rmsDisp = ''
  energyCon = ''
freqSwitch = 0
freqTemp = ''
if trans == "list":
  frequencies = ["0.00", "0.00", "0.00", "0.00", "0.00", "0.00"]
  negfreq = 0
  zeroPointE = '0.000000'
```

```
  thermE = '0.000000'
  enthalpyE = '0.000000'
  gibbsE = '0.000000'
  zeroPointESUM = '0.000000'
  thermESUM = '0.000000'
  enthalpyESUM = '0.000000'
  gibbsESUM = '0.000000'
  totalS = '0.000000'
  elecS = '0.000000'
  rotS = '0.000000'
  transS = '0.000000'
  vibS = '0.000000'
else:
  frequencies = ["0.00", "0.00", "0.00", "0.00", "0.00", "0.00"]
  negfreq = 0
  zeroPointE = 0.000000
  thermE = 0.000000
  enthalpyE = 0.000000
  gibbsE = 0.000000
  zeroPointESUM = 0.000000
  thermESUM = 0.000000
  enthalpyESUM = 0.000000
  gibbsESUM = 0.000000
  totalS = 0.000000
  elecS = 0.000000
  rotS = 0.000000
  transS = 0.000000
  vibS = 0.000000
jobDone = 0
memSwitch = 0
f = open(logfile)
fileList = f.readlines()
f.close()
for i, var in enumerate(fileList):
  #Find the Terachem Version
  if 'TeraChem v' in var:
    programVersion = "TeraChem " + var.split()[2]
  #Find the chk file
  elif 'Scratch directory:' in var:
    chk = var.split(':')[-1].strip()
  #Find the nproc used
  elif 'CUDA devices' in var:
    nproc = var.split()[1]
  #Find the mem used
```

```
elif 'GPU Memory Available:' in var:
  mem = var.split(':')[1].strip()
#Find the job configuration used
elif "Method:" in var:
  configLines.append("method=" + var.split()[-1])
elif "Using dynamic DFT grids." in var:
  configLines.append("dynamicgrid=yes")
elif "Basis set:" in var:
  configLines.append("basis=" + var.split()[-1])
elif "Maximum number of SCF iterations:" in var:
  configLines.append("maxit=" + var.split()[-1])
elif "Max number of optimization cycles:" in var:
  configLines.append("nstep=" + var.split()[-1])
elif "Optimization will be performed" in var:
  configLines.append("min_coordinates=" + var.split()[-2])


elif 'RUNNING GEOMETRY OPTMIZATION' in var:
    optSwitch = 1
elif 'modredundant' in fileList[i]:
    modSwitch = 1
elif "RUNNING THERMOCHEMISTRY ANALYSIS" in fileList[i]:
    freqSwitch = 1
#Check to see if modredundant is in the config
elif modSwitch == 1:
  if 'The following ModRedundant input section has been read:' in var:
    for j in range(1,20):
      if len(fileList[i+j]) > 2:
        modLines.append(fileList[i+j].strip())
      else:
        break
#Get pointgroup and stoic
if 'Framework group' in var:
  pointStoic  = var.split()[-1]
  point = pointStoic.split('[')[0]
elif 'Stoichiometry' in var:
  stoic = var.split()[-1]
#Get charge and multiplicity
elif 'Spin multiplicity:' in var:
  multi = var.split()[-1]
elif 'Total charge:' in var:
  charge = var.split()[-1]
#Find basis functions
elif 'Total orbitals:' in var:
```

```
  basisFunc = fileList[i].split()[-1]
#Get SCF Energy and predicted change
elif 'FINAL ENERGY:' in var:
  scfEnergy = var.split()[-2]
elif 'Predicted change in Energy=' in var:
  predEChange = var.strip().split('=')[-1]
#Optimization parse
elif optSwitch == 1:
  if 'Converged!' in var and 'converged' in fileList[i+1]:
    optComplete = 1
  if printType == "none":
    if 'Testing convergence  in cycle' in var:
      optStep = var.split()[-1]
    #elif 'Energy change' in var and 'ratio' not in var:
      energyCon = fileList[i+1].strip().split()
      if energyCon[-1] == "no":
        energyCon[-1] = '\033[1;31mNO!\033[1;0m'
      elif energyCon[-1] == "yes":
        energyCon[-1] = '\033[1;32mYES\033[1;0m'
    elif 'Max grad' in var:
      maxForce = var.rstrip().split()
      if maxForce[-1] == "no":
        maxForce[-1] = '\033[1;31mNO!\033[1;0m'
      elif maxForce[-1] == "yes":
        maxForce[-1] = '\033[1;32mYES\033[1;0m'
    elif 'RMS grad' in var:
      rmsForce = var.rstrip().split()
      if rmsForce[-1] == "no":
        rmsForce[-1] = '\033[1;31mNO!\033[1;0m'
      elif rmsForce[-1] == "yes":
        rmsForce[-1] = '\033[1;32mYES\033[1;0m'
    elif 'Max step' in var:
      maxDisp = var.rstrip().split()
      if maxDisp[-1] == "no":
        maxDisp[-1] = '\033[1;31mNO!\033[1;0m'
      elif maxDisp[-1] == "yes":
        maxDisp[-1] = '\033[1;32mYES\033[1;0m'
    elif 'RMS step' in var:
      rmsDisp = var.rstrip().split()
      if rmsDisp[-1] == "no":
        rmsDisp[-1] = '\033[1;31mNO!\033[1;0m'
      elif rmsDisp[-1] == "yes":
        rmsDisp[-1] = '\033[1;32mYES\033[1;0m'
  elif printType == "long" or printType == "extra":
```

```
        if 'Testing convergence  in cycle' in var:
          optStep = var.split()[2].strip()
          if 'Energy' not in fileList[i+1]:
            energyCon.append(["0.0000", "0.0000", "0.0000", "0.0000", "0.0000",
"0.0000", "0.0000", "\033[1;31mNO!\033[1;0m"])
            #energyCon.append(["0.0000", "0.0000", "0.0000", "0.0000", "0.0000",
"0.0000", "0.0000", "\033[1;31mNO!\033[1;0m"])
            maxDisp.append(["0.0000", "0.0000", "0.0000", "0.0000", "0.0000",
"0.0000", "0.0000", "\033[1;31mNO!\033[1;0m"])
            rmsDisp.append(["0.0000", "0.0000", "0.0000", "0.0000", "0.0000",
"0.0000", "0.0000", "\033[1;31mNO!\033[1;0m"])
          else:
            energyCon.append(list(fileList[i+1].rstrip().split()))
          if energyCon[-1][-1] == "no":
            energyCon[-1][-1] = '\033[1;31mNO!\033[1;0m'
          elif energyCon[-1][-1] == "yes":
            energyCon[-1][-1] = '\033[1;32mYES\033[1;0m'
        elif 'Max grad' in var and 'component' not in var:
          maxForce.append(list(var.rstrip().split()))
          if maxForce[-1][-1] == "no":
            maxForce[-1][-1] = '\033[1;31mNO!\033[1;0m'
          elif maxForce[-1][-1] == "yes":
            maxForce[-1][-1] = '\033[1;32mYES\033[1;0m'
        elif 'RMS grad' in var:
          rmsForce.append(list(var.rstrip().split()))
          if rmsForce[-1][-1] == "no":
            rmsForce[-1][-1] = '\033[1;31mNO!\033[1;0m'
          elif rmsForce[-1][-1] == "yes":
            rmsForce[-1][-1] = '\033[1;32mYES\033[1;0m'
        elif 'Max step' in var:
          maxDisp.append(list(var.rstrip().split()))
          if maxDisp[-1][-1] == "no":
            maxDisp[-1][-1] = '\033[1;31mNO!\033[1;0m'
          elif maxDisp[-1][-1] == "yes":
            maxDisp[-1][-1] = '\033[1;32mYES\033[1;0m'
        elif 'RMS step' in var:
          rmsDisp.append(list(var.rstrip().split()))
          if rmsDisp[-1][-1] == "no":
            rmsDisp[-1][-1] = '\033[1;31mNO!\033[1;0m'
          elif rmsDisp[-1][-1] == "yes":
            rmsDisp[-1][-1] = '\033[1;32mYES\033[1;0m'


    #Frequency and
```

```
if freqSwitch == 1:
  if 'Temperature' in var:
    freqTemp = var.strip()
  #elif 'Vibrational temperatures:' in var:
  #  frequencies = var.strip().split(':')[-1].strip()
  elif "Thermochemical analysis" in var:
    if frequencies[0] == "0.00":
      frequencies = []
    frequencies.append(str(fileList[i+3].split()[2].strip()))
    frequencies.append(str(fileList[i+4].split()[2].strip()))
    frequencies.append(str(fileList[i+5].split()[2].strip()))
    frequencies.append(str(fileList[i+6].split()[2].strip()))
    frequencies.append(str(fileList[i+7].split()[2].strip()))
    for i in frequencies:
      line = float(i)
      if line < 0:
        negfreq += 1
  elif 'total ZPE' in var:
    zeroPointE = float(var.strip().split()[-2])
  elif 'total E vib' in var:
    enthalpyE = float(var.strip().split()[-2])
    #thermE = str(var.strip().split()[-2])
  elif 'total S vib' in var:
    vibS = float(var.strip().split()[-2])
  #  enthalpyE = str(var.strip().split()[-1])
  #elif 'Thermal correction to Gibbs Free Energy' in var:
  #  gibbsE = str(var.strip().split()[-1])
  #elif 'Sum of electronic and zero-point Energies' in var:
  #  zeroPointESUM = str(var.strip().split()[-1])
  #elif 'Sum of electronic and thermal Energies' in var:
  #  thermESUM = str(var.strip().split()[-1])
  #elif 'Sum of electronic and thermal Enthalpies' in var:
  #  enthalpyESUM = str(var.strip().split()[-1])
  #elif 'Sum of electronic and thermal Free Energies' in var:
  #  gibbsESUM = str(var.strip().split()[-1])
  #  totalS = str(fileList[i+4].strip().split()[-1])
  #  elecS = str(fileList[i+5].strip().split()[-1])
  #  transS = str(fileList[i+6].strip().split()[-1])
  #  rotS = str(fileList[i+7].strip().split()[-1])
  #  vibS = str(fileList[i+8].strip().split()[-1])
if 'Job finished:' in var and len(fileList) - i < 10:
  jobDone = 1
elif 'Job finished:' in var and i - len(fileList) < 10:
  jobDone = 2
```

```
  if trans == "translate":
    #Printed output list
    #printLines = ['\033[1;44m
\033[1;0m']
    printLines = ['Analyzing Terachem Output File: ' + logfile]
    printLines.append('Using ' + str(programVersion))
    printLines.append('[#GPUs=' + nproc + '  Memory=' + mem + '  Scratch
Dir=' + chk + ']')

printLines.append('=========================================
==================================')

  elif trans == "archive":
    #Initial information
    printLines.append("Supporting Information: " + logfile)
    printLines.append("-----------------------------------------------------------------------
----")
    printLines.append("Using: " + programVersion)

printLines.append("=========================================
==================================")

  if trans == "archive" or trans == "translate":
    #Print config
    configLinestmp = ' '.join(str(e) for e in configLines)
    segments = list()
    while len(configLinestmp) > 0:
        segments.append( configLinestmp[:78] )
        configLinestmp = configLinestmp[78:]
    for line in segments:
      printLines.append(line)
    #printLines.append(' '.join(str(e) for e in configLines))

    #Modredundant output
    if modSwitch == 1:
      for line in modLines:
        printLines.append(line)

    #Print pointgroup and stoichiometry
    printLines.append('-----------------------------------------------------------------------
----')
    #printLines.append('Pointgroup=' + point + '\tStoichiometry=' + stoic + '\t' +
pointStoic)
```

```
   #Print Charge Multi and BasisFunc
   printLines.append('Charge = ' + charge + '\tMultiplicity = ' + multi + '\tBasis
= ' + basisFunc)
   printLines.append('--------------------------------------------------------------------------
----')

   #Print Energy
   if freqSwitch == 0:
     printLines.append('SCF Energy = ' + scfEnergy ) #+ '\tPredicted Change =
' + predEChange)
     printLines.append('--------------------------------------------------------------------------
-----')


   #Optimization output
   if optSwitch == 1:
     if optComplete == 1 and optStep != 0:
       printLines.append('\033[1;32mOptimization completed.\033[0;0m  ---------
------------------  Optimization step: ' + optStep)
     elif optComplete == 1 and optStep == 0:
       printLines.append('\033[1;32mOptimization completed.\033[0;0m')
     elif optComplete == 0 and optStep != 0:
       printLines.append('\033[1;31mOptimization incomplete.\033[0;0m  --------
------------------  Optimization step: ' + optStep)
     elif optComplete == 0 and optStep == 0:
       printLines.append('\033[1;31mOptimization incomplete.\033[0;0m')
     if len(maxForce) > 0 and printType == "none":
       printLines.append('Item      Max Val.    Criteria    Pass?      RMS Val.
Criteria    Pass?')
       printLines.append('Energy    ' + energyCon[1] + ' ll ' + energyCon[3] + '
' + energyCon[-1])
       printLines.append('Force     ' + maxForce[2] + ' ll ' + maxForce[4] + '    ' +
maxForce[-1] + '      ' + rmsForce[2] + ' ll ' + rmsForce[4] + '    ' + rmsForce[-1])
       printLines.append('Disp      ' + maxDisp[2] + ' ll ' + maxDisp[4] + '    ' +
maxDisp[-1] + '      ' + rmsDisp[2] + ' ll ' + rmsDisp[4] + '    ' + rmsDisp[-1])
       printLines.append('--------------------------------------------------------------------------
-------')
     elif len(maxForce) > 0 and printType == "long":
       printLines.append('Opt Step:   Energy       Force [Max ll RMS]
Displacement [Max ll RMS]')
       for i in range(len(maxForce)):
         printLines.append(" " + str(i+1) + " " + energyCon[i][1] + "(" +
energyCon[i][-1] + ") [" + maxForce[i][2] + "(" + maxForce[i][-1] + ")ll" +
```

```
rmsForce[i][2] + "(" + rmsForce[i][-1] + ")] [" + maxDisp[i][2] + "(" + maxDisp[i][-
1] + ")ll" + rmsDisp[i][2] + "(" + rmsDisp[i][-1] + ")]")
        printLines.append('----------------------------------------------------------------------------
-------')
      elif len(maxForce) > 0 and printType == "extra":
        printLines.append('Opt Step:   Energy       Force [Max ll RMS]
Displacement [Max ll RMS]')
        if len(maxForce) > 5:
          lastLines = len(maxForce) - 5
        else:
          lastLines = 0
        for i in range(lastLines,len(maxForce)):
          printLines.append(" " + str(i+1) + " " + energyCon[i][1] + "(" +
energyCon[i][-1] + ") [" + maxForce[i][2] + "(" + maxForce[i][-1] + ")ll" +
rmsForce[i][2] + "(" + rmsForce[i][-1] + ")] [" + maxDisp[i][2] + "(" + maxDisp[i][-
1] + ")ll" + rmsDisp[i][2] + "(" + rmsDisp[i][-1] + ")]")
        printLines.append('----------------------------------------------------------------------------
-------')

  if trans == "archive":

    printLines.append("    Atomic        Coordinates (Angstroms)")
    printLines.append("    Type:           X       Y       Z")
    printLines.append('----------------------------------------------------------------------------
----')
    printLines.append("GEOM DATA!")

  if trans == "translate" or trans == "archive":
    #Frequency output
    if freqSwitch == 1 and enthalpyE != '':
      printLines.append('Statistical Thermodynamic Analysis for ' + logfile)
      printLines.append(freqTemp)

printLines.append('==========================================
==================================')
      #printLines.append('SCF Energy=                                    ' +
scfEnergy)
      printLines.append('Zero-point correction (ZPE)=           ' + str(zeroPointE)
+ '  J/mol')# + zeroPointESUM)
      #printLines.append('Internal Energy (U)=                ' + thermE + '  J/mol'
+ thermESUM)
      printLines.append('Enthalpy (H)=                       ' + str(enthalpyE) + '
')# + enthalpyESUM)
```

```
      #printLines.append('Gibbs Free Energy (G)=                ' + gibbsE + '
' + gibbsESUM)
      #printLines.append('Entropy (S) [Cal/Mol-Kelvin]=          ' + totalS)
      #printLines.append('Entropy (S): electronic=              ' + elecS)
      #printLines.append('Entropy (S): translational=           ' + transS)
      #printLines.append('Entropy (S): rotational=              ' + rotS)
      printLines.append('Entropy (S): vibrational=             ' + str(vibS) + '
J/mol/K')
      printLines.append('Frequencies: ' + frequencies[0] + "  " + frequencies[1] +
"  " + frequencies[2] + "  " + frequencies[3] + "  " + frequencies[4] )
      if negfreq == 1:
        printLines.append('\033[1;33m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')
      elif negfreq >= 2:
        printLines.append('\033[1;31m             !!!Warning there were ' +
str(negfreq) + ' negative frequencies!!!\033[0;m')
      printLines.append('----------------------------------------------------------------------
-----')

  if trans == "translate":
    #Print end of file for long and extra
    if printType == "extra" or printType == "long":
      for i in range((len(fileList)-10), len(fileList)):
        printLines.append(fileList[i].strip())
    #Completed job
    if jobDone == 1:

printLines.append('==========================================
==================================')
      printLines.append('\033[1;32m##################             JOB
COMPLETED             ##################\033[0;m')

printLines.append('==========================================
==================================')
    elif jobDone == 2:

printLines.append('==========================================
==================================')
      printLines.append('\033[1;31m!!!!!!!!!!!!!!!!!!           !!!JOB FAILED!!!
!!!!!!!!!!!!!!!!!!\033[0;m')

printLines.append('==========================================
==================================')
```

```
  elif trans == "list":
    line = scfEnergy + "  "
    line += zeroPointESUM + "  " + thermESUM + "  " + enthalpyESUM + "  " +
gibbsESUM + "  "
    if negfreq == 0:
      line += '\033[1;32m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    elif negfreq == 1:
      line += '\033[1;33m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    elif negfreq >= 2:
      line += '\033[1;31m' + frequencies[0] + "  " + frequencies[1] + '\033[1;0m' +
"  "
    line += basisFunc + "  " + pointStoic + "  " + stoic + "  "
    if jobDone == 0:
      line += logfile.split("/")[-1]
    elif jobDone == 1:
      filename  = logfile.split("/")[-1]
      line += '\033[1;32m' + filename + '\033[0;0m'
    elif jobDone == 2:
      filename  = logfile.split("/")[-1]
      line += '\033[1;31m' + filename + '\033[0;0m'
    printLines.append(line)

  if trans != "archive":
    return printLines
  if trans == "archive":
    entropyESUM =  str(float(vibS)/1000/2625.5)
    enthalpyESUM =  str(float(enthalpyE)/1000/2625.5)
    entropyEHart = (float(vibS)/1000/2625.5 )
    enthalpyEHart = ((enthalpyE)/1000/2625.5)
    if len(freqTemp) > 0:
      gibbsE = (float(vibS)/1000/2625.5 * float(freqTemp.split()[1])) +
((enthalpyE)/1000/2625.5)
      gibbsESUM = gibbsE
    else:
      gibbsE = 0
      gibbsESUM = 0
    tableLines = []
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," +
str(zeroPointE) + ",=" + str(entropyEHart)  + "+RC[-2],=" + str(enthalpyEHart)
```

```
+ "+RC[-3],=" + str(gibbsE) + "+RC[-4],=RC[-1]-MIN(C[-1]),=RC[-
1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy + "," +
str(zeroPointE) + "," + str(thermESUM) + "," + str(enthalpyESUM) + "," +
str(gibbsESUM) + ",=RC[-1]-MIN(C[-1]),=RC[-1]*627.5095")
    tableLines.append(logfile.split("/")[-1] + "," + scfEnergy)
    return printLines, tableLines
```

1.2 EtaLibPersistentOTS.py:

```
#! /usr/bin/env python2.7

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```
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#   OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN
ANY WAY OUT OF THE USE
#   OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF
SUCH DAMAGE.

import os
from sys import *
from EtaLibAtom import *
from EtaNUMPYLib import *
import time
import shutil
from numpy import *

###=========================================================
==========================================================#
##
### --- Atom class --- ###
class PersistentOTS(object):
  def __init__(self):
    ### --- OPT Variables --- ###
    self.stepNumber = 300
    self.maxopt = 25
    self.breaktype = ""
    self.breakpoint = 0.000
    self.breakatoms = []
    self.optimized = False
    self.kill = False
    self.inputNumAtoms = 0
    self.shortenStepSize = 0

    ### --- Scan File Variables --- ###
    self.scanType = ''
    self.atomList = []
    self.scan = 0
    self.ts = 0
    self.minorTS = 0
    self.scanLength = 0
    self.scanStepNow = 0
```

```
self.scanSize = 0
self.scanSizeNOW = 0
self.waitSize = 0
self.breakpoint = 0.000
self.breakatoms = []
self.minTSScanVar = 'none'

### --- (TS-)SCAN Variables --- ###
self.minTSScanSize = 0.000
self.scanEnergy = []
self.tsscanEnergy = []

### --- Molecule Variables --- ###
self.finalenergy = 0
self.finalForce = 0
self.finalDisp = 0
self.allEnergy = []
self.allForce = []
self.numAtoms = 0
self.charge = 0
self.multi = 1
self.inputNumAtoms = 0

### --- Input File Variables (mostly for G0X) --- ###
self.QMconfig = []
self.QMconfigORIG = []
self.QMcomment = ''
self.QMcommentORIG = ''
self.QMendlines = []
self.QMendlinesORIG = []
self.TCscratchDir = ''

### --- Geometry holders (Atom class) --- ###
self.inputGeomAtom = []
self.finalGeomAtom = []
self.trajectoryGeomAtom = []
self.highestGeomAtom = []
self.ZMATAtom = []

### --- PersistentOTS variables --- ###
self.baseinput = ''
self.baselog = ''
self.joblog = ''
self.scratchdir = ''
```

```
    self.trajectoryfile = ''
    self.scanfile = ''
    self.outScanFile = ''
    self.linearScanFile = ''
    self.program = "nPersistentOTS.py"
    self.inputfile = ''
    self.outfile = ''
    self.jobname = ''
    self.pwdirectory = ''
    self.jobtype = ''
    self.QMtype = ''
    self.path2QM = ''
    self.debug = 0
    self.test = 0
    self.verbose = 0



#Constants
auToAngstrom = 1.889725988579
hartreeTokcalmol = 627.509469
hartreeToeV = 27.21138386
kcalmolTokjoulemol = 4.184


### --- Setup and reset all the variables --- ###
def EtaPOTS_resetVariables(POTS):
  ### --- OPT Variables --- ###
  #POTS.stepNumber = 300
  #POTS.maxopt = 25
  POTS.breaktype = ''
  POTS.breakpoint = 0.000
  POTS.breakatoms = []
  POTS.optimized = False
  #POTS.kill = False
  POTS.inputNumAtoms = 0
  POTS.shortenStepSize = 0

  ### --- Scan File Variables --- ###
  POTS.scanType = ''
  POTS.atomList = []
  POTS.scan = 0
  POTS.ts = 0
  POTS.minorTS = 0
```

```
POTS.scanLength = 0
POTS.scanStepNow = 0
POTS.scanSize = 0
POTS.scanSizeNOW = 0
POTS.waitSize = 0
POTS.breakpoint = 0.000
POTS.breakatoms = []
POTS.minTSScanVar = 'none'

### --- (TS-)SCAN Variables --- ###
POTS.minTSScanSize = 0.000
#POTS.scanEnergy = []
#POTS.tsscanEnergy = []

### --- Molecule Variables --- ###
POTS.finalenergy = 0
POTS.finalForce = 0
POTS.finalDisp = 0
POTS.allEnergy = []
POTS.allForce = []
#POTS.numAtoms = 0
#POTS.charge = 0
#POTS.multi = 1
POTS.inputNumAtoms = 0

### --- Input File Variables (mostly for G0X) --- ###
POTS.QMconfig = []
#POTS.QMconfigORIG = []
POTS.QMcomment = ''
#POTS.QMcommentORIG = ''
POTS.QMendlines = []
#POTS.QMendlinesORIG = []
POTS.TCscratchDir = ''

### --- Geometry holders (Atom class) --- ###
POTS.inputGeomAtom = []
POTS.finalGeomAtom = []
POTS.trajectoryGeomAtom = []
#POTS.highestGeomAtom = []
POTS.ZMATAtom = []

### --- PersistentOTS variables --- ###
#POTS.baseinput = ''
#POTS.baselog = ''
```

```
  #POTS.joblog = ''
  #POTS.scratchdir = ''
  #POTS.trajectoryfile = ''
  #POTS.scanfile = ''
  #POTS.outScanFile = ''
  #POTS.linearScanFile = ''
  #POTS.program = "nPersistentOTS.py"
  #POTS.inputfile = ''
  #POTS.outfile = ''
  #POTS.jobname = ''
  #POTS.pwdirectory = ''
  #POTS.jobtype = ''
  #POTS.QMtype = ''
  #POTS.path2QM = ''
  #POTS.debug = 0
  #POTS.test = 0
  return POTS



### --- FUNCTIONS --- ###
#################################################################
#################################################################
### --- Parse the scan file  --- ###
def EtaPOTS_parseScanFile(POTS):
  if POTS.debug >= 1:
    print "parseScanFile"
  f = open(POTS.scanfile, 'r')
  scanList = f.readlines()
  f.close()
  for var in scanList:
    line = var.split('=')
    if line[0].strip() == "#STEPSIZE":
      POTS.scanSize = float(line[1].strip())
    elif line[0].strip() == "#SCAN":
      if line[1].split()[0].upper() == "YES":
        POTS.scan = 1
    elif line[0].strip() == "#TS":
      if line[1].split()[0].upper() == "YES":
        POTS.ts = 1
      if line[1].split()[0].upper() == "DYN":
        POTS.ts = 2
    elif line[0].strip() == "#SCANLENGTH":
      POTS.scanLength = int(line[1].split()[0])
```

```
    elif line[0].strip() == "#SCANSTEPNOW":
      POTS.scanStepNow = int(line[1].split()[0])
    elif line[0].strip() == "#MINTSSCANSIZE":
      POTS.minTSScanVar = str(line[1].split()[0].lower())
    elif line[0].strip() == "#WAIT":
      POTS.waitSize = int(line[1].split()[0])
    elif line[0].strip() == "#VARIABLE":
      line2 = line[1].split()
      POTS.scanType = line2[0].lower()
      for i in range(1, len(line2)):
        POTS.atomList.append(int(line2[i]))
    elif line[0].strip() == "#BREAKPOINT":
      line2 = line[1].split()
      POTS.breakpoint = float(line2[0])
      for i in range(1, len(line2)):
        POTS.breakatoms.append(int(line2[i]))
    elif line[0].strip() == "#MINORTS":
      if line[1].split()[0].upper() == "ONE":
        POTS.minorTS = 0
      if line[1].split()[0].upper() == "YES":
        POTS.minorTS = 2
      if line[1].split()[0].upper() == "NO":
        POTS.minorTS = 3
    if POTS.QMtype == "Terachem":
      if var.strip() != '':
        line2 = var.strip().split()
        if line2[0].strip() == "#TCSCRDIR":
          POTS.TCscratchDir = line2[1][1:]
  if POTS.scan == 0:
    EtaPOTS_printWrite(["The scan feature is turned off in the scan text file.",
                        "Please turn this on (#SCAN=yes) if you want this feature."],
POTS.verbose, POTS.joblog)
  if POTS.debug >= 1:
    print POTS.scanSize
    print POTS.scan
    print POTS.ts
    print POTS.scanLength
    print POTS.scanStepNow
    print POTS.minTSScanVar
    print POTS.waitSize
    print POTS.scanType
    print POTS.atomList
    print POTS.breakpoint
    print POTS.breakatoms
```

```
    print POTS.minorTS
    print POTS.TCscratchDir

  return POTS

### --- Parse the scan file  --- ###
def EtaPOTS_makeTempScanFile(POTS):
  if POTS.debug >= 1:
    print "makeTempScanFile"
  if os.path.isfile("Scan.txt"):
    if POTS.QMtype == "G09" or POTS.QMtype == "G03":
      for i in os.listdir(os.getcwd()):
        if i.endswith(".com"):
          ofile = "Scan-" + Eta_basename(i, ".com") + ".txt"
          shutil.copyfile("Scan.txt", ofile)
          print ofile
    elif POTS.QMtype == "Turbomole":
      for i in os.listdir(os.getcwd()):
        if i.endswith(".Turbomole"):
          ofile = Eta_basename(i, ".Turbomole") + "/Scan-" + Eta_basename(i,
".Turbomole") + ".txt"
          shutil.copyfile("Scan.txt", ofile)
          print ofile
      for i in os.listdir(os.getcwd()):
        if i.endswith(".tmol"):
          ofile = "Scan-" + Eta_basename(i, ".tmol") + ".txt"
          shutil.copyfile("Scan.txt", ofile)
          print ofile
    elif POTS.QMtype == "Terachem":
      for i in os.listdir(os.getcwd()):
        if i.endswith(".tc"):
          ofile = "Scan-" + Eta_basename(i, ".tc") + ".txt"
          shutil.copyfile("Scan.txt", ofile)
          print ofile
    elif POTS.QMtype.upper() == "JAGUAR":
      for i in os.listdir(os.getcwd()):
        if i.endswith(".in"):
          ofile = "Scan-" + Eta_basename(i, ".in") + ".txt"
          shutil.copyfile("Scan.txt", ofile)
          print ofile
    shutil.move("Scan.txt", "Scan.distributed")
  else:
    f = open("Scan.txt", 'w')
    print "#SCAN = YES/NO"
```

```
    print "#TS = YES/DYN/NO"
    print "#VARIABLE = bond/angle/dihedral 1 2 3 4"
    print "#SCANLENGTH = 30"
    print "#SCANSTEPNOW = 0"
    print "#STEPSIZE = -0.05"
    print "#MINTSSCANSIZE = loose/none/tight/verytight"
    print "#WAIT = 0"
    print "#BREAKPOINT: 2.3 2 4"
    print "#MINORTS = YES/ONE/NO"
    print "#TCSCRDIR = ./scr-h2o"
    print
"============================================================
=================="
    print "Edit the new Scan.txt file and rerun nPersistantOTS.py -T and the
Scan.txt "
    print "will be distributed for all input files."
    #Write the temp scan file
    f.write("#SCAN = YES\n")
    f.write("#TS = YES\n")
    f.write("#VARIABLE = bond 1 2\n")
    f.write("#SCANLENGTH = 30\n")
    f.write("#SCANSTEPNOW = 0\n")
    f.write("#STEPSIZE = -0.05\n")
    f.write("#MINTSSCANSIZE = none\n")
    f.write("#WAIT = 0\n")
    f.write("#BREAKPOINT: 2.3 2 4\n")
    f.write("#MINORTS = ONE\n")
    f.write("#TCSCRDIR = \n")
    f.close()
  return POTS

### --- Write the final geom to the SCAN xyz file. This can be visualized by
molden or others--- ###
def EtaPOTS_printWrite(list, verbose, file):
  f = open(file, "a")
  for i in list:
    if verbose == 1:
      print i
    elif verbose == 3:
      print i.center(80, ' ')
    f.write(str(i) + "\n")
  f.close()
  return
```

```
### --- Write the final geom to the SCAN xyz file. This can be visualized by
molden or others--- ###
def EtaPOTS_writeFinalGeomtoSCAN(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["writeTrajectory"], POTS.verbose, POTS.joblog)
  #List of ALL
  f = open(POTS.trajectoryfile, 'a')
  for i in range(len(POTS.trajectoryGeomAtom)):
    #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
    if isinstance(ifilelol[i], Atom):
      line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + \
            "  " + str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
    #else print the string (number of atoms or comment line)
    else:
      line = str(ifilelol[i])
    f.write(line + "\n")
  f.close()
  return


### --- Write the final geom to the SCAN xyz file. This can be visualized by
molden or others--- ###
def EtaPOTS_writeFinalGeomtoSCAN(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["writeFinalGeomtoSCAN"], POTS.verbose,
POTS.joblog)
  #List of ALL
  scangeom = []
  #List of Bond Angle Dihedral info
  scanBAD = []
  if os.path.isfile(POTS.outScanFile):
    #Grab the scan geometries Bond Angle Dihedral (BAD) numbers
    f = open(POTS.outScanFile, 'r')
    for line in f:
      scangeom.append(line)
      if line.rstrip().split()[0] == "Energy:":
        scanBAD.append(float(line.rstrip().split()[3]))
    f.close()
    #Output the Geometries
    usedgeom = 0
    f = open(POTS.outScanFile, 'w+')
    for i in range(len(scanBAD)):
```

```
    if float(POTS.finalGeomAtom[1].rstrip().split()[3]) < float(scanBAD[i]) and
usedgeom == 0:
      usedgeom = 1
      #Write finalgeom
      for j in range(len(POTS.finalGeomAtom)):
        #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
        if isinstance(POTS.finalGeomAtom[j], Atom):
          line = POTS.finalGeomAtom[j].e + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[j].x)) + "  " + \
              str("{:.6f}".format(POTS.finalGeomAtom[j].y)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[j].z))
        #else print the string (number of atoms or comment line)
        else:
          line = str(POTS.finalGeomAtom[j])
        f.write(line + "\n")
      #Write scangeom
      for j in range(len(scangeom)):
        if j >= (len(POTS.finalGeomAtom) * i) and j <
(len(POTS.finalGeomAtom) * (i + 1)):
          f.write(scangeom[j])
    else:
      #Write scangeom
      for j in range(len(scangeom)):
        if j >= (len(POTS.finalGeomAtom) * i) and j <
(len(POTS.finalGeomAtom) * (i + 1)):
          f.write(scangeom[j])
  if usedgeom == 0:
    #Write finalgeom
    for j in range(len(POTS.finalGeomAtom)):
      #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
      if isinstance(POTS.finalGeomAtom[j], Atom):
        line = POTS.finalGeomAtom[j].e + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[j].x)) + "  " + \
            str("{:.6f}".format(POTS.finalGeomAtom[j].y)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[j].z))
      #else print the string (number of atoms or comment line)
      else:
        line = str(POTS.finalGeomAtom[j])
      f.write(line + "\n")
 else:
  f = open(POTS.outScanFile, 'w+')
  #Write finalgeom
```

```
    for j in range(len(POTS.finalGeomAtom)):
      #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
      if isinstance(POTS.finalGeomAtom[j], Atom):
        line = POTS.finalGeomAtom[j].e + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[j].x)) + "  " + \
              str("{:.6f}".format(POTS.finalGeomAtom[j].y)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[j].z))
      #else print the string (number of atoms or comment line)
      else:
        line = str(POTS.finalGeomAtom[j])
      f.write(line + "\n")
  f.close()
  return


### --- Write the final geom to the SCAN xyz file. This can be visualized by
molden or others--- ###
def EtaPOTS_writeFinalGeomtoSCANLinear(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["writeFinalGeomtoSCANLinear"], POTS.verbose,
POTS.joblog)
  if os.path.isfile(POTS.linearScanFile):
    f = open(POTS.linearScanFile, 'a')
  else:
    f = open(POTS.linearScanFile, 'w+')
  #Write finalgeom
  for i in range(len(POTS.finalGeomAtom)):
    #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
    if isinstance(POTS.finalGeomAtom[i], Atom):
      line = POTS.finalGeomAtom[i].e + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].x)) + "  " + \
            str("{:.6f}".format(POTS.finalGeomAtom[i].y)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].z))
    #else print the string (number of atoms or comment line)
    else:
      line = str(POTS.finalGeomAtom[i])
    f.write(line + "\n")
  f.close()
  return

### --- Write the final geom to the SCAN xyz file. This can be visualized by
molden or others--- ###
```

```
def EtaPOTS_writeHighGeom(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["writeHighGeom"], POTS.verbose, POTS.joblog)
  if os.path.isfile(POTS.scratchdir + "/HIGHEST-" + POTS.jobname + ".xyz"):
    shutil.move(POTS.scratchdir + "/HIGHEST-" + POTS.jobname + ".xyz",
POTS.scratchdir + "/SECOND-" + POTS.jobname + ".xyz")
  f = open(POTS.scratchdir + "/HIGHEST-" + POTS.jobname + ".xyz", 'w+')
  #Write finalgeom
  for i in range(len(POTS.finalGeomAtom)):
    #if the instance is in Atom form print the 'element X-Coord Y-Coord Z-
Coord'
    if isinstance(POTS.finalGeomAtom[i], Atom):
      line = POTS.finalGeomAtom[i].e + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].x)) + "  " + \
            str("{:.6f}".format(POTS.finalGeomAtom[i].y)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].z))
    #else print the string (number of atoms or comment line)
    else:
      line = str(POTS.finalGeomAtom[i])
    f.write(line + "\n")
  f.close()
  return

### --- Grabs the highest energy geometry held in the SCRATCH folder  ---
###
def EtaPOTS_saveHighestGeom(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["saveHighestGeom",
                        "Saving this geometry as the highest."], POTS.verbose,
POTS.joblog)
  POTS.highestGeomAtom = [0] * len(POTS.finalGeomAtom)
  for i in range(len(POTS.finalGeomAtom)):
    if i <= 1:
      POTS.highestGeomAtom[i] = POTS.finalGeomAtom[i]
    elif i >= 2:
      POTS.highestGeomAtom[i] = Atom()
      POTS.highestGeomAtom[i].e           = POTS.finalGeomAtom[i].e
      POTS.highestGeomAtom[i].en          = POTS.finalGeomAtom[i].en
      POTS.highestGeomAtom[i].x           = POTS.finalGeomAtom[i].x
      POTS.highestGeomAtom[i].y           = POTS.finalGeomAtom[i].y
      POTS.highestGeomAtom[i].z           = POTS.finalGeomAtom[i].z
      POTS.highestGeomAtom[i].int         = POTS.finalGeomAtom[i].int
      POTS.highestGeomAtom[i].en          = POTS.finalGeomAtom[i].en
```

```
    POTS.highestGeomAtom[i].neighbors     =
POTS.finalGeomAtom[i].neighbors
    POTS.highestGeomAtom[i].neighborsdist =
POTS.finalGeomAtom[i].neighborsdist
    POTS.highestGeomAtom[i].nearest       = POTS.finalGeomAtom[i].nearest
    POTS.highestGeomAtom[i].nearestdist   =
POTS.finalGeomAtom[i].nearestdist
    POTS.highestGeomAtom[i].hybridization =
POTS.finalGeomAtom[i].hybridization
    POTS.highestGeomAtom[i].charge        = POTS.finalGeomAtom[i].charge
    POTS.highestGeomAtom[i].string        = POTS.finalGeomAtom[i].string
    POTS.highestGeomAtom[i].atomtype      =
POTS.finalGeomAtom[i].atomtype
 return POTS

### --- Grabs the highest energy geometry held in the SCRATCH folder  ---
###
def EtaPOTS_grabHighestGeom(POTS):
 if POTS.debug >= 1:
  EtaPOTS_printWrite(["grabHighestGeom"], POTS.verbose, POTS.joblog)
 for i in range(len(POTS.highestGeomAtom)):
  if i <= 1:
    POTS.highestGeomAtom[i] = POTS.finalGeomAtom[i]
  elif i >= 2:
    POTS.finalGeomAtom[i] = Atom()
    POTS.finalGeomAtom[i].e           = POTS.highestGeomAtom[i].e
    POTS.finalGeomAtom[i].en          = POTS.highestGeomAtom[i].en
    POTS.finalGeomAtom[i].x           = POTS.highestGeomAtom[i].x
    POTS.finalGeomAtom[i].y           = POTS.highestGeomAtom[i].y
    POTS.finalGeomAtom[i].z           = POTS.highestGeomAtom[i].z
    POTS.finalGeomAtom[i].int         = POTS.highestGeomAtom[i].int
    POTS.finalGeomAtom[i].en          = POTS.highestGeomAtom[i].en
    POTS.finalGeomAtom[i].neighbors     =
POTS.highestGeomAtom[i].neighbors
    POTS.finalGeomAtom[i].neighborsdist =
POTS.highestGeomAtom[i].neighborsdist
    POTS.finalGeomAtom[i].nearest       = POTS.highestGeomAtom[i].nearest
    POTS.finalGeomAtom[i].nearestdist   =
POTS.highestGeomAtom[i].nearestdist
    POTS.finalGeomAtom[i].hybridization =
POTS.highestGeomAtom[i].hybridization
    POTS.finalGeomAtom[i].charge        = POTS.highestGeomAtom[i].charge
    POTS.finalGeomAtom[i].string        = POTS.highestGeomAtom[i].string
```

```
    POTS.finalGeomAtom[i].atomtype     =
POTS.highestGeomAtom[i].atomtype
  return POTS

#  if os.path.isfile(POTS.scratchdir + "/HIGHEST-" + POTS.jobname + ".xyz"):
#    a_list = []
#    the_file = open(POTS.scratchdir + "/HIGHEST-" + POTS.jobname +
".xyz",'r')
#    for line in the_file:
#      a_list.append(line.rstrip())
#    the_file.close()
#    for i in range(len(a_list)):
#      if i <= 1:
#        POTS.finalGeomAtom[i] = a_list[i]
#      elif i >= 2:
#        line = a_list[i].split()
#        POTS.finalGeomAtom[i] = Atom()
#        POTS.finalGeomAtom[i].e = line[0]
#        #POTS.finalGeomAtom[i].en = Eta_getElementNum(a_list[j][0])
#        POTS.finalGeomAtom[i].x = float(line[1])
#        POTS.finalGeomAtom[i].y = float(line[2])
#        POTS.finalGeomAtom[i].z = float(line[3])
#  else:
#    EtaPOTS_printWrite(["Highest geom file does not exist."], POTS.verbose,
POTS.joblog)
#  return POTS

### --- Grabs a previous nth geometry from a xyz file. geomNum  --- ###
def EtaPOTS_grabPreviousGeom(POTS, geomnum):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["grabPreviousGeom"], POTS.verbose, POTS.joblog)
  a_list = []
  the_file = open(POTS.linearScanFile,'r')
  for line in the_file:
    a_list.append(line.rstrip())
  the_file.close()
  #Extract the final geometry from the trajectory
  POTS.finalGeomAtom = [0] * (POTS.trajectoryGeomAtom[0] + 2)
  for i in range(len(a_list)-(geomnum * len(POTS.finalGeomAtom)), len(a_list)
- ((geomnum - 1) * len(POTS.finalGeomAtom))):
    j = i - (len(a_list)-(geomnum * len(POTS.finalGeomAtom)))
    line = a_list[j].split()
    if j <= 1:
      POTS.finalGeomAtom[j] = a_list[i]
```

```
    elif j >= 2:
      POTS.finalGeomAtom[j] = Atom()
      POTS.finalGeomAtom[j].e = line[0]
      #POTS.finalGeomAtom[i].en = Eta_getElementNum(a_list[j][0])
      POTS.finalGeomAtom[j].x = float(line[1])
      POTS.finalGeomAtom[j].y = float(line[2])
      POTS.finalGeomAtom[j].z = float(line[3])
  return POTS

### --- Make a backup copy of the original geom in Atom form --- ###
def EtaPOTS_makeGeomBackup(POTS):
  backupGeom = [0] * (len(POTS.finalGeomAtom))
  backupGeom[0] = POTS.finalGeomAtom[0]
  backupGeom[1] = POTS.finalGeomAtom[1]
  for i in range(2,len(POTS.finalGeomAtom)):
    backupGeom[i] = Atom()
    #EtaPOTS_printWrite([POTS.finalGeomAtom[i].e], POTS.verbose,
POTS.joblog)
    backupGeom[i].e            = POTS.finalGeomAtom[i].e
    backupGeom[i].en           = POTS.finalGeomAtom[i].en
    backupGeom[i].x            = POTS.finalGeomAtom[i].x
    backupGeom[i].y            = POTS.finalGeomAtom[i].y
    backupGeom[i].z            = POTS.finalGeomAtom[i].z
    backupGeom[i].int          = POTS.finalGeomAtom[i].int
    backupGeom[i].en           = POTS.finalGeomAtom[i].en
    backupGeom[i].neighbors     = POTS.finalGeomAtom[i].neighbors
    backupGeom[i].neighborsdist = POTS.finalGeomAtom[i].neighborsdist
    backupGeom[i].nearest       = POTS.finalGeomAtom[i].nearest
    backupGeom[i].nearestdist   = POTS.finalGeomAtom[i].nearestdist
    backupGeom[i].hybridization = POTS.finalGeomAtom[i].hybridization
    backupGeom[i].charge        = POTS.finalGeomAtom[i].charge
    backupGeom[i].string        = POTS.finalGeomAtom[i].string
    backupGeom[i].atomtype      = POTS.finalGeomAtom[i].atomtype

  return backupGeom

### --- Given a number and a list, how many entries in the list are smaller
than the given number? --- ###
def EtaPOTS_numbersmaller(number, list):
  numsmall = 0
  for i in list:
    if number < i:
      numsmall += 1
  return numsmall
```

```
### --- Given a number and a list, how many entries in the list are larger than
the given number? --- ###
def EtaPOTS_numberlarger(number, list):
  numlarge = 0
  for i in list:
    if number > i:
      numlarge += 1
  return numlarge

### --- Move the atoms of interest to the front of the file for subsequent
changes --- ###
def EtaPOTS_renumberFix(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["renumberFix"], POTS.verbose, POTS.joblog)
  #Place the original locations into each atom as an int for unfixing the
geometry
  for i in range(2, len(POTS.finalGeomAtom)):
    POTS.finalGeomAtom[i].int = i
  #Make a backup geom to work from
  oldfinalGeomAtom = EtaPOTS_makeGeomBackup(POTS)
  #oldfinalGeomAtom = POTS.finalGeomAtom
  #EtaPOTS_printgeom(oldfinalGeomAtom)
  #Move the atoms of interest to the tom of the molecule file in the order they
are listed
  # (needed for accurate angle and diherdral SCANs)
  for i in range(len(POTS.atomList)):
    for j in range(2, len(POTS.finalGeomAtom)):
      if j-1 == POTS.atomList[i]:
        POTS.finalGeomAtom[i+2].e           = oldfinalGeomAtom[j].e
        POTS.finalGeomAtom[i+2].en          = oldfinalGeomAtom[j].en
        POTS.finalGeomAtom[i+2].x           = oldfinalGeomAtom[j].x
        POTS.finalGeomAtom[i+2].y           = oldfinalGeomAtom[j].y
        POTS.finalGeomAtom[i+2].z           = oldfinalGeomAtom[j].z
        POTS.finalGeomAtom[i+2].int         = oldfinalGeomAtom[j].int
        POTS.finalGeomAtom[i+2].en          = oldfinalGeomAtom[j].en
        POTS.finalGeomAtom[i+2].neighbors    =
oldfinalGeomAtom[j].neighbors
        POTS.finalGeomAtom[i+2].neighborsdist =
oldfinalGeomAtom[j].neighborsdist
        POTS.finalGeomAtom[i+2].nearest      = oldfinalGeomAtom[j].nearest
        POTS.finalGeomAtom[i+2].nearestdist  =
oldfinalGeomAtom[j].nearestdist
```

```
        POTS.finalGeomAtom[i+2].hybridization =
oldfinalGeomAtom[j].hybridization
        POTS.finalGeomAtom[i+2].charge       = oldfinalGeomAtom[j].charge
        POTS.finalGeomAtom[i+2].string       = oldfinalGeomAtom[j].string
        POTS.finalGeomAtom[i+2].atomtype     = oldfinalGeomAtom[j].atomtype
  #EtaPOTS_printgeom(POTS.finalGeomAtom)
  #For all other atoms move them down the appropriate number of places
  for i in range(2, len(POTS.finalGeomAtom)):
     if i-1 not in POTS.atomList:
        j = EtaPOTS_numbersmaller(i-1, POTS.atomList)
        #k = EtaPOTS_numberlarger(i-1, POTS.atomList)
        POTS.finalGeomAtom[i+j].e            = oldfinalGeomAtom[i].e
        POTS.finalGeomAtom[i+j].en           = oldfinalGeomAtom[i].en
        POTS.finalGeomAtom[i+j].x            = oldfinalGeomAtom[i].x
        POTS.finalGeomAtom[i+j].y            = oldfinalGeomAtom[i].y
        POTS.finalGeomAtom[i+j].z            = oldfinalGeomAtom[i].z
        POTS.finalGeomAtom[i+j].int          = oldfinalGeomAtom[i].int
        POTS.finalGeomAtom[i+j].en           = oldfinalGeomAtom[i].en
        POTS.finalGeomAtom[i+j].neighbors    = oldfinalGeomAtom[i].neighbors
        POTS.finalGeomAtom[i+j].neighborsdist =
oldfinalGeomAtom[i].neighborsdist
        POTS.finalGeomAtom[i+j].nearest      = oldfinalGeomAtom[i].nearest
        POTS.finalGeomAtom[i+j].nearestdist  =
oldfinalGeomAtom[i].nearestdist
        POTS.finalGeomAtom[i+j].hybridization =
oldfinalGeomAtom[i].hybridization
        POTS.finalGeomAtom[i+j].charge       = oldfinalGeomAtom[i].charge
        POTS.finalGeomAtom[i+j].string       = oldfinalGeomAtom[i].string
        POTS.finalGeomAtom[i+j].atomtype     = oldfinalGeomAtom[i].atomtype
  #EtaPOTS_printgeom(POTS.finalGeomAtom)
  return POTS

### --- Move the atoms of interest back to the correct locations--- ###
def EtaPOTS_renumberUnFix(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["renumberUnFix"], POTS.verbose, POTS.joblog)
  oldfinalGeomAtom = EtaPOTS_makeGeomBackup(POTS)
  #EtaPOTS_printgeom(oldfinalGeomAtom)
  #Using the original location saved in oldfinalGeomAtom[i].int place the atoms
back in their correct locations
  for i in range(2, len(POTS.finalGeomAtom)):
    j = oldfinalGeomAtom[i].int
    POTS.finalGeomAtom[j].e            = oldfinalGeomAtom[i].e
    POTS.finalGeomAtom[j].en           = oldfinalGeomAtom[i].en
```

```
    POTS.finalGeomAtom[j].x           = oldfinalGeomAtom[i].x
    POTS.finalGeomAtom[j].y           = oldfinalGeomAtom[i].y
    POTS.finalGeomAtom[j].z           = oldfinalGeomAtom[i].z
    POTS.finalGeomAtom[j].int         = oldfinalGeomAtom[i].int
    POTS.finalGeomAtom[j].en          = oldfinalGeomAtom[i].en
    POTS.finalGeomAtom[j].neighbors     = oldfinalGeomAtom[i].neighbors
    POTS.finalGeomAtom[j].neighborsdist = oldfinalGeomAtom[i].neighborsdist
    POTS.finalGeomAtom[j].nearest       = oldfinalGeomAtom[i].nearest
    POTS.finalGeomAtom[j].nearestdist   = oldfinalGeomAtom[i].nearestdist
    POTS.finalGeomAtom[j].hybridization = oldfinalGeomAtom[i].hybridization
    POTS.finalGeomAtom[j].charge        = oldfinalGeomAtom[i].charge
    POTS.finalGeomAtom[j].string        = oldfinalGeomAtom[i].string
    POTS.finalGeomAtom[j].atomtype      = oldfinalGeomAtom[i].atomtype
  #EtaPOTS_printgeom(POTS.finalGeomAtom)
  return POTS

###
def EtaPOTS_generateMinTSSCANSize(POTS):
  #Set the minimum step size allowed if non was set manually
  if POTS.minTSScanVar.lower().strip() == 'loose':
    x = 100
    if POTS.scanType == "bond":
      POTS.minTSScanSize =
round(x/100.0/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGe
omAtom[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "angle":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "dihedral":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
  elif POTS.minTSScanVar.lower().strip() == 'none':
    x = 50
    if POTS.scanType == "bond":
      POTS.minTSScanSize =
round(x/100.0/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGe
```

```
omAtom[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "angle":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "dihedral":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
  elif POTS.minTSScanVar.lower().strip() == 'tight':
    x = 25
    if POTS.scanType == "bond":
      POTS.minTSScanSize =
round(x/100.0/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGe
omAtom[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "angle":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "dihedral":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
  elif POTS.minTSScanVar.lower().strip() == 'verytight':
    x = 5
    if POTS.scanType == "bond":
      POTS.minTSScanSize =
round(x/100.0/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGe
omAtom[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "angle":
```

```
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
    elif POTS.scanType == "dihedral":
      POTS.minTSScanSize =
round(x/(float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAt
om[POTS.atomList[0]+1].e))) +
float(Eta_getElementMass(Eta_getElementNum(POTS.finalGeomAtom[POTS
.atomList[0]+1].e)))), 4)
  #elif POTS.minTSScanVar.lower() == 'var':
  #  if POTS.scanType == "bond":
  #    POTS.minTSScanSize = 0.001
  #  elif POTS.scanType == "angle":
  #    POTS.minTSScanSize = 0.1
  #  elif POTS.scanType == "dihedral":
  #    POTS.minTSScanSize = 0.1
  #Safe gaurd in case the user mispelled or mistyped the minTSScanVar
keyword
  if POTS.minTSScanSize == 0.0000:
    EtaPOTS_printWrite(["You must have mispelled the #MINTSSCANSIZE
keyword",
                        "Your input was: " + POTS.minTSScanVar], POTS.verbose,
POTS.joblog)
    #                    "The options are:",
    #                    "loose = ",
    #                    "none = ",
    #                    "tight = ",
    #                    "verytight = ",
    #                    "We will now be using: superveryubertight"], POTS.verbose,
POTS.joblog)
    if POTS.scanType == "bond":
      POTS.minTSScanSize = 0.001
    elif POTS.scanType == "angle":
      POTS.minTSScanSize = 0.1
    elif POTS.scanType == "dihedral":
      POTS.minTSScanSize = 0.1
  return POTS

### --- Logic for how the step size and geometry to be used should be. --- ###
def EtaPOTS_scanTSLogic(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["scanTSLogic"], POTS.verbose, POTS.joblog)
```

```
  #energyList = []
  ###Change the step number in the scan text file
  POTS.scanStepNow += 1
  if POTS.scanStepNow >= POTS.scanLength:
    EtaPOTS_printWrite(["The scan has completed " +
str(POTS.scanStepNow) + " of " + str(POTS.scanLength) + " steps.",\
                        "The job will stop now."], POTS.verbose, POTS.joblog)
    POTS.scan = 0
    POTS.kill = True
  #Start Logic for SCAN
  elif POTS.scan == 1:
    #Check for the scan energy file and open if it exists
    if os.path.isfile(POTS.scratchdir + "/scan-" + POTS.jobname + "-
energy.txt"):
      the_file = open(POTS.scratchdir + "/scan-" + POTS.jobname + "-
energy.txt", 'a')
      the_file.write(str(float(POTS.finalenergy)) + "\n")
      the_file.close()
      if POTS.test == 1:
        the_file = open(POTS.scratchdir + "/scan-" + POTS.jobname + "-
energy.txt", 'r')
        for line in the_file:
          POTS.scanEnergy.append(float(line.strip()))
        the_file.close()
        print POTS.scanEnergy
        print float(POTS.finalenergy) - POTS.scanEnergy[-2]
      else:
        #Save the final energy to the scan energies list
        POTS.scanEnergy.append(float(POTS.finalenergy))
      #Print the energy
      EtaPOTS_printWrite(["Last Energy: " + str(POTS.scanEnergy[-2]) + "
Difference: " + str(float(POTS.finalenergy) - float(POTS.scanEnergy[-2]))],
POTS.verbose, POTS.joblog)
      ##Grab the highest energy from the list
      #if os.path.isfile(POTS.scratchdir + "/HIGHEST-" + POTS.jobname +
".xyz"):
      #  the_file = open(POTS.scratchdir + "/HIGHEST-" + POTS.jobname +
".xyz", 'r')
      #  for line in the_file:
      #    if "Energy" in line:
      #      var = line.strip().split()
      #      highestE = var[-1]
      #else:
      #  highestE = POTS.scanEnergy[-1]
```

```
    ###Start logic for TS-SCAN
    if POTS.ts >= 1:
      POTS.tsscanEnergy.append(float(POTS.finalenergy))
    if POTS.ts == 1: # and POTS.waitSize < POTS.scanStepNow:
      #Check for a previous minor TS
      for i in range(len(POTS.scanEnergy) - 2):
        if POTS.scanEnergy[i] > POTS.scanEnergy[i + 1] and
POTS.scanEnergy[i + 1] < POTS.scanEnergy[i + 2] and POTS.minorTS == 0:
          POTS.minorTS = 1
      EtaPOTS_printWrite(["Running TS-SCAN job."], POTS.verbose,
POTS.joblog)
      #if POTS.breakpoint != 0:
      #  print "YEP NEED TO FIX THIS!!"

      #Start logic for TS-SCAN
      if POTS.ts == 1 and POTS.waitSize < POTS.scanStepNow and
POTS.breakpoint == 0:
        #Did this energy equal the last one?
        if POTS.tsscanEnergy[-1] == POTS.tsscanEnergy[-2]:
          EtaPOTS_printWrite(["The energy did not change.",
                              "The job will now be terminated."], POTS.verbose,
POTS.joblog)
          kill = True
          scan = 0
        ### --- For jobs that have run 2 steps
        elif len(POTS.scanEnergy) == 2:  #Step ONE in the TS-SCAN.
          #Did we go down in energy?
          if POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2]:  #Did the first
step go the correct direction?
            EtaPOTS_printWrite(["The energy decreased and we assume we are
going the wrong way.",
                                "We will now turn around from the first geometry."],
POTS.verbose, POTS.joblog)
            #POTS = EtaPOTS_grabPreviousGeom(POTS, 1)  #Grab the first
geometry (or second back from current)
            POTS = EtaPOTS_grabHighestGeom(POTS)
            POTS.scanSize = -POTS.scanSize
          #Did we go up in energy?
          elif POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2]:
            EtaPOTS_printWrite(["The energy is increasing and we assume we
are approaching the TS geometry.",
                                "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
```

```
            EtaPOTS_writeHighGeom(POTS)
            POTS = EtaPOTS_saveHighestGeom(POTS)
          ### --- For jobs that have run 3 steps
          elif len(POTS.scanEnergy) == 3:  #Step TWO in the TS-SCAN.
            #Did we go down twice in a row?
            if POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] < POTS.tsscanEnergy[-3]:
              EtaPOTS_printWrite(["We turned around and that didn't work.",
                          "Most likely we were close but took to far of an initial
step size.",
                          "We will now turn back around and take a smaller step
size."], POTS.verbose, POTS.joblog)
              #POTS = EtaPOTS_grabPreviousGeom(POTS, 2)  #Grab the first
geom (or third one back from the current)
              POTS = EtaPOTS_grabHighestGeom(POTS)
              POTS.scanSize = -POTS.scanSize / 3
            #Did we go down after going up and we are allowing minor TSs?
            elif POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] > POTS.tsscanEnergy[-3] and (POTS.minorTS == 0
or POTS.minorTS == 2):
              EtaPOTS_printWrite(["The energy decreased from the last step.",
                          "One more step to see if we found a minor TS."],
POTS.verbose, POTS.joblog)
            #Did we go down after going up and we don't want to allow minor
TSs?
            elif POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] > POTS.tsscanEnergy[-3] and (POTS.minorTS == 1
or POTS.minorTS == 3):
              EtaPOTS_printWrite(["The energy decreased from the last step.",
                          "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
              POTS = EtaPOTS_grabHighestGeom(POTS)
              POTS.scanSize = -POTS.scanSize / 3
              del POTS.tsscanEnergy[-1]
            #Did we go up at all?
            elif POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2]:
              EtaPOTS_printWrite(["The energy is increasing and we assume we
are approaching the TS geometry.",
                          "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
              EtaPOTS_writeHighGeom(POTS)
              POTS = EtaPOTS_saveHighestGeom(POTS)
            ### WE WILL NOW OUTPUT THE GEOMETRY TO THE SCAN-
SCRATCH FOLDER BELOW
```

```
        ### --- For jobs that have run more than 3 steps
        elif len(POTS.scanEnergy) > 3:
          #Did we turn around twice and it was all down hill from the initial
geom? If so turn around and take a smaller step size
          if POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] < POTS.tsscanEnergy[-3] and POTS.tsscanEnergy[-
3] < POTS.tsscanEnergy[-4]:
            EtaPOTS_printWrite(["Wow that was a bad idea.",
                        "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
            #POTS = EtaPOTS_grabPreviousGeom(POTS, 3)
            POTS = EtaPOTS_grabHighestGeom(POTS)
            POTS.scanSize = -POTS.scanSize / 3
            del POTS.tsscanEnergy[-1]
            del POTS.tsscanEnergy[-1]
            del POTS.tsscanEnergy[-1]
          #Did we drop in energy twice in a row and were we comming from a
high energy state? Better go back to the high energy state
          elif POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] < POTS.tsscanEnergy[-3] and POTS.tsscanEnergy[-
3] > POTS.tsscanEnergy[-4]:
            EtaPOTS_printWrite(["That extra step forward to see if we found a
minor TS was a bad idea.",
                        "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
            #POTS = EtaPOTS_grabPreviousGeom(POTS, 2)
            POTS = EtaPOTS_grabHighestGeom(POTS)
            POTS.scanSize = -POTS.scanSize / 3
            del POTS.tsscanEnergy[-1]
            del POTS.tsscanEnergy[-1]
          #Did we drop in energy but it is the first time in recent history? If so
check to see if it is a minor TS (if we havent found one yet already)
          elif POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] > POTS.tsscanEnergy[-3] and (POTS.minorTS == 0
or POTS.minorTS == 2):
            EtaPOTS_printWrite(["The energy decreased from the last step.",
                        "One more step to see if we found a minor TS."],
POTS.verbose, POTS.joblog)
          #Did we drop in energy but it is the first time in recent history? If so
check to see if it is a minor TS (if we havent found one yet already)
          elif POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] > POTS.tsscanEnergy[-3] and POTS.minorTS == 3:
            EtaPOTS_printWrite(["You have specified that you wish not to check
for minor TSs.",
```

```
                    "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
          #POTS = EtaPOTS_grabPreviousGeom(POTS, 1)
          POTS = EtaPOTS_grabHighestGeom(POTS)
          POTS.scanSize = -POTS.scanSize / 3
          del POTS.tsscanEnergy[-1]
        #Did we drop in energy but it is the first time in recent history? AND
did we already find a minor TS? Better go back and try again
        elif POTS.tsscanEnergy[-1] < POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] > POTS.tsscanEnergy[-3] and POTS.minorTS == 1:
          EtaPOTS_printWrite(["The energy is decreasing and we have
already looked for a minor TS.",
                    "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
          #POTS = EtaPOTS_grabPreviousGeom(POTS, 1)
          POTS = EtaPOTS_grabHighestGeom(POTS)
          POTS.scanSize = -POTS.scanSize / 3
          del POTS.tsscanEnergy[-1]
        #Did we increase in energy after going back down twice? Must be
comming of a geometry change
        elif POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] < POTS.tsscanEnergy[-3] and POTS.tsscanEnergy[-
3] < POTS.tsscanEnergy[-4]:
          #If this is the higher that the last high then save as high otherwise
grab the highest geom
          if POTS.tsscanEnergy[-1] > POTS.highestGeomAtom[1].split()[1]:
            EtaPOTS_printWrite(["The energy is increasing and we assume we
are approaching the TS geometry.",
                    "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
            EtaPOTS_writeHighGeom(POTS)
            POTS = EtaPOTS_saveHighestGeom(POTS)
            del POTS.tsscanEnergy[-2]
            del POTS.tsscanEnergy[-2]
          else:
            EtaPOTS_printWrite(["The energy increased but it isn't the best
geometry.",
                    "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
            POTS = EtaPOTS_grabHighestGeom(POTS)
            POTS.scanSize = -POTS.scanSize / 3
            del POTS.tsscanEnergy[-1]
            del POTS.tsscanEnergy[-1]
            del POTS.tsscanEnergy[-1]
```

```
        #Did we increase in energy after going back down
        elif POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] < POTS.tsscanEnergy[-3] and POTS.tsscanEnergy[-
3] > POTS.tsscanEnergy[-4] and (POTS.minorTS == 0 or POTS.minorTS ==
2):
          EtaPOTS_printWrite(["We found a minor TS and are saving this
geometry as the highest energy.",
                              "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
          #POTS = EtaPOTS_grabPreviousGeom(POTS, 2)
          EtaPOTS_writeHighGeom(POTS)
          POTS = EtaPOTS_saveHighestGeom(POTS)
          del POTS.tsscanEnergy[-2]
        elif POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] < POTS.tsscanEnergy[-3] and POTS.tsscanEnergy[-
3] > POTS.tsscanEnergy[-4] and (POTS.minorTS == 1 or POTS.minorTS ==
3):
          if POTS.tsscanEnergy[-1] > POTS.highestGeomAtom[1].split()[1] and
((POTS.finalGeomAtom[1].split()[-1] - POTS.highestGeomAtom[1].split()[-1]) -
(2 * POTS.scanSize)) < 0.0001:
            EtaPOTS_printWrite(["The energy is increasing and we found a
better geometry.",
                                "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
            EtaPOTS_writeHighGeom(POTS)
            POTS = EtaPOTS_saveHighestGeom(POTS)
            del POTS.tsscanEnergy[-2]
          else:
            EtaPOTS_printWrite(["The energy increased but it isn't the best
geometry.",
                                "Going back to a more reasonable geometry, taking a
smaller step size, and turning around."], POTS.verbose, POTS.joblog)
            POTS = EtaPOTS_grabHighestGeom(POTS)
            POTS.scanSize = -POTS.scanSize / 3
            del POTS.tsscanEnergy[-1]
            del POTS.tsscanEnergy[-1]
        #Did we increase in energy twice in a row? Carry on.
        elif POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2] and
POTS.tsscanEnergy[-2] > POTS.tsscanEnergy[-3] and POTS.tsscanEnergy[-
3] > POTS.tsscanEnergy[-4]:
          EtaPOTS_printWrite(["The energy is increasing and we assume we
are approaching the TS geometry.",
                              "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
```

```
            EtaPOTS_writeHighGeom(POTS)
            POTS = EtaPOTS_saveHighestGeom(POTS)
          ### WE WILL NOW OUTPUT THE GEOMETRY TO THE SCAN-
SCRATCH FOLDER BELOW
          #If the step size is below the minimum but above half of the minimum
then make it the minimum and continue
          #if POTS.scanEnergy[-1] < POTS.scanEnergy[-2]:
          if (abs(POTS.scanSize) <= POTS.minTSScanSize and
abs(POTS.scanSize) > POTS.minTSScanSize/2):
            if POTS.scanSize >= 0:
              POTS.scanSize = POTS.minTSScanSize
            else:
              POTS.scanSize = -POTS.minTSScanSize
          #If the step size is below the minimum and below or equal to half of
the minimum then quit
          elif abs(POTS.scanSize) < POTS.minTSScanSize:
            EtaPOTS_printWrite(["Scan step size has dropped below the
threshold.",
                                "This scan will now be terminated."], POTS.verbose,
POTS.joblog)
            POTS.scan = 0
            POTS.kill = True
        #If the wait number is greater than the step now then wait
        elif POTS.ts == 1 and POTS.waitSize > POTS.scanStepNow:
          EtaPOTS_printWrite(["Waiting " + str(POTS.waitSize -
POTS.scanStepNow) + " steps till TS-SCAN starts."], POTS.verbose,
POTS.joblog)
        #If the wait number is equal to the step now then stop waiting next time
        elif POTS.ts == 1 and POTS.waitSize == POTS.scanStepNow:
          EtaPOTS_printWrite(["TS-SCAN will start next step."], POTS.verbose,
POTS.joblog)
      #If dynamic is on then check if the energy is increasing and if so turn of
dynamic and turn on ts
      elif POTS.ts == 2:
        EtaPOTS_printWrite(["Dynamic TS is turned on. The direction and step
size will not change till the energy increases."], POTS.verbose, POTS.joblog)
        if POTS.tsscanEnergy[-1] > POTS.tsscanEnergy[-2]:
          EtaPOTS_printWrite(["The energy is increasing and we assume we are
approaching the TS geometry.",
                              "Dynamic TS will now be turned off.",
                              "No changes to the step size will be made. Carry on."],
POTS.verbose, POTS.joblog)
          POTS.ts = 1
```

```
    #If this is step is higher in energy than the last then export it to the
HIGHEST- file
    if POTS.scanEnergy[-1] > POTS.scanEnergy[-2] and POTS.breakpoint ==
0 and POTS.ts == 0:
      highestE = POTS.scanEnergy[-1]
      if POTS.highestGeomAtom == []:
         POTS = EtaPOTS_saveHighestGeom(POTS)
      elif highestE > POTS.highestGeomAtom[1][-1]:
        EtaPOTS_printWrite(["This is the highest energy geometry as of yet."],
POTS.verbose, POTS.joblog)
        EtaPOTS_writeHighGeom(POTS)
        POTS = EtaPOTS_saveHighestGeom(POTS)
      #notHighest = 0
      #for line in POTS.scanEnergy:
      #  if highestE < line:
      #    notHighest = 1
      #if notHighest == 0:
      #  EtaPOTS_printWrite(["This is the highest energy geometry as of yet."],
POTS.verbose, POTS.joblog)
      #  EtaPOTS_writeHighGeom(POTS)
      #  EtaPOTS_saveHighestGeom(POTS)
   #If said scan energy file does not exist make one and start adding to it
   else:
    EtaPOTS_printWrite(["There is no known energy data about previous
steps.",
                        "Creating this file now."], POTS.verbose, POTS.joblog)
    the_file = open(POTS.scratchdir + "/scan-" + POTS.jobname + "-
energy.txt", 'w+')
    the_file.write(str(POTS.finalenergy) + "\n")
    the_file.close()
    #Save the final energy to the scan energies list
    POTS.scanEnergy.append(float(POTS.finalenergy))
    EtaPOTS_printWrite(["Energy :" + str(POTS.finalenergy)], POTS.verbose,
POTS.joblog)
    #Export the first optimized geometry
    POTS = EtaPOTS_saveHighestGeom(POTS)
    if POTS.ts >= 1:
      EtaPOTS_writeHighGeom(POTS)
      POTS.tsscanEnergy.append(float(POTS.finalenergy))


##################################################################
##################
   ###Change the geometry for the next step
```

```
    if POTS.debug >= 1:
      EtaPOTS_printWrite(["bondangledihedral"], POTS.verbose, POTS.joblog)
    #Move the atoms of interest around
    POTS = EtaPOTS_renumberFix(POTS)
    #Using internal convert the xyz into a z-matrix
    POTS = EtaPOTS_getzmat(POTS)
    if POTS.verbose == 1:
      EtaPOTS_printzmat(POTS.ZMATAtom)
    if POTS.scanType == "bond":
      #Grap the bond length now
      bondnow = POTS.ZMATAtom[1].dist # zmatlol[1][2]
      EtaPOTS_printWrite(["Bond length was: " + str(bondnow) + ", it will be
changed by " + str(POTS.scanSize)], POTS.verbose, POTS.joblog)
      #Change the bond length acording to the .tc file then replace the old bond
length for this new one
      bondmath = bondnow + POTS.scanSize
      EtaPOTS_printWrite(["Bond length now is: " + str(bondmath)],
POTS.verbose, POTS.joblog)
      POTS.ZMATAtom[1].dist = bondmath # zmatlol[1][2]
      if bondmath < 0.5:
        POTS.scan = 0
        EtaPOTS_printWrite(["The bond of interest crossed 0.5 angstroms.",\
                    "This is unreasonable and the job will be stopped.",\
                    "Are you doing nuclear chemistry?"], POTS.verbose,
POTS.joblog)
    elif POTS.scanType == "angle":
      #Grap the bond length now
      anglenow = POTS.ZMATAtom[2].angle # zmatlol[2][4]
      EtaPOTS_printWrite(["Angle was: " + str(anglenow) + ", it will be changed
by " + str(POTS.scanSize)], POTS.verbose, POTS.joblog)
      #Change the bond length acording to the .tc file then replace the old bond
length for this new one
      anglemath = anglenow + POTS.scanSize
      EtaPOTS_printWrite(["Angle now is: " + str(anglemath)], POTS.verbose,
POTS.joblog)
      POTS.ZMATAtom[2].angle = anglemath # zmatlol[2][4]
      #If the new angle will exceed 180 degrees then the scan size will be
reversed for the next step.
      if anglenow <= 180 and anglemath >= 180: # or (anglenow >= -180 and
anglemath <= -180):
        POTS.scanSize = -POTS.scanSize
        EtaPOTS_printWrite(["The angle of interest crossed 180 degrees and
the scan step size has been reversed.",\
                    "This will allow for the accurate continuation of this scan.",\
```

```
                    "Original step size:\t" + str(-POTS.scanSize),\
                    "New step size:\t" + str(POTS.scanSize)], POTS.verbose,
POTS.joblog)
    #If the new angle will exceed 0 degrees then the scan size will be
reversed for the next step.
    if anglenow >= 0 and anglemath <= 0:
      POTS.scanSize = -POTS.scanSize
      EtaPOTS_printWrite(["The angle of interest crossed 0 degrees and the
scan step size has been reversed.",\
                    "This will allow for the accurate continuation of this scan.",\
                    "Original step size:\t" + str(-POTS.scanSize),\
                    "New step size:\t" + str(POTS.scanSize)], POTS.verbose,
POTS.joblog)
  elif POTS.scanType == "dihedral":
    #Grap the bond length now
    dihedralnow = POTS.ZMATAtom[3].dihedral # zmatlol[3][6]
    EtaPOTS_printWrite(["Dihedral was: " + str(dihedralnow) + ", it will be
changed by " + str(POTS.scanSize)], POTS.verbose, POTS.joblog)
    #Change the bond length acording to the .tc file then replace the old bond
length for this new one
    dihedralmath = dihedralnow + POTS.scanSize
    EtaPOTS_printWrite(["Dihedral now is: " + str(dihedralmath)],
POTS.verbose, POTS.joblog)
    POTS.ZMATAtom[3].dihedral = dihedralmath # zmatlol[3][6]
  if POTS.verbose == 1:
    EtaPOTS_printzmat(POTS.ZMATAtom)
  #Convert the augmented z-matrix to a xyz
  POTS = EtaPOTS_getXYZfromZMAT(POTS)
  #Move the atoms back to their original locations
  POTS = EtaPOTS_renumberUnFix(POTS)
  #if POTS.debug >= 2:
  #    outputFixUnfixGeom(unfixgeom)

  #Open the scanfile and read it into a list
  the_file = open(POTS.scanfile, 'r')
  scanFileList = the_file.readlines()
  the_file.close()
  #Make sure that the variable names and values are separated correctly
  for i, line in enumerate(scanFileList):
    if "=" in line:
      line2 = line.replace("=","  = ")
      scanFileList[i] = line2
  #Open the scanfile for writing it back in with changes
  f = open(POTS.scanfile, 'w+')
```

```
    for line in scanFileList:
      if line.rstrip().split()[0] == "#SCAN" and POTS.scan == 0:
        f.write("#SCAN = NO - DONE\n")
      elif line.rstrip().split()[0] == "#TS" and POTS.ts == 0:
        f.write("#TS = NO\n")
      elif line.rstrip().split()[0] == "#SCANLENGTH" and POTS.scan == 0:
        f.write("#SCANLENGTH = 0\n")
      elif line.rstrip().split()[0] == "#STEPSIZE":
        f.write("#STEPSIZE = " + str(POTS.scanSize) + "\n")
      elif line.rstrip().split()[0] == "#SCANSTEPNOW":
        f.write("#SCANSTEPNOW = " + str(POTS.scanStepNow) + "\n")
      else:
        f.write(line.replace("  =  ", " = "))
    EtaPOTS_printWrite(["Steps:\t\t" + str(POTS.scanLength),
                        "Step number:\t" + str(POTS.scanStepNow),
                        "Wait number:\t" + str(POTS.waitSize),
                        "Step size:\t" + str(POTS.scanSize)], POTS.verbose,
POTS.joblog)
    if POTS.ts >= 1:
      EtaPOTS_printWrite(["Minimum step size:\t+/- " +
str(POTS.minTSScanSize)], POTS.verbose, POTS.joblog)
    if POTS.scan == 0:
      POTS.kill = True
  return POTS


###Depreciated function. This is now a part of scanTSLogic
### --- Changes the geometries by converting them to zmatrix making
changes to the file them converting them back to xyz --- ###
def EtaPOTS_bondangledihedral(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["bondangledihedral"], POTS.verbose, POTS.joblog)
  #Move the atoms of interest around
  POTS = EtaPOTS_renumberFix(POTS)
  #Using internal convert the xyz into a z-matrix
  POTS = EtaPOTS_getzmat(POTS)
  if POTS.verbose == 1:
    EtaPOTS_printzmat(POTS.ZMATAtom)
  if POTS.scanType == "bond":
    #Grap the bond length now
    bondnow = POTS.ZMATAtom[1].dist # zmatlol[1][2]
    EtaPOTS_printWrite(["Bond length was: " + str(bondnow), "It will be
changed by " + str(POTS.scanSize)], POTS.verbose, POTS.joblog)
```

```
    #Change the bond length acording to the .tc file then replace the old bond
length for this new one
    bondmath = bondnow + POTS.scanSize
    EtaPOTS_printWrite(["Bond length now is: " + str(bondmath)],
POTS.verbose, POTS.joblog)
    POTS.ZMATAtom[1].dist = bondmath # zmatlol[1][2]
    if bondmath < 0:
      POTS.scan = 0
      EtaPOTS_printWrite(["The bond of interest crossed 0 angstroms.",\
                    "This is unreasonable and the job will be stopped."],
POTS.verbose, POTS.joblog)
  elif POTS.scanType == "angle":
    #Grap the bond length now
    anglenow = POTS.ZMATAtom[2].angle # zmatlol[2][4]
    EtaPOTS_printWrite(["Angle was: " + str(anglenow), "It will be changed by "
+ str(POTS.scanSize)], POTS.verbose, POTS.joblog)
    #Change the bond length acording to the .tc file then replace the old bond
length for this new one
    anglemath = anglenow + POTS.scanSize
    EtaPOTS_printWrite(["Angle now is: " + str(anglemath)], POTS.verbose,
POTS.joblog)
    POTS.ZMATAtom[2].angle = anglemath # zmatlol[2][4]
    #If the new angle will exceed 180 degrees then the scan size will be
reversed for the next step.
    if anglenow <= 180 and anglemath >= 180: # or (anglenow >= -180 and
anglemath <= -180):
      POTS.scanSize = -POTS.scanSize
      EtaPOTS_printWrite(["The angle of interest crossed 180 degrees and the
scan step size has been reversed.",\
                    "This will allow for the accurate continuation of this scan."],
POTS.verbose, POTS.joblog)
    #If the new angle will exceed 0 degrees then the scan size will be reversed
for the next step.
    if anglenow >= 0 and anglemath <= 0:
      POTS.scanSize = -POTS.scanSize
      EtaPOTS_printWrite(["The angle of interest crossed 0 degrees and the
scan step size has been reversed.",\
                    "This will allow for the accurate continuation of this scan."],
POTS.verbose, POTS.joblog)
  elif POTS.scanType == "dihedral":
    #Grap the bond length now
    dihedralnow = POTS.ZMATAtom[3].dihedral # zmatlol[3][6]
    EtaPOTS_printWrite(["Dihedral was: " + str(dihedralnow), "It will be
changed by " + str(POTS.scanSize)], POTS.verbose, POTS.joblog)
```

```
    #Change the bond length acording to the .tc file then replace the old bond
length for this new one
    dihedralmath = dihedralnow + POTS.scanSize
    EtaPOTS_printWrite(["Dihedral now is: " + str(dihedralmath)],
POTS.verbose, POTS.joblog)
    POTS.ZMATAtom[3].dihedral = dihedralmath # zmatlol[3][6]
  if POTS.verbose == 1:
    EtaPOTS_printzmat(POTS.ZMATAtom)
  #Using internal convert the z-matrix to a xyz
  POTS = EtaPOTS_getXYZfromZMAT(POTS)
  #Move the atoms back to their original locations
  POTS = EtaPOTS_renumberUnFix(POTS)
  #if POTS.debug >= 2:
  #       outputFixUnfixGeom(unfixgeom)
  return POTS

### --- Convert coordinates to distance/angle/dihedral --- ###
def EtaPOTS_getzmat(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["getzmat"], POTS.verbose, POTS.joblog)
  #Make the ZMATAtom only as long as the atoms in the finalGeomAtom list
  POTS.ZMATAtom = [0] * (len(POTS.finalGeomAtom) - 2)
  #Iterate only throught the atoms and not the first two lines
  for i in range(2, len(POTS.finalGeomAtom)):
    #Make each ZMATAtom entry the class ZMAT_Atom and give it the
elemental information
    POTS.ZMATAtom[i-2] = ZMAT_Atom()
    POTS.ZMATAtom[i-2].e = POTS.finalGeomAtom[i].e
    #If it is after the first atom give it the distance from the last atom
    if i > 2:
      POTS.ZMATAtom[i-2].atomdist = i - 3
      POTS.ZMATAtom[i-2].dist = Eta_getdistance(i-1, i, POTS.finalGeomAtom)
    #If it is at least the third atom give it the angle from the last two atoms
    if i > 3:
      POTS.ZMATAtom[i-2].atomangle = i - 4
      POTS.ZMATAtom[i-2].angle = Eta_getangle(i-2, i-1, i,
POTS.finalGeomAtom)
    #If it is at least the fourth atom give it the dihedral from the last three atoms
    if i > 4:
      POTS.ZMATAtom[i-2].atomdihedral = i - 5
      POTS.ZMATAtom[i-2].dihedral = Eta_getdihedral(i-3, i-2, i-1, i,
POTS.finalGeomAtom)
  return POTS
```

```
### --- Get the XYZ coordinates from distance, angle and dihedral data ---
###
def EtaPOTS_getXYZfromZMAT(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["getXYZfromZMAT"], POTS.verbose, POTS.joblog)
  line = []
  x = 0
  y = 0
  z = 0
  xyzgeom = []
  for i in range(len(POTS.ZMATAtom)):
    ### Set up the variables to be used for the function
    #at4 = i
    if i > 0:
      dist = float(POTS.ZMATAtom[i].dist)
      at3 = int(POTS.ZMATAtom[i].atomdist)
    if i > 1:
      angle = float(POTS.ZMATAtom[i].angle)
      angleRad = radians(angle) # * math.pi / 180
      at2 = int(POTS.ZMATAtom[i].atomangle)
    if i > 2:
      dihedral = float(POTS.ZMATAtom[i].dihedral)
      dihedralRad = radians(dihedral) # * math.pi / 180
      at1 = int(POTS.ZMATAtom[i].atomdihedral)

    ### Start to place the atoms in their locations
    #First atom get put at the origin
    if i == 0:
      x = 0.00000
      y = 0.00000
      z = 0.00000
    #Second atom gets put on the x axis
    elif i == 1:
      x = dist
      y = 0.00000
      z = 0.00000
    #Third atom is put on the xz plane with some trig
    elif i == 2:
      a = xyzgeom[at3][1]
      b = dist
      x = a + (dist * cos(math.pi - angleRad))
      y = 0.00000
      z = -dist * sin(math.pi - angleRad)
```

```
   #Fourth and later atoms are placed by using vector math, of which I
understand only slightly
   elif i >= 3:
      ####The at4 x,y,z coordinates from spherical coord
      Sx = dist * sin(angleRad) * cos(dihedralRad)
      Sy = -dist * sin(angleRad) * sin(dihedralRad) #For some reason I need to
have a negative here to get the correct sign in the output..... weird
      Sz = dist * cos(angleRad)
      at4L = [Sx, Sy, Sz]
      ###Finding the angle theta
      #Make the list of lists for the three point (z-axis, origin, and translated
atom 2) needed for an angle calculation
      Z32 = [[0, 0, 0, 1],  [0, 0, 0, 0],  [0, xyzgeom[at2][1] - xyzgeom[at3][1],
xyzgeom[at2][2] - xyzgeom[at3][2], xyzgeom[at2][3] - xyzgeom[at3][3]]]
      #Get theta using the getangle function
      theta = radians(Eta_getangle(0, 1, 2, Z32))
      ###Rodrigues' rotation formula
      #Create the vectprs needed to calculate k
      vector3 = array([xyzgeom[at3][1], xyzgeom[at3][2], xyzgeom[at3][3]])
      vector2 = array([xyzgeom[at2][1], xyzgeom[at2][2], xyzgeom[at2][3]])
      vector0 = array([0, 0, 1])
      #Calculate k for the Rodrigues rotation formula
      k = cross((vector2-vector3), vector0)/linalg.norm(cross((vector2-vector3),
vector0))
      #Generate an array for translated 1
      T1 = [(xyzgeom[at1][1]-xyzgeom[at3][1]), (xyzgeom[at1][2]-
xyzgeom[at3][2]), (xyzgeom[at1][3]-xyzgeom[at3][3])]
      #Calculate the Rodrigues rotation matrix
      RR23T1 = dot(T1, cos(theta)) + dot(cross(k,T1), sin(theta)) +
dot(dot(k,(dot(k,T1))), (1-cos(theta)))
      #Make the list of lists for the four points (x-axis, z-axis, origin, and rotated
translated 1) needed for a dihedral calculation
      XZ31 = [[0, 1, 0, 0], [0, 0, 0, 1], [0, 0, 0, 0], [0, RR23T1[0], RR23T1[1],
RR23T1[2]]]
      #Get phi using the getdihedral function
      phi = radians(Eta_getdihedral(0,1,2,3,XZ31))
      ###Rotation matrix
      #Create the array for the rotation matrix including dihedral phi
      RM = array([[cos(phi), sin(phi), 0], [-sin(phi), cos(phi), 0], [0, 0, 1]])
      #Calculate the dot product of the rotation matrix and the coordinates for 4
(from spherical)
      RM4 = dot(RM, at4L)
      #Calculate the rotated coordinates of the rotated coordinates of atom 4
```

```
      RRN23RM4 = dot(RM4, cos(-theta)) + dot(cross(k,RM4), sin(-theta)) +
dot(dot(k,(dot(k,RM4))), (1-cos(-theta)))
      #Final coordinates that are rotated, rotated and translated
      x = RRN23RM4[0] + xyzgeom[at3][1]
      y = RRN23RM4[1] + xyzgeom[at3][2]
      z = RRN23RM4[2] + xyzgeom[at3][3]
    #Putting everything into a list to send back
    line.append(POTS.ZMATAtom[i].e)
    line.append(x)
    line.append(y)
    line.append(z)
    xyzgeom.append(list(line))
    line[:] = []
  #Add the first two lines to the newgeom lol
  for i in range(len(xyzgeom)):
    #EtaPOTS_printWrite([xyzgeom[i]], POTS.verbose, POTS.joblog)
    POTS.finalGeomAtom[i+2].e = str(xyzgeom[i][0])
    POTS.finalGeomAtom[i+2].x = float(xyzgeom[i][1])
    POTS.finalGeomAtom[i+2].y = float(xyzgeom[i][2])
    POTS.finalGeomAtom[i+2].z = float(xyzgeom[i][3])
  return POTS


### --- Function to easily print out a geom using the atom class for debuging -
-- ###
def EtaPOTS_printgeom(geom):
  for i in range(len(geom)):
    if isinstance(geom[i], Atom):
      line = geom[i].e + "  " + str("{:.6f}".format(geom[i].x)) + \
            "  " + str("{:.6f}".format(geom[i].y)) + "  " + str("{:.6f}".format(geom[i].z))
    #else print the string (number of atoms or comment line)
    else:
      line = str(geom[i])
    EtaPOTS_printWrite([line], POTS.verbose, POTS.joblog)
  return

### --- Function to easily print out a geom using the atom class for debuging -
-- ###
def EtaPOTS_printzmat(zmat):
  for i in range(len(zmat)):
    if isinstance(zmat[i], ZMAT_Atom):
      line = zmat[i].e + "  " + str(zmat[i].atomdist) + "  " +
str("{:.6f}".format(zmat[i].dist)) + \
```

```
          "  " + str(zmat[i].atomangle) + "  " + str("{:.6f}".format(zmat[i].angle)) +
\
          "  " + str(zmat[i].atomdihedral) + "  " +
str("{:.6f}".format(zmat[i].dihedral))
    #else print the string (number of atoms or comment line)
    else:
      line = str(geom[i])
    EtaPOTS_printWrite([line], POTS.verbose, POTS.joblog)
  return

### --- G0X FUNCTIONS --- ###
##############################################################
##########################################################
### --- Parses the input G0X file --- ###
def EtaPOTS_parseInputG0X(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["parseInputG0X"], POTS.verbose, POTS.joblog)
  POTS.QMconfig = []
  POTS.QMcomment = ""
  POTS.charge = 0
  POTS.multi = 1
  POTS.initialGeomAtom = []
  initialgeom = []
  POTS.QMendlines = []
  inputNumAtoms = 0
  emptyline = 0
  endline = "no"
  the_file = open(POTS.baseinput, 'r')
  for line in the_file:
    if line.strip() == "" and endline == "no":
      emptyline += 1
    if line.strip() != '' and emptyline == 0:
      POTS.QMconfig.append(line.strip())
    if line.strip() != '' and emptyline == 1:
      POTS.QMcomment = line.strip()
    if line.strip() != '' and emptyline == 3:
      initialgeom.append(line.strip())
      inputNumAtoms += 1
    if line.strip() != '' and emptyline == 2:
      POTS.charge = int(line.split()[0])
      POTS.multi = int(line.split()[1])
      emptyline += 1
    if line.strip() != '' and emptyline == 4:
      endline = "yes"
```

```
      emptyline += 1
    if emptyline >= 5:
      POTS.QMendlines.append(line.strip())
  POTS.numAtoms = inputNumAtoms
  POTS.initialGeomAtom = [0] * (POTS.numAtoms + 2)
  POTS.initialGeomAtom[0] = inputNumAtoms
  POTS.initialGeomAtom[1] = POTS.QMcomment
  for i, var in enumerate(initialgeom):
    line = var.split()
    POTS.initialGeomAtom[i+2] = Atom()
    POTS.initialGeomAtom[i+2].e = line[0]
    POTS.initialGeomAtom[i+2].en = Eta_getElementNum(line[0])
    POTS.initialGeomAtom[i+2].x = float(line[1])
    POTS.initialGeomAtom[i+2].y = float(line[2])
    POTS.initialGeomAtom[i+2].z = float(line[3])
  #TODO make sure no other "opt"s get caught in this...
  #Set the maxcycles for opt to 25 if larger than 100
  rewrite = False
  for i, line in enumerate(POTS.QMconfig):
    sub = line.split()
    for subline in sub:
      if "opt=(" in subline and "maxcycle" in subline:
        subsubline = subline.split(",")
        for var in subsubline:
          if "maxcycle=" in var:
            POTS.maxopt = int(var.split('=')[-1].replace(')',''))
            if POTS.maxopt > 100:
              EtaPOTS_printWrite(["The max number of optimization cycles was
too low.",\
                                  "It has now been set to 25."], POTS.verbose,
POTS.joblog)
              POTS.QMconfig[i] = line.replace("maxcycle=" + str(POTS.maxopt),
"maxcycle=25")
              rewrite = True
      elif "opt=(" in subline and "maxcycle" not in subline:
            POTS.QMconfig[i] = line.replace("opt=(", "opt=(maxcycle=25,")
            rewrite = True
      elif "opt" in subline:
            POTS.QMconfig[i] = line.replace("opt", "opt=(maxcycle=25) ")
            rewrite = True
  if rewrite == True:
    POTS.maxopt = 25
    POTS.finalGeomAtom = [0] * len(POTS.initialGeomAtom)
    for i in range(len(POTS.initialGeomAtom)):
```

```
    if i <= 1:
      POTS.finalGeomAtom[i] = POTS.initialGeomAtom[i]
    elif i >= 2:
      POTS.finalGeomAtom[i] = Atom()
      POTS.finalGeomAtom[i].e           = POTS.initialGeomAtom[i].e
      POTS.finalGeomAtom[i].en          = POTS.initialGeomAtom[i].en
      POTS.finalGeomAtom[i].x           = POTS.initialGeomAtom[i].x
      POTS.finalGeomAtom[i].y           = POTS.initialGeomAtom[i].y
      POTS.finalGeomAtom[i].z           = POTS.initialGeomAtom[i].z
  EtaPOTS_rebuildG0XCOM(POTS)
  POTS.finalGeomAtom = []
 return POTS

### --- Parses the geometry and energy created by G0X and gives back the
trajectory in a list of lists --- ###
def EtaPOTS_parseOutputG0X(POTS):
 if POTS.debug >= 1:
  EtaPOTS_printWrite(["parseOutputG0X"], POTS.verbose, POTS.joblog)
 a_list = []
 f_list = []
 geom = 0
 force = 0
 numAtoms = 0
 POTS.allEnergy = []
 POTS.trajectoryGeomAtom = []
 the_file = open(POTS.baselog, 'r')
 for idx, line in enumerate(the_file):
  if line.strip() != '':
    if line.split()[0] == 'SCF':
      POTS.allEnergy.append(float(line.split()[4]))
    if line.split()[0] == "Maximum" and line.split()[1] == "Displacement":
      POTS.finalDisp = float(line.split()[2])
    if line.split()[0] == 'NAtoms=':
      POTS.numAtoms = int(line.split()[1])
    if "---------------------------------------------" in line and geom >= 6:
      geom = 0
    if geom >= 1:
      geom += 1
    if line.strip() == "Standard orientation:":
      geom = 1
    if geom >= 5:
      a_list.append(line)
    #Get forces
    if "---------------------------------------------" in line and force >= 5:
```

```
      force = 0
    if force >= 1:
      force += 1
    if "Forces (Hartrees/Bohr)" in line:
      force = 1
    if force >= 4:
      f_list.append(line)
    #Get charge and multiplicity
    elif 'Multiplicity' in line:
      chargeMulti = line.split()
      POTS.charge = chargeMulti[2]
      POTS.multi = chargeMulti[-1]
  the_file.close()
  #Get the final energy from the energy list
  POTS.finalenergy = float(POTS.allEnergy[-1])
  a_listDd = [x for x in a_list if "----------------------------------------------------" not in
x]

##################################################################
########
  #Create the trajectory
  POTS.trajectoryGeomAtom = [0] * (len(a_listDd)/POTS.numAtoms *
(POTS.numAtoms + 2))
  skip = 0
  for i in range(len(a_listDd)):
    if i % POTS.numAtoms == 0 and i/POTS.numAtoms !=
len(POTS.allEnergy):
      POTS.trajectoryGeomAtom[i+skip] = int(POTS.numAtoms)
      POTS.trajectoryGeomAtom[i+skip+1] = "Energy: " +
str(POTS.allEnergy[i/POTS.numAtoms])
      skip = skip + 2
    elif i % POTS.numAtoms == 0 and i/POTS.numAtoms >=
len(POTS.allEnergy):
      POTS.trajectoryGeomAtom[i+skip] = int(POTS.numAtoms)
      POTS.trajectoryGeomAtom[i+skip+1] = "Energy: " + str(POTS.allEnergy[-
1])
      skip = skip + 2
    line = a_listDd[i].split()
    POTS.trajectoryGeomAtom[i+skip] = Atom()
    POTS.trajectoryGeomAtom[i+skip].e = Eta_getElementName(int(line[1]))
    POTS.trajectoryGeomAtom[i+skip].en = int(line[0])
    POTS.trajectoryGeomAtom[i+skip].x = float(line[3])
    POTS.trajectoryGeomAtom[i+skip].y = float(line[4])
    POTS.trajectoryGeomAtom[i+skip].z = float(line[5])
```

```
#############################################################
########
  #Extract the final geometry from the trajectory
  POTS.finalGeomAtom = [0] * (POTS.trajectoryGeomAtom[0] + 2)
  for i in range(len(POTS.finalGeomAtom)):
    j = len(POTS.trajectoryGeomAtom) - len(POTS.finalGeomAtom) + i
    if i <= 1:
      POTS.finalGeomAtom[i] = POTS.trajectoryGeomAtom[j]
    elif i >= 2:
      POTS.finalGeomAtom[i] = Atom()
      POTS.finalGeomAtom[i].e = POTS.trajectoryGeomAtom[j].e
      POTS.finalGeomAtom[i].en = POTS.trajectoryGeomAtom[j].en
      POTS.finalGeomAtom[i].x = POTS.trajectoryGeomAtom[j].x
      POTS.finalGeomAtom[i].y = POTS.trajectoryGeomAtom[j].y
      POTS.finalGeomAtom[i].z = POTS.trajectoryGeomAtom[j].z

#############################################################
########
  #Extract the final forces
  POTS.allForce = [0] * (POTS.numAtoms)
  for i in range(len(POTS.allForce)):
    j = len(f_list) - len(POTS.allForce) + i
    line = f_list[j].strip().split()
    POTS.allForce[i] = line[2] + "  " + line[3] + "  " + line[4]
  return POTS

### --- G0X Optimization Logic --- ###
def EtaPOTS_OPTLogicG0X(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["OPTLogicG0X"], POTS.verbose, POTS.joblog)
  #EtaPOTS_printWrite(["BEGIN OPT LOGIC!"
  ### --- Logic for how the step size and geometry to be used should be. ---
###
  # Check to see if smaller step sizes are needed.
  EtaPOTS_printWrite(["Checking for jitter in the energies."], POTS.verbose,
POTS.joblog)
  jitter = 0
  f = open(POTS.scratchdir + "/optenergies-" + POTS.jobname + ".txt", "a")
  for i, line in enumerate(POTS.allEnergy):
    f.write(str(line) + "\n")
    if i > len(POTS.allEnergy) / 2:
      if (POTS.allEnergy[i] < POTS.allEnergy[i - 1] and POTS.allEnergy[i - 1] >
POTS.allEnergy[i - 2]) or (
```

```
        POTS.allEnergy[i] > POTS.allEnergy[i - 1] and POTS.allEnergy[i - 1] <
POTS.allEnergy[i - 2]):
       jitter += 1
  if jitter > len(POTS.allEnergy) / 4:
    EtaPOTS_printWrite(["Jitters in last half of OPT: " + str(jitter)],
POTS.verbose, POTS.joblog)
    #+ " > " + str(len(allEnergy)/4) + "\n")
    EtaPOTS_printWrite(["Due to the jitter in energies from the last OPT
iteration,",
                        "the step size of the optimization algorithm will be shortened."],
POTS.verbose, POTS.joblog)
    POTS.shortenStepSize = 1

  #Check to see if the job ran too long.
  f = open(POTS.scratchdir + "/optenergies-" + POTS.jobname + ".txt", "r")
  fileEnergyList = f.readlines()
  if len(fileEnergyList) > POTS.stepNumber:
    POTS.kill = True
    EtaPOTS_printWrite(["This job will end due to: exhausted all optimization
steps."], POTS.verbose, POTS.joblog)
  f.close()

  #Check to see if the job finished optimization.
  count = 0
  f = open(POTS.baselog, "r")
  for line in reversed(open(POTS.baselog).readlines()):
    if "Normal termination" in line or "Optimization completed" in line:
      if POTS.jobtype == 'SCAN' or POTS.jobtype == 'TS-SCAN':
        POTS.optimized = True
        EtaPOTS_printWrite(["This job will continue due to: 'Normal termination'
and/or 'Optimization Complete'."], POTS.verbose, POTS.joblog)
      else:
        POTS.kill = True
        EtaPOTS_printWrite(["This job will end due to: 'Normal termination'
and/or 'Optimization Complete'."], POTS.verbose, POTS.joblog)
      break
    count += 1
    if count > 1000:
      break

  #Check if a 'break' has occured
  breakLogic = 0
  line = POTS.QMcomment.split()
  for var in line:
```

```
    if POTS.breaktype == "bond" and breakLogic == 4:
      POTS.breakpoint = float(var)
      breakLogic = 0
    elif POTS.breaktype == "angle" and breakLogic == 5:
      POTS.breakpoint = float(var)
      breakLogic = 0
    elif POTS.breaktype == "dihedral" and breakLogic == 6:
      POTS.breakpoint = float(var)
      breakLogic = 0
    elif breakLogic >= 2:
      POTS.breakatoms.append(int(var))
      breakLogic += 1
    elif breakLogic == 1:
      POTS.breaktype = var
      breakLogic += 1
    if var == "Break:":
      breakLogic = 1
  if POTS.breaktype != "":
    EtaPOTS_printWrite(["Break point logic implemented.",
                        "Checking if " + str(POTS.breaktype) + " " +
str(POTS.breakatoms) + " are within " + str(POTS.breakpoint) + "."],
POTS.verbose, POTS.joblog)

  #Break point logic implementation
  if POTS.breaktype == "bond":
    if POTS.breakpoint < Eta_getdistance(POTS.breakatoms[0] - 1,
POTS.breakatoms[1] - 1, POTS.finalGeomAtom):
      POTS.kill = True
      EtaPOTS_printWrite(["This job will end due to: a break point failure."],
POTS.verbose, POTS.joblog)
  elif POTS.breaktype == "angle":
    if POTS.breakpoint < Eta_getangle(POTS.breakatoms[0] - 1,
POTS.breakatoms[1] - 1, POTS.breakatoms[2] - 1, POTS.finalGeomAtom):
      POTS.kill = True
      EtaPOTS_printWrite(["This job will end due to: a break point failure."],
POTS.verbose, POTS.joblog)
  elif POTS.breaktype == "dihedral":
    if POTS.breakpoint < Eta_getdihedral(POTS.breakatoms[0] - 1,
POTS.breakatoms[1] - 1, POTS.breakatoms[2] - 1, POTS.breakatoms[3] - 1,
                          POTS.finalGeomAtom):
      POTS.kill = True
      EtaPOTS_printWrite(["This job will end due to: a break point failure."],
POTS.verbose, POTS.joblog)
```

```
  #Stepsize logic implementation
  iop = 0
  newsub = 0
  if POTS.shortenStepSize == 1 and POTS.kill == False and POTS.optimized
== False:
    for i, line in enumerate(POTS.QMconfig):
      if "iop(1/8=" in line:
        var = line.split()
        iop = 1
        for sub in var:
          if "iop(1/8=" in sub:
            EtaPOTS_printWrite(["Your step size was: " + str(sub)],
POTS.verbose, POTS.joblog)
            newsub = "iop(1/8=" + str(int(round(float(sub.split("=")[1].split(")")[0]) *
.75))) + ")"
            EtaPOTS_printWrite(["It will now be: " + str(newsub)], POTS.verbose,
POTS.joblog)
            POTS.QMconfig[i] = line.replace(sub, newsub)
    if iop == 0:
      for i, line in enumerate(POTS.QMconfig):
        if "opt=(" in line:
          EtaPOTS_printWrite(["We are now implementing a smaller step size of
iop(1/8=18)"], POTS.verbose, POTS.joblog)
          POTS.QMconfig[i] = line + " iop(1/8=18)"

  #Implement speedups for G09/G03
  if POTS.kill == False and POTS.optimized == False:
    for i, line in enumerate(POTS.QMconfig):
      if "opt=(" in line and "guess=read" not in line:
        EtaPOTS_printWrite(["We are now implementing guess=read for the
next iteration."], POTS.verbose, POTS.joblog)
        POTS.QMconfig[i] = line + " guess=read"
    for i, line in enumerate(POTS.QMconfig):
      if "opt=(" in line and "readfc" not in line:
        EtaPOTS_printWrite(["We are now implementing readfc for the next
iteration."], POTS.verbose, POTS.joblog)
        var = line.split()
        for sub in var:
          if "opt=(" in sub:
            newsub = sub[:-1] + ",readfc)"
            POTS.QMconfig[i] = line.replace(sub, newsub)

  #Kill logic implementation
  #if POTS.kill == True:
```

```
  #  POTS.QMcomment = "!KILL! " + POTS.QMcomment
  return POTS


### --- Output the G09 com file for subsequent computation --- ###
def EtaPOTS_rebuildG0XCOM(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["rebuildG0XCOM"], POTS.verbose, POTS.joblog)
  #Output the new geometry in G09 input format
  datetime = (time.strftime("%Y.%m.%d-%H:%M:%S"))
  #Backup .com file
  if os.path.exists(POTS.baseinput):
    if os.path.isfile(POTS.baseinput):
      shutil.copyfile(POTS.baseinput, POTS.scratchdir + "/Previous_Files/" +
datetime + "-" + POTS.jobname + ".com")
  #Backup .chk file
  if os.path.exists(POTS.jobname + ".chk"):
    if os.path.isfile(POTS.jobname + ".chk"):
      shutil.copyfile(POTS.jobname + ".chk",
                      POTS.scratchdir + "/Previous_Files/" + datetime + "-" +
POTS.jobname + ".chk")
  #Backup .log file
  if os.path.exists(POTS.baselog):
    if os.path.isfile(POTS.baselog):
      shutil.copyfile(POTS.baselog, POTS.scratchdir + "/Previous_Files/" +
datetime + "-" + POTS.jobname + ".log")
  f = open(POTS.baseinput, "w+")
  #for line in beginText:
  for line in POTS.QMconfig:
    f.write(line + "\n")
  f.write("\n")
  f.write(POTS.QMcomment + "\n")
  f.write("\n")
  f.write(str(POTS.charge) + "  " + str(POTS.multi) + "\n")
  for i in range(len(POTS.finalGeomAtom)):
    if i >= 2:
      f.write(POTS.finalGeomAtom[i].e + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].x)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].y)) + "  " +
str("{:.6f}".format(POTS.finalGeomAtom[i].z)) + "\n")
  #for line in endText:
  f.write("\n")
  for line in POTS.QMendlines:
    f.write(line + "\n")
```

```
  f.close
  return



### --- JAGUAR FUNCTIONS --- ###
#################################################################
#################################################################
### --- Parses the input G0X file --- ###
def EtaPOTS_parseInputJaguar(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["parseInputJaguar"], POTS.verbose, POTS.joblog)
  POTS.QMconfig = []
  POTS.QMcomment = ""
  POTS.charge = 0
  POTS.multi = 1
  POTS.initialGeomAtom = []
  POTS.numAtoms = 0
  initialgeom = []
  POTS.QMendlines = []
  xyzline = 0
  the_file = open(POTS.baseinput, 'r')
  for line in the_file:
    if xyzline == 0 and "&zmat" in line:
      xyzline = 1
    elif xyzline == 0:
      POTS.QMconfig.append(line)
    elif xyzline == 1 and "&" in line:
      xyzline = 2
    elif xyzline == 1:
      initialgeom.append(line)
      POTS.numAtoms += 1
    elif xyzline == 2:
      POTS.QMendlines.append(line)
  POTS.initialGeomAtom = [0] * (POTS.numAtoms + 2)
  POTS.initialGeomAtom[0] = POTS.numAtoms
  POTS.initialGeomAtom[1] = POTS.QMcomment
  for i, var in enumerate(initialgeom):
    line = var.split()
    POTS.initialGeomAtom[i+2] = Atom()
    POTS.initialGeomAtom[i+2].e = ''.join([j for j in line[0] if not j.isdigit()])
```

```
    POTS.initialGeomAtom[i+2].en =
Eta_getElementNum(POTS.initialGeomAtom[i+2].e)
    POTS.initialGeomAtom[i+2].x = float(line[1])
    POTS.initialGeomAtom[i+2].y = float(line[2])
    POTS.initialGeomAtom[i+2].z = float(line[3])
    #Set the maxcycles for opt to 25 if larger than 100
  #for i, line in enumerate(POTS.QMconfig):
  #  sub = line.split()
  #  for subline in sub:
  #    if "opt=" in subline:
  #      subsubline = subline.split(",")
  #      for var in subsubline:
  #        if "maxcycle=" in var:
  #          POTS.maxopt = int(var.split('=')[-1].replace(')',''))
  #          if POTS.maxopt > 100:
  #            EtaPOTS_printWrite(["The max number of optimization cycles was
too low.",\
  #                               "It has now been set to 25."], POTS.verbose,
POTS.joblog)
  #            POTS.QMconfig[i] = line.replace("maxcycle=" + str(POTS.maxopt),
"maxcycle=25")
  #            POTS.finalGeomAtom = [0] * len(POTS.initialGeomAtom)
  #            POTS.maxopt = 25
  #            for i in range(len(POTS.initialGeomAtom)):
  #              if i <= 1:
  #                POTS.finalGeomAtom[i] = POTS.initialGeomAtom[i]
  #              elif i >= 2:
  #                POTS.finalGeomAtom[i] = Atom()
  #                POTS.finalGeomAtom[i].e           = POTS.initialGeomAtom[i].e
  #                POTS.finalGeomAtom[i].en          = POTS.initialGeomAtom[i].en
  #                POTS.finalGeomAtom[i].x           = POTS.initialGeomAtom[i].x
  #                POTS.finalGeomAtom[i].y           = POTS.initialGeomAtom[i].y
  #                POTS.finalGeomAtom[i].z           = POTS.initialGeomAtom[i].z
  #            EtaPOTS_rebuildG0XCOM(POTS)
  #            POTS.finalGeomAtom = []
  return POTS

### --- Parses the geometry and energy created by G0X and gives back the
trajectory in a list of lists --- ###
def EtaPOTS_parseOutputJaguar(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["parseOutputJaguar"], POTS.verbose, POTS.joblog)
  a_list = []
  f_list = []
```

```
  force = 0
  #numAtoms = 0
  collectgeom = 0
  POTS.allEnergy = []
  POTS.trajectoryGeomAtom = []
  the_file = open(POTS.baselog, 'r')
  for idx, line in enumerate(the_file):
    #Grab charge and multiplicity
    if 'net molecular charge:' in line:
      POTS.charge = line.rstrip().split()[-1]
    elif 'multiplicity' in line:
      POTS.multi = line.rstrip().split()[-1]
    elif 'SCFE:' in line:
      POTS.allEnergy.append(line.strip().split("hartrees")[0].split()[-1])
    elif 'new geometry:' in line or 'final geometry:' in line:
      collectgeom = 1
      POTS.numAtoms = 0
    elif len(line.strip()) == 0:
      collectgeom = 0
    elif collectgeom == 1 and 'angstroms' not in line and 'atom' not in line:
      a_list.append(line)
      POTS.numAtoms = POTS.numAtoms + 1
    #Get the max displacement
    elif line.split()[0] == "displacement" and line.split()[1] == "maximum:":
      POTS.finalDisp = float(line.split()[2])
    #Get forces
    if "-------------" in line and force >= 6:
      force = 0
    if force >= 1:
      force += 1
    if "forces (hartrees/bohr)" in line:
      force = 1
    if force >= 5:
      f_list.append(line)

  the_file.close()
  #Get the final energy from the energy list
  POTS.finalenergy = float(POTS.allEnergy[-1])
  a_listDd = [x for x in a_list if "----------------------------------------------------" not in
x]

##################################################################
########
  #Create the trajectory
```

```
  POTS.trajectoryGeomAtom = [0] * (len(a_listDd)/POTS.numAtoms *
(POTS.numAtoms + 2))
  skip = 0
  for i in range(len(a_listDd)):
    if i % POTS.numAtoms == 0 and i/POTS.numAtoms !=
len(POTS.allEnergy):
      POTS.trajectoryGeomAtom[i+skip] = int(POTS.numAtoms)
      POTS.trajectoryGeomAtom[i+skip+1] = "Energy: " +
str(POTS.allEnergy[i/POTS.numAtoms])
      skip = skip + 2
    elif i % POTS.numAtoms == 0 and i/POTS.numAtoms >=
len(POTS.allEnergy):
      POTS.trajectoryGeomAtom[i+skip] = int(POTS.numAtoms)
      POTS.trajectoryGeomAtom[i+skip+1] = "Energy: " + str(POTS.allEnergy[-
1])
      skip = skip + 2
    line = a_listDd[i].split()
    POTS.trajectoryGeomAtom[i+skip] = Atom()
    POTS.trajectoryGeomAtom[i+skip].e = ''.join([j for j in line[0] if not j.isdigit()])
    POTS.trajectoryGeomAtom[i+skip].en =
Eta_getElementNum(POTS.trajectoryGeomAtom[i+skip].e)
    POTS.trajectoryGeomAtom[i+skip].x = float(line[1])
    POTS.trajectoryGeomAtom[i+skip].y = float(line[2])
    POTS.trajectoryGeomAtom[i+skip].z = float(line[3])

##################################################################
########
  #Extract the final geometry from the trajectory
  POTS.finalGeomAtom = [0] * (POTS.trajectoryGeomAtom[0] + 2)
  for i in range(len(POTS.finalGeomAtom)):
    j = len(POTS.trajectoryGeomAtom) - len(POTS.finalGeomAtom) + i
    if i <= 1:
      POTS.finalGeomAtom[i] = POTS.trajectoryGeomAtom[j]
    elif i >= 2:
      POTS.finalGeomAtom[i] = Atom()
      POTS.finalGeomAtom[i].e = POTS.trajectoryGeomAtom[j].e
      POTS.finalGeomAtom[i].en = POTS.trajectoryGeomAtom[j].en
      POTS.finalGeomAtom[i].x = POTS.trajectoryGeomAtom[j].x
      POTS.finalGeomAtom[i].y = POTS.trajectoryGeomAtom[j].y
      POTS.finalGeomAtom[i].z = POTS.trajectoryGeomAtom[j].z

##################################################################
########
  #Extract the final forces
```

```
  POTS.allForce = [0] * (POTS.numAtoms)
  for i in range(len(POTS.allForce)):
    j = len(f_list) - len(POTS.allForce) + i
    line = f_list[j].strip().split()
    POTS.allForce[i] = line[2] + "  " + line[3] + "  " + line[4]
  return POTS

### --- G0X Optimization Logic --- ###
def EtaPOTS_OPTLogicJaguar(POTS):
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["OPTLogicJaguar"], POTS.verbose, POTS.joblog)
  #Check to see if the job finished optimization.
  count = 0
  f = open(POTS.baselog, "r")
  for line in reversed(open(POTS.baselog).readlines()):
    if "**           Geometry optimization complete           **" in line:
      if POTS.jobtype == 'SCAN' or POTS.jobtype == 'TS-SCAN':
        POTS.optimized = True
        EtaPOTS_printWrite(["This job will continue due to: 'Normal termination'
and/or 'Optimization Complete'."], POTS.verbose, POTS.joblog)
      else:
        POTS.optimized = True
        POTS.kill = True
        EtaPOTS_printWrite(["This job will end due to: 'Normal termination'
and/or 'Optimization Complete'."], POTS.verbose, POTS.joblog)
      break
    count += 1
    if count > 100000:
      break

  ### Check for jitter in the energy
  EtaPOTS_printWrite(["Checking for jitter in the energies."], POTS.verbose,
POTS.joblog)
  jitter = 0
  f = open(POTS.scratchdir + "/optenergies-" + POTS.jobname + ".txt", "a")
  for i, line in enumerate(POTS.allEnergy):
    f.write(str(line) + "\n")
    if i > len(POTS.allEnergy) / 2:
      if (POTS.allEnergy[i] < POTS.allEnergy[i - 1] and POTS.allEnergy[i - 1] >
POTS.allEnergy[i - 2]) or (
          POTS.allEnergy[i] > POTS.allEnergy[i - 1] and POTS.allEnergy[i - 1] <
POTS.allEnergy[i - 2]):
        jitter += 1
  if jitter > len(POTS.allEnergy) / 4 and POTS.optimized == False:
```

```
    EtaPOTS_printWrite(["Jitters in last half of OPT: " + str(jitter)],
POTS.verbose, POTS.joblog)
    #+ " > " + str(len(allEnergy)/4) + "\n")
    EtaPOTS_printWrite(["Due to the jitter in energies from the last OPT
iteration,",
                        "the step size of the optimization algorithm will be shortened."],
POTS.verbose, POTS.joblog)
    POTS.shortenStepSize = 1

  #Check to see if the job ran too long.
  f = open(POTS.scratchdir + "/optenergies-" + POTS.jobname + ".txt", "r")
  fileEnergyList = f.readlines()
  if len(fileEnergyList) > POTS.stepNumber:
    POTS.kill = True
    EtaPOTS_printWrite(["This job will end due to: exhausted all optimization
steps."], POTS.verbose, POTS.joblog)
  f.close()


  #Check if a 'break' has occured
  breakLogic = 0
  line = POTS.QMcomment.split()
  for var in line:
    if POTS.breaktype == "bond" and breakLogic == 4:
      POTS.breakpoint = float(var)
      breakLogic = 0
    elif POTS.breaktype == "angle" and breakLogic == 5:
      POTS.breakpoint = float(var)
      breakLogic = 0
    elif POTS.breaktype == "dihedral" and breakLogic == 6:
      POTS.breakpoint = float(var)
      breakLogic = 0
    elif breakLogic >= 2:
      POTS.breakatoms.append(int(var))
      breakLogic += 1
    elif breakLogic == 1:
      POTS.breaktype = var
      breakLogic += 1
    if var == "Break:":
      breakLogic = 1
  if POTS.breaktype != "":
    EtaPOTS_printWrite(["Break point logic implemented.",
```

```
                    "Checking if " + str(POTS.breaktype) + " " +
str(POTS.breakatoms) + " are within " + str(POTS.breakpoint) + "."],
POTS.verbose, POTS.joblog)

  #Break point logic implementation
  if POTS.breaktype == "bond":
    if POTS.breakpoint < Eta_getdistance(POTS.breakatoms[0] - 1,
POTS.breakatoms[1] - 1, POTS.finalGeomAtom):
      POTS.kill = True
      EtaPOTS_printWrite(["This job will end due to: a break point failure."],
POTS.verbose, POTS.joblog)
  elif POTS.breaktype == "angle":
    if POTS.breakpoint < Eta_getangle(POTS.breakatoms[0] - 1,
POTS.breakatoms[1] - 1, POTS.breakatoms[2] - 1, POTS.finalGeomAtom):
      POTS.kill = True
      EtaPOTS_printWrite(["This job will end due to: a break point failure."],
POTS.verbose, POTS.joblog)
  elif POTS.breaktype == "dihedral":
    if POTS.breakpoint < Eta_getdihedral(POTS.breakatoms[0] - 1,
POTS.breakatoms[1] - 1, POTS.breakatoms[2] - 1, POTS.breakatoms[3] - 1,
                          POTS.finalGeomAtom):
      POTS.kill = True
      EtaPOTS_printWrite(["This job will end due to: a break point failure."],
POTS.verbose, POTS.joblog)


  #### TODO grab the rerun file for the speedup
  ### Implement speedups for Jaguar
  #Read in the restart file and get all the goods
  if POTS.kill == False and POTS.optimized == False:
    POTS.QMconfig = []
    POTS.QMendlines = []
    POTS.QMcomment = ""
    POTS.numAtoms = 0
    initialgeom = []
    xyzline = 0
    the_file = open(POTS.pwdirectory + "/restart.in", 'r')
    for line in the_file:
      if xyzline == 2:
        POTS.QMendlines.append(line)
      elif xyzline == 1 and "&" in line:
        xyzline = 2
      elif xyzline == 0 and "&zmat" in line:
        xyzline = 1
```

```
    elif "MAEFILE:" in line:
      POTS.QMcomment = line.strip()
    elif xyzline == 0:
      POTS.QMconfig.append(line)
  the_file.close()
  #Stepsize logic implementation
  iop = 0
  newsub = 0
  if POTS.shortenStepSize == 1:
    for i, line in enumerate(POTS.QMconfig):
      if "trust=" in line:
        var = line.split()
        iop = 1
        for sub in var:
          if "trust=" in sub:
            EtaPOTS_printWrite(["Your step size was: " + str(sub)],
POTS.verbose, POTS.joblog)
            newsub = "trust=" + str(int(round(float(sub.split("=")[1].split(")")[0]) *
.75)))
            EtaPOTS_printWrite(["It will now be: " + str(newsub)],
POTS.verbose, POTS.joblog)
            POTS.QMconfig[i] = line.replace(sub, newsub)
    if iop == 0:
      for i, line in enumerate(POTS.QMconfig):
        if "&gen" in line:
          EtaPOTS_printWrite(["We are now implementing a smaller step size
of trust=0.2"], POTS.verbose, POTS.joblog)
          POTS.QMconfig[i] = line + "trust=0.2\n"

  #for i, line in enumerate(POTS.QMconfig):
  #  if "&gen" in line and "readfc" not in line:
  #    EtaPOTS_printWrite(["We are now implementing readfc for the next
iteration."], POTS.verbose, POTS.joblog)
  #    var = line.split()
  #    for sub in var:
  #      if "opt=(" in sub:
  #        newsub = sub[:-1] + ",readfc)"
  #        POTS.QMconfig[i] = line.replace(sub, newsub)
  return POTS


### --- Output the G09 com file for subsequent computation --- ###
def EtaPOTS_rebuildJaguarIN(POTS):
  if POTS.debug >= 1:
```

```
    EtaPOTS_printWrite(["rebuildJaguarIN"], POTS.verbose, POTS.joblog)
  #Output the new geometry in Jaguar input format
  datetime = (time.strftime("%Y.%m.%d-%H:%M:%S"))
  #Backup .in file
  if os.path.exists(POTS.baseinput):
    if os.path.isfile(POTS.baseinput):
      shutil.copyfile(POTS.baseinput, POTS.scratchdir + "/Previous_Files/" +
datetime + "-" + POTS.inputfile)
  #Backup .log file
  if os.path.exists(POTS.jobname + ".log"):
    if os.path.isfile(POTS.jobname + ".log"):
      shutil.copyfile(POTS.jobname + ".log",
                  POTS.scratchdir + "/Previous_Files/" + datetime + "-" +
POTS.jobname + ".log")
  #Backup .out file
  if os.path.exists(POTS.baselog):
    if os.path.isfile(POTS.baselog):
      shutil.copyfile(POTS.baselog, POTS.scratchdir + "/Previous_Files/" +
datetime + "-" + POTS.jobname + ".out")

  #print ofile
  f = open(POTS.baseinput, "w+")
  for i, var in enumerate(POTS.QMconfig):
    f.write(var)
  f.write("&zmat\n")
  for i in range(2, len(POTS.finalGeomAtom)):
    line = str(POTS.finalGeomAtom[i].e) + str(i-1) + " " +
str(POTS.finalGeomAtom[i].x) + " " + str(POTS.finalGeomAtom[i].y) + " " +
str(POTS.finalGeomAtom[i].z)
    f.write(line + "\n")
  f.write("&\n")
  for i, var in enumerate(POTS.QMendlines):
    f.write(var)
  f.close()
  return


#################################################################
### END OF LIBRARY
#################################################################
```

1.3 ETANUMPYLIB.PY:

```
#! /usr/bin/env python2.7

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SUCH DAMAGE.

### --- Special Acknowledgments --- ###
# Joshua J. Kincaid made the z-matrix to xyz conversion function possible.
# Without his help several scripts/programs would be useless.
# Thank you for your assistance Joshua.

import os
from sys import *
import math
from EtaLibAtom import *
from numpy import *
from decimal import *

####=========================================================
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###
#### --- Atom class --- ###
#class Atom(object):
#  def __init__(self):
#    #Hold the string for the element
#    self.e = ''
#    #Hold the int for the element
#    self.en = int(0)
#    #Hold the float for the x coordinate
#    self.x = float(0)
#    #Hold the float for the y coordinate
#    self.y = float(0)
#    #Hold the float for the z coordinate
#    self.z = float(0)
#    #Hold a list of the neighbors
#    self.neighbors = []
#    #Hold a list of the distances for the neighbors
#    self.neighborsdist = []
#    #Hold the int for the atom nearest to this one
```

```
#    self.nearest = int(0)
#    #Hold a string for hybridization for this atom
#    self.hybridization = ''
#    #Hold an int/float for the charge of this atom
#    self.charge = float(0)
#    #Hold an int
#    self.int = 0
#    #Hold a string
#    self.string = ''
#    #Hold a string for the atomtype of this atom
#    self.atomtype = ''


### --- Functions to get geometric data --- ###
###============================================================
============================================================#
##

### --- Distance function --- ###
def Eta_getdistance(at1, at2, lol):
  if isinstance(lol[at1], Atom):
    atom1 = array([lol[at1].x, lol[at1].y, lol[at1].z])
    atom2 = array([lol[at2].x, lol[at2].y, lol[at2].z])
  else:
    atom1 = array([float(lol[at1][1]), float(lol[at1][2]), float(lol[at1][3])])
    atom2 = array([float(lol[at2][1]), float(lol[at2][2]), float(lol[at2][3])])
  vector1 = atom2-atom1
  dist = linalg.norm(vector1)
  #print dist
  return dist

### --- Angle function --- ###
def Eta_getangle(at1, at2, at3, lol):
  if isinstance(lol[at1], Atom):
    # put positions in array
    atom1 = array([lol[at1].x, lol[at1].y, lol[at1].z])
    atom2 = array([lol[at2].x, lol[at2].y, lol[at2].z])
    atom3 = array([lol[at3].x, lol[at3].y, lol[at3].z])
  else:
    atom1 = array([float(lol[at1][1]), float(lol[at1][2]), float(lol[at1][3])])
    atom2 = array([float(lol[at2][1]), float(lol[at2][2]), float(lol[at2][3])])
    atom3 = array([float(lol[at3][1]), float(lol[at3][2]), float(lol[at3][3])])
  # making appropriate vectors and normals
  vector1 = atom1-atom2
```

```
  vector2 = atom3-atom2
  angle =
arccos(dot(vector1,vector2)/(linalg.norm(vector1)*linalg.norm(vector2)))
  #print degrees(angle)
  return degrees(angle)

### --- Dihedral angle function --- ###
def Eta_getdihedral(at1, at2, at3, at4, lol):
  if isinstance(lol[at1], Atom):
    # put positions in array
    atom1 = array([lol[at1].x, lol[at1].y, lol[at1].z])
    atom2 = array([lol[at2].x, lol[at2].y, lol[at2].z])
    atom3 = array([lol[at3].x, lol[at3].y, lol[at3].z])
    atom4 = array([lol[at4].x, lol[at4].y, lol[at4].z])
  else:
    atom1 = array([float(lol[at1][1]), float(lol[at1][2]), float(lol[at1][3])])
    atom2 = array([float(lol[at2][1]), float(lol[at2][2]), float(lol[at2][3])])
    atom3 = array([float(lol[at3][1]), float(lol[at3][2]), float(lol[at3][3])])
    atom4 = array([float(lol[at4][1]), float(lol[at4][2]), float(lol[at4][3])])
  # making appropriate vectors and normals
  vector1 = atom2-atom1
  vector2 = atom3-atom2
  plane1 = cross(vector1,vector2)
  vector3 = atom2-atom3
  vector4 = atom4-atom3
  plane2 = cross(vector3,vector4)
  # finding dihedral angle
  dihedral = arccos(-
dot(plane1,plane2)/(linalg.norm(plane1)*linalg.norm(plane2)))
  # checking the sign of the dihedral then displaying result
  if dot(plane1,vector4) > 0:
    #print degrees(dihedral)
    return  degrees(dihedral)
  else:
    #print -degrees(dihedral)
    return - degrees(dihedral)


### --- TWO STRUCTURE Distance function --- ###
def Eta_TWOSTRUCTUREgetdistance(at1, at2, lol1, lol2):
  #if isinstance(lol1[at1], Atom):
  atom1 = array([lol1[at1].x, lol1[at1].y, lol1[at1].z])
  atom2 = array([lol2[at2].x, lol2[at2].y, lol2[at2].z])
  #else:
```

```
  #  atom1 = array([float(lol1[at1][1]), float(lol1[at1][2]), float(lol1[at1][3])])
  #  atom2 = array([float(lol2[at2][1]), float(lol2[at2][2]), float(lol2[at2][3])])
  vector1 = atom2-atom1
  dist = linalg.norm(vector1)
  #print dist
  return dist


### --- Distance function TWOSTRUCTURE --- ###
def Eta_TWOSTRUCTUREgetdistance(at1, at2, lol1, lol2):
  if isinstance(lol1[at1], Atom):
    atom1 = array([lol1[at1].x, lol1[at1].y, lol1[at1].z])
    atom2 = array([lol2[at2].x, lol2[at2].y, lol2[at2].z])
  else:
    atom1 = array([float(lol1[at1][1]), float(lol1[at1][2]), float(lol1[at1][3])])
    atom2 = array([float(lol2[at2][1]), float(lol2[at2][2]), float(lol2[at2][3])])
  vector1 = atom2-atom1
  dist = linalg.norm(vector1)
  #print dist
  return dist

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##

### --- Bond elucidation section --- ###
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##
### --- Get bonds --- ###
def Eta_getBonds(fileAtom):
  iFileAtomNum = fileAtom[0]
  iFileName = fileAtom[1]
  covBonds = []
  covHBonds = []
  covTMBonds = []
  nearestNeighbor = []
  neighborStart = [0, 1000000]
  #Iterate through the file
  for i, linei in enumerate(fileAtom):
    #Set a placeholder for the nearest neighbor
    nearestNeighbor.append(list(neighborStart))
    #Iterate throught the file again
    for j, linej in enumerate(fileAtom):
```

```
      if i !=j:
        distij = Eta_getdistance(i+2, j+2)
        if j > i:
          if distij <= 2.25 and fileAtom[i+2][0] != 1 and fileAtom[j+2][0] != 1 and
((getElementName(fileAtom[i+2][0]).lower() not in elementLarge) and
(getElementName(fileAtom[j+2][0]).lower() not in elementLarge)):
            distList = [i+1, j+1, distij]
            covBonds.append(distList)
            #print str(i+2) + "\t" + str(j+2) + "\t" + str(distij)
          elif distij <= 1.3 and (fileAtom[i+2][0] == 1 or fileAtom[j+2][0] == 1):
            distList = [i+1, j+1, distij]
            covHBonds.append(distList)
          elif distij <= 3 and ((getElementName(fileAtom[i+2][0]).lower() in
elementLarge) and (getElementName(fileAtom[j+2][0]).lower() in
elementLarge)):
            distList = [i+1, j+1, distij]
            covTMBonds.append(distList)
        if distij < nearestNeighbor[i][1]:
          nearestNeighbor[i][0] = j + 1
          nearestNeighbor[i][1] = distij
  ### --- Remove hydrogen bonds from bond list --- ###
  for i in range(0,len(covHBonds)):
    if (covHBonds[i][0] != nearestNeighbor[covHBonds[i][0]][0]) and
(covHBonds[i][1] != nearestNeighbor[covHBonds[i][0]][0]):
      del covHBonds[i]
  #print "Covalent bonds to Hydrogen:"
  #print covHBonds
  #print "Covalent bonds between \"heavy\" atoms."
  #print covBonds
  #print "Covalent bonds between TM atoms."
  #print covTMBonds
  #print nearestNeighbor
  return fileAtom

### --- Build a list that contains all atoms starting with at1
#  on one side of the molecule that is opposite the other atom atm2
def Eta_buildbondlist(at1, at2, filelol):
  bondedlist = [1,2,3,4]
  return bondedlist

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### --- ZMAT to XYZ to ZMAT conversion section --- ###
###=============================================================
============================================================#
##

### --- get the distance, angle and dihedrals for a Z-matrix --- ###
# This function is iteratable through a file, allowing for:
# 1. grabbing of a single atoms's distance, angle and dihedral
# 2. double ended zmatrix files
# 3. complex zmatrix files dependent on bonding
# You must give the (up to) 4 atoms nessecary to get the zmat for the atom
def Eta_getzmat(i, j, k, l, ifilelol):
  #If the line i is in Atom format find the relevant distance, angle, and dihedral
  if isinstance(ifilelol[i], Atom):
    line = []
    line.append(i-1)
    line.append(ifilelol[i].e)
    #If the atom is not the first in the file get the distance to the last atom
    if i > 2:
      line.append(j-1)
      dist = Eta_getdistance(j, i, ifilelol)
      line.append(dist)
    #If the atom is not the first or second in the file get the angle to the last two
atoms
    if i > 3:
      line.append(k-1)
      angle = Eta_getangle(k, j, i, ifilelol)
      line.append(angle)
    #If the atom is not the first, second, or third in the file get the dihedral to the
last three atoms
    if i > 4:
      line.append(l-1)
      dihedral = Eta_getdihedral(l, k, j, i, ifilelol)
      line.append(dihedral)
  #If not an Atom (ie first two lines) print them back out
  else:
    line = []
    line.append(ifilelol[i])
  line.append(-1)
  line.append(-1)
  line.append(-1)
  line.append(-1)
  line.append(-1)
  line.append(-1)
```

```
  line.append("\n")
  return line

### --- Get the XYZ coordinates from distance, angle and dihedral data ---
###
def Eta_getXYZfromZMAT(zmatLOL):
  xyzLOL = ["0"] * len(zmatLOL)
  xyzLOL[0] = zmatLOL[0][0]
  xyzLOL[1] = zmatLOL[1][0]
  for i in range(2, len(zmatLOL)):
    ### Set up the variables to be used for the function
    dist = float(zmatLOL[i][3])
    angle = float(zmatLOL[i][5])
    dihedral = float(zmatLOL[i][7])
    angleRad = radians(angle)  # * math.pi / 180
    dihedralRad = radians(dihedral)  # * math.pi / 180
    at1 = int(zmatLOL[i][6]) + 1
    at2 = int(zmatLOL[i][4]) + 1
    at3 = int(zmatLOL[i][2]) + 1
    at4 = int(zmatLOL[i][0]) + 1
    x = 0
    y = 0
    z = 0

    ### Start to place the atoms in their locations
    if at4 == 2:
      x = 0.00000
      y = 0.00000
      z = 0.00000

    elif at4 == 3:
      x = dist
      y = 0.00000
      z = 0.00000

    elif at4 == 4:
      a = xyzLOL[at3].x
      b = dist
      x = a + (dist * cos(math.pi - angleRad))
      y = 0.00000
      z = -dist * sin(math.pi - angleRad)

    elif at4 >= 5:
      ####The at4 x,y,z coordinates from spherical coord
```

```
    Sx = dist * sin(angleRad) * cos(dihedralRad)
    Sy = -dist * sin(angleRad) * sin(dihedralRad)  #For some reason I need to
have a negative here to get the correct sign in the output..... weird
    Sz = dist * cos(angleRad)
    at4L = [Sx, Sy, Sz]

    ###Finding the angle theta
    #Make the list of lists for the three point (z-axis, origin, and translated
atom 2) needed for an angle calculation
    Z32 = [[0, 0, 0, 1], [0, 0, 0, 0],
          [0, xyzLOL[at2].x - xyzLOL[at3].x, xyzLOL[at2].y - xyzLOL[at3].y,
xyzLOL[at2].z - xyzLOL[at3].z]]
    #Get theta using the getangle function
    theta = radians(Eta_getangle(0, 1, 2, Z32))
    #print "theta: " +str(theta)

    ###Rodrigues' rotation formula
    #Create the vectors needed to calculate k
    vector3 = array([xyzLOL[at3].x, xyzLOL[at3].y, xyzLOL[at3].z])
    vector2 = array([xyzLOL[at2].x, xyzLOL[at2].y, xyzLOL[at2].z])
    vector0 = array([0, 0, 1])
    #Calculate k for the Rodrigues rotation formula
    k = cross((vector2 - vector3), vector0) / linalg.norm(cross((vector2 -
vector3), vector0))
    #Generate an array for translated 1
    T1 = [(xyzLOL[at1].x - xyzLOL[at3].x), (xyzLOL[at1].y - xyzLOL[at3].y),
(xyzLOL[at1].z - xyzLOL[at3].z)]
    #Calculate the Rodrigues rotation matrix
    RR23T1 = dot(T1, cos(theta)) + dot(cross(k, T1), sin(theta)) + dot(dot(k,
(dot(k, T1))), (1 - cos(theta)))
    #Make the list of lists for the four points (x-axis, z-axis, origin, and rotated
translated 1) needed for a dihedral calculation
    XZ31 = [[0, 1, 0, 0], [0, 0, 0, 1], [0, 0, 0, 0], [0, RR23T1[0], RR23T1[1],
RR23T1[2]]]
    #Get phi using the getdihedral function
    phi = radians(Eta_getdihedral(0, 1, 2, 3, XZ31))

    ###Rotation matrix
    #Create the array for the rotation matrix including dihedral phi
    RM = array([[cos(phi), sin(phi), 0], [-sin(phi), cos(phi), 0], [0, 0, 1]])
    #Calculate the dot product of the rotation matrix and the coordinates for 4
(from spherical)
    RM4 = dot(RM, at4L)
    #Calculate the rotated coordinates of the rotated coordinates of atom 4
```

```
      RRN23RM4 = dot(RM4, cos(-theta)) + dot(cross(k, RM4), sin(-theta)) +
dot(dot(k, (dot(k, RM4))), (1 - cos(-theta)))
      #Final coordinates that are rotated, rotated and translated
      x = RRN23RM4[0] + xyzLOL[at3].x
      y = RRN23RM4[1] + xyzLOL[at3].y
      z = RRN23RM4[2] + xyzLOL[at3].z
    #Putting everything into a Atom list to send back
    xyzLOL[i] = Atom()
    xyzLOL[i].e = zmatLOL[i][1]
    xyzLOL[i].en = Eta_getElementNum(zmatLOL[i][1])
    xyzLOL[i].x = x
    xyzLOL[i].y = y
    xyzLOL[i].z = z
  return xyzLOL

### --- Generate a list of lists for the zmatrix of the structure --- ###
def Eta_genZMATbasic(ifilelol):
  zmatlol = []
  for i in range(0, len(ifilelol)):
    linetemp = Eta_getzmat(i, i-1, i-2, i-3, ifilelol)
    zmatlol.append(linetemp)
  return zmatlol

def Eta_genZMATdoublesided(ifilelol, list1, list2):
  zmatlol = []
  for i in range(0, len(ifilelol)):
    linetemp = Eta_getzmat(i, i-1, i-2, i-3, ifilelol)
    zmatlol.append(linetemp)
  return zmatlol


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2. ηTRASLATE SCRIPTS:

2.1 NTRANSLATE-XYZ-DIHANGDIST.PY:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
from EtaNUMPYLib import *

if argv[1] == "-h":
  print "<input file>.xyz atom1 atom2 atom3 atom4"
  sys.exit(0)
### --- Arguments --- ###
ifile = argv[1]
atomTemp = " ".join(sys.argv[2:] + ["-1", "-1", "-1", "-1"])
atoms = atomTemp.split()
atom1 = int(atoms[0])
atom2 = int(atoms[1])
atom3 = int(atoms[2])
atom4 = int(atoms[3])

### Display input and output file name passed as the args
#print ("Input file : %s and output file: %s" % (ifile,ofile) )

### --- Open parent file --- ###
ifilelol = Eta_XYZ_LOL(ifile)

### --- Print out the distance, angle, or dihedral --- ###
if atom3 == -1:
        print ifile + ": " + str(Eta_getdistance(atom1+1, atom2+1, ifilelol))
elif atom4 == -1:
        print ifile + ": " +  str(Eta_getangle(atom1+1, atom2+1, atom3+1,
ifilelol))
elif atom4 >= 0:
        print ifile + ": " +  str(Eta_getdihedral(atom1+1, atom2+1, atom3+1,
atom4+1, ifilelol))
```

```
#################################################################
### END OF SCRIPT
#################################################################
```

2.2 nTranslate-XYZ-Remove_Atom.py:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
from decimal import *


### --- Arguments --- ###
program = "nTranslate-XYZ-Remove_Atom.py"
ifile = ''
ofile = ''
deleteAtoms = []
allindir =0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:o:a:dh")
except getopt.GetoptError:
  print program + " -i <inputfile.xyz> -o <outputfile.xyz> -a <delete_atom> -d
(all in dir)"
  sys.exit(2)
###############################
# o == option
# a == argument passed to the o
###############################
for o, a in myopts:
  if o == '-i':
    ifile = a
  elif o == '-o':
    ofile = a
  elif o == '-a':
    deleteAtoms.append(int(a))
  elif o == '-d':
    allindir = 1
  elif o == '-h':
    print program + " -i <inputfile.xyz> -o <outputfile.xyz> -d <delete_atom>"
    sys.exit(0)
```

```
  else:
    print("Usage: %s -i <inputfile.xyz> -o <outputfile.xyz> -d <delete_atom>" %
sys.argv[0])
    sys.exit(0)

if allindir == 0:
  ### --- Open parent file --- ###
  ifilelol = Eta_XYZ_LOL(ifile)

  ### --- Output file in Z-matrix format --- ###
  f = open(ofile, 'w+')
  f.write(str(ifilelol[0] - len(deleteAtoms)) + "\n")
  f.write(ifilelol[1] + "\n")
  for i in range(2, len(ifilelol)):
    if i - 1 not in deleteAtoms:
      line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
      f.write(line + "\n")
    else:
      print "Removing atom: " + str(i - 1)
  f.close()

elif allindir == 1:
  Eta_makeDir("REMOVED")
  for i in os.listdir(os.getcwd()):
    if i.endswith(".xyz"):
      ifile = i
      ofile = "REMOVED/" + ifile
      print i

      ### --- Open parent file --- ###
      ifilelol = Eta_XYZ_LOL(ifile)

      ### --- Output file in Z-matrix format --- ###
      f = open(ofile, 'w+')
      f.write(str(ifilelol[0] - len(deleteAtoms)) + "\n")
      f.write(ifilelol[1] + "\n")
      for i in range(2, len(ifilelol)):
        if i - 1 not in deleteAtoms:
          line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
          f.write(line + "\n")
        else:
          print "Removing atom: " + str(i - 1)
```

```
    f.close()

#################################################################
### END OF SCRIPT
#################################################################
```

2.3 nTranslate-XYZ-Renumber.py:

```
#!/usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
from EtaNUMPYLib import *
from decimal import *
from numpy import *


### --- Arguments --- ###
program = "nTranslate-XYZ-Renumber.py"
mainfile = ""
debug = 0
autofind = 0
atomNum = -1

#Define what type of job we will be running
if len(argv) == 1:
  argv.append("-a")
  autofind = 1
elif argv[1] == "-h":
  print
"============================================================
============================================"
  print program + "<main file>.xyz -a <auto select> -h\n"\

"============================================================
============================================\n\n"\
      "This script will renumber all the xyz files within the current directory to a
specified key structure.\n" \
      "\n" \
      "If any of the structures within the directory are larger than the specified
key file,\n" \
      "any unmatched atoms will be appended to the end of the file.\n" \
      "\n" \
      "All renumbered files are saved in the folder \"RENUMBERED\" including
the key structure.\n"\
```

```
      "\n" \
      "If you do not specify a structure the smallest one will be chosen for
you."
  sys.exit(0)
else:
  mainfile = argv[1]

### --- Make RENUMBERED folder --- ###
if not os.path.exists("RENUMBERED"): os.makedirs("RENUMBERED")

### --- If asked to do so iterate through the folder for other .xyz files and find
the smallest one --- ###
if autofind == 1:
  for i in os.listdir(os.getcwd()):
    if i.endswith(".xyz"):
      f = open(i, "r")
      for j, line in enumerate(f):
        if j >= 1:
          break
        elif atomNum == -1:
          atomNum = int(line)
          mainfile = i
        elif int(line.strip()) < atomNum:
          atomNum = int(line)
          mainfile = i
      f.close()

### --- Open parent file --- ###
mainfileAtom = Eta_XYZ_LOL(mainfile)

print "Renumbering all structures to " + mainfile + "."

#Output the main file to the renumbered folder
Eta_outputXYZ("RENUMBERED/" + mainfile, mainfileAtom)

#Iterate through the folder for other .xyz files
for i in os.listdir(os.getcwd()):
  if i.endswith(".xyz") and i != mainfile:
    ifile = i

    #Print out the current job for the user
    print ifile

    #Get the XYZ lol/Atom data from the child file (ifile)
```

```
    childfileAtom = Eta_XYZ_LOL(ifile)

    #Build a holder for the Atom data and copy the first two lines
    if len(childfileAtom) > len(mainfileAtom):
      ofileAtom = [0] * len(childfileAtom)
    else:
      ofileAtom = [0] * len(mainfileAtom)
    ofileAtom[0] = childfileAtom[0]
    ofileAtom[1] = childfileAtom[1]

    #Make a holder for matched and unmatched atom numbers to use later
    matchedatoms = []
    matchedatomsdist = []
    unmatchedatoms = []

    #Build a holder for the distance matrix
    distanceMatrix = [[0 for x in xrange(len(childfileAtom)-2)] for x in
xrange(len(mainfileAtom)-2)]

    #Build the distance matrix
    for j in range(2, len(mainfileAtom)):
      for k in range(2, len(childfileAtom)):
        distanceMatrix[j-2][k-2] = Eta_TWOSTRUCTUREgetdistance(j, k,
mainfileAtom, childfileAtom)

    #Find the best nearest neighbor and if not already used
    for j in range(len(mainfileAtom) - 2):
      nearestNeighbor = 0
      nearestNeighborDist = distanceMatrix[j][0]
      for k in range(1, len(childfileAtom)-2):
        if distanceMatrix[j][k] < nearestNeighborDist:
          nearestNeighborDist = distanceMatrix[j][k]
          nearestNeighbor = k

      if nearestNeighbor + 2 not in matchedatoms:
        #ofileAtom[j+2] = childfileAtom[nearestNeighbor + 2]
        matchedatoms.append(nearestNeighbor + 2)
        matchedatomsdist.append(nearestNeighborDist)

      elif nearestNeighbor + 2 in matchedatoms:
        for l in range(len(matchedatoms)):
          #print str(l) + "   " + str(matchedatoms[l]) + "  " +
str(matchedatomsdist[l])
```

```
        if nearestNeighbor + 2 == matchedatoms[l] and nearestNeighborDist <
matchedatomsdist[l]:
          #ofileAtom[j+2] = childfileAtom[nearestNeighbor + 2]
          matchedatoms[l] = nearestNeighbor + 2
          matchedatomsdist[l] = nearestNeighborDist

   #Iterate throught the matched atom list and add them to the end on the ofile
atom/lol
   for k in range(len(matchedatoms)):
     #print unmatchedatoms[k]
     ofileAtom[2 + k] = childfileAtom[matchedatoms[k]]

   #Iterate through the child file and if an atom is not matched add it to the
unmatched atom list
   for k in range(2, len(childfileAtom)):
     if k not in matchedatoms:
       #print k
       unmatchedatoms.append(k)

   #Iterate throught the unmatched atom list and add them to the end on the
ofile atom/lol
   for k in range(len(unmatchedatoms)):
     #print unmatchedatoms[k]
     ofileAtom[len(matchedatoms) + 2 + k] = childfileAtom[unmatchedatoms[k]]

   #Output the newly renumbered file to the renumbered folder
   Eta_outputXYZ("RENUMBERED/" + ifile, ofileAtom)

#################################################################
### END OF SCRIPT
#################################################################
```

2.4 nTranslate-New-Second-Line.py:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
from decimal import *


### --- Arguments --- ###
program = "nTranslate-New-Second-Line.py"
ifile = ''
ofile = ''
secondLine = ''
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:o:dh")
except getopt.GetoptError:
  print program + " -i <inputfile.xyz> -o <outputfile.xyz> -d <all xyz in dir>"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-i':
    ifile = a
  elif o == '-o':
    ofile = a
  elif o == '-d':
    allInDir = 1
  elif o == '-h':
    print program + " -i <inputfile.xyz> -o <outputfile.xyz> -d <all xyz in dir>"
    sys.exit(0)
  else:
    print("Usage: %s -i <inputfile.xyz> -o <outputfile.xyz> -d <all xyz in dir>" %
sys.argv[0])
```

```
    sys.exit(0)

if allInDir == 0:
  ### --- Open parent file --- ###
  ifilelol = Eta_XYZ_LOL(ifile)
  secondLine = ofile
  ### --- Output file in Z-matrix format --- ###
  f = open(ofile, 'w+')
  f.write(str(ifilelol[0]) + "\n")
  f.write(secondLine + "\n")
  for i in range(2, len(ifilelol)):
    line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
    f.write(line + "\n")
  f.close()
elif allInDir == 1:
  ### --- Make directories if they do not exist --- ###
  Eta_makeDir("RENAMED")
  for i in os.listdir(os.getcwd()):
    if i.endswith(".xyz"):
      ifile = i
      ofiletmp = ifile.split(".")
      ofile = ""
      for i in range(len(ofiletmp)):
        if i != len(ofiletmp) - 1:
          ofile += ofiletmp[i] + "."
        elif i == len(ofiletmp) - 1:
          ofile += "xyz"
      secondLine = ofile
      #Print out the names
      print ifile + " ----> RENAMED/" + ofile
      ### --- Open parent file --- ###
      ifilelol = Eta_XYZ_LOL(ifile)
      ### --- Output file in Z-matrix format --- ###
      f = open("RENAMED/" + ofile, 'w+')
      f.write(str(ifilelol[0]) + "\n")
      f.write(secondLine + "\n")
      for i in range(2, len(ifilelol)):
        line = ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
        f.write(line + "\n")
      f.close()

#############################################################
```

```
### END OF SCRIPT
#################################################################
```

2.5 nTranslate-Change-Geom-XYZ.py:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
from EtaNUMPYLib import *
from decimal import *
from numpy import *

### --- Arguments --- ###
program = "nTranslate-Change-Geom-XYZ.py"
debug = 0
ifile = ''
ofile = ''
printfile = 0
bond_angle_dihedral = []
newvalue = ''
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:o:b:v:phd", ["bad=", "var="])
except getopt.GetoptError:
  print program + " -i <inputfile.xyz> -o <outputfile.zmat> -b or --
bad=<bond/angle/dihedral atom numbers>   -v or --newvalue=<new geometric
value> "
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-i':
    ifile = a
  elif o == '-o':
    ofile = a
  elif o == '--bad' or o == '-b':
    for item in a.split():
```

```
      bond_angle_dihedral.append(int(item))
  elif o == '--newvalue' or o == '-v':
    newvalue = a
  elif o == '-p':
    printfile = 1
  elif o == '-d':
    allInDir = 1
  elif o == '-D':
    debug += 1
  elif o == '-h':
    print program + " -i <inputfile.xyz> -o <outputfile.zmat> --
bad=<bond/angle/dihedral atom numbers>  --newvalue=<new geometric
value> "
    sys.exit(0)
  else:
    print("Usage: %s  -i <inputfile.xyz> -o <outputfile.zmat> --
bad=<bond/angle/dihedral atom numbers>  --newvalue=<new geometric
value> " % sys.argv[0])
    sys.exit(0)


def runChange(ifile, ofile, bond_angle_dihedral):
  ### --- Open parent file --- ###
  ifilelol = Eta_XYZ_LOL(ifile)

  ### --- Renumber atoms to put the atoms of interest in the
  ifilelol_renumbered = Eta_renumberbasic(ifilelol, bond_angle_dihedral)

  ##Change the bond/angle/dihedral of interest
  #if len(bond_angle_dihedral) == 2:
  #  list1 = Eta_buildbondlist(bond_angle_dihedral[0], bond_angle_dihedral[1],
ifilelol)
  #  list2 = Eta_buildbondlist(bond_angle_dihedral[1], bond_angle_dihedral[0],
ifilelol)
  #elif len(bond_angle_dihedral) == 3:
  #  list1 = Eta_buildbondlist(bond_angle_dihedral[1], bond_angle_dihedral[2],
ifilelol)
  #  list2 = Eta_buildbondlist(bond_angle_dihedral[2], bond_angle_dihedral[1],
ifilelol)
  #elif len(bond_angle_dihedral) == 4:
  #  list1 = Eta_buildbondlist(bond_angle_dihedral[1], bond_angle_dihedral[2],
ifilelol)
  #  list2 = Eta_buildbondlist(bond_angle_dihedral[2], bond_angle_dihedral[1],
ifilelol)
```

```
  ### --- Generate a list of lists for the zmatrix of the structure --- ###
  zmatlol = []
  for i in range(0, len(ifilelol_renumbered)):
    linetemp = Eta_getzmat(i, i-1, i-2, i-3, ifilelol_renumbered)
    zmatlol.append(linetemp)

  #Change the bond/angle/dihedral of interest
  if len(bond_angle_dihedral) == 2:
    zmatlol[3][3] = newvalue
  elif len(bond_angle_dihedral) == 3:
    zmatlol[4][5] = newvalue
  elif len(bond_angle_dihedral) == 4:
    zmatlol[5][7] = newvalue

  #Grab the XYZ from the now changed zmat
  ifilelol_renumbered_fixed = Eta_getXYZfromZMAT(zmatlol)

  ### --- RE-Renumber atoms to put the atoms of interest in the
  #Iterate through the bond_angle_dihedral list and put them back to their
locations
  for i, atom in enumerate(bond_angle_dihedral):
    ifilelol[atom + 1] = ifilelol_renumbered_fixed[i+2]
  #Iterate throught the ifilelol and add the rest of the file to the renumbered
  usedBAD = 0
  for i in range(2, len(ifilelol)):
    if i-1 not in bond_angle_dihedral:
      ifilelol[i] = ifilelol_renumbered_fixed[i + len(bond_angle_dihedral) -
usedBAD]
    else:
      usedBAD = usedBAD + 1

  ### --- Output  format --- ###
  Eta_outputXYZ(ofile, ifilelol)

  ### --- Print out the xyz from the zmatrix --- ###
  if printfile == 1:
    for i in range(len(ifilelol)):
      if i <= 1:
        print ifilelol[i]
      else:
        print ifilelol[i].e + "  " + str("{:.6f}".format(ifilelol[i].x)) + "  " +
str("{:.6f}".format(ifilelol[i].y)) + "  " + str("{:.6f}".format(ifilelol[i].z))
```

```
  return

try:
  if allInDir == 1:
    for i in os.listdir(os.getcwd()):
      if i.endswith(".xyz"):
        ifile = i
        #ofile = "OUT-" + i
        ofile = Eta_basename(ifile, ".xyz") + "-OUT.xyz"
        print ifile + " ----> " + ofile
        runChange(ifile, ofile, bond_angle_dihedral)
  else:
    print ifile + " ----> " + ofile
    runChange(ifile, ofile, bond_angle_dihedral)
except:
  print "Something failed. Make sure the/a xyz file(s) exists."

#################################################################
### END OF SCRIPT
#################################################################
```

2.6 nTranslate-XYZ-XXInput.py:

2.6.1 nTranslate-XYZ-G09Input.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
from sys import *
import sys
import getopt
from EtaLibAtom import *

# ## --- Arguments --- ###
program = "nTranslate-XYZ-G09Input.py"
#Grab the first argument from the command and use that as the snippet
try:
  snippet = sys.argv[1]
except IndexError:
  snippet = "-h"
#If help is wanted allow the skipping of a snippet
if snippet == "-h":
  argv.append("-h")
  argv.append("-h")
#If interactive mode is wanted allow the skipping of a snippet
if snippet == "-i":
  argv.append("-i")
  argv.append("-i")
#Unless the charge is stated via the -c argument the charge will be assumed
to be 0
charge = 0
chargeset = False
#Unless the multiplicity is stated via the -m argument the multiplicity will be
assumed to be 1
multi = 1
multiset = False
modred = []
writemod = 0
ionicCM = ""
ionicswitch = 0
debug = 0
interactive = 0
```

```
### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "c:m:dih", ["mod=", "ionic="])
except getopt.GetoptError:
  print program + " <snippet> -c <charge> -m <multiplicity> --
mod=\"constraint\" --ionic=reg/mno -d"
  sys.exit(2)
###############################
# o == option
# a == argument passed to the o
###############################
for o, a in myopts:
  if o == '-c':
    charge = a
    chargeset = True
  elif o == '-m':
    multi = a
    multiset = True
  elif o == '-d':
    debug += 1
  elif o == '--mod':
    modred.append(a)
    writemod = 1
  elif o == '--ionic':
    ionicCM = a
    ionicswitch = 1
  elif o == '-i':
    interactive = 1
  elif o == '-h':
    print program + "' <snippet> -c <charge> -m <multiplicity> --
mod=\"constraint\" --ionic=reg/mno -d'"
    sys.exit(0)
  else:
    print("Usage: %s  <snippet> -c <charge> -m <multiplicity> --
mod=\"constraint\" --ionic=reg/mno -d" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print "Charge: " + str(charge)
  print "Multiplicity: " + str(multi)
  print "Snippet: " + snippet
  print "Modredundant Variable: "
  print modred
```

```
### --- OK Now setup the input variables for the first time --- ###
G0XInput = InputArguments()

#if interactive == 1:
#  G0XInput = Eta_interactiveConfig
#else:
#  #Grab the snippet information
#  G0XInput = Eta_parseSnippetG0X(snippet, G0XInput)

### --- Make NEWJOBS folder --- ###
if not os.path.exists("NEWJOBS.G0X"): os.makedirs("NEWJOBS.G0X")

### --- Open and parse the xyz files in the folder --- ###
print "Currently Translating:"
for i in os.listdir(os.getcwd()):
  if i.endswith(".xyz"):
    ifile = i
    print i

    if debug >= 2:
      print snippet

    #Parse XYZ file into a list of lists
    ifilelol = Eta_XYZ_LOL(ifile)

    ### Copy the charge, multi and modredundant lines to the G0XInput
    if len(modred) > 0:
      G0XInput.writemod = 1
    for line in modred:
      G0XInput.modred.append(line)
    if chargeset == True:
      print "YES"
      G0XInput.charge = charge
    if multiset == True:
      G0XInput.multi = multi

    ### --- Calculate charge from file --- ###
    if ionicswitch == 1:
      G0XInput.charge = Eta_ionic(ionicswitch, ionicCM, ifilelol)

    ### --- Generate the ECP list for files if needed --- ###
    if interactive == 0:
      G0XInput = Eta_parseSnippetG0X(snippet, G0XInput)
```

```
    if G0XInput.writeecp == 1:
      G0XInput.config, G0XInput.ecplines = Eta_G0XECP(G0XInput.ecp,
G0XInput.config, ifilelol)

    if G0XInput.writecloseecp == 1:
      G0XInput.closelines, G0XInput.closeecplines =
Eta_G0XECP(G0XInput.closeecp, G0XInput.closelines, ifilelol)

    ### --- Out put the G0X input files --- ###
    Eta_outputG0X(ifile, G0XInput, ifilelol)

    ### --- RESET THE VARIABLES --- ###
    G0XInput = Eta_resetInputVariables(G0XInput)


#################################################################
### END OF SCRIPT
#################################################################
```

2.6.2 nTranslate-XYZ-JaguarInput.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import sys
from sys import *
import getopt
from EtaLibAtom import *

# ## --- Arguments --- ###
program = "nTranslate-XYZ-JaguarInput.py"
#Grab the first argument from the command and use that as the snippet
try:
  snippet = sys.argv[1]
except IndexError:
  snippet = "-h"
#If help is wanted allow the skipping of a snippet
if snippet == "-h":
  argv.append("-h")
  argv.append("-h")
#Unless the charge is stated via the -s argument the charge will be assumed
to be 0
charge = 0
#Unless the multiplicity is stated via the -m argument the multiplicity will be
assumed to be 1
multi = 1
modred = []
writemod = 0
ionicCM = ""
ionicswitch = 0
debug = 0


### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "c:m:dh", ["mod=", "ionic="])
except getopt.GetoptError:
  print program + " <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d"
  sys.exit(2)
###############################
# o == option
```

```
# a == argument passed to the o
##############################
for o, a in myopts:
  if o == '-c':
    charge = a
  elif o == '-m':
    multi = a
  elif o == '-d':
    debug += 1
  elif o == '--mod':
    modred.append(a)
    writemod = 1
  elif o == '--ionic':
    ionicCM = a
    ionicswitch = 1
  elif o == '-h':
    print program + ''' <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d'''
    sys.exit(0)
  else:
    print("Usage: %s  <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print "Charge: " + charge
  print "Multiplicity: " + multi
  print "Snippet: " + snippet
  print "Modredundant Variable: "
  print modred

#Grab the snippet information
config, ecp, closelines, writeecp, writeclose = Eta_parseSnippet(snippet)

if debug >= 1:
  print "Configuration:"
  print config
  print "ECP Input: " + ecp
  print "Additional Lines: "
  print closelines

### --- Make NEWJOBS folder --- ###
if not os.path.exists("NEWJOBS.JAG"): os.makedirs("NEWJOBS.JAG")
```

```
### --- Open and parse the xyz files in the folder --- ###
print "Currently Translating:"
for i in os.listdir(os.getcwd()):
  if i.endswith(".xyz"):
    ifile = i
    print i
    #Parse XYZ file into a list of lists
    ifilelol = Eta_XYZ_LOL(ifile)

    ### --- Calculate charge from file --- ###
    if ionicswitch == 1:
      charge = Eta_ionic(ionicswitch, ionicCM, ifilelol)

    ### --- Out put the G0X input files --- ###
    Eta_outputJaguar(ifile, config, charge, multi, writemod, modred, writeecp,
[], writeclose, closelines, ifilelol)




#################################################################
### END OF SCRIPT
#################################################################
```

2.6.3 nTranslate-XYZ-TCInput.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

# ## --- Arguments --- ###
program = "nTranslate-XYZ-TCInput.py"
#Grab the first argument from the command and use that as the snippet
try:
  snippet = sys.argv[1]
except IndexError:
  snippet = "-h"
#If help is wanted allow the skipping of a snippet
if snippet == "-h":
  argv.append("-h")
  argv.append("-h")
#Unless the charge is stated via the -s argument the charge will be assumed
to be 0
charge = 0
#Unless the multiplicity is stated via the -m argument the multiplicity will be
assumed to be 1
multi = 1
modred = []
writemod = 0
ionicCM = ""
ionicswitch = 0
debug = 0
#Constants
auToAngstrom = 1.889725988579

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "c:m:dh", ["mod=", "ionic="])
except getopt.GetoptError:
  print program + " <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d"
  sys.exit(2)
```

```
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-c':
    charge = a
  elif o == '-m':
    multi = a
  elif o == '-d':
    debug += 1
  elif o == '--mod':
    modred.append(int(a))
    writemod = 1
  elif o == '--ionic':
    ionicCM = a
    ionicswitch = 1
  elif o == '-h':
    print program + "' <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d"'
    sys.exit(0)
  else:
    print("Usage: %s  <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print "Charge: " + charge
  print "Multiplicity: " + multi
  print "Snippet: " + snippet
  print "Modredundant Variable: "
  print modred

#Grab the snippet information
config, ecp, closelines, writeecp, writeclose = Eta_parseSnippet(snippet)

if debug >= 1:
  print "Configuration:"
  print config
  print "ECP Input: " + ecp
  print "Additional Lines: "
  print closelines

### --- Make NEWJOBS folder --- ###
```

```
if not os.path.exists("NEWJOBS.TC"): os.makedirs("NEWJOBS.TC")

### --- Open and parse the xyz files in the folder --- ###
print "Currently Translating:"
for i in os.listdir(os.getcwd()):
  if i.endswith(".xyz"):
    ifile = i
    print i
    #Parse XYZ file into a list of lists
    ifilelol = Eta_XYZ_LOL(ifile)

    ### --- Calculate charge from file --- ###
    if ionicswitch == 1:
      charge = Eta_ionic(ionicswitch, ionicCM, ifilelol)

    ### --- Out put the G0X input files --- ###
    Eta_outputTC(ifile, config, charge, multi, writemod, modred, writeecp, [],
writeclose, closelines, ifilelol)



#################################################################
### END OF SCRIPT
#################################################################
```

2.6.4 nTranslate-XYZ-TMInput.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

# ## --- Arguments --- ###
program = "nTranslate-XYZ-TMInput.py"
#Grab the first argument from the command and use that as the snippet
try:
  snippet = sys.argv[1]
except IndexError:
  snippet = "-h"
#If help is wanted allow the skipping of a snippet
if snippet == "-h":
  argv.append("-h")
  argv.append("-h")
#Unless the charge is stated via the -s argument the charge will be assumed
to be 0
charge = 0
#Unless the multiplicity is stated via the -m argument the multiplicity will be
assumed to be 1
multi = 1
modred = []
writemod = 0
ionicCM = ""
ionicswitch = 0
debug = 0
#Constants
auToAngstrom = 1.889725988579

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "c:m:dh", ["mod=", "ionic="])
except getopt.GetoptError:
  print program + " <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d"
  sys.exit(2)
```

```
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-c':
    charge = a
  elif o == '-m':
    multi = a
  elif o == '-d':
    debug += 1
  elif o == '--mod':
    modred.append(int(a))
    writemod = 1
  elif o == '--ionic':
    ionicCM = a
    ionicswitch = 1
  elif o == '-h':
    print program + "' <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d"'
    sys.exit(0)
  else:
    print("Usage: %s  <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print "Charge: " + charge
  print "Multiplicity: " + multi
  print "Snippet: " + snippet
  print "Modredundant Variable: "
  print modred

#Grab the snippet information
config, ecp, closelines, writeecp, writeclose = Eta_parseSnippet(snippet)

if debug >= 1:
  print "Configuration:"
  print config
  print "ECP Input: " + ecp
  print "Additional Lines: "
  print closelines

### --- Make NEWJOBS folder --- ###
```

```
if not os.path.exists("NEWJOBS.TM"): os.makedirs("NEWJOBS.TM")

### --- Open and parse the xyz files in the folder --- ###
print "Currently Translating:"
for i in os.listdir(os.getcwd()):
  if i.endswith(".xyz"):
    ifile = i
    print i
    #Parse XYZ file into a list of lists
    ifilelol = Eta_XYZ_LOL(ifile)

    ### --- Calculate charge from file --- ###
    if ionicswitch == 1:
      charge = Eta_ionic(ionicswitch, ionicCM, ifilelol)

    ### --- Out put the G0X input files --- ###
    Eta_outputTM(ifile, config, charge, multi, writemod, modred, writeecp, [],
writeclose, closelines, ifilelol)



#################################################################
### END OF SCRIPT
#################################################################
```

2.7 nTranslate-XXOutput-XXInput.py:

2.7.1 nTranslate-G0XOutput-G0XInput.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
from sys import *
import sys
import getopt
from EtaLibAtom import *

# ## --- Arguments --- ###
program = "nTranslate-G0XOutput-G0XInput.py"
#Grab the first argument from the command and use that as the snippet
try:
  snippet = sys.argv[1]
except IndexError:
  snippet = "-h"
#If help is wanted allow the skipping of a snippet
if snippet == "-h":
  argv.append("-h")
  argv.append("-h")
#If interactive mode is wanted allow the skipping of a snippet
if snippet == "-i":
  argv.append("-i")
  argv.append("-i")
#Unless the charge is stated via the -c argument the charge will be assumed
to be 0
charge = 0
chargeset = False
#Unless the multiplicity is stated via the -m argument the multiplicity will be
assumed to be 1
multi = 1
multiset = False
modred = []
writemod = 0
ionicCM = ""
ionicswitch = 0
debug = 0
interactive = 0
```

```
### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "c:m:dih", ["mod=", "ionic="])
except getopt.GetoptError:
  print program + " <snippet> -c <charge> -m <multiplicity> --
mod=\"constraint\" --ionic=reg/mno -d"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-c':
    charge = a
    chargeset = True
  elif o == '-m':
    multi = a
    multiset = True
  elif o == '-d':
    debug += 1
  elif o == '--mod':
    modred.append(a)
    writemod = 1
  elif o == '--ionic':
    ionicCM = a
    ionicswitch = 1
  elif o == '-i':
    interactive = 1
  elif o == '-h':
    print program + "' <snippet> -c <charge> -m <multiplicity> --
mod=\"constraint\" --ionic=reg/mno -d'"
    sys.exit(0)
  else:
    print("Usage: %s  <snippet> -c <charge> -m <multiplicity> --
mod=\"constraint\" --ionic=reg/mno -d" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print "Charge: " + str(charge)
  print "Multiplicity: " + str(multi)
  print "Snippet: " + snippet
  print "Modredundant Variable: "
  print modred
```

```
### --- OK Now setup the input variables for the first time --- ###
G0XInput = InputArguments()

#if interactive == 1:
#  G0XInput = Eta_interactiveConfig
#else:
#  #Grab the snippet information
#  G0XInput = Eta_parseSnippetG0X(snippet, G0XInput)

### --- Make NEWJOBS folder --- ###
if not os.path.exists("NEWJOBS.G0X"): os.makedirs("NEWJOBS.G0X")

### --- Open and parse the xyz files in the folder --- ###
print "Currently Translating:"
for i in os.listdir(os.getcwd()):
  if i.endswith(".log"):
    ifile = i
    print i

    if debug >= 2:
      print snippet

    #Parse XYZ file into a list of lists
    ifilelol, G0XInput.charge, G0XInput.multi = Eta_parseOutputG0X(ifile)

    ### Copy the charge, multi and modredundant lines to the G0XInput
    if len(modred) > 0:
      G0XInput.writemod = 1
    for line in modred:
      G0XInput.modred.append(line)
    if chargeset == True:
      print "YES"
      G0XInput.charge = charge
    if multiset == True:
      G0XInput.multi = multi

    ### --- Calculate charge from file --- ###
    if ionicswitch == 1:
      G0XInput.charge = Eta_ionic(ionicswitch, ionicCM, ifilelol)

    ### --- Generate the ECP list for files if needed --- ###
    if interactive == 0:
      G0XInput = Eta_parseSnippetG0X(snippet, G0XInput)
```

```
    if G0XInput.writeecp == 1:
      G0XInput.config, G0XInput.ecplines = Eta_G0XECP(G0XInput.ecp,
G0XInput.config, ifilelol)

    if G0XInput.writecloseecp == 1:
      G0XInput.closelines, G0XInput.closeecplines =
Eta_G0XECP(G0XInput.closeecp, G0XInput.closelines, ifilelol)

    ### --- Out put the G0X input files --- ###
    Eta_outputG0X(ifile, G0XInput, ifilelol)

    ### --- RESET THE VARIABLES --- ###
    G0XInput = Eta_resetInputVariables(G0XInput)


#################################################################
### END OF SCRIPT
#################################################################
```

2.7.2 nTranslate-JaguarOutput-JaguarInput.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

# ## --- Arguments --- ###
program = "nTranslate-XYZ-JaguarInput.py"
#Grab the first argument from the command and use that as the snippet
try:
  snippet = sys.argv[1]
except IndexError:
  snippet = "-h"
#If help is wanted allow the skipping of a snippet
if snippet == "-h":
  argv.append("-h")
  argv.append("-h")
#Unless the charge is stated via the -s argument the charge will be assumed
to be 0
charge = 0
#Unless the multiplicity is stated via the -m argument the multiplicity will be
assumed to be 1
multi = 1
modred = []
writemod = 0
ionicCM = ""
ionicswitch = 0
debug = 0


### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "c:m:dh", ["mod=", "ionic="])
except getopt.GetoptError:
  print program + " <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d"
  sys.exit(2)
###############################
```

```
# o == option
# a == argument passed to the o
##############################
for o, a in myopts:
  if o == '-c':
    charge = a
  elif o == '-m':
    multi = a
  elif o == '-d':
    debug += 1
  elif o == '--mod':
    modred.append(a)
    writemod = 1
  elif o == '--ionic':
    ionicCM = a
    ionicswitch = 1
  elif o == '-h':
    print program + ''' <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d'''
    sys.exit(0)
  else:
    print("Usage: %s  <snippet> -c <charge> -m <multiplicity> --mod
\"constraint\" --ionic=reg/mno -d" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print "Charge: " + charge
  print "Multiplicity: " + multi
  print "Snippet: " + snippet
  print "Modredundant Variable: "
  print modred

#Grab the snippet information
config, ecp, closelines, writeecp, writeclose = Eta_parseSnippet(snippet)

if debug >= 1:
  print "Configuration:"
  print config
  print "ECP Input: " + ecp
  print "Additional Lines: "
  print closelines

### --- Make NEWJOBS folder --- ###
if not os.path.exists("NEWJOBS.JAG"): os.makedirs("NEWJOBS.JAG")
```

```
### --- Open and parse the xyz files in the folder --- ###
print "Currently Translating:"
for i in os.listdir(os.getcwd()):
  if i.endswith(".out"):
    ifile = i
    print i
    #Parse XYZ file into a list of lists
    ifilelol, charge, multi = Eta_parseOutputJaguar(ifile)

    ### --- Calculate charge from file --- ###
    if ionicswitch == 1:
      charge = Eta_ionic(ionicswitch, ionicCM, ifilelol)

    ### --- Out put the G0X input files --- ###
    Eta_outputJaguar(ifile, config, charge, multi, writemod, modred, writeecp,
[], writeclose, closelines, ifilelol)


#################################################################
### END OF SCRIPT
#################################################################
```

2.8 nTranslate-XXOutput-SCREWER-XYZ.py:

2.8.1 nTranslate-G0XOutput-SCREWER-XYZ.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
import time
import shutil

### --- Arguments --- ###
program = "nTranslate-G0XOutput-SCREWER-XYZ.py"
ifile = ''
ofile = ''
allInDir = 0
trajectory = 0
geometry = 0
vibration = 1
negative = False
numAtoms = 0
finalenergy = 0
finalgeom = []
multiplyer = float(1.000)

#Grab the first argument from the command and use that as the input file
try:
  ifile = sys.argv[1]
except IndexError:
  ifile = "-h"
#If help is wanted allow the skipping of a input file
if ifile == "-h":
  argv.append("-h")
  argv.append("-h")
if ifile == "-d":
  argv.append("-d")
  argv.append("-d")
```

```
### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "dnv:m:h")
except getopt.GetoptError:
  print program + " <input file (G0X log)> -v (vib. number) -d (all in dir) -n
(negative vibration vectors) -m <multiplyer>"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-v':
    vibration = int(a)
  elif o == '-d':
    allInDir = 1
  elif o == '-n':
    negative = True
  elif o == '-m':
    multiplyer = float(a)
  elif o == '-h':
    print program + " <input file (G0X log)> -v (vib. number) -d (all in dir) -n
(negative vibration vectors) -m <multiplyer>"
    sys.exit(0)
  else:
    print("Usage: %s  <input file (G0X log)> -v (vib. number) -d (all in dir) -n
(negative vibration vectors) -m <multiplyer>" % sys.argv[0])
    sys.exit(0)

#Make SCREWERed directory
Eta_makeDir("SCREWERed")

def G0X_Screwer(ifile):
  #Print some information to the screen
  print "A new XYZ file will be generated from " + ifile
  print "and will be augmented by the vibrational frequency " + str(vibration) +
"."

  #Extract the last geometry from the G0X log file
  ifilelol, charge, multi = Eta_parseOutputG0X(ifile)

  #Grab the xyz changes for the SCREWERing and place them all into one big
list
  freqswitch = 0
```

```
  freqwrite = 0
  writecount = -1
  freqlist = []
  the_file = open(ifile, 'r')
  for idx, line in enumerate(the_file):
    #print line
    if line.strip() != '':
      if line.split()[0] == 'NAtoms=':
        numAtoms = int(line.split()[1])
      if 'Low frequencies' in line:
        freqswitch = 1
      elif line.split()[0] == 'Frequencies' and freqswitch == 1:
        for i in range(numAtoms * 3):
          freqlist.append(0.0000)
      elif line.split()[0] == 'Atom' and freqswitch == 1:
        freqwrite = 1
      elif freqwrite == 1:
        if len(line.split()) < 11:
          freqwrite = 0
          writecount = writecount + (numAtoms * 3)
        else:
          freqlist[writecount + int(line.split()[0]) + (numAtoms * 0)] = line.split()[2]
+ " " + line.split()[3] + " " + line.split()[4]
          freqlist[writecount + int(line.split()[0]) + (numAtoms * 1)] = line.split()[5]
+ " " + line.split()[6] + " " + line.split()[7]
          freqlist[writecount + int(line.split()[0]) + (numAtoms * 2)] = line.split()[8]
+ " " + line.split()[9] + " " + line.split()[10]

  #Generate ofile name
  ofiletmp = ifile.split(".")
  ofile = ""
  for i in range(len(ofiletmp)):
    if i != len(ofiletmp) - 1:
      ofile += ofiletmp[i] + "."
    elif i == len(ofiletmp) - 1:
      ofile += "xyz"
  print ifile + " ----> " + ofile
  #Move the X Y and Z coordinates with regard to the vibrational mode of
interest
  for i in range(2, len(ifilelol)):
    ifilelol[i].x = ifilelol[i].x + (multiplyer * float(freqlist[((vibration-1) * numAtoms)
+ i - 2].split()[0]))
    ifilelol[i].y = ifilelol[i].y + (multiplyer * float(freqlist[((vibration-1) * numAtoms)
+ i - 2].split()[1]))
```

```
    ifilelol[i].z = ifilelol[i].z + (multiplyer * float(freqlist[((vibration-1) * numAtoms)
+ i - 2].split()[2]))

  #Ouput the geometry(ies) to the ofile
  Eta_outputXYZ("SCREWERed/" + ofile, ifilelol)
  return

if negative == True:
  multiplyer = -1 * multiplyer
else:
  multiplyer = multiplyer


if allInDir == 1:
  for i in os.listdir(os.getcwd()):
    if i.endswith(".log"):
      ifile = i
      G0X_Screwer(ifile)
else:
  G0X_Screwer(ifile)


#################################################################
### END OF SCRIPT
#################################################################
```

2.9 NXT.PY:

2.9.1 nGT.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Arguments --- ###
program = "nGT.py"
#Grab the first argument from the command and use that as the snippet
try:
  logfile = sys.argv[1]
except IndexError:
  logfile = "-h"
#If help is wanted allow the skipping of a snippet
if logfile == "-h":
  argv.append("-h")
  argv.append("-h")
if logfile == "-a":
  argv.append("-a")
  argv.append("-a")
debug = 0
printType = "none"
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "dhlea")
except getopt.GetoptError:
  print program + " <log file> -d -a -e -l"
  sys.exit(2)
###############################
# o == option
# a == argument passed to the o
###############################
for o, a in myopts:
  if o == '-d':
```

```
    debug += 1
  elif o == '-l':
    printType = "long"
  elif o == '-e':
    printType = "extra"
  elif o == '-a':
    allInDir = 1
  elif o == '-h':
    print program + "' <log file> -d -a -e -l'"
    sys.exit(0)
  else:
    print("Usage: %s  <log file> -d -a -e -l" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print logfile
  printLines = Eta_TranslateG0XOutput(logfile, "translate", printType)
  for line in printLines:
    print line

try:
  if allInDir == 1:
    for i in os.listdir(os.getcwd()):
      if i.endswith(".log"):
        logfile = i
        print
"##################################################################
#################"
        printLines = Eta_TranslateG0XOutput(logfile, "translate", printType)
        for line in printLines:
          print line
  else:
    printLines = Eta_TranslateG0XOutput(logfile, "translate", printType)
    for line in printLines:
      print line
except:
  print "Something failed. Make sure the/a log file exists."

##################################################################
### END OF SCRIPT
##################################################################
```

2.9.2 nJT.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *


### --- Arguments --- ###
program = "nJT.py"
#Grab the first argument from the command and use that as the snippet
try:
  logfile = sys.argv[1]
except IndexError:
  logfile = "-h"
#If help is wanted allow the skipping of a snippet
if logfile == "-h":
  argv.append("-h")
  argv.append("-h")
if logfile == "-a":
  argv.append("-a")
  argv.append("-a")
debug = 0
printType = "none"
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "dhela")
except getopt.GetoptError:
  print program + " <log file> -d -e -l -a"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-d':
    debug += 1
```

```
  elif o == '-l':
    printType = "long"
  elif o == '-e':
    printType = "extra"
  elif o == '-a':
    allInDir = 1
  elif o == '-h':
    print program + "' <log file> -d -l -e -a'"
    sys.exit(0)
  else:
    print("Usage: %s  <log file> -d -l -e -a" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print logfile

try:
  if allInDir == 1:
    for i in os.listdir(os.getcwd()):
      if i.endswith(".out"):
        logfile = i
        print
"################################################################
#################"
        printLines = Eta_TranslateJaguarOutput(logfile, "translate", printType)
        for line in printLines:
          print line
  else:
    printLines = Eta_TranslateJaguarOutput(logfile, "translate", printType)
    for line in printLines:
        print line
except:
  print "Something failed. Make sure the/a log file exists."


################################################################
### END OF SCRIPT
################################################################
```

2.9.3 nTCT.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Arguments --- ###
program = "nTCT.py"
#Grab the first argument from the command and use that as the snippet
try:
  logfile = sys.argv[1]
except IndexError:
  logfile = "-h"
#If help is wanted allow the skipping of a snippet
if logfile == "-h":
  argv.append("-h")
  argv.append("-h")
if logfile == "-a":
  argv.append("-a")
  argv.append("-a")
debug = 0
printType = "none"
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "dhela")
except getopt.GetoptError:
  print program + " <log file> -d -l -e -a"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-d':
    debug += 1
  elif o == '-l':
```

```
    printType = "long"
  elif o == '-e':
    printType = "extra"
  elif o == '-a':
    allInDir = 1
  elif o == '-h':
    print program + "' <log file> -d -l -e -a'"
    sys.exit(0)
  else:
    print("Usage: %s  <log file> -d -l -e -a" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print logfile

try:
  if allInDir == 1:
    for i in os.listdir(os.getcwd()):
      if i.endswith(".log"):
        logfile = i
        print
"##############################################################
#################"
        printLines = Eta_TranslateTCOutput(logfile, "translate", printType)
        for line in printLines:
          print line
  else:
    printLines = Eta_TranslateTCOutput(logfile, "translate", printType)
    for line in printLines:
      print line
except:
  print "Something failed. Make sure the/a log file exists."


##############################################################
### END OF SCRIPT
##############################################################
```

2.9.4 nTMT.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Arguments --- ###
program = "nTMT.py"
#Grab the first argument from the command and use that as the snippet
try:
  logfile = sys.argv[1]
except IndexError:
  logfile = "-h"
#If help is wanted allow the skipping of a snippet
if logfile == "-h":
  argv.append("-h")
  argv.append("-h")
if logfile == "-a":
  argv.append("-a")
  argv.append("-a")
debug = 0
printType = "none"
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "dhela")
except getopt.GetoptError:
  print program + " <log file> -d -l -e -a"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-d':
    debug += 1
  elif o == '-l':
```

```
    printType = "long"
  elif o == '-e':
    printType = "extra"
  elif o == '-a':
    allInDir = 1
  elif o == '-h':
    print program + "' <log file> -d -l -e -a'"
    sys.exit(0)
  else:
    print("Usage: %s  <log file> -d -l -e -a" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print logfile

#try:
if allInDir == 1:
  for i in os.listdir(os.getcwd()):
    if i.endswith(".Turbomole"):
      for j in os.listdir(i):
        if j.endswith(".log"):
          logfile = i + "/" + j
          print
"#################################################################
#################"
          printLines = Eta_TranslateTMOutput(logfile, "translate", printType)
          for line in printLines:
            print line
else:
  printLines = Eta_TranslateTMOutput(logfile, "translate", printType)
  for line in printLines:
    print line
#except:
#  print "Something failed. Make sure the/a log file exists."


#################################################################
### END OF SCRIPT
#################################################################
```

2.10 nXList.py:

2.10.1 nGList.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *



print "-------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------
---"
print "SCF              ZPE         Internal       Enthalpy       Gibbs          Freq1
Freq2   NBasis PntGrp Stoichiometry       File Name     "
print "-------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------
---"

pwd = os.getcwd()
for i in os.listdir(pwd):
  if i.endswith(".log"):
    logfile = i
    printLines = Eta_TranslateG0XOutput(logfile, "list", "none")
    for line in printLines:
      print line

#################################################################
### END OF SCRIPT
#################################################################
```

2.10.2 nJList.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *


print "-------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------
---"
print "SCF             ZPE         Internal       Enthalpy       Gibbs         Freq1
Freq2   NBasis PntGrp Stoichiometry       File Name     "
print "-------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------
---"

pwd = os.getcwd()
for i in os.listdir(pwd):
  if i.endswith(".out"):
    logfile = i
    printLines = Eta_TranslateJaguarOutput(logfile, "list", "none")
    for line in printLines:
      print line

#################################################################
### END OF SCRIPT
#################################################################
```

2.10.3 nTCList.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *



print "-------------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------------
---"
print "SCF             ZPE         Internal       Enthalpy       Gibbs          Freq1
Freq2   NBasis PntGrp Stoichiometry       File Name     "
print "-------------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------------
---"

pwd = os.getcwd()
for i in os.listdir(pwd):
  if i.endswith(".log"):
    logfile = i
    printLines = Eta_TranslateTCOutput(logfile, "list", "none")
    for line in printLines:
      print line

#################################################################
### END OF SCRIPT
#################################################################
```

2.10.4 nTMList.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *


print "-------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------
---"
print "SCF             ZPE         Internal       Enthalpy       Gibbs         Freq1
Freq2   NBasis PntGrp Stoichiometry       File Name     "
print "-------------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------------
---"

pwd = os.getcwd()
for i in os.listdir(pwd):
  if i.endswith(".Turbomole"):
    for j in os.listdir(i):
      if j.endswith(".log"):
        logfile = i + "/" + j
        printLines = Eta_TranslateTMOutput(logfile, "list", "none")
        for line in printLines:
          print line



#############################################################
### END OF SCRIPT
#############################################################
```

2.11 nXArchive.py:

2.11.1 nGArchive.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Make NEWJOBS folder --- ###
if not os.path.exists("ARCHIVE"): os.makedirs("ARCHIVE")
if not os.path.exists("ARCHIVE/PUB"): os.makedirs("ARCHIVE/PUB")
if not os.path.exists("ARCHIVE/TABLE"): os.makedirs("ARCHIVE/TABLE")
f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
if not os.path.exists("ARCHIVE/XYZ"): os.makedirs("ARCHIVE/XYZ")
if not os.path.exists("ARCHIVE/JOBLOG"):
os.makedirs("ARCHIVE/JOBLOG")
if not os.path.exists("ARCHIVE/LOG"): os.makedirs("ARCHIVE/LOG")
if not os.path.exists("ARCHIVE/INPUT"): os.makedirs("ARCHIVE/INPUT")

pwd = os.getcwd()
#Archive each log file
for i in os.listdir(pwd):
  if i.endswith(".log"):
    basefile = i.replace(".log", "", 1)
    logfile = i
    print "Archiving " + basefile
    #Grab the final geometry and the translated output for the pub file
    finalgeom, charge, multi = Eta_parseOutputG0X(logfile)
    printLines, tableLines = Eta_TranslateG0XOutput(logfile, "archive", "none")
    #Output the pub files
    f = open("ARCHIVE/PUB/" + basefile + ".pub", "w")
    for line in printLines:
      if "GEOM DATA!" in line:
```

```
        for j in range(len(finalgeom)):
          #if j <= 1:
          #  print finalgeom[i]
          if j >= 2:
            f.write(Eta_getElementName(Eta_getElementNum(str(finalgeom[j].e)))
+ "      " + str(finalgeom[j].x) + "      " + str(finalgeom[j].y) + "      " +
str(finalgeom[j].z) + "\n")
      else:
        f.write(line + "\n")
    f.close()
    #Output the Table files
    for j, line in enumerate(tableLines):
      if j == 0:
        f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "a")
        f.write(line + "\n")
        f.close()
      elif j == 1:
        f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "a")
        f.write(line + "\n")
        f.close()
      elif j == 2:
        f = open("ARCHIVE/TABLE/Table-Energy-SCF.txt", "a")
        f.write(line + "\n")
        f.close()
    #Output the final geometry in xyz format
    Eta_outputXYZ("ARCHIVE/XYZ/" + basefile + ".xyz", finalgeom)


#################################################################
### END OF SCRIPT
#################################################################
```

2.11.2 nJArchive.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Make NEWJOBS folder --- ###
if not os.path.exists("ARCHIVE"): os.makedirs("ARCHIVE")
if not os.path.exists("ARCHIVE/PUB"): os.makedirs("ARCHIVE/PUB")
if not os.path.exists("ARCHIVE/TABLE"): os.makedirs("ARCHIVE/TABLE")
f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
if not os.path.exists("ARCHIVE/XYZ"): os.makedirs("ARCHIVE/XYZ")
if not os.path.exists("ARCHIVE/JOBLOG"):
os.makedirs("ARCHIVE/JOBLOG")
if not os.path.exists("ARCHIVE/LOG"): os.makedirs("ARCHIVE/LOG")
if not os.path.exists("ARCHIVE/INPUT"): os.makedirs("ARCHIVE/INPUT")

pwd = os.getcwd()
#Archive each log file
for i in os.listdir(pwd):
  if i.endswith(".out"):
    basefile = i.replace(".out", "", 1)
    logfile = i
    print "Archiving " + basefile
    #Grab the final geometry and the translated output for the pub file
    finalgeom, charge, multi = Eta_parseOutputG0X(logfile)
    printLines, tableLines = Eta_TranslateG0XOutput(logfile, "archive", "none")
    #Output the pub files
    f = open("ARCHIVE/PUB/" + basefile + ".pub", "w")
    for line in printLines:
      if "GEOM DATA!" in line:
        for j in range(len(finalgeom)):
          #if i <= 1:
```

```
        #  print finalgeom[i]
        if j >= 2:
          f.write(Eta_getElementName(Eta_getElementNum(str(finalgeom[j].e)))
+ "      " + str(finalgeom[j].x) + "      " + str(finalgeom[j].y) + "      " +
str(finalgeom[j].z) + "\n")
      else:
        f.write(line + "\n")
    f.close()
    #Output the Table files
    for j, line in enumerate(tableLines):
      if j == 0:
        f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "a")
        f.write(line + "\n")
        f.close()
      elif j == 1:
        f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "a")
        f.write(line + "\n")
        f.close()
      elif j == 2:
        f = open("ARCHIVE/TABLE/Table-Energy-SCF.txt", "a")
        f.write(line + "\n")
        f.close()
    #Output the final geometry in xyz format
    Eta_outputXYZ("ARCHIVE/XYZ/" + basefile + ".xyz", finalgeom)


#################################################################
### END OF SCRIPT
#################################################################
```

2.11.3 nTCArchive.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Make NEWJOBS folder --- ###
if not os.path.exists("ARCHIVE"): os.makedirs("ARCHIVE")
if not os.path.exists("ARCHIVE/PUB"): os.makedirs("ARCHIVE/PUB")
if not os.path.exists("ARCHIVE/TABLE"): os.makedirs("ARCHIVE/TABLE")
f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
if not os.path.exists("ARCHIVE/XYZ"): os.makedirs("ARCHIVE/XYZ")
if not os.path.exists("ARCHIVE/JOBLOG"):
os.makedirs("ARCHIVE/JOBLOG")
if not os.path.exists("ARCHIVE/LOG"): os.makedirs("ARCHIVE/LOG")
if not os.path.exists("ARCHIVE/INPUT"): os.makedirs("ARCHIVE/INPUT")

pwd = os.getcwd()
#Archive each log file
for i in os.listdir(pwd):
  if i.endswith(".log"):
    basefile = i.replace(".log", "", 1)
    logfile = i
    f = open(i, "r")
    for line in f:
      if 'Scratch directory:' in line:
        optimfile = line.split()[-1] + "/optim.xyz"
        f.close()
        break
    print "Archiving " + basefile
    #Grab the final geometry and the translated output for the pub file
    finalgeom = Eta_parseOptimTerachem(optimfile)
    printLines, tableLines = Eta_TranslateTCOutput(logfile, "archive", "none")
```

```
    #Output the pub files
    f = open("ARCHIVE/PUB/" + basefile + ".pub", "w")
    for line in printLines:
      if "GEOM DATA!" in line:
        for j in range(len(finalgeom)):
          #if j <= 1:
          #  print finalgeom[i]
          if j >= 2:
            f.write(Eta_getElementName(Eta_getElementNum(str(finalgeom[j].e)))
+ "      " + str(finalgeom[j].x) + "       " + str(finalgeom[j].y) + "       " +
str(finalgeom[j].z) + "\n")
      else:
        f.write(line + "\n")
    f.close()
    #Output the Table files
    for j, line in enumerate(tableLines):
      if j == 0:
        f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "a")
        f.write(line + "\n")
        f.close()
      elif j == 1:
        f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "a")
        f.write(line + "\n")
        f.close()
      elif j == 2:
        f = open("ARCHIVE/TABLE/Table-Energy-SCF.txt", "a")
        f.write(line + "\n")
        f.close()
    #Output the final geometry in xyz format
    Eta_outputXYZ("ARCHIVE/XYZ/" + basefile + ".xyz", finalgeom)


#################################################################
### END OF SCRIPT
#################################################################
```

2.11.4 nTMArchive.py

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Make NEWJOBS folder --- ###
if not os.path.exists("ARCHIVE"): os.makedirs("ARCHIVE")
if not os.path.exists("ARCHIVE/PUB"): os.makedirs("ARCHIVE/PUB")
if not os.path.exists("ARCHIVE/TABLE"): os.makedirs("ARCHIVE/TABLE")
f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "w")
f.write("File_Name,SCF,ZPE,T*S,H,G,dG(Hart),dG(kcal/mol)\n")
f.close()
if not os.path.exists("ARCHIVE/XYZ"): os.makedirs("ARCHIVE/XYZ")
if not os.path.exists("ARCHIVE/JOBLOG"):
os.makedirs("ARCHIVE/JOBLOG")
if not os.path.exists("ARCHIVE/LOG"): os.makedirs("ARCHIVE/LOG")
if not os.path.exists("ARCHIVE/INPUT"): os.makedirs("ARCHIVE/INPUT")

pwd = os.getcwd()
#Go into each Turbomole folder
for i in os.listdir(pwd):
  if i.endswith(".Turbomole"):
    #Archive each log file
    for j in os.listdir(i):
      if j.endswith(".log"):
        #Get the basename for the logfile
        basefile = j.replace(".log", "", 1)
        logfile = i + "/" + j
        print "Archiving " + basefile
        #Grab the final geometry and the translated output for the pub file
        finalgeom, charge, multi = Eta_parseOutputTM(logfile)
        printLines, tableLines = Eta_TranslateTMOutput(logfile, "archive",
"none")
        #Output the pub files
```

```
        f = open("ARCHIVE/PUB/" + basefile + ".pub", "w")
        for line in printLines:
          if "GEOM DATA!" in line:
            for k in range(len(finalgeom)):
              #if k <= 1:
              #  print finalgeom[i]
              if k >= 2:

f.write(Eta_getElementName(Eta_getElementNum(str(finalgeom[k].e))) + "
" + str(finalgeom[k].x) + "      " + str(finalgeom[k].y) + "      " +
str(finalgeom[k].z) + "\n")
          else:
            f.write(line + "\n")
        f.close()
        #Output the Table files
        for k, line in enumerate(tableLines):
          if k == 0:
            f = open("ARCHIVE/TABLE/Table-Energy-Equationed.txt", "a")
            f.write(line + "\n")
            f.close()
          elif k == 1:
            f = open("ARCHIVE/TABLE/Table-Energy-Totals.txt", "a")
            f.write(line + "\n")
            f.close()
          elif j == 2:
            f = open("ARCHIVE/TABLE/Table-Energy-SCF.txt", "a")
            f.write(line + "\n")
            f.close()
        #Output the final geometry in xyz format
        Eta_outputXYZ("ARCHIVE/XYZ/" + basefile + ".xyz", finalgeom)


#################################################################
### END OF SCRIPT
#################################################################
```

3. PSIENTIFIC SCRIPTS:

3.1 NDEPROTONATE.PY:

```
#! /usr/bin/env python2.7

###### LICENSE ######

#Eta_Scripts default imports
import os
import math
from sys import *
import sys
import getopt
from decimal import *
import shutil
from EtaLibAtom import *
from EtaNUMPYLib import *

#Script specific imports
from itertools import *
import time

### --- Arguments --- ###
program = "nDeprotonate.py"
ifile = ''
ofile = ''
verbose = 0
debug = 0
template = 0
start_time = time.time()


# Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:p:hvtdD")
except getopt.GetoptError:
  print program + " -i <inputfile.map>"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-i':
```

```
    ifile = a
  elif o == '-p':
    deprotonations = int(a)
  elif o == '-h':
    print program + "-i <inputfile.map>"
    sys.exit(0)
  elif o == '-v':
    verbose = 1
  elif o == '-d':
    debug = 1
  elif o == '-D':
    debug = 2
  elif o == '-t':
    template = 1
  else:
    print("Usage: %s -i inputfile.map" % sys.argv[0])
    sys.exit(0)

if template == 1:
  print "#Input file name"
  print "input = .xyz"
  print "#Output folder and name"
  print "output = "
  print "#Number of deprotonations"
  print "deprotonations = 1"
  print "#Protons to delete"
  print "$PROTONS"
  print "4 6     <-- Hydrogens 4 and 6 are equivalent"
  print "8 9 10  <-- Hydrogens 8 9 & 10 are equivalent"
  print "$ENDPROTONS"
  sys.exit(0)

### --- Open input file and parse into variable --- ###
f = open(ifile)
inputList = f.readlines()
f.close()

protonSwitch = "off"
protons = []
protonsTemp = []
symDifProtons = 0
totalProtons = 0
protonsList = []
```

```
for var in inputList:
  line = var.split()
  if line[0] == "$PROTONS":
    protonSwitch = "on"
  if line[0] == "$ENDPROTONS":
    protonSwitch = "off"
  elif line[0] == "input":
    parentFile = line[2]
  elif line[0] == "output":
    outputFolder = line[2]
  elif line[0] == "deprotonations":
    deprotonations = int(line[2])
  if protonSwitch == "on":
    if line[0][0] != "$" and line[0][0] != "#":
      for i in range(len(line)):
        protonsList.append(int(line[i]))
        protonsTemp.append(int(line[i]))
        totalProtons = totalProtons + 1
      symDifProtons = symDifProtons + 1
      protons.append(list(protonsTemp))
      protonsTemp[:] = []

### --- Script specific functions --- ###
##################################################################
####################

### --- get the error of two different numbers --- ###
def getErrorDist(a, b):
  error = ((a + b) / 2 / deprotonations) * 0.10
  #print "DIST"
  #print str((a+b)/2) + " " + str(abs(a-b)) + " " + str(error)
  return error


def getErrorDih(a, b):
  error = ((a + b) / 2 / deprotonations) * 0.10
  #print "DIH"
  #print str((a+b)/2) + " " + str(abs(a-b)) + " " + str(error)
  return error

### --- if all the items in a list are the same return true --- ###
def all_same(items):
  return all(x == items[0] for x in items)
```

```
### --- "find" a target item in a list and return the index --- ###
def find(target, listoi):
  for i, lst in enumerate(listoi):
    for j, item in enumerate(lst):
      if item == target:
        return (i, j)
  return (None, None)

##############################################################
####################

### --- Make the output folder --- ###
Eta_makeDir(outputFolder)

### --- Open parent file --- ###
ifilelol = Eta_XYZ_LOL(parentFile)

### --- Get bonds --- ###
covBonds = []
covHBonds = []
covTMBonds = []
nearestNeighbor = []
neighborStart = [0, 1000000]

### --- Generate bond lists --- ###
for i in range(0, int(ifilelol[0])):
  nearestNeighbor.append(list(neighborStart))
  for j in range(0, int(ifilelol[0])):
    if i != j:
      distij = Eta_getdistance(i + 2, j + 2, ifilelol)
      if j > i:
        if distij <= 2.25 and ifilelol[i + 2].e != 1 and ifilelol[j + 2].e != 1 and (
          (ifilelol[i + 2].e.lower() not in elementLarge) or (
          ifilelol[j + 2].e.lower() not in elementLarge)):
          ifilelol[i + 2].neighbors.append(j + 1)
          ifilelol[j + 2].neighbors.append(i + 1)
          ifilelol[i + 2].neighborsdist.append(distij)
          ifilelol[j + 2].neighborsdist.append(distij)
        elif distij <= 3 and ((ifilelol[i + 2].e.lower() in elementLarge) and (
          ifilelol[j + 2].e.lower() in elementLarge)):
          ifilelol[i + 2].neighbors.append(j + 1)
          ifilelol[j + 2].neighbors.append(i + 1)
          ifilelol[i + 2].neighborsdist.append(distij)
          ifilelol[j + 2].neighborsdist.append(distij)
```

```
        elif distij <= 1.3 and (ifilelol[i + 2].e == 1 or ifilelol[j + 2].e == 1):
          ifilelol[i + 2].neighbors.append(j + 1)
          ifilelol[j + 2].neighbors.append(i + 1)
          ifilelol[i + 2].neighborsdist.append(distij)
          ifilelol[j + 2].neighborsdist.append(distij)
  ifilelol[i + 2].nearest = ifilelol[i + 2].neighbors[0]
  for k in range(len(ifilelol[i + 2].neighbors) - 1):
    if ifilelol[i + 2].neighborsdist[k] > ifilelol[i + 2].neighborsdist[k + 1]:
      ifilelol[i + 2].nearest = ifilelol[i + 2].neighbors[k + 1]

### --- Algorythm to find all the possible and chemically relavent combinations
--- ###
### --- Generate all combinations WITHOUT replacements --- ###
permutationsList = list(combinations(protonsList, deprotonations))
#print "permutationsList list:"
#print permutationsList

# Permutations time elapsed
elapsed_time = time.time() - start_time
print "Permutations time elapsed: " + str(elapsed_time)

### --- Setup the lists for holding all the data --- ###
permutationsListofIndex = []
permutationsListofIndexAndLast = []
permutationsDuplicates = []
permutationsDeduplicated = []

### --- Iterate through the list of permutations and build an index identifier list
and and index plus last atom number list --- ###
a_list = []
for i in range(0, len(permutationsList)):
  if debug == 1 and float(i) * 100 % len(permutationsList) == 0:
    print "Building permutations list " + str(float(i) / len(permutationsList) * 100)
+ " %"
  for j in range(0, len(permutationsList[i])):
    #Bring back the list index for the list of list number What index is 5 in?
    a_list.append(find(permutationsList[i][j], protons)[0])
  #Append the new list to the permutationsListofIndex list
  permutationsListofIndex.append(list(a_list))
  #Append the last atom number to the list
  a_list.append(permutationsList[i][len(permutationsList[i]) - 1])
  permutationsListofIndexAndLast.append(list(a_list))
  a_list[:] = []
  loiduplicate = 0
```

```
  ### --- Iterate through the identifiers and remove chemically duplicate
deprotonations --- ###
  for k in range(i):
    #             ### --- Check if the identifier lists are identical and remove one
and set the "list of index" (loi) duplicate switch --- ###
    #             if permutationsListofIndex[k] == permutationsListofIndex[i] and
permutationsListofIndex[k][-1] == permutationsListofIndex[i][0] and
loiduplicate == 0:
    #                     print str(permutationsList[k]) + " " +
str(permutationsList[i]) + " " + str(permutationsListofIndex[k]) + " " +
str(permutationsListofIndex[i])
    #                     loiduplicate = 1
    #                     #print "yes"
    #                     permutationsList[i] = [-1]
    #                     break
    #             ### --- Check if the identifier plus atom number lists are identical
and if not reset the "list of index" (loi) duplicate switch --- ###
    #             elif permutationsListofIndex[k] != permutationsListofIndex[i] :
    #                     loiduplicate = 0
    #                     #print "no"
    ### --- Check if the identifier plus atom number lists are identical  and
remove one--- ###
    if permutationsListofIndexAndLast[k] == permutationsListofIndexAndLast[i]:
      permutationsList[i] = [-1]
      break

#### --- Iterate through the identifiers and remove chemically duplicate
deprotonations --- ###
#for i in range(len(permutationsListofIndexAndLast)):
#       if debug == 1 and float(i) * 100 % len(permutationsList) == 0:
#               print "Parsing permutations list " +
str(float(i)/len(permutationsListofIndexAndLast)*100) + " %"
#       for j in range(i+1, len(permutationsListofIndexAndLast)):
#               ### --- Check if the identifier lists are identical and remove one
and set the "list of index" (loi) duplicate switch --- ###
#               if permutationsListofIndex[i] == permutationsListofIndex[j] and
permutationsListofIndex[i][-1] == permutationsListofIndex[i][0] and loiduplicate
== 0:
#                       print str(permutationsList[i]) + " " + str(permutationsList[j])
+ " " + str(permutationsListofIndex[i]) + " " + str(permutationsListofIndex[j])
#                       loiduplicate = 1
#                       #print "yes"
#                       permutationsList[j] = [-1]
```

```
#                 ### --- Check if the identifier plus atom number lists are identical
and remove one--- ###
#                 if permutationsListofIndexAndLast[i] ==
permutationsListofIndexAndLast[j]:
#                         permutationsList[j] = [-1]
#                         #print str(permutationsListofIndexAndLast[i]) + "\t" +
str(permutationsListofIndexAndLast[j])
#                 ### --- Check if the identifier plus atom number lists are identical
and if not reset the "list of index" (loi) duplicate switch --- ###
#                 elif permutationsListofIndex[i] != permutationsListofIndex[j] :
#                         loiduplicate = 0
#                         #print "no"
#print permutationsListofIndex
#print permutationsListofIndexAndLast
#print permutationsList
#print permutationsList

# Math dedup time elapsed
elapsed_time = time.time() - start_time
print "Math dedup time elapsed: " + str(elapsed_time)

### --- make a new deduplicated list without the removed list entries (those
which had [-1]) --- ###
permutationsDeduplicatedNoGeom = [x for x in permutationsList if x != [-1]]

### --- List all the sums of distances and dihedrals for future removal of
degenerate deprotonations --- ###
if deprotonations > 1:
  geomdist = []
  geomdih = []
  for i in range(len(permutationsDeduplicatedNoGeom)):
    dist = 0
    dih = 0
    for j in range(len(permutationsDeduplicatedNoGeom[i])):
      if ifilelol[permutationsDeduplicatedNoGeom[i][j - 1] + 1].nearest + 1 !=
ifilelol[
            permutationsDeduplicatedNoGeom[i][j] + 1].nearest + 1:
        dih += Eta_getdihedral(permutationsDeduplicatedNoGeom[i][j - 1] + 1,
                    ifilelol[permutationsDeduplicatedNoGeom[i][j - 1] + 1].nearest
+ 1,
                    ifilelol[permutationsDeduplicatedNoGeom[i][j] + 1].nearest +
1,
                    permutationsDeduplicatedNoGeom[i][j] + 1, ifilelol)
      else:
```

```
        permutationsDeduplicatedNoGeom[i] = [-1]
        break
      dist += Eta_getdistance(permutationsDeduplicatedNoGeom[i][j - 1] + 1,
permutationsDeduplicatedNoGeom[i][j] + 1,
                        ifilelol)
    geomdist.append(dist)
    geomdih.append(dih)

  ### --- Look through the dist and dihedral lists and if they are within a cut-off
they are degenerate. --- ###
  for i in range(len(permutationsDeduplicatedNoGeom)):
    for k in range(i + 1, len(permutationsDeduplicatedNoGeom)):
      #if abs(geomdist[i-1] - geomdist[i]) <= getError(geomdist[i-1], geomdist[i])
and abs(geomdih[i-1] - geomdih[i]) <= getError(geomdih[i-1], geomdih[i]):
      #if abs(geomdist[i-1] - geomdist[i]) <= 0.05*deprotonations and
abs(geomdih[i-1] - geomdih[i]) <= 5*deprotonations:
      if abs(geomdist[i - 1] - geomdist[k - 1]) <= getErrorDist(geomdist[i - 1],
geomdist[k - 1]) and abs(
                geomdih[i - 1] - geomdih[k - 1]) <= getErrorDih(geomdih[i - 1],
geomdih[k - 1]):
        permutationsDeduplicatedNoGeom[k - 1] = [-1]
        geomdist[k - 1] = -1
        geomdih[k - 1] = -1
  geomdistDeduped = [x for x in geomdist if x != -1]
  geomdihDeduped = [x for x in geomdih if x != -1]

### --- Look to see that two hydrogens are not on the same oxegen --- ###
#         for i in range(len(permutationsDeduplicatedNoGeom)):
#                   if permutationsDeduplicatedNoGeom[i][0] != -1:
#                             if
ifilelol[permutationsDeduplicatedNoGeom[i][0]+1].nearest ==
ifilelol[permutationsDeduplicatedNoGeom[i][1]+1].nearest:
#                                       permutationsDeduplicatedNoGeom[j] = [-1]

### --- make a new deduplicated list without the removed list entries (those
which had [-1]) --- ###
permutationsDeduplicated = [x for x in permutationsDeduplicatedNoGeom if x
!= [-1]]

# Geom dedup time elapsed
elapsed_time = time.time() - start_time
print "Geom dedup time elapsed: " + str(elapsed_time)
```

```
### --- Print out data regarding the number of permutations (non degenerate
states) --- ###
print "Permutations (total: " + str(len(permutationsDeduplicated)) + ") for
deprotonated geometries:"
if verbose == 1:
  print permutationsDeduplicated
print "Output deprotonated files in " + str(outputFolder) + "."

### --- Output the permutations in xyz files --- ###
parentFileAtomNum = ifilelol[0]
newFileAtomNum = parentFileAtomNum - deprotonations
for i in range(0, len(permutationsDeduplicated)):
  newFileName = str(outputFolder) + "-" + str(deprotonations) + "-" + str(i +
1).zfill(
    len(str(len(permutationsDeduplicated)))) + ".xyz"
  f = open(outputFolder + "/" + newFileName, 'w+')
  f.write(str(newFileAtomNum) + "\n")
  f.write(str(newFileName) + "\n")
  if verbose == 1 or debug == 1:
    print "Permutation: " + str(i + 1)
    print "Removing atom(s): " + str(permutationsDeduplicated[i])
    if deprotonations > 1:
      print str(geomdistDeduped[i]) + " " + str(geomdihDeduped[i])
  linetemp = []
  for j in range(0, int(parentFileAtomNum)):
    if j + 1 not in permutationsDeduplicated[i]:
      linetemp.append(ifilelol[j + 2].e)
      linetemp.append(ifilelol[j + 2].x)
      linetemp.append(ifilelol[j + 2].y)
      linetemp.append(ifilelol[j + 2].z)
      line = '    '.join(str(e) for e in linetemp) + "\n"
      linetemp[:] = []
      f.write(line)
    else:
      if debug == 1:
        linetemp.append(ifilelol[j + 2].e)
        linetemp.append(ifilelol[j + 2].x)
        linetemp.append(ifilelol[j + 2].y)
        linetemp.append(ifilelol[j + 2].z)
        print '    '.join(str(e) for e in linetemp)
        linetemp[:] = []
  f.close()
# total time elapsed
elapsed_time = time.time() - start_time
```

```
print "Total time elapsed: " + str(elapsed_time)

#################################################################
### END OF SCRIPT
#################################################################
```

3.2 nDist-Int-Splitter.py:

```
#! /usr/bin/env python2.7

###### LICENSE ######

#Eta_Scripts default imports
import os
import math
from sys import *
import sys
import getopt
from decimal import *
import shutil
from EtaLibAtom import *
from EtaNUMPYLib import *

#Script specific imports
from itertools import *
import time

### --- Arguments --- ###
program = "nDist-Int-Splitter.py"
ifile = ''
ofile = ''
outputFolder = ''
parentFile = ''
verbose = 0
debug = 0
template = 0
start_time = time.time()
allInDir = 0

# Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:p:hvtdD")
except getopt.GetoptError:
  print program + " -i <inputfile.map> -d"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-i':
```

```
    ifile = a
  elif o == '-p':
    deprotonations = int(a)
  elif o == '-h':
    print program + "-i <inputfile.map>"
    sys.exit(0)
  elif o == '-v':
    verbose = 1
  elif o == '-d':
    allInDir = 1
  elif o == '-D':
    debug += 1
  elif o == '-t':
    template = 1
  else:
    print("Usage: %s -i inputfile.map" % sys.argv[0])
    sys.exit(0)

if template == 1:
  print "#Input file name"
  print "input = .xyz"
  print "#Output folder and name"
  print "output = "
  print "#Molecule sections"
  print "$SECTIONS       <-- Each line is it's own section"
  print "1 2 3 4 5 6     <-- Atoms 4 and 6 are one section"
  print "7-10            <-- Atoms 7 through 10 are a different section"
  print "$ENDSECTIONS"
  sys.exit(0)

### --- Open input file and parse into variable --- ###
f = open(ifile)
inputList = f.readlines()
f.close()

sectionSwitch = "off"
sections = []
sectionsTemp = []
totalSections = 0
lineTemp = []
sectionLine = []

for var in inputList:
  line = var.split()
```

```
  if line[0] == "$SECTIONS":
    sectionSwitch = "on"
  if line[0] == "$ENDSECTIONS":
    sectionSwitch = "off"
  elif line[0] == "input":
    parentFile = line[2]
  elif line[0] == "output":
    outputFolder = line[2]
  if sectionSwitch == "on":
    if line[0][0] != "$" and line[0][0] != "#":
      for i in line:
        lineTemp.append(i)
        #print i
      totalSections = totalSections + 1
      sectionsTemp.append(list(lineTemp))
      lineTemp[:] = []

### --- Expand upon the parentDeleteTemp list if
# there are certain characters to denote multiple atoms.
###
for i in range(len(sectionsTemp)):
  for j in range(len(sectionsTemp[i])):
    if "-" in str(sectionsTemp[i][j]):  #Use the '-' symbol to denote all atoms
between the former and latter
      line = str(sectionsTemp[i][j]).split('-')
      start = int(line[0])
      for k in xrange(int(line[0]), int(line[1]) + 1):
        #print k
        sectionLine.append(k)
    if "-" not in str(sectionsTemp[i][j]):  #If not one of the special symbols just
add it to the final list
      sectionLine.append(int(sectionsTemp[i][j]))
  sections.append(list(sectionLine))
  sectionLine[:] = []

#print sections

#### --- Script specific functions --- ###
##########################################################################
####################

### --- Print out some general data --- ###
print "Breaking up " + parentFile + " into " + str(len(sections)) + " sections with
atoms of:"
```

```
for i in range(len(sections)):
  line = ""
  for j in sections[i]:
    line += str(j) + " "
  print line
print "The output folder is: ./" + outputFolder
print
"###############################################################
######################"
#### --- Make the output folder --- ###
Eta_makeDir(outputFolder)

#### --- Open parent file --- ###
ifilelol = Eta_XYZ_LOL(parentFile)

### --- Algorythm to find all the possible section combinations --- ###
### --- Generate all combinations WITHOUT replacements!
### --- For instance if there are 3 or 4 sections to your molecule you
### --- need to grab all the single, doubles and possibly triples.
permutationsList = []
for i in range(len(sections)-1):
  permutationsListTemp = list(combinations(range(len(sections)), i+1))
  for i in permutationsListTemp:
    permutationsList.append(i)
#print "permutationsList list:"
#print permutationsList

### --- Output the permutations in xyz files --- ###
print "Building and writing file:"
for i in range(len(permutationsList)):
  ofile = ""
  for j in range(len(permutationsList[i])):
    #print permutationsList[i][j]
    ofile += "S" + str(permutationsList[i][j]+1) + "-"
  ofile += parentFile
  print ofile
  atomList = []
  for j in range(len(permutationsList[i])):
    #print sections[permutationsList[i][j]]
    for k in sections[permutationsList[i][j]]:
      atomList.append(k)
  #print atomList
  f = open(outputFolder + "/" + ofile, "w")
  f.write(str(len(atomList)) + "\n")
```

```
  f.write(ofile + "\n")
  for j in atomList:
    f.write(ifilelol[j+1].e + "  " + str("{:.6f}".format(ifilelol[j+1].x)) + "  " +
str("{:.6f}".format(ifilelol[j+1].y)) + "  " + str("{:.6f}".format(ifilelol[j+1].z)) + "\n")
  f.close()

#################################################################
### END OF SCRIPT
#################################################################
```

3.3 nTranslate-Change-Geom-XYZ.py:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *
from EtaNUMPYLib import *
from EtaLibPersistentOTS import *
from decimal import *
from numpy import *

### --- Arguments --- ###
program = "nTranslate-Change-Geom-XYZ.py"
debug = 0
ifile = ''
ofile = ''
printfile = 0
bond_angle_dihedral = []
newvalue = ''
allInDir = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:o:b:v:phd", ["bad=", "var="])
except getopt.GetoptError:
  print program + " -i <inputfile.xyz> -o <outputfile.zmat> -b or --
bad=<bond/angle/dihedral atom numbers>   -v or --newvalue=<new geometric
value> "
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-i':
    ifile = a
  elif o == '-o':
    ofile = a
  elif o == '--bad' or o == '-b':
```

```
    for item in a.split():
      bond_angle_dihedral.append(int(item))
  elif o == '--newvalue' or o == '-v':
    newvalue = a
  elif o == '-p':
    printfile = 1
  elif o == '-d':
    allInDir = 1
  elif o == '-D':
    debug += 1
  elif o == '-h':
    print program + " -i <inputfile.xyz> -o <outputfile.zmat> --
bad=<bond/angle/dihedral atom numbers>  --newvalue=<new geometric
value> "
    sys.exit(0)
  else:
    print("Usage: %s  -i <inputfile.xyz> -o <outputfile.zmat> --
bad=<bond/angle/dihedral atom numbers>  --newvalue=<new geometric
value> " % sys.argv[0])
    sys.exit(0)

print ifile + " ----> " + ofile

### --- OK Now setup the variables for the first time --- ###
POTS = PersistentOTS()

POTS.verbose = 1
POTS.joblog = "log"
POTS.debug = 0
POTS.finalGeomAtom = Eta_XYZ_LOL(ifile)

EtaPOTS_printgeom(POTS.finalGeomAtom)

#Change the bond/angle/dihedral of interest
if len(bond_angle_dihedral) == 2:
  POTS.scanType = "bond"
elif len(bond_angle_dihedral) == 3:
  POTS.scanType = "angle"
elif len(bond_angle_dihedral) == 4:
  POTS.scanType = "dihedral"

for i in range(len(bond_angle_dihedral)):
  POTS.atomList.append(int(bond_angle_dihedral[i]))
```

```
#Change the geometry for the next step
POTS = EtaPOTS_bondangledihedral(POTS)

EtaPOTS_printgeom(POTS.finalGeomAtom)
```

3.4 NMAP.PY:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from decimal import *
import shutil
from EtaLibAtom import *


### --- Arguments --- ###
program = "nMAP.py"
ifile = ''
ofile = ''
debug = 0
writeTemplateMap = 0
triangle = 0

# Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:tThD")
except getopt.GetoptError:
  print program + " -i <inputfile.map> -t <print out template map file> -T <only
build the triangle of the posible combinations>"
  sys.exit(2)
###############################
# o == option
# a == argument passed to the o
###############################
for o, a in myopts:
  if o == '-i':
    ifile = a
  elif o == '-D':
    debug += 1
  elif o == '-t':
    writeTemplateMap = 1
  elif o == '-T':
    triangle = 1
  elif o == '-h':
```

```
    print program + " -i <inputfile.map> -t <print out template map file> -T <only
build the triangle of the posible combinations>"
    sys.exit(0)
  else:
    print("Usage: %s -i inputfile.map -t <print out template map file> -T <only
build the triangle of the posible combinations>" % sys.argv[0])
    sys.exit(0)

if writeTemplateMap == 1:
  print "#Input file"
  print "parentFolder = "
  print "#Library folder to use"
  print "childFolder = "
  print "#Output folder"
  print "outputFolder = "
  print "#Base name for files"
  print "baseName = "
  print "#End name for files"
  print "endName = "
  print "#Quatfit location"
  print "quatfit = /opt/apps/Quatfit/quatfit"
  print "#List of atoms to align to"
  print "parent = "
  print "child = "
  print "weights = "
  print "#List of atoms to delete from the input (parent) file"
  print "deleteParent = "
  print "deleteChild = "
  sys.exit(0)

### Display input and output file name passed as the args
#print ("Input file : %s and output file: %s" % (ifile,ofile) )

### --- Open input settings file and parse into variable --- ###
f = open(ifile)
inputList = f.readlines()
f.close()

### --- Set up variables for the settings file --- ###
parentFolder = ''
childFolder = ''
outputFolder = ''
alignParent = []
alignChild = []
```

```
alignWeights = []
parentDelete = []
parentDeleteTemp = []
childDelete = []
childDeleteTemp = []
quatfit = "quatfit"
baseName = ''
endName = ""


### --- Parse line by line the settings file --- ###
for var in inputList:
  line = var.split()
  if line[0] == "parentFolder":
    parentFolder = str(line[-1])
  elif line[0] == "childFolder":
    childFolder = str(line[-1])
  elif line[0] == "outputFolder":
    outputFolder = str(line[-1])
  elif line[0] == "baseName":
    baseName = str(line[-1])
  elif line[0] == "endName":
    endName = str(line[-1])
  elif line[0] == "quatfit":
    quatfit = str(line[-1])
  elif line[0] == "parent":
    for i in range(len(line)):  #For multiple entries add them to a list
      if i >= 2:
        alignParent.append(line[i])
  elif line[0] == "child":
    for i in range(len(line)):
      if i >= 2:
        alignChild.append(line[i])
  elif line[0] == "weights":
    for i in range(len(line)):
      if i >= 2:
        alignWeights.append(line[i])
  elif line[0] == "deleteParent":
    for i in range(len(line)):
      if i >= 2:
        parentDeleteTemp.append(line[i])
  elif line[0] == "deleteChild":
    for i in range(len(line)):
      if i >= 2:
```

```
      childDeleteTemp.append(line[i])


### --- Expand upon the parentDeleteTemp list if
# there are certain characters to denote multiple atoms.
###
for i in range(len(parentDeleteTemp)):
  if "-" in str(parentDeleteTemp[i]):  #Use the '-' symbol to denote all atoms
between the former and latter
    line = str(parentDeleteTemp[i]).split('-')
    start = int(line[0])
    for j in xrange(int(line[0]), int(line[1]) + 1):
      #print j
      parentDelete.append(j)
  if "-" not in str(parentDeleteTemp[i]):  #If not one of the special symbols just
add it to the final list
    parentDelete.append(int(parentDeleteTemp[i]))
for i in range(len(childDeleteTemp)):
  if "-" in str(childDeleteTemp[i]):  #Use the '-' symbol to denote all atoms
between the former and latter
    line = str(childDeleteTemp[i]).split('-')
    start = int(line[0])
    for j in xrange(int(line[0]), int(line[1]) + 1):
      #print j
      childDelete.append(j)
  if "-" not in str(childDeleteTemp[i]):  #If not one of the special symbols just
add it to the final list
    childDelete.append(int(childDeleteTemp[i]))


### --- Make the output folder --- ###
Eta_makeDir(outputFolder)
Eta_makeDir(outputFolder + "/temp")


### --- Make the align files for quatfit. --- ###
if len(alignWeights) < len(alignParent):
  for i in range(len(alignParent)):
    alignWeights.append(1)
f = open(outputFolder + "/align.txt", "w+")
f.write(str(len(alignParent)) + "\n")
for i in range(len(alignParent)):
```

```
  linetemp = str(alignParent[i]) + " " + str(alignChild[i]) + " " +
str(alignWeights[i]) + "\n"  #ie. 3 4 1 (atoms 3 and 4 will be aligned with a
weight of 1)
  f.write(linetemp)
f.close()
f = open(outputFolder + "/alignparent.txt", "w+")
f.write(str(len(alignParent)) + "\n")
for i in range(len(alignParent)):
  linetemp = str(alignParent[i]) + " " + str(alignParent[i]) + " " +
str(alignWeights[i]) + "\n"  #ie. 3 4 1 (atoms 3 and 4 will be aligned with a
weight of 1)
  f.write(linetemp)
f.close()


### --- Align the parent files before aligning the substrates to them --- ###
### Purely for aesthetics and does not change the final outcome
mainParent = ""
print "Aligning parent strutures:"
for aF in os.listdir(parentFolder):
  if aF.endswith(".xyz"):
    parentFile = parentFolder + "/" + aF
    if mainParent == "":
      mainParent = parentFile
    else:
      print "Aligning " + parentFile + " to " + mainParent
      os.system(quatfit + " -r" + mainParent + " -f " + parentFile + " -p " +
outputFolder + "/alignparent.txt -o "+ parentFile + ".tmp >/dev/null")
      shutil.move(parentFile + ".tmp", parentFile)


### --- If the parents and children are the same or triangle is enforced only
run the triangle of matches --- ###
if parentFolder == childFolder or triangle == 1:
  print "Running only the triangle TRIANGLE!"
  ### --- Iterating through the parent files in the parent folder and children files
in the children folder making lists --- ###
  parentFileList = []
  childFileList = []
  for pF in os.listdir(parentFolder):
    if pF.endswith(".xyz"):
      parentFileList.append(parentFolder + "/" + pF)
  for cF in os.listdir(childFolder):
    if cF.endswith(".xyz"):
```

```
      childFileList.append(cF)
  ### --- Iterate through the lists just made and align and merge them
  for i in range(len(parentFileList)):
    parentFile = parentFileList[i]
    parentfilelol = Eta_XYZ_LOL(parentFile)
    for j in range(i, len(childFileList)):
      childFile = childFileList[j]
      childFileTemp = outputFolder + "/temp/" + childFile

      print "Aligning " + parentFile + " and " + childFile
      ### Running program outside the script. ###
      if debug == 1:
        os.system(
          quatfit + " -r" + parentFile + " -f " + childFolder + "/" + childFile + " -p " +
outputFolder
          + "/align.txt -o " + childFileTemp)
        print
"++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++"
      else:
        os.system(
          quatfit + " -r" + parentFile + " -f " + childFolder + "/" + childFile + " -p " +
outputFolder
          + "/align.txt -o " + childFileTemp + " >/dev/null")

      ### --- Open child library file and input each line into a list --- ###
      libfilelol = Eta_XYZ_LOL(childFileTemp)

      ### --- Get new file length --- ###
      newFileAtomNum = int(parentfilelol[0]) + int(libfilelol[0]) - len(parentDelete)
- len(childDelete)
      if baseName == "":
        if endName == "":
          newFileName = ''.join(parentfilelol[1]) + "-" + ''.join(libfilelol[1]) + ".xyz"
        else:
          newFileName = ''.join(parentfilelol[1]) + "-" + ''.join(libfilelol[1]) + "-" +
endName + ".xyz"
      else:
        if endName == "":
          newFileName = baseName + "-" + ''.join(parentfilelol[1]) + "-" +
''.join(libfilelol[1]) + ".xyz"
        else:
          newFileName = baseName + "-" + ''.join(parentfilelol[1]) + "-" + ''.join(
            libfilelol[1]) + "-" + endName + ".xyz"
```

```
      print "Exporting " + newFileName
      ### --- Output file WITHOUT parentDelete atoms and with the childFile
atoms --- ###
      f = open(outputFolder + "/" + newFileName, 'w+')
      f.write(str(newFileAtomNum) + "\n")
      f.write(str(newFileName)[:-4] + "\n")
      for i in range(0, int(parentfilelol[0])):
        if i + 1 not in parentDelete:
          linetemp = parentfilelol[i + 2].e + "  " + str("{:.6f}".format(parentfilelol[i +
2].x)) + "  " + str("{:.6f}".format(parentfilelol[i + 2].y)) + "  " +
str("{:.6f}".format(parentfilelol[i + 2].z)) + "\n"
          #linetemp = '     '.join(str(e) for e in parentfilelol[i + 2]) + "\n"
          f.write(linetemp)
      for i in range(0, int(libfilelol[0])):
        if i + 1 not in childDelete:
          linetemp = libfilelol[i + 2].e + "  " + str("{:.6f}".format(libfilelol[i + 2].x)) + "
" + str("{:.6f}".format(libfilelol[i + 2].y)) + "  " + str("{:.6f}".format(libfilelol[i +
2].z)) + "\n"
          #linetemp = '     '.join(str(e) for e in libfilelol[i + 2]) + "\n"
          f.write(linetemp)
      f.close()


##############################################

else:
  for pF in os.listdir(parentFolder):
    if pF.endswith(".xyz"):
      parentFile = parentFolder + "/" + pF
      ### --- Iterating through a folder of files --- ###
      for i in os.listdir(childFolder):
        if i.endswith(".xyz"):
          childFile = i
          print "Aligning " + pF + " and " + i
          ### Running program outside the script. ###
          if debug == 1:
            os.system(
              quatfit + " -r" + parentFile + " -f " + childFolder + "/" + childFile + " -p "
+ outputFolder
              + "/align.txt -o " + outputFolder + "/temp/" + childFile)
            print
"++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++"
          else:
```

```
          os.system(
            quatfit + " -r" + parentFile + " -f " + childFolder + "/" + childFile + " -p "
+ outputFolder
            + "/align.txt -o " + outputFolder + "/temp/" + childFile + " >/dev/null")

    ### --- Open parent file and input each line into a list --- ###
    parentfilelol = Eta_XYZ_LOL(parentFile)

    ### --- Iterating through a folder of files --- ###
    for i in os.listdir(outputFolder + "/temp"):
      if i.endswith(".xyz"):
        childFile = outputFolder + "/temp/" + i
        #print childFile
        ### --- Open child library file and input each line into a list --- ###
        libfilelol = Eta_XYZ_LOL(childFile)
        ### --- Get new file length --- ###
        newFileAtomNum = int(parentfilelol[0]) + int(libfilelol[0]) -
len(parentDelete) - len(childDelete)
        if baseName == "":
          if endName == "":
            newFileName = ''.join(parentfilelol[1]) + "-" + ''.join(libfilelol[1]) + ".xyz"
          else:
            newFileName = ''.join(parentfilelol[1]) + "-" + ''.join(libfilelol[1]) + "-" +
endName + ".xyz"
        else:
          if endName == "":
            newFileName = baseName + "-" + ''.join(parentfilelol[1]) + "-" +
''.join(libfilelol[1]) + ".xyz"
          else:
            newFileName = baseName + "-" + ''.join(parentfilelol[1]) + "-" + ''.join(
              libfilelol[1]) + "-" + endName + ".xyz"
        print "Exporting " + newFileName
        ### --- Output file WITHOUT parentDelete atoms and with the childFile
atoms --- ###
        f = open(outputFolder + "/" + newFileName, 'w+')
        f.write(str(newFileAtomNum) + "\n")
        f.write(str(newFileName)[:-4] + "\n")
        for i in range(0, int(parentfilelol[0])):
          if i + 1 not in parentDelete:
            linetemp = parentfilelol[i + 2].e + "  " + str("{:.6f}".format(parentfilelol[i
+ 2].x)) + "  " + str("{:.6f}".format(parentfilelol[i + 2].y)) + "  " +
str("{:.6f}".format(parentfilelol[i + 2].z)) + "\n"
            #linetemp = '     '.join(str(e) for e in parentfilelol[i + 2]) + "\n"
            f.write(linetemp)
```

```
        for i in range(0, int(libfilelol[0])):
          if i + 1 not in childDelete:
            linetemp = libfilelol[i + 2].e + "  " + str("{:.6f}".format(libfilelol[i + 2].x))
+ "  " + str("{:.6f}".format(libfilelol[i + 2].y)) + "  " + str("{:.6f}".format(libfilelol[i +
2].z)) + "\n"
            #linetemp = '     '.join(str(e) for e in libfilelol[i + 2]) + "\n"
            f.write(linetemp)
        f.close()


#################################################################
### END OF SCRIPT
#################################################################
```

3.5 nPERSISTENTOTS.PY:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from decimal import *
import shutil
from EtaLibAtom import *
from EtaNUMPYLib import *
from EtaLibPersistentOTS import *

### --- Arguments --- ###
program = "nPersistentOTS.py"
inputfile = ''
outfile = ''
jobname = ''
pwdirectory = ''
jobtype = ''
QMtype = ''
path2QM = ''
cpus = 1
debug = 0
test = 0
maketemplate = False

### --- OK Now setup the variables for the first time --- ###
#EtaPOTS_resetVariables()
POTS = PersistentOTS()

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "i:o:n:d:t:j:p:c:hDTv", ["template"])
except getopt.GetoptError:
  print program + " -i <input file> -o <output file> -n <job name> -d <directory>
-t <QM code> -j <job type> -p <path to QM code> -h (print help)"
  sys.exit(2)
###############################
# o == option
# a == argument passed to the o
```

```
################################
for o, a in myopts:
  if o == '-i':
    POTS.inputfile = a
  elif o == '-o':
    POTS.outfile = a
  elif o == '-n':
    POTS.jobname = a
  elif o == '-d':
    POTS.pwdirectory = a
  elif o == '-t':
    POTS.QMtype = a
  elif o == '-j':
    POTS.jobtype = a
  elif o == '-p':
    POTS.path2QM = a
  elif o == '-c':
    cpus = a
  elif o == '-D':
    POTS.debug += 1
  elif o == '-T':
    POTS.test = 1
  elif o == '-v':
    POTS.verbose = 1
  elif o == '--template':
    maketemplate = True
  elif o == '-h':
    print program + " -idjtjphD"
    print "-----------------------------------------------------------------------------------------------
--------------------"
    print "       -i       (H2O.com)          | Input file."
    print "                                   |   For Turbomole jobs you will
specify the define input file."
    print "                                   |   For Gaussian jobs you will specify
the .com/.inp file."
    print "                                   |   For Terachem jobs you will
specify the configuration file."
    print "                                   | "
    print "       -o       (H2O.log)          | Output file."
    print "                                   |   Usually the .log or .out file."
    print "                                   | "
    print "       -n       (H2O)              | Job name. "
    print "                                   |   Needs to be unique from other
jobs in the same directory."
```

```
   print "                                    l   All outputs will have this string in
their names."
   print "                                    l"
   print "       -d       (/home/user/H2O_OPT)    l Directory where files will be
saved/updated."
   print "                                    l   If you are running the job on a
cluster, this can be the originating "
   print "                                    l   folder of the input and output files.
This way updates can be "
   print "                                    l   propogated from the node's local
drive every iteration of the job."
   print "                                    l "
   print "       -t       (G09)               l QM code used (Gaussian
(G03/G09), Turbomole (TM), Terachem (TC))"
   print "                                    l   Indicating the type of QM code
used allows for correct parsing of "
   print "                                    l   output and input files."
   print "                                    l"
   print "       -j       (OPT)               l Job type (OPT, SCAN, TS-SCAN)"
   print "                                    l   OPT: "
   print "                                    l   Run subsequent iterations of the
input file while updating "
   print "                                    l   the geometry. Useful for very long
or difficult optimizations."
   print "                                    l   SCAN: "
   print "                                    l   In conjunction with a 'Scan'
configuration file, this will"
   print "                                    l   run subsequent positionally
restrained optimizations (POPT)"
   print "                                    l   until the number of steps has
been fulfilled."
   print "                                    l   TS-SCAN: "
   print "                                    l   In conjunction with a 'Scan'
configuration file, this will"
   print "                                    l   run subsequent positionally
restrained optimizations (POPT)"
   print "                                    l   with added logic to take smaller
scanning step sizes and "
   print "                                    l   the ability to reverse the direction
of the scan to find the "
   print "                                    l   optimal input geometry for a TS
search."
   print "                                    l   "
   print "       -p       (/share/apps/Gaussian)    l Path to the QM code"
```

```
    print "                                        |    "
    print "        -h                              | Print this help screen"
    print "                                        | "
    print "-------------------------------------------------------------------------------------------
--------------------"
    print "Example: " + program + " -i H2O.com -o H2O.log -n H20 -d
/home/user/H2O_OPT -t G09 -j OPT -p /share/apps/Gaussian"
    sys.exit(0)
  else:
    print(
    "Usage: %s -i <input file> -o <output file> -n <job name> -d <directory> -t
<QM code> -j <job type> -p <path to QM code> -h (print help)" %
    sys.argv[0])
    sys.exit(0)

if maketemplate == True:
  EtaPOTS_makeTempScanFile(POTS)
  sys.exit(0)

##############################################################
########
### START OF SCRIPT
##############################################################
########
###Start off
POTS.kill = False
###Set up variables
POTS.baseinput = POTS.pwdirectory + "/" + POTS.inputfile
POTS.baselog = POTS.pwdirectory + "/" + POTS.outfile
POTS.joblog = POTS.pwdirectory + "/" + POTS.jobname + ".joblog"
POTS.scratchdir = POTS.pwdirectory + "/SCRATCH-" + POTS.jobname
POTS.trajectoryfile = POTS.scratchdir + "/TRAJECTORY-" + POTS.jobname
+ ".xyz"
POTS.scanfile = POTS.pwdirectory + "/Scan-" + POTS.jobname + ".txt"
POTS.outScanFile = POTS.pwdirectory + "/SCAN-" + POTS.jobname + ".xyz"
POTS.linearScanFile = POTS.scratchdir + "/LINEAR-SCAN-" +
POTS.jobname + ".xyz"

EtaPOTS_printWrite(["##############################################
#####################################",
                    "",
                    "                ***********************************************",
                    "                          nPersistentOTS.py",
                    "                ***********************************************",
```

```
            "",
            " Copyright (c) 2014, Thomas J. L. Mustard, O. Maduka Ogba,
Paul Ha-Yeon Cheong",
            "",
            "                        PHYC Group",
            "                  Oregon State University",
            "                    College of Science",
            "                  Department of Chemistry",
            "                     153 Gilbert Hall",
            "                    Corvallis OR, 97331",
            "              E-mail:  mustardt@onid.orst.edu",
            "                   Ph.  (541)-737-2081",
            "                http://phyc.chem.oregonstate.edu/",
            "",

"##################################################################
###################",
            "",
            "  All rights reserved.",
            "",
            "  Redistribution and use in source and binary forms, with or
without",
            "  modification, are permitted provided that the following
conditions are met:",
            "",
            "  * Redistributions of source code must retain the above
copyright notice, this",
            "    list of conditions and the following disclaimer.",
            "",
            "  * Redistributions in binary form must reproduce the above
copyright notice,",
            "    this list of conditions and the following disclaimer in the
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            "    and/or other materials provided with the distribution.",
            "",
            "  * Neither the name of the {organization} nor the names of its",
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            "    this software without specific prior written permission.",
            "",
            "  THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT
HOLDERS AND CONTRIBUTORS \"AS IS\"",
            "  AND ANY EXPRESS OR IMPLIED WARRANTIES,
INCLUDING, BUT NOT LIMITED TO, THE",
```

```
                "  IMPLIED WARRANTIES OF MERCHANTABILITY AND
FITNESS FOR A PARTICULAR PURPOSE ARE",
                "  DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT
HOLDER OR CONTRIBUTORS BE LIABLE",
                "  FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL,
EXEMPLARY, OR CONSEQUENTIAL",
                "  DAMAGES (INCLUDING, BUT NOT LIMITED TO,
PROCUREMENT OF SUBSTITUTE GOODS OR",
                "  SERVICES; LOSS OF USE, DATA, OR PROFITS; OR
BUSINESS INTERRUPTION) HOWEVER",
                "  CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER
IN CONTRACT, STRICT LIABILITY,",
                "  OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE)
ARISING IN ANY WAY OUT OF THE USE",
                "  OF THIS SOFTWARE, EVEN IF ADVISED OF THE
POSSIBILITY OF SUCH DAMAGE.",
                "",

"#############################################################
###################"], POTS.verbose, POTS.joblog)

###Start the loop
while POTS.kill == False:
  EtaPOTS_printWrite(["",
                  "QM used for job: " + str(POTS.QMtype),
                  "Type of job: " + str(POTS.jobtype),
                  ""], POTS.verbose, POTS.joblog)
  if debug >= 1:
    EtaPOTS_printWrite([POTS.baseinput,
                    POTS.baselog,
                    POTS.scratchdir,
                    POTS.trajectoryfile,
                    POTS.scanfile,
                    POTS.outScanFile], POTS.verbose, POTS.joblog)

#############################################################
########
  ### --- #Make required directories if needed --- ###
  if POTS.debug >= 1:
    EtaPOTS_printWrite(["makeDirectories"], POTS.verbose, POTS.joblog)
  Eta_makeDir(POTS.scratchdir)
  Eta_makeDir(POTS.scratchdir + "/Previous_Files")
```

```
##########################################################################
  ### --- Grab the last configuration from the input file --- ###
  if POTS.QMtype == "G09" or POTS.QMtype == "G03":
    POTS = EtaPOTS_parseInputG0X(POTS)
  elif POTS.QMtype == "Turbomole":
    EtaPOTS_printWrite(["Not sure what to due here.", POTS.verbose,
POTS.joblog])
  elif POTS.QMtype == "Terachem":
    EtaPOTS_printWrite(["Not sure what to due here.", POTS.verbose,
POTS.joblog])
  elif POTS.QMtype.upper() == "JAGUAR":
    POTS = EtaPOTS_parseInputJaguar(POTS)
  #Save the original configurations of the file
  if POTS.QMconfigORIG == []:
    for i in POTS.QMconfig:
      POTS.QMconfigORIG.append(i)
  if POTS.QMcommentORIG == '':
    POTS.QMcommentORIG = POTS.QMcomment
  if POTS.QMendlinesORIG == []:
    for i in POTS.QMendlines:
      POTS.QMendlinesORIG.append(i)

  if POTS.test != 1:
    ### Run the QM code ###
    ### G09
    if POTS.QMtype == "G09":
      EtaPOTS_printWrite(["Running G09"], POTS.verbose, POTS.joblog)
      try:
        os.system("g09 < " + POTS.baseinput + " > " + POTS.baselog)
      except getopt.GetoptError:
        EtaPOTS_printWrite(["Gaussian09 Failed!!!!"], POTS.verbose,
POTS.joblog)
    ### G03
    elif POTS.QMtype == "G03":
      EtaPOTS_printWrite(["Running G03"], POTS.verbose, POTS.joblog)
      try:
        os.system("g03 < " + POTS.baseinput + " > " + POTS.baselog)
      except getopt.GetoptError:
        EtaPOTS_printWrite(["Gaussian03 Failed!!!!"], POTS.verbose,
POTS.joblog)
    ### Turbomole
    elif POTS.QMtype == "Turbomole":
```

```
      EtaPOTS_printWrite(["Running Turbomole Jobex"], POTS.verbose,
POTS.joblog)
      try:
        os.system("jobex -ri -c 300 -v -outfile " + POTS.baselog)
      except getopt.GetoptError:
        EtaPOTS_printWrite(["Turbomole Failed!!!!"], POTS.verbose,
POTS.joblog)
    ### Terachem
    elif POTS.QMtype == "Terachem":
      EtaPOTS_printWrite(["Running Terachem"], POTS.verbose, POTS.joblog)
      try:
        os.system("/share/psw/TeraChem/hidden/RUN-TC.sh " +
POTS.baseinput + " >> " + POTS.baselog)
      except getopt.GetoptError:
        EtaPOTS_printWrite(["TeraChem Failed!!!!"], POTS.verbose,
POTS.joblog)
    ### Jaguar
    elif POTS.QMtype.upper() == "JAGUAR":
      EtaPOTS_printWrite(["Running Jaguar"], POTS.verbose, POTS.joblog)
      try:
        os.system("/export/apps/schrodinger2014-2/jaguar run -TPP " + cpus + "
-WAIT -HOST localhost " + POTS.baseinput + " >> " + POTS.baselog)
      except getopt.GetoptError:
        EtaPOTS_printWrite(["Jaguar Failed!!!!"], POTS.verbose, POTS.joblog)


#############################################################
########
  ### --- Grab the last geom from the output file --- ###
  if POTS.QMtype == "G09" or POTS.QMtype == "G03":
    #POTS.trajectoryGeomAtom, POTS.charge, POTS.multi =
Eta_parseOutputG0X_Traj(baselog)  #Parse log file for final geometry
    #POTS.QMconfig, POTS.QMendlines, POTS.charge, POTS.multi,
POTS.inputGeomAtom = Eta_parseInputG0X(baseinput)
    POTS = EtaPOTS_parseOutputG0X(POTS)  #Parse log file for final
geometry
    POTS = EtaPOTS_parseInputG0X(POTS)
  elif POTS.QMtype == "Turbomole":
    #POTS.trajectoryGeomAtom, POTS.charge, POTS.multi =
Eta_parseOutputTM_Traj(baselog)  #Parse log file for final geometry
    POTS = Eta_parseOutputTM_Traj(POTS)  #Parse log file for final geometry
  elif POTS.QMtype == "Terachem":
    #POTS.trajectoryGeomAtom = Eta_parseOptimTerachem_Traj(pwdirectory
+ TCscratchDir + "optim.xyz")  #Parse optim.xyz file for final geometry
```

```
    POTS = EtaPOTS_parseOptimTerachem_Traj(POTS)  #Parse optim.xyz
file for final geometry
  elif POTS.QMtype.upper() == "JAGUAR":
    POTS = EtaPOTS_parseOutputJaguar(POTS)
    POTS = EtaPOTS_parseInputJaguar(POTS)


#################################################################
########
  #Write the trajectory out
  Eta_outputXYZ_Traj(POTS.trajectoryfile, POTS.trajectoryGeomAtom)


#################################################################
########
  ###For OPT jobs
  #if POTS.jobtype == "OPT":

#################################################################
########
  ### --- Output a new input file for the next step in the scan --- ###
  if POTS.QMtype == "G09" or POTS.QMtype == "G03":
    #Decide what the next step should be
    POTS = EtaPOTS_OPTLogicG0X(POTS)
    #Move/convert files for the next computation
    #EtaPOTS_rebuildG0XCOM(POTS)
  elif POTS.QMtype == "Turbomole":
    #Decide what the next step should be
    EtaPOTS_printWrite(["OPT LOGIC HERE!"], POTS.verbose, POTS.joblog)
    POTS = EtaPOTS_OPTLogicTM(POTS)
    #output the fixed geometry
    #outputFixUnfixGeom(POTS.finalGeomAtom)
    #Move/convert files for the next computation
    #EtaPOTS_rebuildTurbomoleTMOL(POTS)
  elif POTS.QMtype == "Terachem":
    #Decide what the next step should be
    EtaPOTS_printWrite(["OPT LOGIC HERE!"], POTS.verbose, POTS.joblog)
    POTS = EtaPOTS_OPTLogicTC(POTS)
    #Move/convert files for the next computation
    #EtaPOTS_rebuildTerachemXYZ(POTS)
    ###For SCAN and TS-SCAN jobs
  elif POTS.QMtype.upper() == "JAGUAR":
    #Decide what the next step should be
    POTS = EtaPOTS_OPTLogicJaguar(POTS)
```

```
   #Move/convert files for the next computation
   #EtaPOTS_rebuildJaguarIN(POTS)

#################################################################
########
  if (POTS.jobtype == "SCAN" or POTS.jobtype == "TS-SCAN") and
POTS.optimized == True:
   if not os.path.isfile(POTS.scanfile):
     EtaPOTS_printWrite(["The scan file nessecary for both the SCAN and TS-
SCAN function does not exist.",
                  "Please include this file and submit again."], POTS.verbose,
POTS.joblog)
     sys.exit(0)
   #Parse the scan file and print out important information
   POTS = EtaPOTS_parseScanFile(POTS)
   POTS = EtaPOTS_generateMinTSSCANSize(POTS)
   EtaPOTS_printWrite(["Atoms to be moved: " + str(POTS.scanType) + "  " +
str(POTS.atomList)], POTS.verbose, POTS.joblog)
   #Update the second line for the SCAN file
   if POTS.scanType == "bond":
     POTS.finalGeomAtom[1] = POTS.finalGeomAtom[1] + "   Bond: " +
str(Eta_getdistance(POTS.atomList[0] + 1,
     POTS.atomList[1] + 1, POTS.finalGeomAtom))
   if POTS.scanType == "angle":
     POTS.finalGeomAtom[1] = POTS.finalGeomAtom[1] + "   Angle: " + str(
     Eta_getangle(POTS.atomList[0] + 1, POTS.atomList[1] + 1,
POTS.atomList[2] + 1, POTS.finalGeomAtom))
   if POTS.scanType == "dihedral":
     POTS.finalGeomAtom[1] = POTS.finalGeomAtom[1] + "   Dihedral: " + str(
     Eta_getdihedral(POTS.atomList[0] + 1, POTS.atomList[1] + 1,
POTS.atomList[2] + 1, POTS.atomList[3] + 1,
     POTS.finalGeomAtom))
   #Write last finalgeom to the SCAN xyz file
   EtaPOTS_writeFinalGeomtoSCAN(POTS)
   EtaPOTS_writeFinalGeomtoSCANLinear(POTS)
   #Decide what the next step should be
   POTS = EtaPOTS_scanTSLogic(POTS)
   ### Implemented in scanTSLogic so that the scan file is updated
   ##Change the geometry for the next step
   #POTS = EtaPOTS_bondangledihedral(POTS)
   #Delete the optimize files if they exist
   Eta_delFile(POTS.scratchdir + "/optenergies-" + POTS.jobname + ".txt")
   #Reset the configuration for the next scan step. This will hasten
optimization if a smaller step size was taken
```

```
    POTS.QMconfig = []
    POTS.QMendlines = []
    for line in POTS.QMconfigORIG:
      POTS.QMconfig.append(line)
    POTS.QMcomment = POTS.QMcommentORIG
    for line in POTS.QMendlinesORIG:
      POTS.QMendlines.append(line)


##############################################################
########
  ### --- Output a new input file for the next step in the OPT/(TS-)SCAN ---
###
  if POTS.QMtype == "G09" or POTS.QMtype == "G03":
    #Move/convert files for the next computation
    EtaPOTS_rebuildG0XCOM(POTS)
  elif POTS.QMtype == "Turbomole":
    #output the fixed geometry
    #outputFixUnfixGeom(unfixgeom)
    #Move/convert files for the next computation
    EtaPOTS_rebuildTurbomoleTMOL(POTS)
  elif POTS.QMtype == "Terachem":
    #Move/convert files for the next computation
    EtaPOTS_rebuildTerachemXYZ(POTS)
  elif POTS.QMtype.upper() == "JAGUAR":
    #Move/convert files for the next computation
    EtaPOTS_rebuildJaguarIN(POTS)

EtaPOTS_printWrite(["##############################################
#####################################"], POTS.verbose, POTS.joblog)
  ### --- RESET THE VARIABLES --- ###
  POTS = EtaPOTS_resetVariables(POTS)
  if POTS.test == 1:
    POTS.kill = True
EtaPOTS_printWrite(["====== END ======",
                    ""], POTS.verbose, POTS.joblog)

##############################################################
### END OF SCRIPT
##############################################################
```

4. ηTRASLATE SCRIPTS:

4.1 NSUBMIT.ALL.G09.CORE=2.PY:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
import math
from sys import *
import sys
import getopt
from EtaLibAtom import *


### --- Arguments --- ###
program = "Submit.All.G09.Core=6-GEN02.py"
#Grab the first argument from the command and use that as the snippet
try:
  inputfile = sys.argv[1]
except IndexError:
  inputfile = "all"
#If help is wanted allow the skipping of a snippet
if inputfile == "-h":
  argv.append("-h")
  argv.append("-h")
elif inputfile == "-d":
  argv.append("-d")
  argv.append("-d")
elif inputfile == "--hold":
  argv.append("--hold")
  argv.append("--hold")
debug = 0
hold = 0

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[2:], "dh", ["hold"])
except getopt.GetoptError:
  print program + " -d --hold"
  sys.exit(2)
###############################
# o == option
# a == argument passed to the o
```

```
##############################
for o, a in myopts:
  if o == '-d':
    debug += 1
  elif o == '--hold':
    hold = 1
  elif o == '-h':
    print program + '" -d --hold'"
    sys.exit(0)
  else:
    print("Usage: %s  -d --hold" % sys.argv[0])
    sys.exit(0)

if debug >= 1:
  print inputfile

############################################################
### --- Job settings --- ###
program = "G09"
nodeprocs = 48 #Number of procs on node
nodemem = 128000 #Total memory on node in MB
nproc = 2 #Number of procs to be used
memory = str(int(math.floor(nodemem/nodeprocs * nproc * 0.90)))
queue = "gen02" #Queue name
EtaDir = os.environ["ETADIR"]

header = EtaDir + "/SGE/headers/Femri.SMP.sget"
snippet = EtaDir + "/SGE/snippets/hidden/G09.sget"

############################################################

for i in os.listdir(os.getcwd()):
  if i.endswith(".com"):
    inputfile = i
    ### --- Get the 'basename' of the file --- ###
    #Assuming the input file ends with '.com'
    #basename = inputfile[::-1].replace('moc.', '')[::-1]
    basename = Eta_basename(inputfile, ".com")

    f = open(inputfile, "r")
    ifileList = f.readlines()
    f.close()

    deleteList = []
```

```
    for i, line in enumerate(ifileList):
      if "%chk=" in line:
        ifileList[i] = "DELETE"
      elif "%nproc=" in line:
        ifileList[i] = "DELETE"
      elif "%mem=" in line:
        ifileList[i] = "DELETE"

    ### --- Clean up the ifileList by removing any chk, mem, and nproc settings
--- ###
    ifileListCLEAN = [x for x in ifileList if x != "DELETE"]

    headerLines = Eta_returnModified(basename, program, queue, nproc,
memory, header)
    snippetLines = Eta_returnModified(basename, program, queue, nproc,
memory, snippet)

    f = open(inputfile, "w")
    f.write("%chk=" + str(basename) + ".chk\n")
    f.write("%mem=" + str(memory) + "MB\n")
    f.write("%nproc=" + str(nproc) + "\n")
    for line in ifileListCLEAN:
      if 'link1' in line.lower():
        f.write(line)
        f.write("%chk=" + str(basename) + ".chk\n")
        f.write("%mem=" + str(memory) + "MB\n")
        f.write("%nproc=" + str(nproc) + "\n")
      else:
        f.write(line)
    f.close()

    f = open(basename + ".sge", "w")
    for line in headerLines:
      f.write(line)
    for line in snippetLines:
      f.write(line)
    f.close()

    if hold == 0:
      os.system("qsub " + basename + ".sge |tee " + basename + ".joblog")
    else:
      print "The job " + basename + ".sge will be made but not submitted."

##############################################################
```

```
### END OF SCRIPT
#################################################################
```

4.2 nSUBMIT HEADER SNIPPET EXAMPLE:

```
#!/bin/zsh

#$ -S /bin/sh

# Give a jobname. This option is used to  append r_ to any jobname starting
with
# numbers instead of alphabets because SGE cannot accept jobname
starting with
# numbers.
#$ -N PROGRAM!-BASENAME!
#
#  The following items pertain to this script
#  Use current working directory
#$ -cwd
#  input           = /dev/null
#  output          = BASENAME!.joblog
#$ -o BASENAME!.joblog
#  error           = Merged with joblog
#$ -j y

# Resources
#$ -pe smp PROCS!
#$ -q QUE!
#$ -l mem_free=MEM!M
#$ -l h_vmem=MEM!M

#  Email address to notify
#$ -M hcheong@mail

#  Notify at beginning and end of job
#$ -m bea

#  Job is not rerunable
#$ -r n

# Application base directory
export APPBASE=/export/apps
export SRIPTBASE=/export/psw
```

4.3 nSUBMIT JOB SNIPPET EXAMPLE:

```
# Initialization for Gaussian09 serial execution
g09root=APPDIR!
mkdir /state/partition1/$USER-BASENAME!-$JOB_ID
GAUSS_SCRDIR=/state/partition1/$USER-BASENAME!-$JOB_ID
export g09root GAUSS_SCRDIR
. $g09root/g09/bsd/g09.profile

echo ""
echo
"_____________________________________________________________________________
_____________________________"
echo "Gaussian09 SGE SUBMISSION SCRIPT"
echo "  Started by USER:      $USER"
echo "  JOB ID:               $JOB_ID"
echo "  APP directory:        $g09root/g09-D.01"
echo "  PWD directory:        $PWD"
echo "  SCRATCH directory:    $GAUSS_SCRDIR"

# Run the Gaussian09 program
echo "  Started on:           " `hostname -s`
echo "  Started at:           " `date`

g09 BASENAME!.com

echo "  Finished at:          " `date`
rm -rvf /state/partition1/$USER-BASENAME!-$JOB_ID
```

5. ηVISUALIZE SCRIPTS:

5.1 NVISUALIZE-PYMOL-XYZ.PY:

```
#! /usr/bin/env python2.7

###### LICENSE ######

import os
from sys import *
import sys
import getopt
from EtaLibAtom import *

### --- Arguments --- ###
program = "nVisualize-Pymol-XYZ.py"
dist = False
EtaDir = os.environ["ETADIR"]
build = "Pymolv1.3-Build.pml"
visual = "Pymolv1.3-Visualize.pml"

### Read command line args
try:
  myopts, args = getopt.getopt(sys.argv[1:], "b:v:dh")
except getopt.GetoptError:
  print program + " -d (generate distances) -h"
  sys.exit(2)
################################
# o == option
# a == argument passed to the o
################################
for o, a in myopts:
  if o == '-d':
    dist = True
  elif o == '-v':
    visual = a
  elif o == '-b':
    build = a
  elif o == '-h':
    print program + " -h"
    sys.exit(0)
  else:
    print("Usage: %s -h" % sys.argv[0])
    sys.exit(0)
```

```
### --- Make the Pymol folder --- ###
Eta_makeDir("Pymol-Picture")

### --- Grab the build and visualize configuration file --- ###
f = open(EtaDir + "/Pymol/snippets/" + build, 'r')
buildlines = f.readlines()
f.close()
f = open(EtaDir + "/Pymol/snippets/" + visual, 'r')
vislines = f.readlines()
f.close()
os.system("cp " + EtaDir + "/Pymol/snippets/Pymolv1.3-Visualize.pml Pymol-
Picture/")



### --- Creat the Visual-Script.pml file --- ###
f = open("Pymol-Picture/Visual-Script.pml", 'w')
f.write("#=========================================\n#Start\n")

### --- Iterating through a folder of files --- ###
for i in os.listdir(os.getcwd()):
  if i.endswith(".xyz"):
    ifile = i
    basename = Eta_basename(ifile, ".xyz")
    os.system("cp "+ basename + ".xyz Pymol-Picture/" + basename +
"_orig.xyz")
    os.system("cp "+ basename + ".xyz Pymol-Picture/" + basename +
"_high.xyz")
    os.system("cp "+ basename + ".xyz Pymol-Picture/" + basename +
"_med.xyz")
    os.system("cp "+ basename + ".xyz Pymol-Picture/" + basename +
"_low.xyz")
    os.system("cp "+ basename + ".xyz Pymol-Picture/" + basename +
"_dat.xyz")
    f.write("load " + basename + "_orig.xyz\n")
    f.write("load " + basename + "_high.xyz\n")
    f.write("load " + basename + "_med.xyz\n")
    f.write("load " + basename + "_low.xyz\n")
    f.write("load " + basename + "_dat.xyz\n")
    f.write("#grouping objects\n")
    f.write("#-------------------------------------------------------------------------------------
-------------------------------------------------\n")
    f.write("group " + basename + ", " + basename + "_orig\n")
    f.write("group " + basename + ", " + basename + "_high\n")
```

```
    f.write("group " + basename + ", " + basename + "_med\n")
    f.write("group " + basename + ", " + basename + "_low\n")
    f.write("group " + basename + ", " + basename + "_dat\n")
    f.write("\n")

    if dist == True:
      f.write("#-------------------------------------------------------------------------------------
-------------------------------------------------\n")
      f.write("#DISTANCE, DISTANCES\n")
      f.write("#Defining distances (dist)\n")
      f.write("distance Distance_HX_" + basename + "_DIST = (elem H) and " +
basename + "_high,  (neighbor elem H) and " + basename + "_high, 2.0;color
Grey, Distance_HX\n")
      f.write("distance Distance_CX_" + basename + "_DIST = (elem C) and " +
basename + "_high, (neighbor elem C) and " + basename + "_high, 2.0;color
Grey, Distance_CX\n")
      f.write("distance Distance_HB_" + basename + "_DIST = (elem B) and " +
basename + "_high, (elem H and neighbor elem B) and " + basename +
"_high, 2.0;color purple, Distance_HB\n")
      f.write("distance Distance_HC_" + basename + "_DIST = (elem C) and " +
basename + "_high, (elem H and neighbor elem C) and " + basename +
"_high, 2.0;color Black, Distance_HC\n")
      f.write("distance Distance_HN_" + basename + "_DIST = (elem N) and " +
basename + "_high, (elem H and neighbor elem N) and " + basename +
"_high, 2.0;color Blue, Distance_HN\n")
      f.write("distance Distance_HO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem H and neighbor elem O) and " + basename +
"_high, 2.0;color Red, Distance_HO\n")
      f.write("distance Distance_HSi_" + basename + "_DIST = (name Si) and "
+ basename + "_high, (elem H and neighbor elem Si) and " + basename +
"_high, 2.0;color Orange, Distance_HSi\n")
      f.write("distance Distance_HP_" + basename + "_DIST = (elem P) and " +
basename + "_high, (elem H and neighbor elem P) and " + basename +
"_high, 2.0;color Orange, Distance_HP\n")
      f.write("distance Distance_HS_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem H and neighbor elem S) and " + basename +
"_high, 2.0;color Orange, Distance_HS\n")
      f.write("distance Distance_BC_" + basename + "_DIST = (elem B) and " +
basename + "_high, (elem C and neighbor elem B) and " + basename +
"_high, 2.0;color Black, Distance_BC\n")
      f.write("distance Distance_BN_" + basename + "_DIST = (elem N) and " +
basename + "_high, (elem B and neighbor elem N) and " + basename +
"_high, 2.0;color Blue, Distance_BN\n")
```

```
    f.write("distance Distance_BO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem B and neighbor elem O) and " + basename +
"_high, 2.0;color Red, Distance_BO\n")
    f.write("distance Distance_CC_" + basename + "_DIST = (elem C) and " +
basename + "_high, (elem C) and " + basename + "_high, 1.6;color Black,
Distance_CC\n")
    f.write("distance Distance_CN_" + basename + "_DIST = (elem N) and " +
basename + "_high, (elem C and neighbor elem N) and " + basename +
"_high, 2.0;color Blue, Distance_CN\n")
    f.write("distance Distance_CO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem C and neighbor elem O) and " + basename +
"_high, 2.0;color Red, Distance_CO\n")
    f.write("distance Distance_CSi_" + basename + "_DIST = (name Si) and "
+ basename + "_high, (elem C and neighbor elem Si) and " + basename +
"_high, 2.0;color Orange, Distance_CSi\n")
    f.write("distance Distance_CP_" + basename + "_DIST = (elem P) and " +
basename + "_high, (elem C and neighbor elem P) and " + basename +
"_high, 2.0;color Orange, Distance_CP\n")
    f.write("distance Distance_CS_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem C and neighbor elem S) and " + basename +
"_high, 2.0;color Orange, Distance_CS\n")
    f.write("distance Distance_NN_" + basename + "_DIST = (elem N) and " +
basename + "_high, (elem N and neighbor elem N) and " + basename +
"_high, 2.0;color Blue, Distance_NN\n")
    f.write("distance Distance_NO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem N neighbor elem O) and " + basename + "_high,
2.0;color Blue, Distance_NO\n")
    f.write("distance Distance_NSi_" + basename + "_DIST = (name Si) and "
+ basename + "_high, (elem N and neighbor elem Si) and " + basename +
"_high, 2.0;color Orange, Distance_NSi\n")
    f.write("distance Distance_NP_" + basename + "_DIST = (elem P) and " +
basename + "_high, (elem N and neighbor elem P) and " + basename +
"_high, 2.0;color Orange, Distance_NP\n")
    f.write("distance Distance_NS_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem N and neighbor elem S) and " + basename +
"_high, 2.0;color Orange, Distance_NS\n")
    f.write("distance Distance_OO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem O and neighbor elem O) and " + basename +
"_high, 2.0;color Red, Distance_OO\n")
    f.write("distance Distance_OSi_" + basename + "_DIST = (name Si) and "
+ basename + "_high, (elem O and neighbor elem Si) and " + basename +
"_high, 2.0;color Orange, Distance_OSi\n")
```

```
    f.write("distance Distance_OP_" + basename + "_DIST = (elem P) and " +
basename + "_high, (elem O and neighbor elem P) and " + basename +
"_high, 2.0;color Orange, Distance_OP\n")
    f.write("distance Distance_OS_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem O and neighbor elem S) and " + basename +
"_high, 2.0;color Orange, Distance_OS\n")
    f.write("distance Distance_PRh_" + basename + "_DIST = (elem P) and "
+ basename + "_high, (name Rh and neighbor elem P) and " + basename +
"_high, 2.5;color Orange, Distance_PRh\n")
    f.write("\n")
    f.write("#----------------------------------------------------------------------------------------
-------------------------------------------------\n")
    f.write("#HYDROGEN-BONDING, H-BOND, H-BONDING\n")
    f.write("#Defining hydrogen bonding distances (h_bond, hbond)\n")
    f.write("set h_bond_cutoff_center, 3.6\n")
    f.write("set h_bond_cutoff_edge, 3.2\n")
    f.write("\n")
    f.write("#----------------------------------------------------------------------------------------
-------------------------------------------------\n")
    f.write("#TRANSITION STATE BONDS (TS, TSS, TS-BOND, TS-BONDS,
TSBOND, TSBONDS)\n")
    f.write("#Defining ts bonds (ts,ts_bond)\n")
    f.write("distance TS_C-C_" + basename + "_DIST = (/////C) and " +
basename + "_high, (/////C) and " + basename + "_high, 3.0\n")
    f.write("\n")
    f.write("#----------------------------------------------------------------------------------------
-------------------------------------------------\n")
    f.write("#STERIC (STERIC, STERICS)\n")
    f.write("#Defining steric interactions between hydrogens (hh, steric,
sterics)\n")
    f.write("distance Steric_HH_21_" + basename + "_DIST = (elem H) and "
+ basename + "_high, (elem H) and " + basename + "_high, 2.1; color Grey,
Steric_HH_21\n")
    f.write("distance Steric_HH_22_" + basename + "_DIST = (elem H) and "
+ basename + "_high, (elem H) and " + basename + "_high, 2.2; color Grey,
Steric_HH_22\n")
    f.write("distance Steric_HH_23_" + basename + "_DIST = (elem H) and "
+ basename + "_high, (elem H) and " + basename + "_high, 2.3; color Grey,
Steric_HH_23\n")
    f.write("distance Steric_HH_24_" + basename + "_DIST = (elem H) and "
+ basename + "_high, (elem H) and " + basename + "_high, 2.4; color Grey,
Steric_HH_24\n")
    f.write("#----------------------------------------------------------------------------------------
-------------------------------------------------\n")
```

```
    f.write("#ELECTROSTATIC (ELECTROSTATIC, ELECTROSTATICS,
ESP, ESPS)\n")
    f.write("#Defining electrostatic interactions and contacts (electrostatic,
esp, esc)\n")
    f.write("select XH_32, /////H and (neighbor /////N or neighbor /////O or
neighbor /////S)\n")
    f.write("distance Classic_ESP_NH_32_" + basename + "_DIST = /////N,
XH_32, 3.2; color Navy_Blue, Classic_ESP_NH_*\n")
    f.write("distance Classic_ESP_OH_32_" + basename + "_DIST = /////O,
XH_32, 3.2; color Red, Classic_ESP_OH_*\n")
    f.write("distance Classic_ESP_HX_32_" + basename + "_DIST = XH_32
and " + basename + "_high, (/////N or /////O or /////S) and " + basename +
"_high, 3.2; color Grey, Classic_ESP_HX_*; delete XH_32\n")
    f.write("distance ESP_CH_32_" + basename + "_DIST = (elem C) and " +
basename + "_high, ((elem H) and not (neighbor (elem H))) and " +
basename + "_high, 3.2; color Grey, ESP_CH_*\n")
    f.write("distance ESP_NH_32_" + basename + "_DIST = (elem N) and " +
basename + "_high, ((elem H) and not (neighbor (elem H))) and " +
basename + "_high, 3.2; color Navy_Blue, ESP_NH_*\n")
    f.write("distance ESP_OH_32_" + basename + "_DIST = (elem O) and " +
basename + "_high, ((elem H) and not (neighbor (elem H))) and " +
basename + "_high, 3.2; color Pink, ESP_OH_*\n")
    f.write("distance ESP_SH_32_" + basename + "_DIST = (elem S) and " +
basename + "_high, ((elem H) and not (neighbor (elem H))) and " +
basename + "_high, 3.2; color Yellow, ESP_SH_*\n")
    f.write("distance ESP_BN_32_" + basename + "_DIST = (elem B) and " +
basename + "_high, (elem N) and " + basename + "_high, 3.2; color Pink,
ESP_BN_*\n")
    f.write("distance ESP_OO_32_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem O) and " + basename + "_high, 3.2; color Red,
ESP_OO_*\n")
    f.write("distance ESP_ON_32_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem N) and " + basename + "_high, 3.2; color purple,
ESP_ON_*\n")
    f.write("distance ESP_SS_32_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem S) and " + basename + "_high, 3.2; color sulfur,
ESP_SS_*\n")
    f.write("distance ESP_SO_32_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem O) and " + basename + "_high, 3.2; color violet,
ESP_SO_*\n")
    f.write("distance ESP_SN_32_" + basename + "_DIST = (elem S) and " +
basename + "_high, (elem N) and " + basename + "_high, 3.2; color purple,
ESP_SN_*\n")
```

```
    f.write("distance ESP_ClH_32_" + basename + "_DIST = (name Cl) and "
+ basename + "_high, (elem H) and " + basename + "_high, 3.2; color Green,
ESP_ClH_*\n")
    f.write("\n")
    f.write("#-----------------------------------------------------------------------------------------
-------------------------------------------------\n")
    f.write("distance TMBond_SiO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem S) and " + basename + "_high, 2.5;  Bond_SiO\n")
    f.write("distance TMBond_SnO_" + basename + "_DIST = (elem O) and "
+ basename + "_high, (elem S) and " + basename + "_high, 2.5;
Bond_SnO\n")
    f.write("distance TMBond_ZnO_" + basename + "_DIST = (elem O) and "
+ basename + "_high, (elem Zn) and " + basename + "_high, 2.5;
Bond_ZnO\n")
    f.write("distance TMBond_InO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem In) and " + basename + "_high, 2.5;  Bond_InO\n")
    f.write("distance TMBond_GaO_" + basename + "_DIST = (elem O) and "
+ basename + "_high, (elem Ga) and " + basename + "_high, 2.5;
Bond_GaO\n")
    f.write("distance TMBond_AlO_" + basename + "_DIST = (elem O) and " +
basename + "_high, (elem Al) and " + basename + "_high, 2.5;  Bond_AlO\n")
    f.write("\n")
    f.write("group " + basename + ", *_" + basename + "_DIST\n")
  if dist == True:
    f.write("#-----------------------------------------------------------------------------------------
-------------------------------------------------\n")
    f.write("#Defining all distances\n")
    f.write("distance ALL_MainGroup_Distance = *, *, 1.75, 1; color Black,
ALL_MainGroup_Distance\n")
    f.write("distance ALL_TMGroup_Distance = *, *, 2.6, 1; color Black,
ALL_TMGroup_Distance\n")
    f.write("distance ALL_Distance= *, neighbor, 3.0, 1; color Black,
ALL_Distance\n")


for line in buildlines:
  f.write(line)
for line in vislines:
  f.write(line)

f.close()

os.system("open Pymol-Picture/Visual-Script.pml")
```

```
#################################################################
### END OF SCRIPT
#################################################################
```

5.1.1 PYMOLV1.3-BUILD.PML:

```
#-------------------------------------------------------------------------------------------------------------------------------
#ATOMBOND, ATOMBONDS
#Defining unusual atom bonds
#=============================================================================================
#Iron, IRON, FE, Fe, fe
unbond /////Fe,/////C
distance Bond_FeC = (elem Fe), (elem C), 2.5
color Brown, Bond_FeC
#=============================================================================================
#Unbond In, Ga, Zn, Al, etc with O for amorphous solids
select InL25, elem O within 2.5 of name In
unbond /////In,InL25
delete InL25
select SiL25, elem O within 2.5 of name Si
unbond /////Si,SiL25
delete SiL25
select SnL25, elem O within 2.5 of name Sn
unbond /////Sn,SnL25
delete SnL25
select ZnL25, elem O within 2.5 of name Zn
unbond /////Zn,ZnL25
delete ZnL25
select GaL25, elem O within 2.5 of name Ga
unbond /////Ga,GaL25
delete GaL25
select AlL25, elem O within 2.5 of name Al
unbond /////Al,AlL25
delete AlL25
#=============================================================================================
#Rhodium, RHODIUM, RH, Rh, rh
bond /////Rh,/////P
unbond /////Rh,/////C
distance Bond_RhH = (/////Rh), (elem H), 2.5; color Grape, Bond_RhH
distance Bond_RhC = (/////Rh), (elem C), 2.6; color Grape, Bond_RhC
distance Bond_RhN = (/////Rh), (elem N), 2.5; color Grape, Bond_RhN
distance Bond_RhO = (/////Rh), (elem O), 2.5; color Grape, Bond_RhO
distance Bond_RhF = (elem Rh), (elem F), 3.0; color Grape, Bond_RhF
distance Bond_RhCl = (elem Rh), (elem Cl), 3.0; color Grape, Bond_RhCl
distance Bond_RhBr = (elem Rh), (elem Br), 3.0; color Grape, Bond_RhBr
```

```
#select RhL26, (elem C or elem Cl or elem P) within 2.4 of name Rh
#bond /////Rh,RhL26
#delete RhL26
#select all-original, *_high
#select Rh, elem Rh and all-original
#unbond Rh, all
#delete Rh
#delete all-original
#-------------------------------------------------------------------------------------------------
---------------------------------
#=================================================================
================================
#Palladium, PD, Pd, pd
bond /////Pd,/////P
unbond /////Pd,/////C
distance Bond_PdH = (/////Pd), (elem H), 2.2; color Grape, Bond_PdH
distance Bond_PdC = (/////Pd), (elem C), 2.4; color Grape, Bond_PdC
distance Bond_PdN = (/////Pd), (elem N), 2.4; color Grape, Bond_PdN
distance Bond_PdO = (/////Pd), (elem O), 2.4; color Grape, Bond_PdO
distance Bond_PdF = (elem Pd), (elem F), 3.0; color Grape, Bond_PdF
distance Bond_PdCl = (elem Pd), (elem Cl), 3.0; color Grape, Bond_PdCl
distance Bond_PdBr = (elem Pd), (elem Br), 3.0; color Grape, Bond_PdBr
select PdL26, (elem C) within 2.2 of name Pd
bond /////Pd,PdL26
delete PdL26
select PdL26, (elem Br) within 3.0 of name Pd
bond /////Pd,PdL26
delete PdL26
#=================================================================
================================
#Aluminum, Aluminium, AL, Al, al
select AlL30, (elem O or elem Cl or elem N) within 1.7 of name Al
bond /////Al,AlL30
distance Bond_AlO = (name Al), (/////O), 2.0; color Eggplant, Bond_AlO
distance Bond_AlCl = (name Al), (/////Cl), 1.7; color Eggplant, Bond_AlCl
delete AlL30
#=================================================================
================================
#Gallium, Gauminium, GA, Ga, ga
#select GaL30, (elem O or elem Cl or elem N) within 2.2 of name Ga
#bond /////Ga,GaL30
#distance Bond_GaO = (name Ga), (/////O), 2.2; color Eggplant, Bond_GaO
#distance Bond_GaCl = (name Ga), (/////Cl), 2.2; color Eggplant, Bond_GaCl
#delete GaL30
```

```
#select OH12, elem H within 1.2 of name O
#bond /////O,OH12
#select OO2, elem O within 2.0 of name O
#unbond /////O,/////O

#-------------------------------------------------------------------------------------------------------------------------
#SPHERE, SPHERES, STICK, STICKS, LABEL, LABELS, GAP, GAPS, TEXTURE, TEXTURES
#Setting molecular representations (bonds, atoms, representation, label, dash)
#============================================================================
#sphere (spheres)
show sphere, *_med
show sphere, *_high
show sphere, *_orig
set sphere_scale, 0.25
set sphere_scale, 1.00, *_orig
set sphere_transparency, 0.5, *_orig
disable *_orig
show stick, *_med
show stick, *_high
set stick_radius=0.15, *_high
#============================================================================
#Low Level settings
set lines, *_low
#============================================================================
#dat Level settings
show sticks, *_dat
hide lines, *_dat
set stick_radius, 0.05, *_dat
set stick_color, black, *_dat
set stick_transparency, 0.5, *_dat
#============================================================================
#line (lines)
set line_smooth, 1
#============================================================================
#label (labels)
```

```
set label_font_id, 13
#set label_position (0,0,5)
#set texture_fonts=1
set label_size= 26
set label_color, Black
set label_outline_color, White
set label_distance_digits, 2
set label_angle_digits, 1
set label_dihedral_digits, 1
#set float_labels, 1
set label_shadow_mode, 0
#-------------------------------------------------------------------------------------------------
----------------------------------
#unactivating, disactivating objects and groups
disable Distance_*
disable ALL_*
disable Steric_*
disable ESP_*
disable TMBond_*
disable BOND_*
disable Classic_ESP_*
delete XH_32
```

5.1.2 PYMOLV1.3-VISUALIZE.PML:

```
#-------------------------------------------------------------------------------------------------------------
-----------------------------------
#COLOR, COLORS, COLOUR, COLOURS
#Defining Custom Colors
set_color Almond, [0.94,0.86,0.77]
set_color Antique_Brass, [0.80,0.58,0.46]
set_color Apricot, [0.99,0.85,0.71]
set_color Aquamarine, [0.47,0.86,0.89]
set_color Asparagus, [0.53,0.66,0.42]
set_color Atomic_Tangerine, [1.00,0.64,0.45]
set_color Banana_Mania, [0.98,0.91,0.71]
set_color Beaver, [0.62,0.51,0.44]
set_color Bittersweet, [0.99,0.49,0.43]
set_color Black, [0.14,0.14,0.14]
set_color Blue, [0.12,0.46,1.00]
#set_color Blue, [0.0,0.0,1.0]
set_color Blue_Bell, [0.68,0.68,0.84]
set_color Blue_Green, [0.10,0.62,0.74]
set_color Blue_Violet, [0.45,0.40,0.74]
set_color Blush, [0.87,0.36,0.51]
set_color Brick_Red, [0.80,0.25,0.33]
set_color Brown, [0.71,0.40,0.30]
set_color Burnt_Orange, [1.00,0.50,0.29]
set_color Burnt_Sienna, [0.92,0.49,0.36]
set_color Cadet_Blue, [0.69,0.72,0.78]
set_color Canary, [1.00,1.00,0.60]
set_color Caribbean_Green, [0.11,0.83,0.64]
set_color Carnation_Pink, [1.00,0.67,0.80]
set_color Cerise, [0.87,0.27,0.57]
set_color Cerulean, [0.11,0.67,0.84]
set_color Chestnut, [0.74,0.36,0.35]
set_color Copper, [0.87,0.58,0.46]
set_color Cornflower, [0.60,0.81,0.92]
set_color Cotton_Candy, [1.00,0.74,0.85]
set_color Cyan, [0.0,1.0,0.5]
set_color Dandelion, [0.99,0.86,0.43]
set_color Denim, [0.17,0.42,0.77]
set_color Desert_Sand, [0.94,0.80,0.72]
set_color Eggplant, [0.43,0.32,0.38]
#set_color Eggplant, [0.25,0.0,0.5]
set_color Electric_Lime, [0.11,0.98,0.08]
set_color Fern, [0.44,0.74,0.47]
set_color Forest_Green, [0.43,0.68,0.51]
```

```
set_color Fuchsia, [0.76,0.39,0.77]
set_color Fuzzy_Wuzzy_Brown, [0.80,0.40,0.40]
set_color Gold, [0.91,0.78,0.59]
#set_color Gold, [1.0,1.0,0.0]
set_color Goldenrod, [0.99,0.85,0.46]
set_color Granny_Smith_Apple, [0.66,0.89,0.63]
set_color Grape, [0.5,0.0,1.0]
#set_color Gray, [0.58,0.57,0.55]
set_color Gray, [0.6,0.6,0.6]
#set_color Grey, [0.7,0.7,0.7]
set_color Grey, [0.6,0.6,0.6]
#set_color LGray, [0.9,0.9,0.9]
#set_color LGrey, [0.9,0.9,0.9]
set_color LGray, [0.85,0.85,0.85]
set_color LGrey, [0.85,0.85,0.85]
set_color Green, [0.11,0.67,0.47]
#set_color Green, [0.0,1.0,0.0]
set_color Green_Yellow, [0.94,0.91,0.57]
set_color Hot_Magenta, [1.00,0.11,0.81]
set_color Inch_Worm, [0.70,0.93,0.36]
set_color Indigo, [0.36,0.46,0.80]
set_color Jazzberry_Jam, [0.79,0.22,0.40]
set_color Jungle_Green, [0.23,0.69,0.56]
set_color Laser_Lemon, [0.99,0.99,0.45]
set_color Lavender, [0.99,0.71,0.84]
set_color Macaroni_and_Cheese, [1.00,0.74,0.53]
set_color Magenta, [0.96,0.39,0.69]
set_color Mahogany, [0.80,0.29,0.29]
set_color Manatee, [0.59,0.60,0.67]
set_color Mango_Tango, [1.00,0.51,0.26]
set_color Maroon, [0.78,0.22,0.35]
set_color Mauvelous, [0.94,0.60,0.67]
set_color Melon, [0.99,0.74,0.71]
set_color Midnight_Blue, [0.10,0.28,0.46]
set_color Mountain_Meadow, [0.19,0.73,0.56]
set_color Navy_Blue, [0.10,0.45,0.82]
set_color Neon_Carrot, [1.00,0.64,0.26]
set_color Olive_Green, [0.73,0.72,0.42]
set_color Orange, [1.00,0.46,0.22]
#set_color Orange, [1.0,0.8,0.0]
set_color Orchid, [0.90,0.66,0.84]
set_color Outer_Space, [0.25,0.29,0.30]
set_color Outrageous_Orange, [1.00,0.43,0.29]
set_color Pacific_Blue, [0.11,0.66,0.79]
```

```
set_color Peach, [1.00,0.81,0.67]
set_color Periwinkle, [0.77,0.82,0.90]
set_color Piggy_Pink, [0.99,0.84,0.89]
set_color Pine_Green, [0.08,0.50,0.47]
set_color Pink_Flamingo, [0.99,0.45,0.99]
set_color Pink_Sherbet, [0.97,0.50,0.63]
set_color Plum, [0.56,0.27,0.52]
set_color Purple_Heart, [0.45,0.26,0.78]
set_color Purple_Mountains?_Majesty, [0.62,0.51,0.73]
set_color Purple_Pizzazz, [1.00,0.11,0.81]
set_color Radical_Red, [1.00,0.29,0.42]
set_color Raw_Sienna, [0.84,0.54,0.35]
set_color Razzle_Dazzle_Rose, [1.00,0.28,0.82]
set_color Razzmatazz, [0.89,0.15,0.42]
set_color Red, [0.93,0.13,0.30]
#set_color Red, [1.0,0.0,0.0]
set_color Red_Orange, [1.00,0.33,0.29]
set_color Red_Violet, [0.75,0.27,0.56]
set_color Robin_Egg_Blue, [0.12,0.81,0.80]
set_color Royal_Purple, [0.47,0.32,0.66]
set_color Salmon, [1.00,0.61,0.67]
set_color Scarlet, [0.99,0.16,0.28]
set_color Screamin_Green, [0.46,1.00,0.48]
set_color Sea_Green, [0.62,0.89,0.75]
set_color Sepia, [0.65,0.41,0.31]
set_color Shadow, [0.54,0.47,0.36]
set_color Shamrock, [0.27,0.81,0.64]
set_color Shocking_Pink, [0.98,0.49,0.99]
set_color Silver, [0.80,0.77,0.76]
set_color Sky_Blue, [0.50,0.85,0.92]
set_color Spring_Green, [0.93,0.92,0.75]
set_color Sunglow, [1.00,0.81,0.28]
set_color Sunset_Orange, [0.99,0.37,0.33]
set_color Tan, [0.98,0.65,0.42]
set_color Tickle_Me_Pink, [0.99,0.54,0.67]
set_color Timberwolf, [0.86,0.84,0.82]
set_color Tropical_Rain_Forest, [0.09,0.50,0.43]
set_color Tumbleweed, [0.87,0.67,0.53]
set_color Turquoise_Blue, [0.47,0.87,0.91]
set_color Unmellow_Yellow, [0.99,0.99,0.45]
set_color Violet_(Purple), [0.57,0.43,0.68]
set_color Violet_Red, [0.97,0.33,0.58]
set_color Vivid_Tangerine, [1.00,0.63,0.54]
set_color Vivid_Violet, [0.56,0.31,0.62]
```

```
#set_color White, [0.93,0.93,0.93]
set_color White, [1.0,1.0,1.0]
set_color Wild_Blue_Yonder, [0.64,0.68,0.82]
set_color Wild_Strawberry, [1.00,0.26,0.64]
set_color Wild_Watermelon, [0.99,0.42,0.52]
set_color Wisteria, [0.80,0.64,0.87]
set_color Yellow, [0.99,0.91,0.51]
#set_color Yellow, [1.0,1.0,0.0]
set_color Yellow_Green, [0.77,0.89,0.52]
set_color Yellow_Orange, [1.00,0.71,0.33]

#------------------------------------------------------------------------------------------------
----------------------------------
#ATOMCOLOR, ATOMCOLORS, ATOMCOLOUR, ATOMCOLOURS
#Defining colors of atoms
color Navy_Blue, (elem N)
color Navy_Blue, (name N)
color Brown, (elem Fe)
color Brown, (name Fe)
color Cornflower, (elem D)
color Cornflower, (name D)
color Gold, (elem Au)
color Gold, (name Au)
color Grape, (elem Rh)
color Grape, (name Rh)
color Green, (elem Cl)
color Green, (name Cl)
color Grey, (elem C)
color Grey, (name C)
color Orange, (elem P)
color Orange, (name P)
color Pink, (elem B)
color Pink, (name B)
color Red, (elem O)
color Red, (name O)
color Seafoam, (elem F)
color Seafoam, (name F)
color Silver, (elem Ag)
color Silver, (name Ag)
color LGray, (elem H)
color LGray, (name H)

#------------------------------------------------------------------------------------------------
----------------------------------
```

```
#RAY, FOG, TRACE, LIGHT, ORTHO, ALIAS, ANTI-ALIAS, SPEC
#=============================================================
=================================
#Setting ray settings (ray, fog, trace, light, ortho, alias, spec)
#fog (fogs, depth, depth-cue)
#set fog_start, 0.1
#set ray_trace_fog = 1
#set depth_cue, 1
#unset depth_cue
#=============================================================
=================================
#background (backgrounds)
bg_color White
#=============================================================
=================================
#color space (color-space, color type, color-type)
#space cmyk
space rgb
#=============================================================
=================================
#ortho (orthoscopic, parallax, paralax)
set orthoscopic=1
#=============================================================
=================================
#alias (antialias, anti-alias)
set antialias=2
#=============================================================
=================================
#spec (specular, specs)
#set spec_power=200
#set spec_reflect=0.2
set reflect,1.5
#set specular_intensity=200.0
set specular, 0.25
set spec_count,1
#set two_sided_lighting=1
set light_count,10
#=============================================================
=================================
#ray (raytrace)
set ray_trace_frames, 1
#Most Recent
Change!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

```
set ray_trace_mode, 1
#Most Recent
Change!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
set ray_trace_gain, 0.1
#set ray_trace_gain,4
set ray_opaque_background, off
set opaque_background, off
set bg_rgb=(1.0,1.0,1.0)
#set ray_texture, 1
set ray_shadow_decay_factor, 0.1
set ray_shadow_decay_range, 2
set direct, 0
set shininess, 1
set ambient, 0.1
#==============================================================
=================================
#autocopy
set auto_copy_images=1
#----------------------------------------------------------------------------------------------------
-----------------------------------
#GUI
#Setting gui settings
set internal_gui_width, 250
viewport 1024,1034
set internal_prompt,0

#----------------------------------------------------------------------------------------------------
-----------------------------------
#unknown settings
set cache_frames=0
zoom all, complete=1
center state=0, origin=1

#----------------------------------------------------------------------------------------------------
-----------------------------------
#VAN DER WAALS, VDW for High Level
#Defining custom atom van der waals (vdw) radii.
alter (name Ag) and *_high,vdw=1.72
alter (name Al) and *_high,vdw=2.00
alter (name Ar) and *_high,vdw=1.88
alter (name As) and *_high,vdw=1.85
alter (name Au) and *_high,vdw=1.66
alter (name Br) and *_high,vdw=1.85
```

```
alter (name B) and *_high,vdw=1.65
alter (name C) and *_high,vdw=1.70
alter (name Cd) and *_high,vdw=1.58
alter (name Cl) and *_high,vdw=1.75
alter (name Cu) and *_high,vdw=1.40
alter (name F) and *_high,vdw=1.47
alter (name Fe) and *_high,vdw=1.8
alter (name Ga) and *_high,vdw=1.87
alter (name H) and *_high,vdw=1.20
alter (name He) and *_high,vdw=1.40
alter (name Hg) and *_high,vdw=1.55
alter (name I) and *_high,vdw=1.98
alter (name In) and *_high,vdw=1.93
alter (name K) and *_high,vdw=2.75
alter (name Kr) and *_high,vdw=2.02
alter (name Li) and *_high,vdw=1.82
alter (name Mg) and *_high,vdw=1.73
alter (name N) and *_high,vdw=1.55
alter (name Na) and *_high,vdw=2.27
alter (name Ne) and *_high,vdw=1.54
alter (name Ni) and *_high,vdw=1.63
alter (name O) and *_high,vdw=1.52
alter (name P) and *_high,vdw=1.80
alter (name Pb) and *_high,vdw=2.02
alter (name Pd) and *_high,vdw=1.63
alter (name Pt) and *_high,vdw=1.72
alter (name Rh) and *_high,vdw=2.0
alter (name S) and *_high,vdw=1.80
alter (name Se) and *_high,vdw=1.90
alter (name Si) and *_high,vdw=2.10
alter (name Sn) and *_high,vdw=2.17
alter (name Te) and *_high,vdw=2.06
alter (name Tl) and *_high,vdw=1.96
alter (name U) and *_high,vdw=1.86
alter (name Xe) and *_high,vdw=2.16
alter (name Zn) and *_high,vdw=1.39

#-------------------------------------------------------------------------------------------------------
-----------------------------------
#COPY! for Medium
#VAN DER WAALS, VDW for Med level
#Defining custom atom van der waals (vdw) radii.
#Ligand Sizing
set stick_radius, 0.0501, *_med
```

```
alter elem Ag and *_med,vdw=0.68
alter elem Al and *_med,vdw=0.79
alter elem Ar and *_med,vdw=0.74
alter elem As and *_med,vdw=0.73
alter elem Au and *_med,vdw=0.65
alter elem Br and *_med,vdw=0.73
alter elem B and *_med,vdw=0.65
alter elem C and *_med,vdw=0.67
alter elem Cd and *_med,vdw=0.62
alter elem Cl and *_med,vdw=0.69
alter elem Cu and *_med,vdw=0.55
alter elem F and *_med,vdw=0.58
alter elem Fe and *_med,vdw=0.71
alter elem Ga and *_med,vdw=0.74
alter elem H and *_med,vdw=0.47
alter elem He and *_med,vdw=0.55
alter elem Hg and *_med,vdw=0.61
alter elem I and *_med,vdw=0.78
alter elem In and *_med,vdw=0.76
alter elem K and *_med,vdw=1.08
alter elem Kr and *_med,vdw=0.80
alter elem Li and *_med,vdw=0.72
alter elem Mg and *_med,vdw=0.68
alter elem N and *_med,vdw=0.61
alter elem Na and *_med,vdw=0.89
alter elem Ne and *_med,vdw=0.61
alter elem Ni and *_med,vdw=0.64
alter elem O and *_med,vdw=0.60
alter elem P and *_med,vdw=0.71
alter elem Pb and *_med,vdw=0.80
alter elem Pd and *_med,vdw=0.64
alter elem Pt and *_med,vdw=0.68
alter elem Rh and *_med,vdw=0.79
alter elem S and *_med,vdw=0.71
alter elem Se and *_med,vdw=0.75
alter elem Si and *_med,vdw=0.83
alter elem Sn and *_med,vdw=0.86
alter elem Te and *_med,vdw=0.81
alter elem Tl and *_med,vdw=0.77
alter elem U and *_med,vdw=0.73
alter elem Xe and *_med,vdw=0.85
alter elem Zn and *_med,vdw=0.55
```

```
#====================================================================
====================
#Low Level settings
set lines, *_low

#====================================================================
====================
#dat Level settings
set stick_radius, 0.05, *_dat
set stick_color, black, *_dat
set stick_transparency, 0.5, *_dat

#====================================================================
================================
#line (lines)
set line_smooth, 1
#====================================================================
================================
#label (labels)
set label_font_id, 13
#set label_position (0,0,5)
#set texture_fonts=1
set label_size= -0.3
set label_color, Black
set label_outline_color, White
set label_distance_digits, 2
set label_angle_digits, 1
set label_dihedral_digits, 1
#set float_labels, 1
set label_shadow_mode, 0

#====================================================================
====================
#Measurements
#Bond lengths
set dash_radius, 0
set dash_width, 0

#TMBond lengths
set dash_color, grey40, TMBond*
set dash_radius, 0.15, TMBond*
set dash_length, 1, TMBond*
set dash_width, 1, TMBond*
set dash_gap, 0, TMBond*
```

```
hide labels, TMBond*

#TS
set dash_gap, 0, *_ts
set dash_length, 0.01, *_ts
set dash_color, gray25, *_ts
set dash_radius, 0.101, *_ts

#H-bonding
set dash_color, green, *_h
set dash_radius, 0.05, *_h
set dash_length, 0.001, *_h
set dash_gap, 0.25, *_h

#Interaction
set dash_color, white, *_int
set dash_radius, 0.04, *_int
set dash_length, 0.001, *_int
set dash_gap, 0.25, *_int

#Dihedrals
set dash_color, black, *_dih
set dash_radius, 0.02, *_dih
set dash_length, 0.12, *_dih
set dihedral_length, 1, *_dih
set dash_gap, 0.25, *_dih

#Angles
set dash_gap, 0, *_angle
set angle_color, white, *_angle
set dash_radius, 0.025, *_angle


#-------------------------------------------------------------------------------------------------
---------------------------------
#double bonds, valences, resonance, conjugation
set valence, 1

#-------------------------------------------------------------------------------------------------
---------------------------------
#turning on sequence viewer
set seq_view, 0
set seq_view_label_color, Black
set seq_view_format, 2
```

```
#-------------------------------------------------------------------------------------------------
----------------------------------

#REBUILD, REDRAW, RESET
#Rebuilding graphics
rebuild
recolor
refresh
```