Distribution Agreement

In presenting this thesis as a partial fulfillment of the requirements for a degree from Emory University, I hereby grant to Emory University and its agents the non-exclusive license to archive, make accessible, and display my thesis in whole or in part in all forms of media, now or hereafter now, including display on the World Wide Web. I understand that I may select some access restrictions as part of the online submission of this thesis. I retain all ownership rights to the copyright of the thesis. I also retain the right to use in future works (such as articles or books) all or part of this thesis.

Anjanay Nangia March 30, 2023

Computational Modeling of Oxyradical and Metal-Oxo Reactivity and Selectivity in Hydrogen Atom Transfer Reactions

by

Anjanay Nangia

Dr. Huw M. L. Davies
Adviser

Chemistry

Dr. Huw M. L. Davies

Adviser

Dr. Frank E. McDonald

Committee Member

Dr. Jamal G. Musaev

Committee Member

2023

Computational Modeling of Oxyradical and Metal-Oxo Reactivity and Selectivity in Hydrogen Atom Transfer Reactions

By

Anjanay Nangia

Dr. Huw M. L. Davies

Adviser

An abstract of
a thesis submitted to the Faculty of Emory College of Arts and Sciences
of Emory University in partial fulfillment
of the requirements of the degree of
Bachelor of Science with Honors

Chemistry

2023

Abstract

Computational Modeling of Oxyradical and Metal-Oxo Reactivity and Selectivity in Hydrogen Atom Transfer Reactions
By Anjanay Nangia

Oxyradicals and metal-oxo species have proven to be useful tools in the selective oxidation of C-H bonds. Understanding the reaction mechanisms, reactivities, and selectivities of these oxidations has been an important challenge in physical organic chemistry. A computational study was carried out to explore oxyradical and metal-oxo species to further trace the origins of their patterns in reactivity and selectivity as well as develop analogous models between metal-oxo catalysts and their oxyradical counterparts. Using density functional theory (DFT), the energetics of hydrogen abstraction reactions were probed with tert-butoxy, cumyloxy, and hydroxy radicals, as well as with a ruthenium-oxo bis(bipyridine) species, dubbed the Dubois-Sigman catalyst, and a non-heme iron-oxo PDP species, known as the White-Chen catalyst. It was found that a bimodal Evans-Polanyi relationship, divided by substrate type, was moderately useful in describing the kinetics of this set of oxyradicals and metal-oxo species. A modified Evans-Polanyi relationship, known as the Roberts-Steel equation, was also applied to predict kinetic barriers of both oxyradicals and metal-oxo species. It was found that the Roberts-Steel functional form was unable to capture the variation in kinetics for metal-oxo species and was moderately successful for the range of alkoxy radicals explored in this work. It was suggested that a missing explanatory variable in the regression equation may resolve observed differences. Finally, a distortion-interaction analysis revealed that distortive effects that manifested in the transition-state were mainly explained by developments along the reaction coordinate and correlated well with activation energy barriers. The White-Chen catalyst, uniquely, demonstrated elevated distortive effects in the transition-state more than those seen by other metal-oxo and oxyradical species, that requires further investigation.

Computational Modeling of Oxyradical and Metal-Oxo Reactivity and Selectivity in Hydrogen Atom Transfer Reactions

By

Anjanay Nangia

Dr. Huw M. L. Davies

Adviser

A thesis submitted to the Faculty of Emory College of Arts and Sciences
of Emory University in partial fulfillment
of the requirements of the degree of
Bachelor of Science with Honors

Chemistry

2023

Acknowledgements

I would like to extend my sincerest gratitude to Dr. Ken Houk for inviting me to be a member of his research group at UCLA during a global pandemic in May 2020 and for supporting me in my chemistry research journey long after as a remote undergraduate researcher in his lab. Although I will not be pursuing a Ph.D., I appreciate all the guidance and mentorship you have given me since I joined and know that the skills and knowledge, I have learned will prepare me for my future.

I would also like to extend a thank you to everyone in the Houk lab, especially Jonathan Wong, Dr. Aneta Turlik, Dr. Mark Maskeri, Dr. Guochao Xu, and Dr. Xiangyang Chen for their willingness to help and support me even if we were always 3 hours apart and more than 2,000 miles away.

I owe a huge thanks to Dr. McDonald for helping cultivate my interest in chemistry at Emory in the first place and for being a supportive mentor throughout my college career. In our 203Z class, I remember feeling pushed to think more analytically and outside the box which I genuinely feel has helped me grow as a critical thinker – regardless of whether it involves diagnosing a mechanism or pitching a biotech company's stock for investment. Having you as a professor has undoubtedly been a tremendous blessing. Similarly, I am also grateful for the guidance and mentorship of Professor McCormick – whether it be related to course selection or career advice, your advice has always been an important part of my every semester at Emory.

I would also like to thank Dr. Huw Davies and Dr. Jamal Musaev for serving on my Honors Committee and for their contributions to the NSF Center for C-H Functionalization (CCHF) where my research began three years ago. I would like to especially express my gratitude to Dr. Davies – my honors thesis would not have been a possibility without your enthusiasm and willingness to sponsor my research with Dr. Houk.

Finally, I would like to thank the Hoffman2 cluster at UCLA for their computational resources, the CCHF and Chemistry Summer Undergraduate Research Program (CSURP) for sponsoring two unforgettable summers of research, and most of all, the Department of Chemistry and Emory College for a wonderful four years.

Table of Contents

Schemes

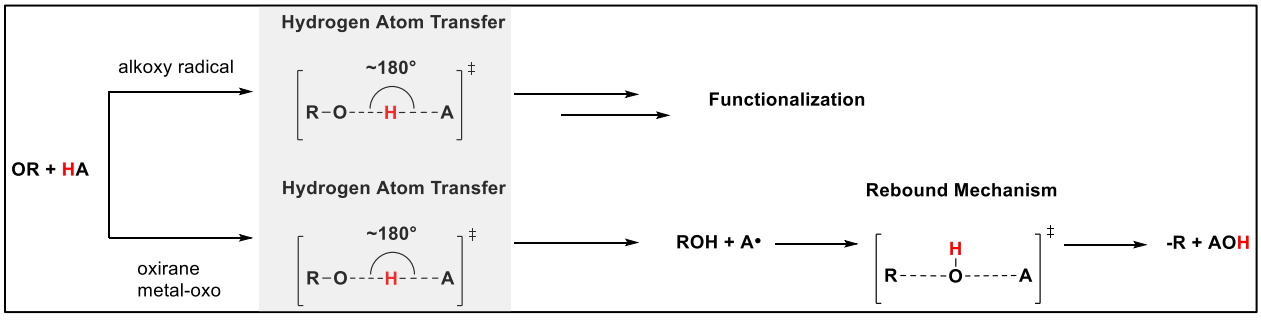
Figures

Tables

1. Introduction

Selective functionalization of inert sp^3 C-H bonds is one of the largest challenges currently being faced in organic chemistry. Oxidations, a type of C-H functionalization reaction where a C-H bond of a substrate is replaced with a C-O bond, are especially important and have been accomplished using radical reagents[1-3], dioxiranes[4-6], and transition metal catalysts[7-10] under mild conditions. These methods have been shown to offer efficient reactivity and great selectivity, even in a late stage synthesis[11,12], demonstrating their importance in developing newer, cheaper, and more diverse synthetic pathways. Oxyradicals, dioxiranes, and metal-oxo catalysts are often the chosen species to perform selective C-H oxidations and, mechanistically, most oxidations are believed to be mediated through a rate-determining step known as a hydrogen-atom-transfer (HAT) reaction that involves the abstraction of the hydrogen atom in the substrate's C-H bond[3,13-15]. In transition-metal catalysts and dioxiranes, this step is typically followed by a "rebound" mechanism leading to a hydroxylated product[14,15]. These pathways are summarized in Scheme 1.

Scheme 1. Alkoxy radicals, oxiranes, and metal-oxo species all participate in a hydrogen atom transfer with their corresponding substrate before functionalization. Metal-oxos and oxiranes experience a "rebound" mechanism which leads to a hydroxylated product.



To better inform the use of these reagents in the context of C-H functionalization, a deeper understanding of the factors that underly reactivity and selectivity patterns of the HAT reaction is required.

The Bell-Evans-Polanyi (BEP) correlation is perhaps the most fundamental and powerful relationship that attempts to address this[16-18]. It relates the activation energy of a reaction to the reaction's overall thermodynamics as seen in Equation 1. Typically, α and β are parameters obtained by linear regression and are positive, implying that a reaction will occur faster when the reaction is more exothermic.

$$\textbf{Equation 1}.\ \Delta H^{\ddagger} = \alpha + \beta \Delta H_{rxn}$$

However, there are limitations to the BEP approach. In Liu et al., HAT reactions with a series of 26 substrates that vary in C-H bond structure and electronics are explored with dimethyl dioxirane (DMDO) and trifluoro dioxirane (TFDO) as abstractors. Through a computational study, the transition state barriers and enthalpy of separated reactants are calculated for each dioxirane species (52 total) and fitted to the BEP relationship shown in Equation 1 to obtain α and β. They subsequently reported that a traditional BEP relationship poorly reproduced kinetic barriers given by a low coefficient of determination[13]. Yet, when the substrate set was divided into two groups – "saturated" and "unsaturated" (where the activated C-H bond is allylic or adjacent to unsaturation), Liu showed that these two classes of C-H bonds separately and independently satisfied a BEP relationship, but together did not. This effect is neither local to DMDO or TFDO nor computational methods. In Bietti et al., it is demonstrated, experimentally, that cumyloxy's (CumO•) HAT transfer reactions with 56 substrates also display bimodal patterns of reactivity such that allylic and benzylic hydrocarbons have distinct correlations from saturated hydrocarbons, alcohols, ethers, diols, amines, and carbamates[19]. This bimodal pattern highlights a weakness of the BEP relationship, which does not adequately capture Bernasconi's

Principle of Non-Perfect Synchronization (PNS). PNS suggests that, in HAT reactions, lagging stabilization appears due to delocalizing effects[20-22]. In other words, PNS implies that the stability of the products, or the thermodynamics of the reaction, is not completely reflected in its kinetics. This "lag" can be attributed to the nonlinear transfer of radical density from the abstractor to the delocalized substrate in the transition state. Hence, for unsaturated substrates that experience delocalization throughout the reaction, we should expect β in equation 1 to be less than 1, whereas for saturated substrates it should be closer to 1. Indeed, this is found in Liu et al. where β is 0.35 and 0.91 for unsaturated and saturated substrates, respectively[13]. This property is also reflected geometrically in the transition-state, where C-H bond breaking distances are found to be shorter for unsaturated substrates. These "earlier" transition-states are a result of stabilization not developing fully and thus "lagging behind" in the transition-state.

To resolve this and other weaknesses, Roberts and Steel propose a modified Bell-Evans-Polanyi relationship[23], which in addition to thermodynamics, introduces polar, steric, and stereoelectronic effects that influence the transition-state and activation energy barrier, as shown in Equation 2:

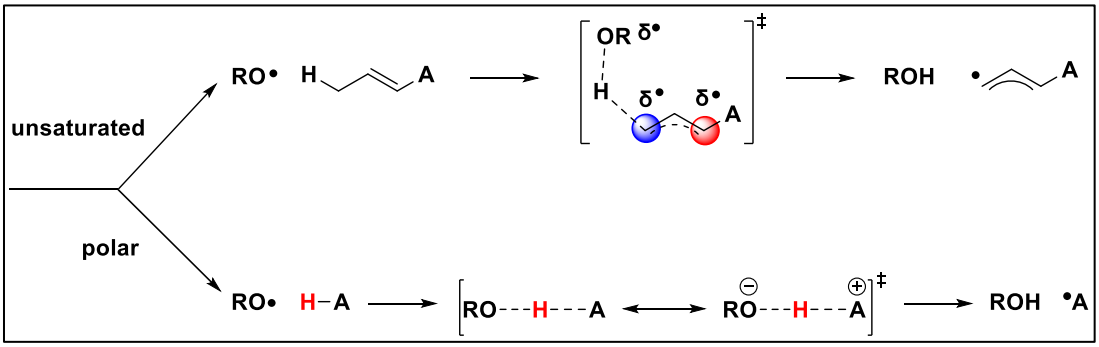
$$\textbf{Equation 2}.\ \Delta H^{\ddagger} = E_0 f + \alpha \Delta H_{rxn}(1-d) + \beta \Delta\chi^2 + \gamma(S_A + S_B)$$

Here, $\Delta H^{\ddagger}$ and ΔH are unchanged but four new terms are included to modulate these new non-thermodynamic effects (*f, d,* $\Delta\chi^2$, and S_X) paired with four associated fitted parameters (E_0, α, β, and γ). In the context of this work, the *f* term is a calculated quantity designed to measure the energetic cost of forming the O-H and stretching the C-H bonds in the transition-state. It is a dimensionless quantity calculated by the bond dissociation energies (BDE) as given in Equation 3:

$$\textbf{Equation 3}.\ f = \frac{BDE_{O-H}BDE_{C-H}}{BDE_{H-H}{}^2}$$

The *d* term serves to introduce PNS and assigns a penalty to $\Delta H^{\ddagger}$, proportional to ΔH_{rxn}, when we expect that stabilization does not develop linearly over the reaction coordinate. It can be described as a binary variable that is set to zero for "saturated" substrates that do not experience conjugative delocalization during the transition-state, and 0.44 for "unsaturated" substrates. The $\Delta\chi^2$ is another calculated quantity that measures the difference in Mulliken electronegativity between the abstractor and the substrate radical. It is sensible that stabilization could be achieved in the transition state when a substrate-abstractor pair differ significantly in electronegativity as the contribution of ionic resonance hybrids become more significant. Indeed, this is also seen experimentally as in Bietti et al., polar effects from electron-rich substrates tend to enhance rate constants when working with nucleophilic radicals. These combined effects are summarized in Scheme 2.

Scheme 2. Demonstration of the delocalization and polar effects in the Roberts-Steel equation. Delocalizing effects that destabilize the transition state arise from the delay in transfer of radical density from •OR to the red carbon. Polar effects that stabilize the transition state arise from the presence of ionic resonance forms that correspond to differences in substrate-abstractor electronegativities.



Finally, S_X describes the deformations in the reactant's and product's radical structures during the reaction and are given to be 0.6 and 0.25 for alkyl and alkoxy radicals, respectively. Of these new terms, *f* and $\Delta\chi^2$, require additional computational calculations as they are not

typically experimentally available, but they are neither computationally expensive nor difficult to identify.

Liu et al. make use of this Roberts-Steel functional form in their subsequent paper[24], demonstrating its efficacy on the same 26 substrates and with an expanded radical set of CH_3O•, tBuO•, CCl_3CH_2O•, and CF_3CH_2O•. They find, additionally, that the *f* and S_X terms have relatively minor contributions in explaining barriers and thus propose an even simpler functional form in Equation 4:

$$\textbf{Equation 4}.\ \Delta H^{\ddagger} = \gamma + \alpha\Delta H_{rxn}(1-d) + \beta\Delta\chi^2$$

Through multivariate linear regression, parameters γ, α, and β are solved from a fitting with the four alkoxy radicals as shown in Equation 5. A strong R^2 of 0.89 is achieved between actual and predicted barriers by the equation (RMSE = 1.06 and MAE = 0.86).

$$\textbf{Equation 5}.\ \Delta H^{\ddagger} = 10.0 + 0.52\Delta H_{rxn}(1-d) - 0.35\Delta\chi^2$$

Interestingly, Equation 5 implies three unique properties: 1) that 52% of the thermodynamic stability in the reaction manifests in the kinetic barriers with *saturated* substrates 2) that approximately 29% (0.52 × 0.56) of the thermodynamic stability in the reaction manifests in the kinetic barriers with *unsaturated* substrates and 3) that 35% of the difference in substrate-abstractor electronegativity contributes towards savings in the kinetic barriers of these reactions.

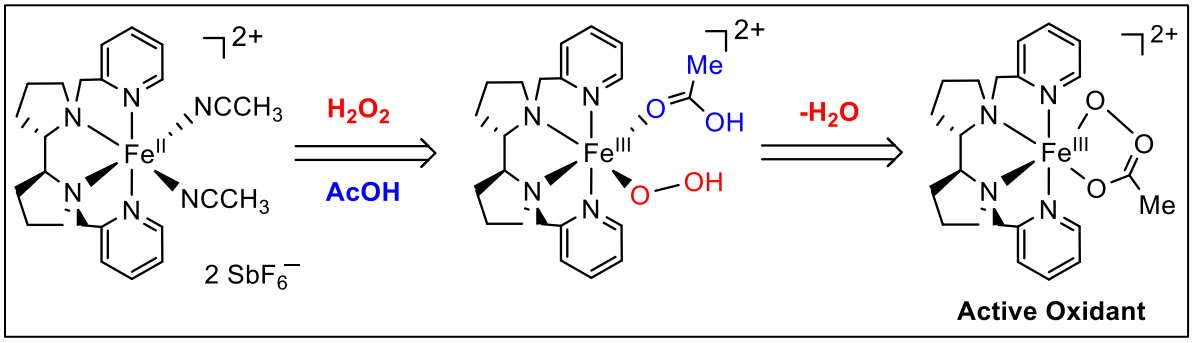
In light of the rising prevalence of using radicals and transition metal catalysts in the functionalization of C(sp^3)-H bonds, we sought to develop a deeper understanding of HAT reactions as well as test the scope of the BEP and Roberts-Steel relationships involving alkoxy radicals and metal-oxo species. The same 26 substrates explored in Liu et al (in Table 1) were chosen once more to sample C-H bonds in a wide range of chemical environments. HO•, CumO•, and tBuO• were selected as representative alkoxy radicals for their utility in performing

HAT reactions[25]. The iron-oxo "White-Chen" catalyst and the ruthenium-oxo "Dubois-Sigman" catalyst were also chosen for this investigation because they are two representative metal-oxo species known for their ability to perform efficient and selective C-H oxidations, especially under mild conditions[7,8].

1.1 Iron-oxo Catalyzed HAT and Hydroxylation

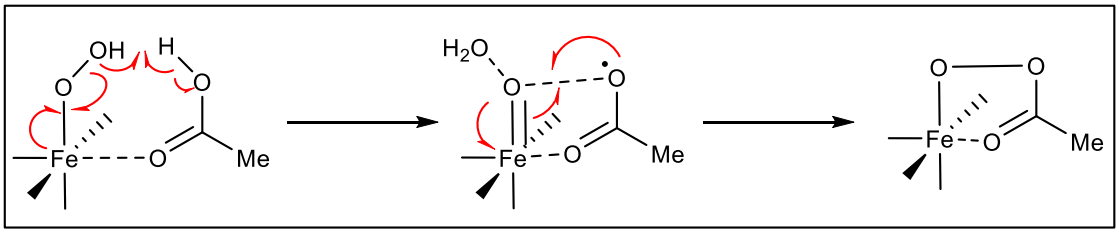
Iron-oxo catalysts have proven instrumental in the site-selective oxidations of aliphatic C-H bonds and the White-Chen catalyst is no exception. The active White-Chen catalyst, as depicted in Figure 1, is a small molecule non-heme iron-oxo catalyst that has been shown to predictably favor electron-rich, unhindered, and strain-relief inducing sp^3 C-H bond sites[7].

Figure 1. The "White-Chen" catalyst. The catalyst is activated in the presence of hydrogen peroxide and acetic acid with the loss of water. The active catalyst is a Fe(III) 2+ iron species.



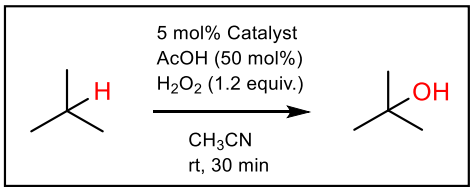
DFT studies have shown that the active iron species is generated, as illustrated in Figure 2, as a doublet with a cyclical geometry between the acetate ligand and the terminal oxygen in its ground-state[26].

Figure 2. The active oxidant is believed to be formed through radical transformations beginning with an iron-hydroperoxo leading to a ferric peracetate species.



Experimentally, it is shown that it is the active oxidant that performs the initial HAT, immediately followed by a "rebound" mechanism that delivers the hydroxy group onto the alkyl radical under the conditions shown in Figure 3[7].

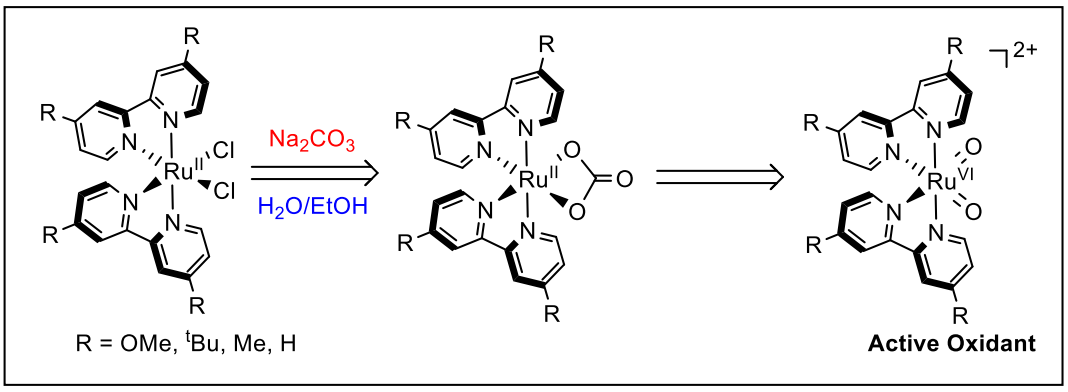
Figure 3. A representative hydroxylation via the iron-oxo catalyst is shown under experimental conditions.



1.2 Ruthenium-oxo Catalyzed HAT and Hydroxylation

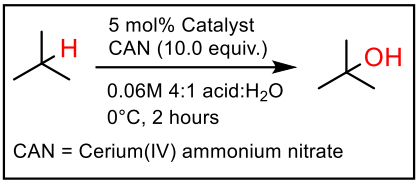
Ruthenium-oxo species have also begun to be recognized as potent and site-selective C-H oxidizing reagents. The Dubois-Sigman catalyst, pictured in Figure 4, is one such example known to discriminate flexibly between structurally disparate substrates. For example, while predisposed to reacting with tertiary or benzylic sites, the Dubois-Sigman catalyst can be tuned to select secondary sites under different acid pK_a conditions[27]. Figure 4 also highlights the tunability of the bipyridine scaffold which can produce an array of sterically and electronically different ruthenium-oxo species.

Figure 4. The "Dubois-Sigman" catalyst. The catalyst is activated in the presence of sodium carbonate, water, and ethanol, proceeding through a ruthenium-carbonato intermediate. This gives way to a Ru(VI) 2+ structure which is believed to be the active oxidant.



Experimentally, it is also the active oxidant that performs the initial HAT, although it is unclear if this is followed by a rebound mechanism or a concerted [3+2] cycloaddition delivering the hydroxy group onto the alkyl radical[28]. Nevertheless, the conditions shown in Figure 5 are typical for such transformations. Notably, reactions are accelerated in the presence of an acid, although it has been shown that hydroxylated product is still generated with MeCN/H_2O (1:1) solvent when run for 3 hours at room temperature[8]. For consistency, MeCN is treated as the standard solvent for all abstractors (metal-oxo and alkoxy radicals) in this work.

Figure 5. A representative hydroxylation via the ruthenium-oxo catalyst is shown under experimental conditions.



2. Results and Discussion

Benchmarking Active Oxidants. As implied by earlier schemes, both the White-Chen and Dubois-Sigman catalysts are characterized by a metal-oxo center bearing a +2 charge. DFT calculations on each catalyst revealed 3 potential ground-state oxidants, **1-3**, for the White-Chen species, and 3 potential oxidants, **4-6**, for the Dubois-Sigman species.

Inspection of Figure 6 reveals that oxidants **1** and **2** have doublet spin ground-states (S = 1/2) and **3** has a quartet (S = 3/2) state. Structurally, **1** and **2** are very similar, where both the C=O bond on the acetate and Fe=O bond are eclipsed, differing only in their O-O bond distance. In this case, **1** has an O-O bond length of 1.45Å whereas **2** has an O-O bond length of 2.02Å. **1** and **3** are also similar, with the C=O bond and Fe=O bond being slightly *gauche* to one another. On a relative energy basis, it is apparent that the most stable White-Chen species is the cyclic doublet isomer, **1**, which is 8.6 kcal/mol and 11.8 kcal/mol lower than **2** and **3**, respectively. This

finding agrees with the precedent found in the literature, and **1** will be considered the active oxidant for this exploration[26].

Figure 6. UB3LYP-D3/def2-TZVPP // UB3LYP-D3/def2-SVP in SMD CH_3CN solvent geometries of **1-6** in various spin states and geometries. Relative energies are given with respect to **1** for geometries **1-3** and with respect to **4** for **4-6**. Hydrogen atoms on each catalyst's skeleton are omitted for clarity.

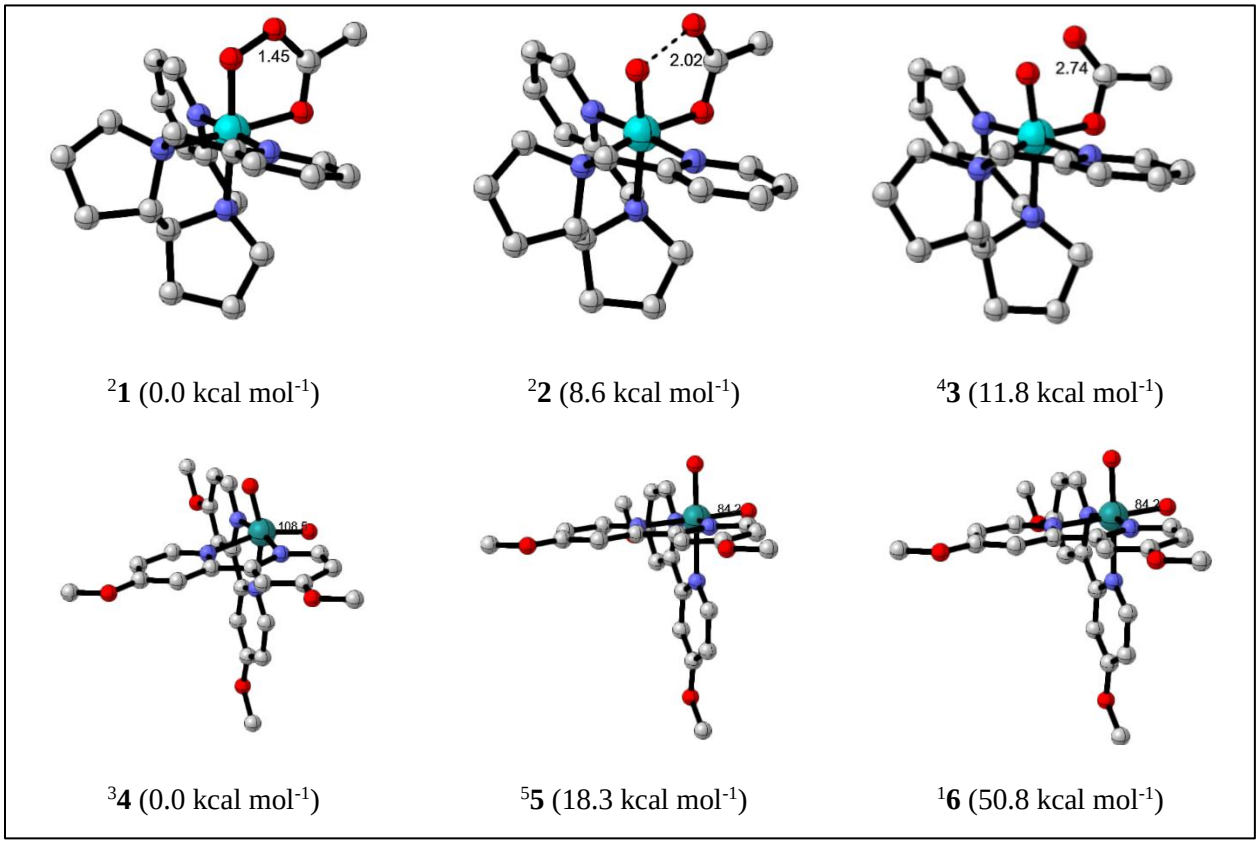
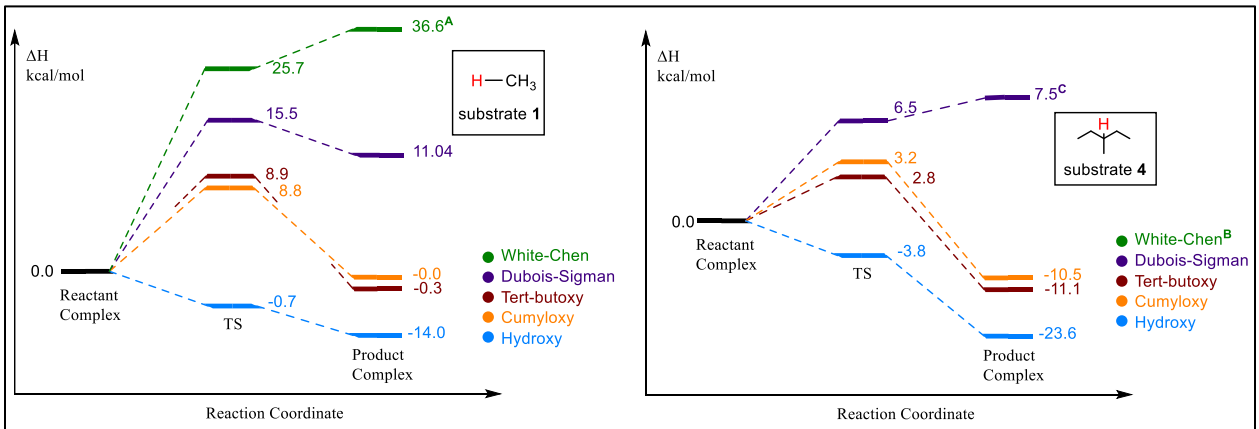


Figure 6 also shows that oxidants **4, 5,** and **6** have triplet (S = 1), quintet (S = 3), and singlet (S = 0) ground-states, respectively. **5** and **6** share identical geometries, differing only in their spin. **4** and **5** differ slightly structurally, where **4** is characterized by having a wider O-Ru-O bond angle (108.5°) compared with **5** (84.2°). On a relative energy basis, the triplet structure, **4**, is the most stable ground-state geometry of the Dubois-Sigman catalyst, as it is 18.3 kcal/mol and 50.8 kcal/mol below the quintet and singlet structures, respectively. For this reason, the triplet structure and spin state will also be considered the active oxidant for this work.

HAT Reaction of Methane and 3-methylpentane. To illustrate the thermodynamics and kinetics of metal-oxo species **1** and **4** to other oxidants, we present Figure 7 which shows the pathway from the optimized reactant complex through the HAT and the subsequent optimized product-complex. Expectedly, the barriers of HAT reactions with metal-oxo species are relatively high, but not prohibitive to occurring under mild conditions, and the reactions generally lead to endothermic substrate radical intermediates. At the same time, HAT reactions with oxyradicals have lower barriers and generally lead exothermically to intermediates. It is also unsurprising that the structural similarities between tert-butoxy and cumyloxy confer similar kinetics and thermodynamics. Hydroxy uniquely demonstrates submerged kinetic barriers and a further exothermic intermediate, potentially suggesting the presence of strong attractive effects or stabilization during the transition-state. Importantly, these submerged kinetic barriers can, in part, be attributed to zero-point energy corrections to single-point energies.

Figure 7. Energy profiles (in kcal/mol) for the hydrogen atom transfer reactions of the White-Chen, Dubois-Sigman catalysts and Tert-butoxy, Cumyloxy, and Hydroxy radicals with methane and 3-methylpentane are given with the abstracted hydrogen depicted in red.



A. The product-complex of White-Chen with methane could not be located, and instead the relative ΔH of the separated products is provided
B. The transition state of White-Chen with 3-methylpentane could not be located and is omitted
C. The product-complex of Dubois-Sigman with 3-methylpentane could not be located, and instead the relative ΔH of the separated products is provided

Reactivities and Selectivities of Abstracting Species. As mentioned previously, we studied the HAT of a variety of 26 substrates containing sp^3 C-H bonds, designed to broadly

sample the chemical space, with our "abstracting group" of 5 different oxyradicals and metal-oxo species. Table 1 summarizes the abstracting group (OR) and the substrates used for this exploration (HA). Figure 8 shows kinetic barriers ranked for each substrate by each abstractor. As previously suggested, kinetic barriers are highest for the metal-oxo abstractors compared to oxyradicals.

Table 1. sp^3 C-H Bonds (in red) for HAT to Oxyradicals and Metal-Oxo Catalysts Studied in this Work. OR shows the "abstracting group" considered, substrates 1-12 are labeled as "saturated", and substrates 13-26 are labeled as "unsaturated" (containing a C-H, which if it were abstracted, would lead to a conjugated radical).

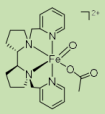
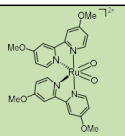
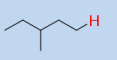
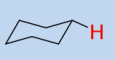
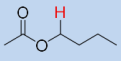
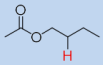
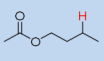
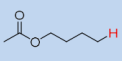
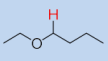
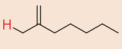
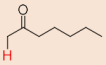
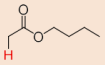
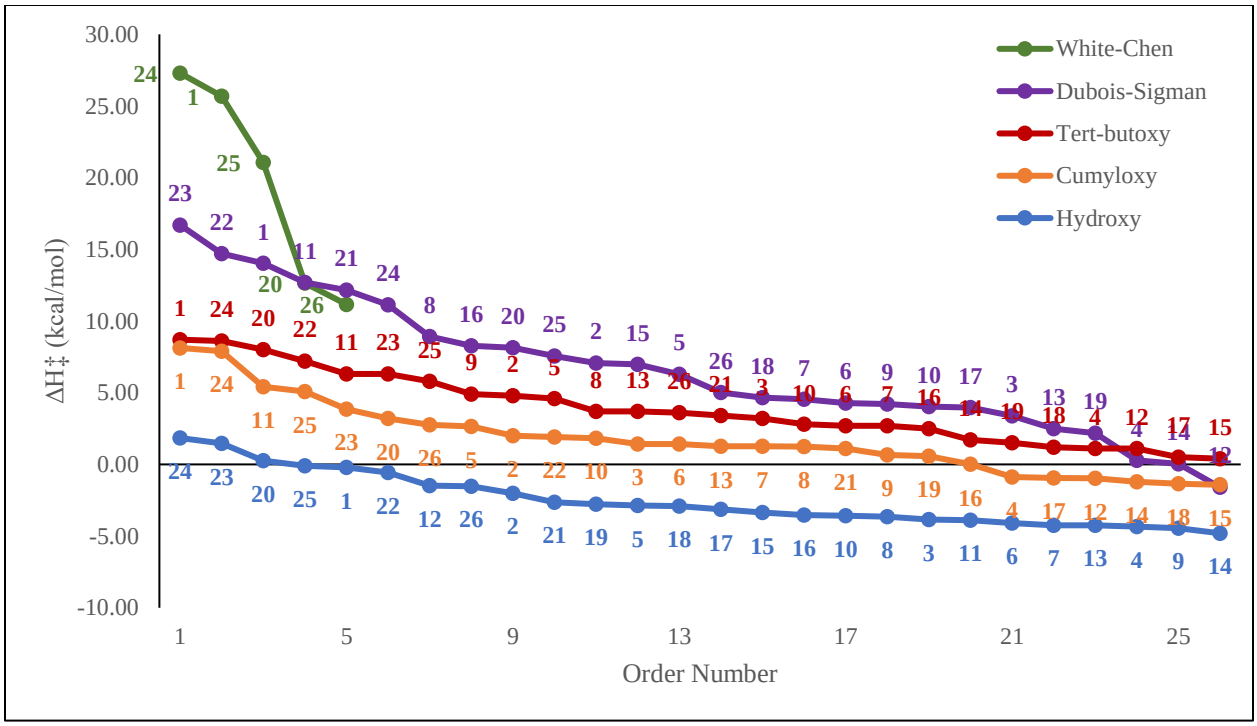
OR =	 *White-Chen*	 *Dubois-Sigman*	tBuO•	CumO•	HO•		
HA = *(saturated)*	 1	 2	 3	 4	 5	 6	 7
	 8	 9	 10	 11	 12		
HA = *(unsaturated)*	 13	 14	 15	 16	 17	 18	 19
	 20	 21	 22	 23	 24	 25	 26

Figure 8. $\Delta H^{\ddagger}$ for HAT from the C-H bonds of substrates shown in Table 1 to the metal-oxo species, White-Chen (green) and Dubois-Sigman (purple), and oxyradicals, tert-butoxy (red), cumyloxy (orange), and hydroxy (blue) ordered from greatest to least with substrates given as data labels. Energies are given in kcal/mol.



Per Table 2, this is consistent with the Bell-Evans-Polanyi principle that higher enthalpies of activation ($\Delta H^{\ddagger}$) are a manifestation of higher enthalpies of reaction (ΔH). For example, the enthalpies of reaction, are on average, higher for metal-oxo catalysts compared with those of oxyradicals. In this way, we show the reactivity increases as follows: White-Chen < Dubois-Sigman < Tert-butoxy < Cumyloxy < Hydroxy.

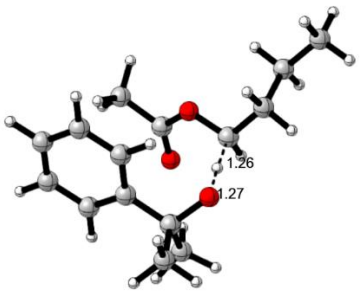
Table 2. Summary statistics with known $\Delta H^{\ddagger}$ and ΔH for HAT from the C-H bonds of substrates are presented. ΔH is calculated from separated reactants and products. Energies are given in kcal/mol.

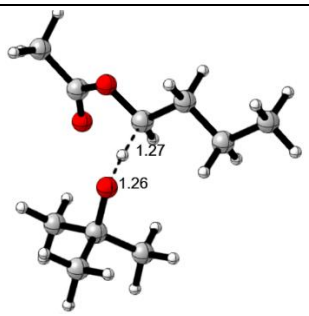
Summary Statistics					
$\Delta H^{\ddagger}$ (kcal/mol)	**White-Chen**	**Dubois-Sigman**	**tBuO•**	**CumO•**	**HO•**
Average	19.6	6.6	3.9	1.8	-2.5
High	27.3	16.7	8.7	8.1	1.8
Low	11.2	-1.6	0.4	-1.4	-4.8
σ_{sample}	7.4	4.7	2.5	2.6	1.9
N =	5	26	26	26	26
ΔH (kcal/mol)	**White-Chen**	**Dubois-Sigman**	**tBuO•**	**CumO•**	**HO•**

Average	25.6	0.2	-10.3	-10.4	-24.5
High	36.6	12.9	1.1	1.2	-12.9
Low	17.1	-13.4	-24.2	-23.5	-37.6
σ_{sample}	7.3	7.0	6.5	6.6	6.6
N =	5	26	26	26	26

Interestingly, between tBuO• and CumO•, two structurally similar radicals, unique patterns of reactivity also emerge. Figure 9, for instance, shows that the HAT of substrates 9 and 22 have discernibly lower barriers for CumO• compared with tBuO•. Structurally, both transition-states are nearly identical in bond distances and their thermodynamics strongly parallel each other. Differences in kinetic barriers arise, however, from additional stability that is afforded in the transition-state to CumO•. We hypothesize that this stability results from dispersive interactions that arise between the phenyl ring face and groups in its proximity.

Figure 9. Transition-state structures of HAT with substrates 9 and 22 by CumO• and tBuO•. Relative energies are quoted with respect to the left structure. All energies are given in kcal/mol.





Substrate 9 ($\Delta\Delta H^{\ddagger}$ = CumO• – tBuO• = -4.2 kcal mol^{-1})

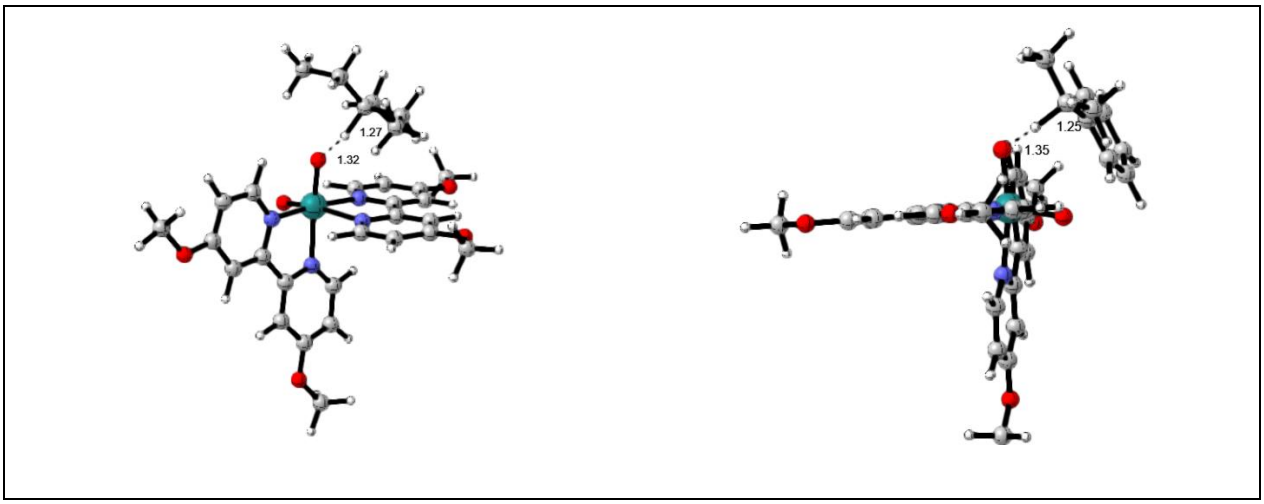
Substrate 9 ($\Delta\Delta H$ = CumO• – tBuO• = -0.1 kcal mol^{-1})

Substrate 22 ($\Delta\Delta H^{\ddagger}$ = CumO• – tBuO• = -5.3 kcal mol^{-1})

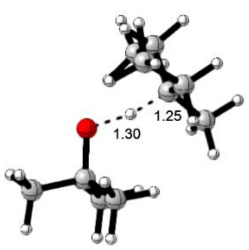
Substrate 22 ($\Delta\Delta H$ = CumO• – tBuO• = -0.1 kcal mol^{-1})

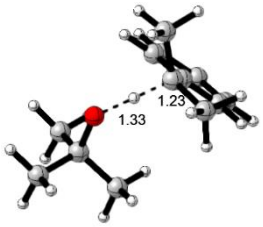
Table 2 also emphasizes idiosyncratic differences between all five abstractors that can be understood in terms of their standard deviations. Here, a low standard deviation implies that an abstractor is not very selective and is unable to effectively distinguish between different sp^3 C-H bond environments. Expectedly, we find higher variation in $\Delta H^{\ddagger}$ barriers for transition-metal catalysts, a result which confers greater selectivity and further explains their place in the C-H activation toolkit. For oxyradicals, on the other hand, although there is substantial variation in their enthalpies of reaction, less than half of it is captured in the variation in kinetic barriers.

Figure 10. Transition-state structures of HAT with substrates 4 and 18 by Dubois-Sigman and tBuO•. Relative energies are quoted with respect to the left structure. All energies are given in kcal/mol.



Dubois-Sigman ($\Delta\Delta H^{\ddagger}$ = Substrate 4 – Substrate 18 = -4.4 kcal mol^{-1})





tBuO• ($\Delta\Delta H^{\ddagger}$ = Substrate 4 – Substrate 18 = 0.1 kcal mol^{-1})

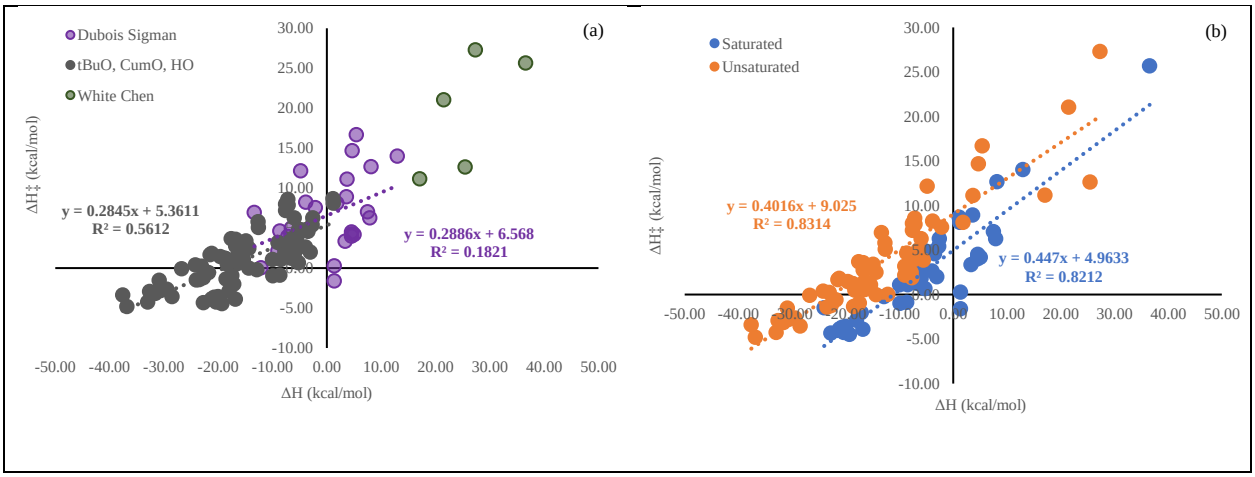
To further reinforce this point, Figure 10 reveals the differences in selectivity between tBuO• and the Dubois-Sigman catalyst. Both substrate 4 and 18 have tertiary sp^3 bonds, but when reacting with the Dubois-Sigman catalyst, there is a clear preference for the tertiary "saturated" C-H bond whereas, for tBuO•, there is no such preference. In fact, for all tertiary C-H bonds explored, the Dubois-Sigman catalyst has the lowest barriers for saturated C-H bonds with a HAT with substrate 4 having the lowest barrier, followed by unsaturated substrates 18 (benzylic), 26 (*tert*-nitrile), and 15 (allylic), in that order. As mentioned earlier, the Dubois-Sigman catalyst selectively reacts with tertiary and benzylic sites, and this finding is consistent with earlier results[27]. Additionally, for longer chain-like structures, it has been shown that deactivating electron-withdrawing groups (EWGs) like nitriles, limit reactivity to the α-carbon, leading to functionalization at 2° positions five to six carbons down the chain, an outcome which aligns with the results presented here. This apparent difference in selectivity could be the result of saturated substrates engaging better in van der Waal interactions with the catalyst's bipyridyl-ring ligands.

Bell-Evans-Polanyi Relationship. As demonstrated prior, the BEP relationship takes the following linear form per Equation 1:

$$\textbf{Equation 1}.\ \Delta H^{\ddagger} = \alpha + \beta \Delta H_{rxn}$$

Figure 11 shows a plot of $\Delta H^{\ddagger}$ vs ΔH for HAT involving the C-H bonds of substrates 1-26 to the five abstractors. The correlations shown in (a) demonstrate a weak BEP relationship, evidenced by the poor R^2 values. For example, for the pooled oxyradicals an R^2 of 0.5612 is found. Likewise, for the Dubois-Sigman catalyst, a worse R^2 of 0.1821 is found, characterized by considerable scattering. Qualitatively, this is consistent with the high degree of variation in $\Delta H^{\ddagger}$ seen earlier in metal-oxo catalysts that also confers their selectivity. However, when resolving this relationship by substrate type in (b), we see stronger relationships. Both saturated and unsaturated substrate kinetic barriers see R^2 of 0.8212 and 0.8314, respectively. As has been shown earlier, in unsaturated substrates, only about 50% of the enthalpy of reaction manifests in the TS. This corresponds with Bernasconi's Principle of Non-Perfect Synchronization with lagging stabilization appearing due to an incompletely delocalized radical developing in the TS. HAT reactions with saturated substrates are usually characterized by having a β close to 1, demonstrating synchronization. Curiously, here, we show that it is closer to 45%, which we believe is a result of more idiosyncratic stabilizing effects that will be explored briefly in the following section.

Figure 11. Plot of $\Delta H^{\ddagger}$ vs ΔH for HAT from the C-H bonds of the substrates shown in Table 1 to the five abstractors. Energies are given in kcal/mol. (a) Graphical display of $\Delta H^{\ddagger}$ vs ΔH shown for White-Chen (in green), Dubois-Sigman (in purple), and all oxyradicals pooled in gray separately. (b) Graphical display with all abstractors pooled demonstrating a bimodal relationship by substrate type (saturated = substrates 1-12 and unsaturated = substrates 13-26).

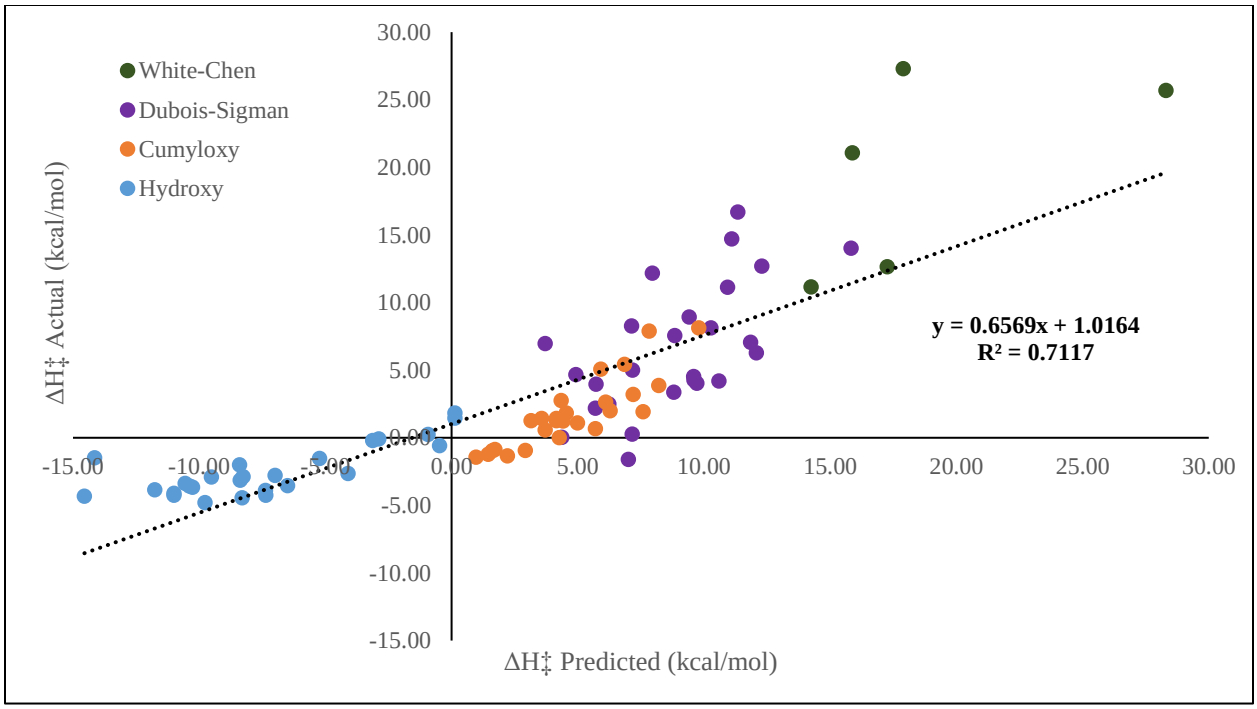


Roberts-Steel Relationship. A Roberts-Steel treatment was also applied to our series of abstractors to demonstrate the relationship's utility in describing a wide range of hydrogen-atom-transfer reactions. Following the simplified Roberts-Steel relationship shown below

$$\textbf{Equation 5}.\ \Delta H^{\ddagger} = 10.0 + 0.52\Delta H_{rxn}(1-d) - 0.35\Delta\chi^2$$

predictions for $\Delta H^{\ddagger}$ could be calculated using the enthalpies of reaction, the classification of substrates as "unsaturated" and "saturated", and the difference in electronegativities between abstractor and substrate.

Figure 12. Plot of $\Delta H^{\ddagger}$ Actual vs $\Delta H^{\ddagger}$ Predicted using Equation 5 of the Roberts-Steel Equation for HAT from the C-H bonds of the substrates shown in Table 1 to four abstractors (all but tert-butoxy). Energies are given in kcal/mol. White-Chen, Dubois-Sigman, Cumyloxy, and Hydroxy energy barriers are presented in green, purple, orange, and blue, respectively.

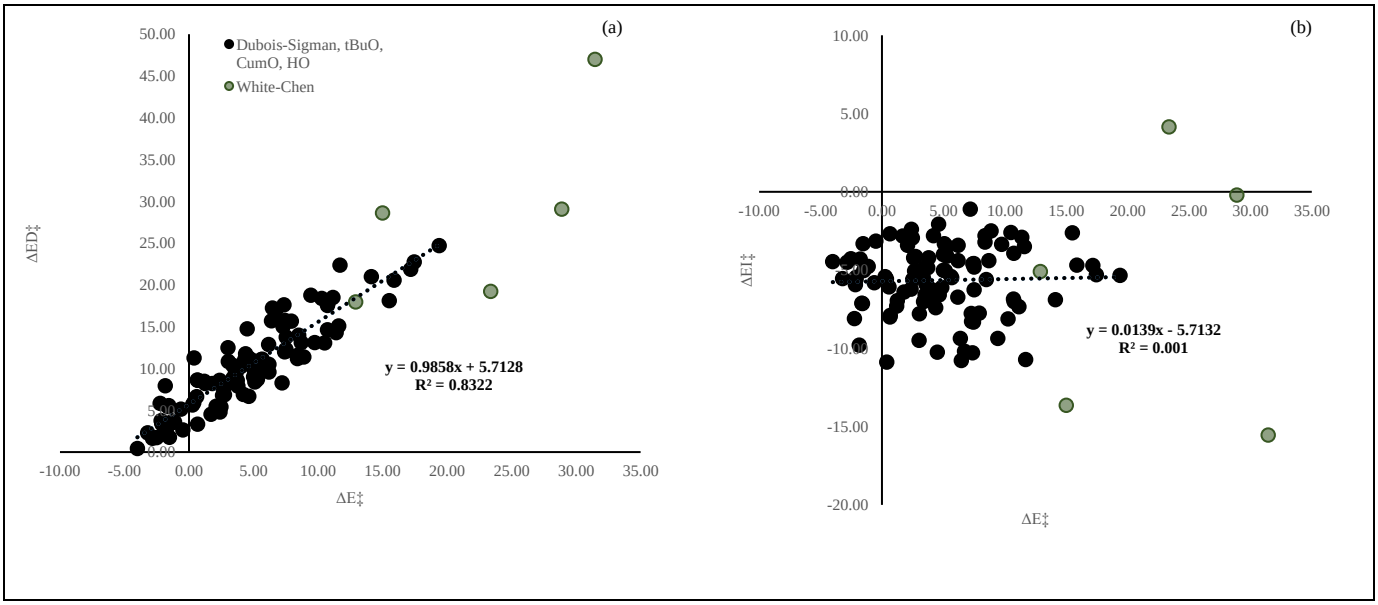


The correlations shown in Figure 12 are a result of plotting actual kinetic barriers against those predicted by the Roberts-Steel equation for our set of abstractors (excluding tert-butoxy as it has recently been shown to obey these Roberts-Steel type kinetics). For the overall set of abstractors, a relatively poor fitting was obtained with an R^2 of 0.7117. Consistent with the broader themes of this work, both metal-oxo species appear to demonstrate more scattering in predictions vs actuals of their kinetic barriers, emphasizing the limitations of the Roberts-Steel equation, as this functional form is unable to describe all the variation in kinetic barriers seen for metal-oxo catalysts. Perhaps the addition of a new term could resolve these deficiencies. For oxyradicals, visually, while there is a tighter spread, it does appear that HO• and CumO• have different kinetics. Nonetheless, it is worth noting that a regression slope of 1 would suggest that predicted barriers align perfectly with actual barriers but for all radicals shown here, a slope of 0.66 is obtained, implying that the Roberts-Steel equation systematically overestimates kinetic barriers. For oxyradicals, this may be a result of either strong attractive forces in the transition-state for

HO• or unique van der Waal interactions arising with CumO•, whereas for metal-oxo species this may result from a missing term that could capture the additional variation/qualities of transition metal catalysts.

Distortion Interaction Analysis. The distortion interaction analysis was also used to explore the origins of reactivities and selectivities in HAT reactions. In this model, the activation energy ($\Delta E^{\ddagger}$) can be described as the sum of the distortion energy ($\Delta E_D^{\ddagger}$), or the energy required to distort the reactants to the transition-state without interacting, and the interaction energy ($\Delta E_I^{\ddagger}$), or the intermolecular interaction between the two distorted fragments. Figure 13 shows the relationships between the activation energy and both interaction and distortion components.

Figure 13. Distortion Interaction Plots with all five abstractors. White-Chen (in green), Dubois-Sigman, tert-butoxy, cumyloxy, and hydroxy (in black). (a) $\Delta E_D^{\ddagger}$ vs $\Delta E^{\ddagger}$. (b) $\Delta E_I^{\ddagger}$ vs $\Delta E^{\ddagger}$. Energies are given in kcal/mol.



A rather modest linear relationship is observed in the regression of distortion energies with activation energies with an $R^2 = 0.83$ of the four core abstractors, whereas essentially no relationship is observed in the regression of interaction energies with activation energies ($R^2 \approx$

0.00). Interestingly, the linear trend in Figure 13a implies that an increase of 1 kcal/mol in the distortion energy is correlated with ≈ 1 kcal/mol increase in the overall activation energy barrier.

Figure 14. $\Delta E_D^{\ddagger}$ vs $r_{C\text{-}H}$ for four abstractors (all but White-Chen). Energies are given in kcal/mol; bond lengths are given in Å.

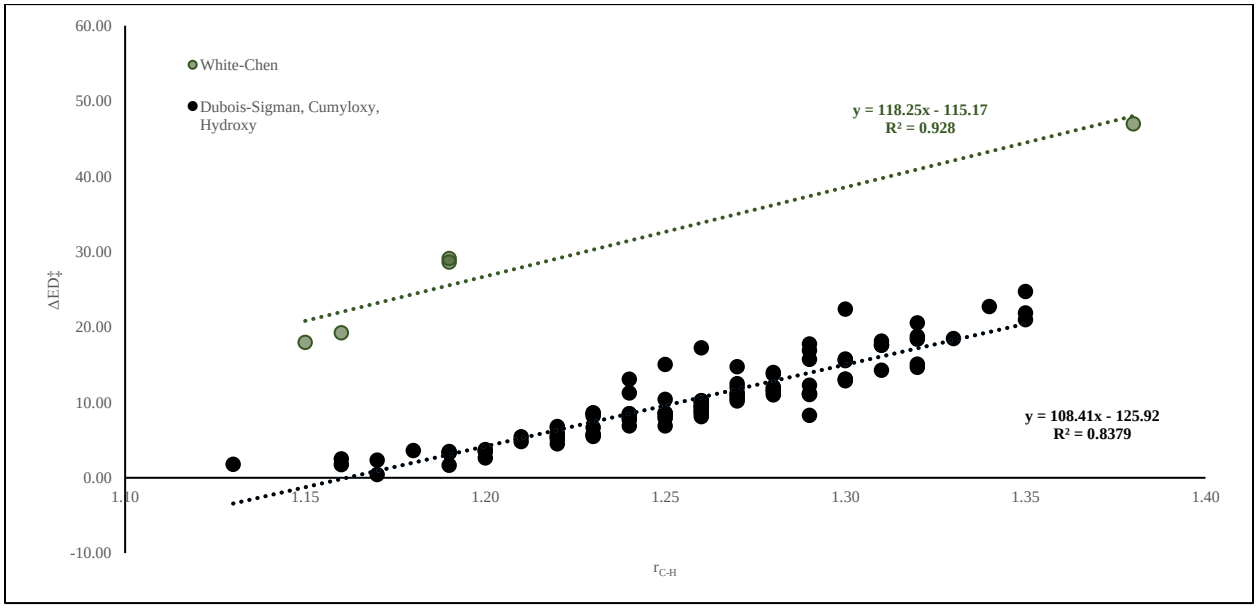
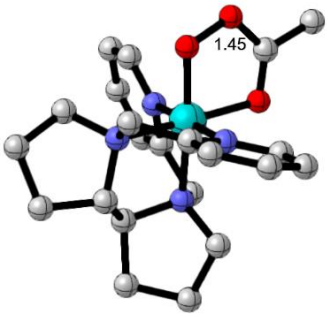
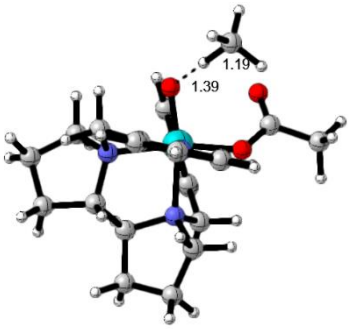
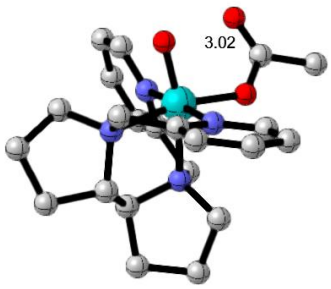


Figure 14 highlights that this parallel trend between distortion energies and activation energies originates from "early" vs "late" -ness in the reaction coordinate. As demonstrated, larger distortion energies are generally observed when the transition-state appears more "product-like", characterized by having a longer C-H bond. Figure 14 also reveals that the White-Chen catalyst still experiences the same trend; however, it experiences a greater energy penalty in distortion energies for the same transition-state geometries. While the sample size for transition-states for the White-Chen catalyst is not large enough to generalize, we hypothesize that this energy penalty in distortion energies may, in part, originate from strong deviations in the catalyst's geometry, shifting from the cyclic structure to the gauche structure as shown in Figure 15.

Figure 15. Ground-state structures of the White-Chen catalyst and its distorted geometry during the transition-state with substrate 1. Relative energies are quoted with respect to the left structure. All energies are given in kcal/mol.







$E_{Ground\text{-}State}$ (0.0 kcal mol^{-1}) **TS Geometry** **$E_{Distorted}$** (24.9 kcal mol^{-1})

3. Conclusion and Future Directions

We have studied the origins of reactivity and selectivity of HAT from sp^3 C-H bonds to different abstracting species including a diverse array of alkoxy radicals and metal-oxo catalysts. Through a computational approach, patterns that have been previously experimentally observed were validated. For example, we have replicated the Dubois-Sigman and White-Chen catalyst's patterns of reactivity and selectivity with the available transition-state geometries. We have also elucidated unique features of the cumyloxy radical, showing that its bulky phenyl group may play a non-trivial role in stabilizing kinetic barriers via van der Waal interactions in the transition-state. Similarly, the Dubois-Sigman catalyst's apparent selectivity for tertiary saturated substrates over unsaturated substrates was proposed to operate via a similar van der Waal and PNS argument. A Bell-Evans-Polanyi relationship was also applied to further explore the origins of reactivities of each abstracting species, especially metal-oxo catalysts. It was shown that bimodal BEP relationships were adequate in describing both oxyradical and metal-oxo barriers. The Roberts-Steel model, previously validated for oxyradicals, was extended to our abstractor set to generate predictions for kinetic barriers, including metal-oxo catalysts for the first time. It was shown that the relationship struggled to capture the variation in activation enthalpy barriers.

These results imply that a more robust model with new and/or higher order terms may be required to fully explain and predict kinetic barriers of more varied abstracting species. To that end, we are currently exploring machine learning fittings as an extension of this work. Finally, it was shown that distortive effects in the transition-state were primarily responsible for explaining activation energy barriers for most abstractors and that these distortive effects stemmed from the "early" and "late"-ness of each transition-state. The White-Chen catalyst experienced disproportionately large distortive effects which may be result of a conformational change during the reaction. However, with a limited sample size of transition-states, it is uncertain whether this is the cause of discrepancies in distortive effects.

4. Supplemental Information

4.1 Procedure for Density Functional Calculations

A. Benchmarking

The coordinates of the White-Chen catalyst were obtained from a previous computational exploration in xyz format[26] which were subsequently converted to gjf using PyMol[29] and Gaussian 16[30]. The structure was then optimized in Gaussian, using the unrestricted B3LYP-D3(BJ) functional and def2-SVP basis set, by varying the Fe-O-O-C dihedral angle and spin-state (doublet, quartet). Structures for the Dubois-Sigman catalyst were obtained from a crystal structure of *cis*-bis(2,2'-Bipyridyl)-dichloro-ruthenium(ii) hydrate[31] and following the replacement of the dichloro-ligands with oxo-ligands and two *para*-OMe substitutions to each bipyridine ligand in Gaussian, the active catalyst was generated computationally and optimized according to the same procedure above, while varying spin states (singlet, triplet, quintet).

B. Optimizations and Single Point Calculations

For all species (White-Chen catalyst, Dubois-Sigman catalyst, tert-Butoxy, cumyloxy, hydroxy), pre-optimizations of ground-state and transition-state geometries were carried out with the Semiempirical Extended Tight-Binding Program Package (xTB)[32].

For oxyradicals (tert-butoxy, cumyloxy, hydroxy), calculations were then performed on these pre-optimized geometries with Gaussian 16 using unrestricted ωB97X-D with the 6-31G(d) basis set. For metal-oxo species (White-Chen catalyst and Dubois-Sigman), calculations were also performed with Gaussian 16 using the unrestricted B3LYP-D3(BJ) functional and def2-SVP basis set with the SMD solvation model for acetonitrile. Frequency analyses were carried out at the same level of theory as the geometry optimization on these stationary points to ensure these structures corresponded to energy minima or saddle points (transition-states).

All geometry optimized structures were further treated with xTB's Conformer-Rotamer Ensemble Sampling Tool (CREST)[33] to identify stable conformer arrangements of ground-state and transition-state structures. For ground-state structures, conformers were sampled using the MF-MD-GC workflow. Transition-state structure conformers invoked the same workflow; however, bond-breaking, and bond-forming distances were constrained.

Single point calculations were also computed in Gaussian 16. For optimized structures with oxyradicals, energies were calculated using the unrestricted ωB97X-D functional with 6-311++G(d,p) basis set. For optimized structures with metal-oxo species, energies were calculated using the unrestricted B3LYP-D3(BJ) functional with def2-TZVPP basis set. Solvent effects were considered for all structures using SMD solvation for acetonitrile. The cost-effectiveness and reliability of ωB97X-D and B3LYP-D3(BJ) has been demonstrated in many studies[26,34-38]. From single point calculations, enthalpies, free energies, enthalpies of activation, and free energies of activation could be obtained from thermal corrections provided by geometry optimizations:

$$\Delta H = \Delta E + H_{corr}$$

$$\Delta G = \Delta E + G_{corr}$$

$$\Delta H^{\ddagger} = \Delta E^{\ddagger} + H_{corr}$$

$$\Delta G^{\ddagger} = \Delta E^{\ddagger} + G_{corr}$$

Here, *E* refers to the single-point-energy calculated for each fragment obtained by the self-consistent procedure (SCF).

C. Procedure for Potential Energy Surface Calculations

To map the potential energy surface of each HAT reaction involving Substrates **1** and **4** with each abstractor, an intrinsic reaction coordinate (IRC) was calculated following both the forward

and reverse direction from the transition-state, using the appropriate level of theory decided for oxyradicals and metal-oxo species including keywords (maxpoints = 20, stepsize = 20, lqa, and iop(1/108=-1)). From the IRC, reactant-complexes and product-complexes were obtained and optimized following the earlier procedure.

Here, it was found that a product-complex intermediate for the White-Chen abstraction of **1** and Dubois-Sigman abstraction of **4** could not be found and instead the structures collapsed to the hydroxylated product.

D. Procedure for Vertical Ionization Potential and Electron Affinity Calculations

Ground-state optimized structures of all oxyradicals, substrate radicals, and metal-oxo species were used to calculate the energies of their corresponding anions and cations via the single-point-energy procedure. These SCF energies were then aggregated to compute the vertical ionization potentials (*VIP*) and vertical electron affinities (*VEA*) as follows:

$$VIP = E_{cation} - E_{radical}$$

$$VEA = E_{radical} - E_{anion}$$

The Mulliken electronegativity (χ) is then computed as the arithmetic average of *VIP* and *VEA*. For its inclusion in the Roberts-Steel equation, the electronegativity of the oxidant is subtracted from the substrate as demonstrated and squared:

$$\Delta\chi^2 = (\chi_{oxidant} - \chi_{substrate})^2$$

E. Procedure for Distortion Interaction Analysis

Transition-state optimized structures of all oxyradical-substrate and metal-oxo substrates were broken into two fragments by removing the forming oxygen-hydrogen bond, resulting in an uncoordinated radical/metal and the substrate. The energies of these fragments were then calculated using single point calculations (UωB97X-D/6-311++G(d,p) for oxyradicals and

UB3LYP-D3(BJ)/def2-TZVPP for metals). Distortion interaction energies were then computed as follows:

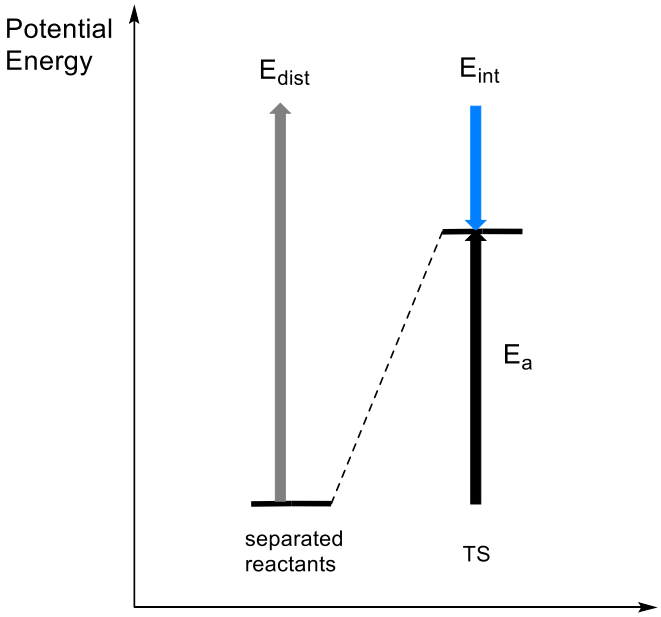
$$\Delta E_{dist}^{\ddagger} = E_{strained} - E_{separated}$$

$$\Delta E^{\ddagger} = E_{TS} - E_{separated}$$

$$\Delta E_{int}^{\ddagger} = \Delta E_{dist}^{\ddagger} - \Delta E^{\ddagger}$$

$E_{strained}$ is obtained from the sum of the SCF energies of the two distorted fragments and $E_{seperated}$ refers to the sum of the SCF energies of the two ground-state participating fragments. Finally, E_{TS} is refers to the SCF energy of the transition-state.

Figure S1. Distortion-Interaction Model where $\Delta E_{int}^{\ddagger}$ is given as the difference between $\Delta E_{dist}^{\ddagger}$ and $\Delta E_{a}^{\ddagger}$, both of which are calculated values from the transition state geometry.



F. Visualizations

All visualizations of optimized structures were generated using CylView[39].

4.2 Thermodynamic and Kinetic Findings

Table S1. E, H correction, G correction for all 26 substrates. Calculations are based on UB3LYP-D3(BJ)/def2-TZVPP // UB3LYP-D3(BJ)/def2-SVP with SMD model in CH_3CN. All energies are given in Hartrees.

	A			**A•**		
	E(UB3LYP)	H Correction	G Correction	E(UB3LYP)	H Correction	G Correction
1	-40.540075	0.048014	0.026851	-39.85922	0.033272	0.009389
2	-237.20828	0.196566	0.155714	-236.5361	0.181794	0.13932
3	-237.20828	0.196566	0.155714	-236.5429	0.181983	0.13876
4	-237.20828	0.196566	0.155714	-236.5466	0.182542	0.138863
5	-237.20828	0.196566	0.155714	-236.5356	0.182001	0.139576
6	-236.0021	0.175842	0.140476	-235.3349	0.161463	0.124827
7	-236.0021	0.175842	0.140476	-235.3349	0.161423	0.124743
8	-386.53221	0.18503	0.137392	-385.8668	0.170862	0.122479
9	-386.53221	0.18503	0.137392	-385.8643	0.1706	0.120911
10	-386.53221	0.18503	0.137392	-385.8653	0.170772	0.123229
11	-386.53221	0.18503	0.137392	-385.8591	0.170312	0.121987
12	-312.45164	0.20261	0.157677	-311.7905	0.1891	0.142765
13	-117.96745	0.082939	0.053839	-117.322	0.07044	0.040525
14	-157.30129	0.11263	0.080512	-156.6623	0.099812	0.065768
15	-196.63988	0.142965	0.106192	-196.0018	0.129081	0.089891
16	-271.70389	0.134645	0.096456	-271.0511	0.121148	0.084912
17	-311.03828	0.164572	0.124201	-310.3904	0.150679	0.109845
18	-350.37281	0.193778	0.150409	-349.7274	0.180064	0.134819
19	-314.63987	0.232223	0.185288	-313.9948	0.218276	0.170678

20	-232.59248	0.119233	0.082175	-231.9306	0.105725	0.06882
21	-232.59248	0.119233	0.082175	-231.9401	0.104624	0.067526
22	-350.59523	0.208035	0.159858	-349.929	0.194775	0.14712
23	-386.53221	0.18503	0.137392	-385.8645	0.17145	0.125098
24	-132.82639	0.04949	0.02094	-132.161	0.035452	0.006622
25	-172.15983	0.07946	0.047183	-171.5038	0.065452	0.031783
26	-211.49447	0.108742	0.07314	-210.8457	0.094983	0.057057

Table S2. $\Delta E^{\ddagger}$, $\Delta H^{\ddagger}$, $\Delta G^{\ddagger}$, ΔH_{rxn}, ΔG_{rxn}, r_{C-H}, r_{O-H} for H-abstraction catalyzed by White-Chen Catalyst. Calculations are based on UB3LYP-D3(BJ)/def2-TZVPP // UB3LYP-D3(BJ)/def2-SVP with SMD model in CH_3CN. All energies are given in kcal/mol. Only the following five barriers could be isolated computationally.

	$\Delta E^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	ΔH_{rxn}	ΔG_{rxn}	r_{O-H}	r_{O-H}
1	28.9	25.7	33.2	36.6	34.1	1.39	1.19
20	15.0	12.6	25.1	25.4	24.8	1.43	1.19
24	31.5	27.3	37.5	27.3	26.4	1.12	1.38
25	23.4	21.1	31.6	21.5	19.9	1.50	1.16
26	12.9	11.2	22.3	17.1	14.9	1.59	1.15

Table S3. $\Delta E^{\ddagger}$, $\Delta H^{\ddagger}$, $\Delta G^{\ddagger}$, ΔH_{rxn}, ΔG_{rxn}, r_{C-H}, r_{O-H} for H-abstraction catalyzed by Dubois-Sigman Catalyst. Calculations are based on UB3LYP-D3(BJ)/def2-TZVPP // UB3LYP-D3(BJ)/def2-SVP with SMD model in CH_3CN. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	ΔH_{rxn}	ΔG_{rxn}	r_{O-H}	r_{C-H}
1	17.2	14.0	24.2	12.9	11.1	1.19	1.35

2	10.3	7.1	19.4	7.5	6.3	1.23	1.32
3	6.4	3.4	15.8	3.3	1.7	1.27	1.29
4	3.0	0.3	13.1	1.3	-0.6	1.32	1.27
5	9.4	6.3	18.5	7.9	6.8	1.23	1.32
6	7.3	4.3	16.4	4.6	3.6	1.27	1.3
7	7.5	4.5	16.5	4.5	3.6	1.26	1.3
8	11.7	8.9	23.9	3.6	3.0	1.27	1.3
9	7.4	4.2	18.4	5.0	3.6	1.24	1.31
10	6.7	4.0	18.6	4.5	4.4	1.26	1.29
11	15.9	12.7	27.6	8.1	7.5	1.22	1.32
12	0.4	-1.6	12.7	1.4	0.3	1.37	1.24
13	4.7	2.5	13.9	-7.8	-8.5	1.33	1.27
14	1.8	0.0	10.2	-12.2	-13.5	1.38	1.23
15	9.7	7.0	18.6	-13.4	-15.0	1.38	1.24
16	10.8	8.3	22.6	-3.9	-2.8	1.29	1.29
17	6.5	4.0	17.3	-7.2	-7.7	1.35	1.26
18	7.3	4.7	18.4	-8.7	-10.0	1.35	1.25
19	4.5	2.2	15.9	-9.0	-9.6	1.32	1.27
20	11.2	8.1	21.2	1.8	1.8	1.22	1.33
21	15.5	12.2	24.4	-4.8	-5.0	1.25	1.31
22	17.5	14.7	30.4	4.7	4.9	1.21	1.34
23	19.4	16.7	32.2	5.4	6.1	1.19	1.35
24	14.1	11.1	22.9	3.7	3.4	1.2	1.35
25	10.7	7.6	19.6	-2.2	-3.2	1.24	1.31
26	7.9	5.0	17.6	-6.6	-8.2	1.27	1.3

Table S4. $\Delta E^{\ddagger}$, $\Delta H^{\ddagger}$, $\Delta G^{\ddagger}$, ΔH_{rxn}, ΔG_{rxn}, $r_{C\text{-}H}$, $r_{O\text{-}H}$ for H-abstraction catalyzed by CumO•. Calculations are based on UωB97X-D/6-311++G(d,p) // UωB97X-D/6-31G(d) with SMD model in CH_3CN. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	ΔH_{rxn}	ΔG_{rxn}	$r_{O\text{-}H}$	$r_{O\text{-}H}$
1	10.7	8.1	17.1	1.2	-0.1	1.19	1.32
2	4.4	2.0	15.9	-3.1	-3.0	1.24	1.28
3	3.6	1.4	14.3	-7.1	-7.7	1.28	1.26
4	1.3	-0.9	12.4	-8.7	-10.5	1.31	1.25
5	4.9	2.6	15.8	-3.9	-3.3	1.24	1.28
6	3.7	1.4	12.7	-6.3	-7.5	1.28	1.25
7	3.6	1.3	13.0	-6.3	-7.5	1.27	1.27
8	3.5	1.2	15.3	-6.6	-6.5	1.27	1.26
9	3.1	0.7	15.2	-5.3	-5.7	1.25	1.27
10	4.0	1.8	17.0	-6.0	-6.4	1.27	1.26
11	7.5	5.4	20.5	-2.7	-2.5	1.24	1.28
12	0.7	-1.0	13.5	-9.9	-10.2	1.35	1.23
13	2.7	1.3	13.7	-18.9	-19.0	1.32	1.24
14	0.3	-1.2	10.7	-22.7	-23.5	1.34	1.23
15	0.6	-1.4	11.6	-23.5	-24.0	1.36	1.22
16	2.4	0.0	14.1	-14.4	-13.2	1.30	1.25
17	1.2	-0.9	13.1	-17.5	-17.1	1.33	1.24
18	0.6	-1.3	12.3	-18.5	-18.8	1.35	1.23
19	2.7	0.6	14.5	-16.5	-15.8	1.32	1.24
20	5.7	3.2	16.9	-9.0	-8.6	1.23	1.29

21	3.4	1.1	14.9	-15.4	-15.3	1.28	1.26
22	4.3	1.9	16.3	-7.7	-6.6	1.23	1.29
23	6.2	3.9	18.9	-5.5	-4.0	1.21	1.30
24	10.5	7.9	18.1	-7.1	-7.5	1.21	1.30
25	7.5	5.1	17.1	-12.6	-13.2	1.24	1.28
26	5.2	2.8	14.7	-16.8	-18.1	1.28	1.26

Table S5. $\Delta E^{\ddagger}$, $\Delta H^{\ddagger}$, $\Delta G^{\ddagger}$, ΔH_{rxn}, ΔG_{rxn}, $r_{C\text{-}H}$, $r_{O\text{-}H}$ for H-abstraction catalyzed by HO•. Calculations are based on UωB97X-D/6-311++G(d,p) // UωB97X-D/6-31G(d) with SMD model in CH_3CN. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	ΔH_{rxn}	ΔG_{rxn}	$r_{O\text{-}H}$	$r_{O\text{-}H}$
1	2.5	-0.2	5.8	-12.9	-15.4	1.25	1.26
2	0.4	-2.0	7.0	-17.2	-18.3	1.31	1.22
3	-2.1	-3.9	5.2	-21.2	-23.0	1.39	1.19
4	-3.2	-4.3	5.0	-22.8	-25.7	1.45	1.17
5	-0.6	-2.9	6.1	-18.0	-18.6	1.32	1.22
6	-2.1	-4.1	3.9	-20.4	-22.7	1.38	1.20
7	-2.2	-4.2	2.9	-20.4	-22.7	1.36	1.20
8	-1.6	-3.7	6.9	-20.7	-21.7	1.32	1.22
9	-2.2	-4.4	5.6	-19.4	-21.0	1.30	1.23
10	-1.6	-3.6	8.5	-20.1	-21.6	1.34	1.21
11	-1.8	-3.9	7.6	-16.8	-17.8	1.28	1.24
12	-1.5	-1.5	7.7	-24.0	-25.5	1.66	1.13
13	-2.8	-4.2	3.2	-33.0	-34.2	1.39	1.19
14	-4.0	-4.8	2.1	-36.8	-38.8	1.45	1.17

15	-2.5	-3.4	4.9	-37.6	-39.2	1.51	1.16
16	-1.5	-3.5	4.9	-28.5	-28.4	1.38	1.20
17	-1.3	-3.1	6.1	-31.6	-32.4	1.40	1.19
18	-1.8	-2.9	6.0	-32.6	-34.0	1.47	1.16
19	-1.1	-2.8	7.7	-30.6	-31.1	1.41	1.18
20	2.5	0.3	9.0	-23.1	-23.9	1.31	1.22
21	-0.5	-2.6	5.7	-29.5	-30.5	1.38	1.20
22	1.7	-0.6	9.0	-21.8	-21.8	1.33	1.22
23	3.6	1.5	11.8	-19.6	-19.2	1.24	1.26
24	4.6	1.8	8.9	-21.2	-22.8	1.28	1.23
25	2.4	-0.1	8.0	-26.7	-28.4	1.33	1.21
26	0.7	-1.5	6.3	-30.9	-33.3	1.39	1.19

Table S6. Computed electronegativites for all radical and metal-oxo species. Calculations for alkoxy radicals are based on UωB97X-D/6-311++G(d, p)//UωB97X-D/6-31G(d). Calculations for all other species are based on UB3LYP-D3(BJ)/def2-TZVPP // UB3LYP-D3(BJ)/def2-SVP with SMD model in CH_3CN. Energies are given in eV.

X•	IE/eV	EA/eV	χ/eV	d
1	6.26	2.78	4.52	0
2	5.30	2.13	3.71	0
3	4.79	1.69	3.24	0
4	4.42	1.48	2.95	0
5	5.30	2.14	3.72	0
6	4.79	1.84	3.31	0

7	4.79	1.84	3.32	0
8	4.99	1.95	3.47	0
9	5.31	2.14	3.73	0
10	4.94	1.83	3.39	0
11	5.38	2.19	3.78	0
12	4.32	1.42	2.87	0
13	5.28	2.85	4.06	0.44
14	4.85	2.51	3.68	0.44
15	4.63	2.39	3.51	0.44
16	4.87	2.93	3.90	0.44
17	4.58	2.68	3.63	0.44
18	4.37	2.48	3.43	0.44
19	5.14	2.74	3.94	0.44
20	6.88	3.68	5.28	0.44
21	6.21	3.33	4.77	0.44
22	6.84	3.66	5.25	0.44
23	6.93	3.66	5.30	0.44
24	7.09	3.91	5.50	0.44
25	6.35	3.45	4.90	0.44
26	5.87	3.13	4.50	0.44
White-Chen	24.72	-12.85	5.94	
Dubois-Sigman	7.48	4.78	6.13	
tBuO•	8.55	3.91	6.23	
CumO•	8.03	4.06	6.05	
HO•	12.83	4.74	8.79	

Table S7. Difference in electronegativities of the moieties A and B ($\Delta\chi_{AB}$). Energies are given in eV. Calculations for alkoxy radicals are based on UωB97X-D/6-311++G(d, p)//UωB97X-D/6-31G(d). Calculations for metal-oxo species are based on UB3LYP-D3(BJ)/def2-TZVPP // UB3LYP-D3(BJ)/def2-SVP with SMD model in CH_3CN.

$\Delta\chi_{AB}$	White-Chen	Dubois-Sigman	tBuO•	CumO•	HO•
1	1.42	1.61	1.71	1.53	4.26
2	2.22	2.42	2.51	2.33	5.07
3	2.70	2.89	2.99	2.81	5.55
4	2.99	3.18	3.28	3.10	5.84
5	2.22	2.41	2.51	2.33	5.06
6	2.62	2.81	2.91	2.73	5.47
7	2.62	2.81	2.91	2.73	5.47
8	2.46	2.66	2.75	2.57	5.31
9	2.21	2.40	2.50	2.32	5.06
10	2.55	2.74	2.84	2.66	5.40
11	2.15	2.34	2.44	2.26	5.00
12	3.06	3.26	3.35	3.17	5.91
13	1.87	2.06	2.16	1.98	4.72
14	2.26	2.45	2.55	2.37	5.11
15	2.43	2.62	2.72	2.54	5.28
16	2.04	2.23	2.33	2.15	4.89
17	2.30	2.50	2.59	2.41	5.15
18	2.51	2.70	2.80	2.62	5.36
19	2.00	2.19	2.29	2.11	4.85

20	0.66	0.85	0.95	0.77	3.50
21	1.17	1.36	1.46	1.28	4.02
22	0.68	0.88	0.97	0.79	3.53
23	0.64	0.83	0.93	0.75	3.49
24	0.43	0.62	0.72	0.54	3.28
25	1.04	1.23	1.33	1.15	3.89
26	1.44	1.63	1.73	1.55	4.29

Table S8. $\Delta E^{\ddagger}$, $\Delta E_d^{\ddagger}$, and $\Delta E_{int}^{\ddagger}$ for H-abstraction catalyzed by White-Chen Catalyst. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta E_D^{\ddagger}$	$\Delta E_I^{\ddagger}$
1	28.9	29.1	-0.2
20	15.0	28.6	-13.6
24	31.5	47.0	-15.5
25	23.4	19.2	4.1
26	12.9	18.0	-5.1

Table S9. $\Delta E^{\ddagger}$, $\Delta E_d^{\ddagger}$, and $\Delta E_{int}^{\ddagger}$ for H-abstraction catalyzed by Dubois-Sigman Catalyst. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta E_D^{\ddagger}$	$\Delta E_I^{\ddagger}$
1	17.2	21.9	-4.7
2	10.3	18.4	-8.1
3	6.4	15.7	-9.4
4	3.0	12.5	-9.5

5	9.4	18.8	-9.4
6	7.3	15.6	-8.3
7	7.5	15.8	-8.3
8	11.7	22.4	-10.7
9	7.4	17.6	-10.3
10	6.7	16.9	-10.2
11	15.9	20.6	-4.7
12	0.4	11.3	-10.9
13	4.7	11.2	-6.6
14	1.8	8.2	-6.4
15	9.7	13.1	-3.4
16	10.8	17.8	-7.0
17	6.5	17.2	-10.8
18	7.3	15.0	-7.8
19	4.5	14.8	-10.2
20	11.2	18.5	-7.3
21	15.5	18.1	-2.6
22	17.5	22.7	-5.3
23	19.4	24.7	-5.3
24	14.1	21.0	-6.9
25	10.7	17.6	-6.8
26	7.9	15.7	-7.7

Table S10. $\Delta E^{\ddagger}$, $\Delta E_d^{\ddagger}$, and $\Delta E_{int}^{\ddagger}$ for H-abstraction catalyzed by CumO•. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta E_D^{\ddagger}$	$\Delta E_I^{\ddagger}$
1	10.7	14.7	-3.9
2	4.4	11.8	-7.4
3	3.6	9.5	-5.9
4	1.3	8.2	-6.9
5	4.9	11.0	-6.1
6	3.7	8.6	-4.8
7	3.6	10.2	-6.6
8	3.5	10.1	-6.6
9	3.1	10.8	-7.8
10	4.0	10.2	-6.2
11	7.5	13.8	-6.3
12	0.7	8.6	-7.9
13	2.7	6.9	-4.1
14	0.3	5.7	-5.4
15	0.6	6.6	-6.1
16	2.4	8.6	-6.2
17	1.2	8.5	-7.3
18	0.6	8.6	-8.0
19	2.7	7.7	-5.0
20	5.7	11.1	-5.5
21	3.4	8.8	-5.4
22	4.3	11.1	-6.7
23	6.2	12.9	-6.7
24	10.5	13.1	-2.6

25	7.5	12.1	-4.6
26	5.2	10.2	-5.0

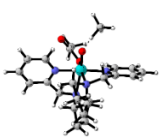
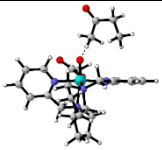
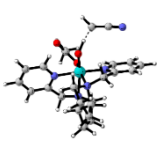
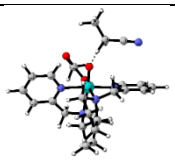
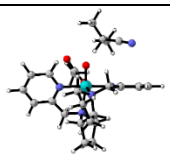
Table S11. $\Delta E^{\ddagger}$, $\Delta E_d^{\ddagger}$, and $\Delta E_{int}^{\ddagger}$ for H-abstraction catalyzed by HO•. All energies are given in kcal/mol.

	$\Delta E^{\ddagger}$	$\Delta E_D^{\ddagger}$	$\Delta E_I^{\ddagger}$
1	2.5	8.1	-5.6
2	0.4	5.9	-5.6
3	-2.1	3.4	-5.5
4	-3.2	2.3	-5.5
5	-0.6	5.2	-5.8
6	-2.1	3.5	-5.6
7	-2.2	3.8	-5.9
8	-1.6	5.6	-7.1
9	-2.2	5.8	-8.1
10	-1.6	5.5	-7.1
11	-1.8	8.0	-9.8
12	-1.5	1.8	-3.3
13	-2.8	1.7	-4.5
14	-4.0	0.4	-4.5
15	-2.5	1.8	-4.3
16	-1.5	3.6	-5.0
17	-1.3	3.5	-4.8
18	-1.8	2.5	-4.3
19	-1.1	3.6	-4.8

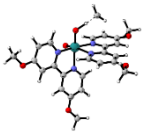
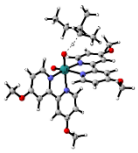
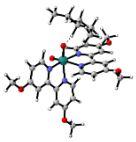
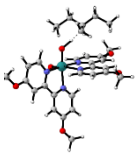
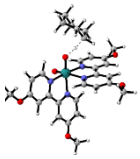
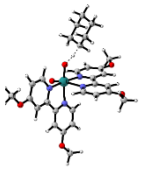
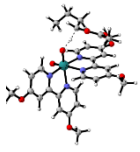
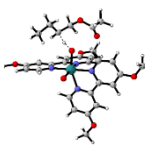
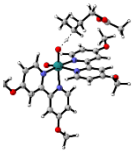
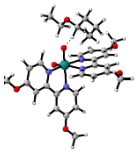
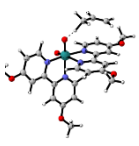
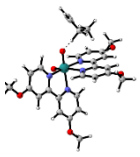
20	2.5	5.4	-2.9
21	-0.5	2.7	-3.1
22	1.7	4.5	-2.8
23	3.6	9.4	-5.9
24	4.6	6.7	-2.1
25	2.4	4.8	-2.4
26	0.7	3.3	-2.7

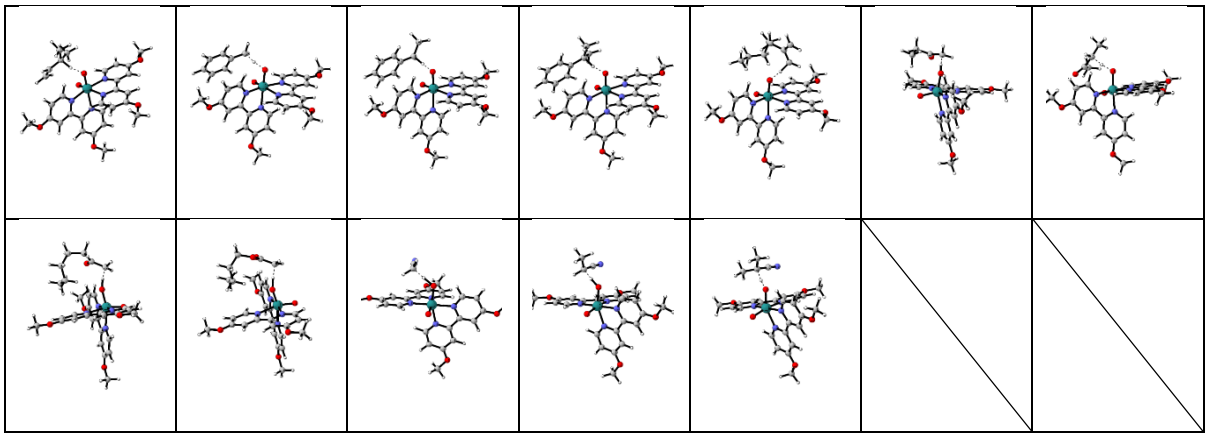
4.3 Transition State Geometries

A. White-Chen

						
1	**20**	**24**	**25**	**26**		

B. Dubois-Sigman

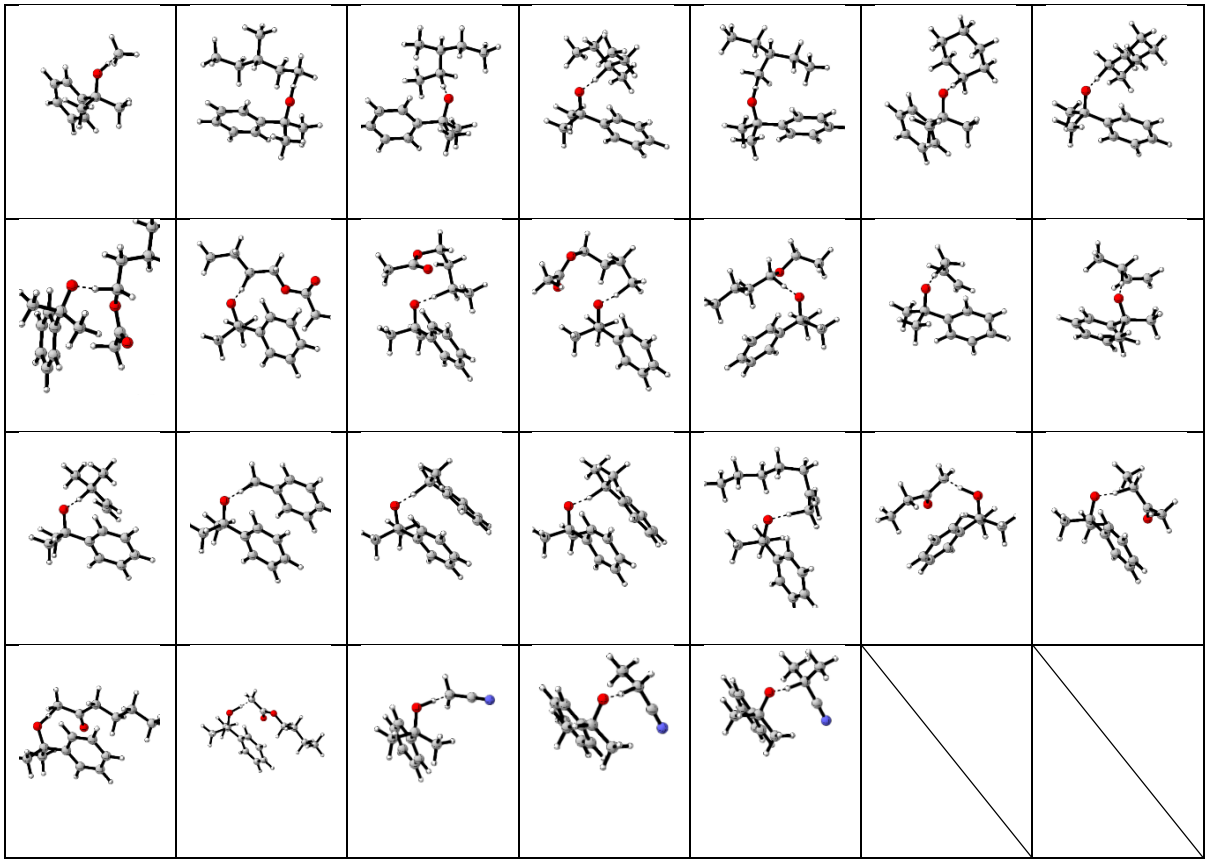
						
						



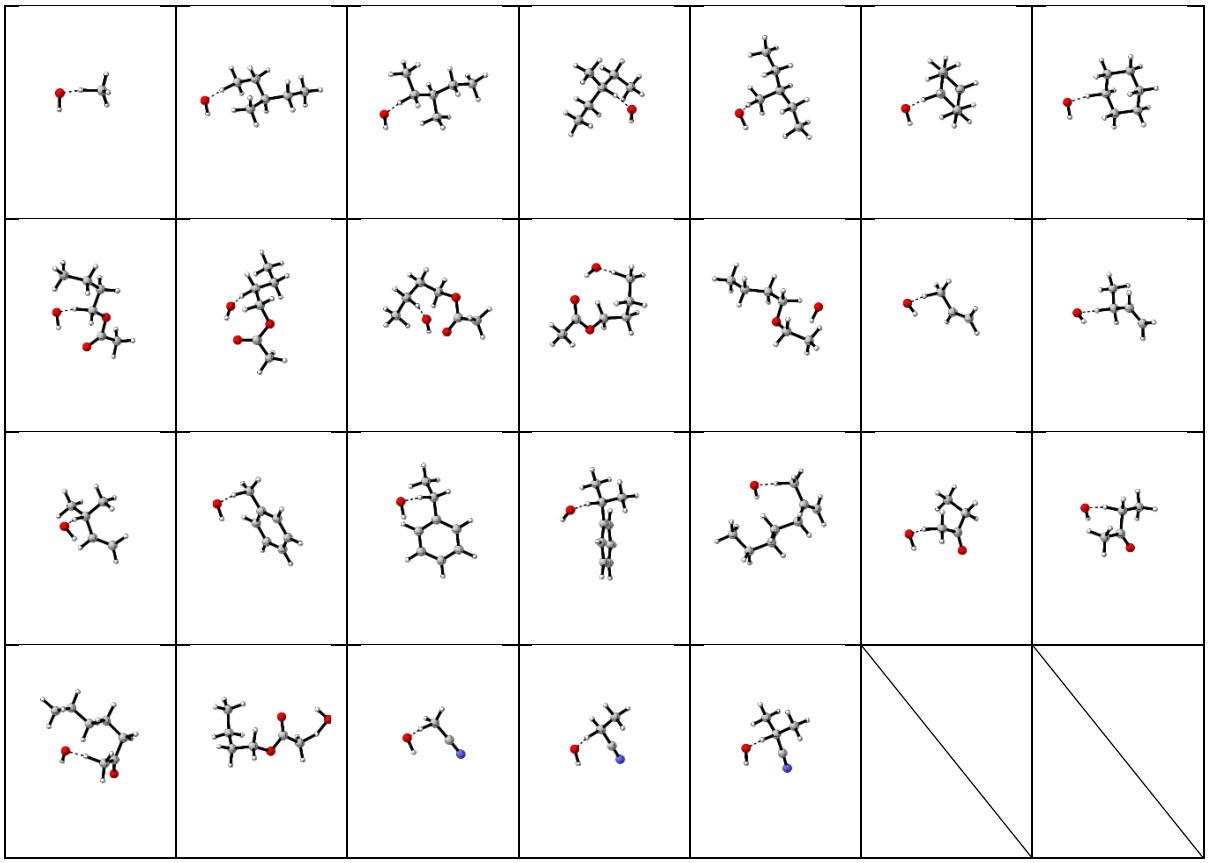
C. Tertbutoxy

Transition-state energies and structures are given in Liu et al[24].

D. Cumyloxy



E. Hydroxy



4.4 Cartesian Coordinates of Ground-State and Transition-state Optimizations

A. Ground-state Benchmarked Structures

Ground-state energies and structures for all substrates are given in Liu et al[24]. Energies and geometries were re-calculated under UB3LYP for transition metal catalysts and are given in Table S1.

^{2}1

Fe	0.035289	0.516911	-0.142523
N	1.994511	0.159821	-0.236233
C	2.788991	0.442944	-1.281836
H	2.299905	0.846304	-2.169058
C	4.160655	0.224505	-1.225599
H	4.780065	0.464498	-2.090687
C	4.711833	-0.305868	-0.056539
H	5.784912	-0.496158	0.013002
C	3.875998	-0.597808	1.021878
H	4.265623	-1.020225	1.949017
C	2.512295	-0.341572	0.902331
C	1.512387	-0.563750	1.993689
H	1.827412	-1.384981	2.652148
H	1.431051	0.347277	2.605486
N	0.179118	-0.823344	1.384425
C	-0.879614	-0.860131	2.441975
H	-1.854900	-0.774787	1.952134
H	-0.753520	-0.009645	3.122612
C	-0.733902	-2.238562	3.089676
H	-1.687039	-2.563621	3.528232
H	0.011007	-2.212624	3.897755
C	-0.264785	-3.157035	1.936387
H	-1.063799	-3.835567	1.607232
H	0.588549	-3.777849	2.237607
C	0.126171	-2.204996	0.782289
H	1.116931	-2.438276	0.371089
C	-0.895975	-2.198889	-0.348159
H	-1.898256	-2.068943	0.078359
C	-0.811958	-3.454506	-1.249005
H	-0.130731	-4.189644	-0.798181
H	-1.793234	-3.935269	-1.349315
C	-0.277131	-2.955540	-2.610539
H	0.498436	-3.612660	-3.026791
H	-1.087298	-2.886725	-3.350923
C	0.286891	-1.570657	-2.299226
H	0.336334	-0.883726	-3.152353
H	1.286919	-1.660179	-1.861112
N	-0.624992	-1.018808	-1.251836
C	-1.897869	-0.542717	-1.861446
H	-2.504976	-1.376452	-2.239636
H	-1.642769	0.102809	-2.715584
C	-2.657566	0.261581	-0.852742
C	-4.039614	0.432206	-0.861057

H	-4.642405	-0.081259	-1.611298
C	-4.619081	1.266936	0.095332
H	-5.700433	1.418637	0.108163
C	-3.804794	1.905227	1.034874
H	-4.221803	2.566776	1.795111
C	-2.433971	1.681923	0.994037
H	-1.751965	2.146931	1.706998
N	-1.889240	0.869933	0.072389
O	0.101545	1.646375	-1.574927
O	0.541999	2.126678	0.877401
C	0.827922	3.054681	0.101607
C	1.338139	4.377119	0.546557
H	1.577633	5.024588	-0.304926
H	0.564780	4.849263	1.173217
H	2.230262	4.214896	1.170205
O	0.687692	2.919844	-1.195101

SCF Done: E(UB3LYP)= -2563.062232
Sum of electronic and zero-point Energies= -2562.562397
Sum of electronic and thermal Energies= -2562.536853
Sum of electronic and thermal Enthalpies= -2562.535909
Sum of electronic and thermal Free Energies= -2562.616367

^{2}2

Fe	0.037165	0.517849	-0.320512
N	1.996635	0.129092	-0.355670
C	2.774403	0.300412	-1.437110
H	2.272139	0.611929	-2.353365
C	4.146375	0.088795	-1.376317
H	4.752793	0.232807	-2.271361
C	4.714835	-0.307723	-0.163160
H	5.789097	-0.488871	-0.088047
C	3.895695	-0.472535	0.953640
H	4.299585	-0.781498	1.918607
C	2.529082	-0.233124	0.827451
C	1.555615	-0.314119	1.960345
H	1.882776	-1.053563	2.704174
H	1.498760	0.665469	2.456656
N	0.206851	-0.633954	1.423440
C	-0.825720	-0.510762	2.498327
H	-1.813802	-0.485824	2.027051
H	-0.677369	0.425588	3.049254
C	-0.670988	-1.785006	3.331153
H	-1.612851	-2.036975	3.836948
H	0.096660	-1.651006	4.106748
C	-0.238393	-2.861125	2.307181
H	-1.052806	-3.566493	2.091873
H	0.613576	-3.447639	2.673712
C	0.139792	-2.083868	1.023893
H	1.123722	-2.380229	0.638777
C	-0.892087	-2.238139	-0.085287
H	-1.893588	-2.053170	0.322064
C	-0.808528	-3.606247	-0.804766
H	-0.120248	-4.267197	-0.260010
H	-1.788763	-4.098467	-0.828111
C	-0.286677	-3.303218	-2.227600
H	0.489732	-4.008858	-2.552238
H	-1.102685	-3.343257	-2.963572
C	0.274767	-1.887212	-2.124675
H	0.305309	-1.325797	-3.065692
H	1.280182	-1.906932	-1.691097
N	-0.632091	-1.197916	-1.154213
C	-1.914642	-0.809001	-1.808858
H	-2.519532	-1.690417	-2.059799
H	-1.671705	-0.285103	-2.746001
C	-2.664654	0.119270	-0.906900
C	-4.049239	0.263659	-0.901074
H	-4.658562	-0.359751	-1.556577
C	-4.622536	1.210644	-0.051641
H	-5.706091	1.343987	-0.030622
C	-3.799530	1.982121	0.772879
H	-4.211349	2.730968	1.450415
C	-2.425544	1.780182	0.728392
H	-1.735803	2.342287	1.357749
N	-1.888768	0.863648	-0.093416
O	0.106090	1.303636	-1.747316
O	0.493741	2.087912	0.674978
C	0.783270	3.122461	-0.015386
C	1.191711	4.364346	0.726979
H	1.462205	5.171128	0.036179
H	0.348135	4.676049	1.362254
H	2.042393	4.113076	1.378145
O	0.740341	3.159544	-1.267238

SCF Done: E(UB3LYP)= -2563.047728
Sum of electronic and zero-point Energies= -2562.549014
Sum of electronic and thermal Energies= -2562.523095
Sum of electronic and thermal Enthalpies= -2562.522151
Sum of electronic and thermal Free Energies= -2562.603887

^{4}3

Fe	0.060859	0.498082	-0.416191
N	1.958361	-0.011643	-0.458426
C	2.700824	0.006668	-1.580683
H	2.184970	0.256967	-2.507445
C	4.054882	-0.290970	-1.540289
H	4.634720	-0.277911	-2.463723
C	4.642303	-0.600129	-0.310283
H	5.705304	-0.843018	-0.251767
C	3.860622	-0.597247	0.845158
H	4.283207	-0.831838	1.822866
C	2.508105	-0.285429	0.744399
C	1.579644	-0.181231	1.910320
H	1.886283	-0.864446	2.714036
H	1.615439	0.844453	2.305128
N	0.193799	-0.453520	1.453045
C	-0.793126	-0.092565	2.514992
H	-1.789295	-0.056843	2.060660
H	-0.556254	0.897386	2.921609
C	-0.713776	-1.245461	3.516743
H	-1.648634	-1.334928	4.086236
H	0.099997	-1.076695	4.236551
C	-0.428272	-2.488401	2.642014
H	-1.322797	-3.116799	2.530566
H	0.361344	-3.115791	3.074221
C	0.000646	-1.934385	1.260666
H	0.954258	-2.361464	0.925199
C	-1.052669	-2.158539	0.185350
H	-2.029972	-1.839159	0.565825
C	-1.082004	-3.612988	-0.340927
H	-0.479882	-4.255615	0.315700
H	-2.105805	-4.007240	-0.339803
C	-0.496231	-3.556564	-1.771623
H	0.247296	-4.343717	-1.954247

H	-1.288066	-3.663562	-2.526432
C	0.152368	-2.175801	-1.862908
H	0.227899	-1.756881	-2.872763
H	1.149092	-2.197093	-1.410544
N	-0.725874	-1.303941	-1.017882
C	-1.973516	-0.945212	-1.751749
H	-2.614471	-1.826554	-1.887165
H	-1.690005	-0.574290	-2.748200
C	-2.686443	0.131265	-1.000097
C	-4.060018	0.350994	-1.040653
H	-4.693741	-0.318878	-1.623013
C	-4.590214	1.429621	-0.331494
H	-5.664444	1.624162	-0.351935
C	-3.736959	2.253772	0.405832
H	-4.113359	3.106245	0.972449
C	-2.375359	1.975765	0.416092
H	-1.656922	2.577159	0.972783
N	-1.884585	0.932761	-0.270720
O	0.100366	1.044015	-1.969942
O	0.483280	2.050489	0.450086
C	1.206593	3.059818	-0.061176
C	1.160318	4.272723	0.832746
H	1.841956	5.043019	0.450796
H	0.130401	4.663662	0.856687
H	1.434500	3.995340	1.861594
O	1.823410	2.988544	-1.099096

SCF Done: E(UB3LYP)= -2563.042399
Sum of electronic and zero-point Energies= -2562.544122
Sum of electronic and thermal Energies= -2562.517986
Sum of electronic and thermal Enthalpies= -2562.517042
Sum of electronic and thermal Free Energies= -2562.599876

^{3}4

C	-0.340891	2.078535	0.834707
C	0.359773	-1.916735	1.125205
N	0.520470	1.289890	0.175330
N	-0.517252	-1.241160	0.369024
C	0.065602	2.989696	1.796572
C	-0.022297	-2.655782	2.233352
N	2.055337	-0.352620	-1.216058
N	-2.079412	0.163823	-1.231151
C	1.439008	3.092938	2.086139
C	-1.386600	-2.693237	2.577396
C	2.336459	2.260609	1.387777
C	-2.301018	-1.982806	1.774097
C	1.850658	1.371288	0.444696
C	-1.840734	-1.273313	0.678156
C	2.707570	0.449283	-0.326026
C	-2.716422	-0.500685	-0.224055
C	4.078341	0.358014	-0.165741
C	-4.089214	-0.414445	-0.078307
C	4.813586	-0.569328	-0.932146
C	-4.841157	0.372757	-0.974598
C	4.118584	-1.389788	-1.841187
C	-4.160976	1.056704	-2.000283
C	2.746844	-1.244286	-1.947165
C	-2.787073	0.919402	-2.088738
Ru	-0.012341	-0.102036	-1.396873
H	-1.397465	1.986398	0.581034
H	-0.683140	3.602966	2.294256
H	3.401261	2.335272	1.602010
H	4.607907	0.987741	0.547598
H	4.620107	-2.130407	-2.461342
H	2.169986	-1.859592	-2.638864
H	1.408989	-1.866901	0.833120
H	0.739575	-3.182860	2.804352
H	-3.358501	-2.006570	2.032118
H	-4.607711	-0.943448	0.719751
H	-4.675572	1.683225	-2.726233
H	-2.221896	1.428473	-2.870590
O	6.121633	-0.599921	-0.731487
O	1.966547	3.923105	2.974629
O	-6.149611	0.411284	-0.777553
O	-1.890965	-3.352357	3.610833
C	-1.022794	-4.104327	4.464299
H	-0.508543	-4.896615	3.898338
H	-0.282560	-3.447248	4.946815
H	-1.667499	-4.556063	5.227609
C	-6.974874	1.196729	-1.645006
H	-8.001505	1.066745	-1.282635
H	-6.694618	2.260308	-1.592173
H	-6.899611	0.839762	-2.683776
C	1.114209	4.798615	3.719232
H	0.398930	4.224080	4.328147
H	1.775872	5.376925	4.375081
H	0.570330	5.480749	3.047177
C	6.932564	-1.516981	-1.474127
H	6.640901	-2.556858	-1.260001
H	6.855192	-1.319590	-2.554561
H	7.962814	-1.345987	-1.140198
O	0.091290	1.211415	-2.506309
O	-0.131290	-1.566973	-2.293881

SCF Done: E(UB3LYP)= -1694.810627
Sum of electronic and zero-point Energies= -1692.537625
Sum of electronic and thermal Energies= -1692.505724
Sum of electronic and thermal Enthalpies= -1692.504779
Sum of electronic and thermal Free Energies= -1692.601832

^{5}5

C	-0.522057	2.196678	0.742700
C	0.522027	-2.196713	0.742708
N	0.393225	1.420766	0.139831
N	-0.393240	-1.420790	0.139828
C	-0.203482	3.086326	1.756557
C	0.203430	-3.086359	1.756559
N	2.058470	-0.155321	-1.175032
N	-2.058455	0.155297	-1.175061
C	1.138015	3.179984	2.170051
C	-1.138070	-3.180011	2.170030
C	2.094904	2.364854	1.532597
C	-2.094951	-2.364890	1.532551
C	1.697480	1.501153	0.527548
C	-1.697503	-1.501178	0.527522
C	2.626813	0.615747	-0.202514
C	-2.626816	-0.615751	-0.202540
C	3.983723	0.541463	0.053652
C	-3.983718	-0.541412	0.053649
C	4.793234	-0.330621	-0.702932
C	-4.793206	0.330693	-0.702936
C	4.188745	-1.104656	-1.712259
C	-4.188705	1.104686	-1.712284
C	2.824351	-0.983647	-1.908315

C	-2.824314	0.983638	-1.908344
Ru	0.000010	-0.000025	-1.392496
H	-1.552904	2.104285	0.401184
H	-0.994958	3.685976	2.202128
H	3.135832	2.435841	1.843314
H	4.447684	1.144663	0.832505
H	4.754226	-1.792635	-2.338034
H	2.313039	-1.568480	-2.674031
H	1.552878	-2.104334	0.401202
H	0.994896	-3.686015	2.202145
H	-3.135890	-2.435888	1.843230
H	-4.447685	-1.144576	0.832527
H	-4.754170	1.792675	-2.338063
H	-2.312992	1.568461	-2.674061
O	6.081397	-0.354142	-0.399435
O	1.585866	3.984777	3.123222
O	-6.081370	0.354254	-0.399446
O	-1.585925	-3.984821	3.123181
C	-0.674716	-4.851819	3.805165
H	-0.203925	-5.555681	3.101205
H	0.100698	-4.271477	4.329087
H	-1.275853	-5.406946	4.535239
C	-6.964131	1.223678	-1.116570
H	-7.958172	1.069509	-0.680312
H	-6.662855	2.275201	-0.990803
H	-6.984620	0.963776	-2.186214
C	0.674674	4.851759	3.805251
H	-0.100745	4.271410	4.329156
H	1.275825	5.406847	4.535343
H	0.203886	5.555659	3.101328
C	6.964200	-1.223555	-1.116525
H	6.662967	-2.275087	-0.990729
H	6.984693	-0.963684	-2.186176
H	7.958230	-1.069333	-0.680261
O	0.088429	1.218802	-2.744723
O	-0.088412	-1.218746	-2.744794

SCF Done: E(UB3LYP)= -1694.780962
Sum of electronic and zero-point Energies= -1692.511862
Sum of electronic and thermal Energies= -1692.479754
Sum of electronic and thermal Enthalpies= -1692.478809
Sum of electronic and thermal Free Energies= -1692.576208

^{1}6

C	-0.226024	-1.126889	1.905694
C	0.225997	-1.126964	-1.905712
N	0.590812	-0.345248	1.190004
N	-0.590810	-0.345309	-1.190004
C	0.230004	-2.215520	2.633220
C	-0.230053	-2.215614	-2.633194
N	2.065869	1.300292	-0.323148
N	-2.065837	1.300278	0.323149
C	1.607337	-2.502930	2.614229
C	-1.607383	-2.503028	-2.614141
C	2.458722	-1.665935	1.865720
C	-2.458741	-1.666017	-1.865620
C	1.927843	-0.593473	1.167641
C	-1.927839	-0.593537	-1.167584
C	2.748085	0.333259	0.355294
C	-2.748065	0.333231	-0.355261
C	4.126009	0.251014	0.260570
C	-4.125993	0.251028	-0.260556
C	4.829950	1.170203	-0.544320
C	-4.829925	1.170264	0.544289
C	4.099947	2.151830	-1.242574
C	-4.099907	2.151895	1.242521
C	2.723976	2.177119	-1.096820
C	-2.723934	2.177146	1.096781
Ru	0.000016	1.377233	-0.000024
H	-1.287201	-0.873483	1.896216
H	-0.485039	-2.812928	3.195801
H	3.526139	-1.880392	1.851001
H	4.686022	-0.511019	0.800110
H	4.578178	2.885977	-1.887918
H	2.117194	2.918777	-1.619762
H	1.287174	-0.873551	-1.896287
H	0.484971	-2.813036	-3.195785
H	-3.526157	-1.880475	-1.850868
H	-4.686026	-0.511003	-0.800081
H	-4.578128	2.886075	1.887835
H	-2.117139	2.918806	1.619706
O	6.146546	1.035471	-0.584863
O	2.181547	-3.512548	3.254442
O	-6.146527	1.035573	0.584804
O	-2.181615	-3.512662	-3.254311
C	-1.380477	-4.398090	-4.041886
H	-0.879134	-3.852377	-4.856595
H	-0.631179	-4.908946	-3.417189
H	-2.072681	-5.136029	-4.464527
C	-6.928916	1.939462	1.372683
H	-7.972166	1.630131	1.238075
H	-6.654849	1.867245	2.436659
H	-6.800502	2.974973	1.021423
C	1.380382	-4.397964	4.042004
H	0.631102	-4.908826	3.417292
H	2.072571	-5.135899	4.464677
H	0.879016	-3.852239	4.856690
C	6.928943	1.939317	-1.372783
H	6.654854	1.867074	-2.436751
H	6.800559	2.974842	-1.021552
H	7.972188	1.629966	-1.238184
O	0.265423	2.176446	1.464957
O	-0.265417	2.176362	-1.465045

SCF Done: E(UB3LYP)= -1694.730093
Sum of electronic and zero-point Energies= -1692.526443
Sum of electronic and thermal Energies= -1692.49479
Sum of electronic and thermal Enthalpies= -1692.493845
Sum of electronic and thermal Free Energies= -1692.588785

B. Transition-state Structures

White-Chen Transition-state Structures

1

Fe	0.003351	0.424731	-0.291780
N	1.953236	0.048315	-0.474601
C	2.642464	0.244785	-1.608960
H	2.073190	0.581757	-2.475069
C	4.013456	0.028644	-1.660142
H	4.547472	0.188650	-2.597529
C	4.675772	-0.385874	-0.502072
H	5.752709	-0.565917	-0.514568

C	3.947162	-0.571454	0.672497
H	4.424882	-0.896504	1.597561
C	2.574549	-0.335575	0.656201
C	1.685680	-0.449516	1.852290
H	2.058848	-1.211752	2.549557
H	1.657335	0.511164	2.384793
N	0.305748	-0.763909	1.395128
C	-0.664578	-0.620937	2.525454
H	-1.677320	-0.600204	2.110368
H	-0.479375	0.322354	3.051654
C	-0.461191	-1.886539	3.360509
H	-1.372009	-2.129997	3.923747
H	0.351522	-1.743595	4.086503
C	-0.089902	-2.976793	2.326745
H	-0.915041	-3.684833	2.168267
H	0.782905	-3.557877	2.650122
C	0.210343	-2.217981	1.012510
H	1.169080	-2.519037	0.572567
C	-0.886315	-2.378798	-0.027354
H	-1.862734	-2.208792	0.442626
C	-0.828327	-3.742968	-0.757729
H	-0.107017	-4.400525	-0.253114
H	-1.804454	-4.243191	-0.733515
C	-0.384211	-3.424826	-2.203839
H	0.382704	-4.118602	-2.573399
H	-1.237404	-3.469538	-2.895918
C	0.163619	-2.001622	-2.119634
H	0.139945	-1.433157	-3.056704
H	1.190336	-2.011282	-1.737625
N	-0.701053	-1.332830	-1.100321
C	-2.022256	-0.960208	-1.677017
H	-2.634682	-1.849308	-1.878740
H	-1.843933	-0.444784	-2.631917
C	-2.726347	-0.029337	-0.741462
C	-4.109523	0.104887	-0.665130
H	-4.745406	-0.532620	-1.280552
C	-4.647673	1.059498	0.198860
H	-5.730076	1.182933	0.273407
C	-3.791326	1.850959	0.968487
H	-4.174995	2.607052	1.654359
C	-2.419948	1.661432	0.856875
H	-1.694278	2.237195	1.430133
N	-1.918383	0.735106	0.023059
O	-0.057534	1.107017	-1.824387
O	0.391213	1.906551	0.769490
C	1.281748	2.861293	0.522831
C	1.377066	3.836223	1.675660
H	2.149920	4.586828	1.466851
H	0.405379	4.334159	1.820324
H	1.613479	3.297761	2.606251
O	1.923179	2.963104	-0.502524
C	-1.145052	3.441634	-1.899887
H	-0.582597	2.389697	-1.874645
H	-1.113266	3.830635	-0.875886
H	-2.160607	3.214436	-2.248582
H	-0.554597	4.032179	-2.612665

SCF Done: E(UB3LYP)= -2605.159166
Sum of electronic and zero-point Energies= -2602.979663
Sum of electronic and thermal Energies= -2602.950209
Sum of electronic and thermal Enthalpies= -2602.949264
Sum of electronic and thermal Free Energies= -2603.03891

20

Fe	0.084712	0.159215	0.038993
N	1.268771	1.655482	-0.538019
C	0.966092	2.484675	-1.548194
H	0.045013	2.272919	-2.091072
C	1.789593	3.555722	-1.869202
H	1.521924	4.209085	-2.700413
C	2.943115	3.771986	-1.111197
H	3.609271	4.605991	-1.341553
C	3.237493	2.908813	-0.056674
H	4.128624	3.038402	0.558871
C	2.367811	1.854128	0.211649
C	2.542751	0.890900	1.340932
H	3.608089	0.744618	1.566396
H	2.062607	1.288935	2.245710
N	1.879832	-0.390858	0.985242
C	1.787380	-1.284683	2.179466
H	1.072783	-2.083511	1.955279
H	1.417999	-0.715232	3.039875
C	3.195765	-1.862357	2.335178
H	3.164167	-2.832820	2.848521
H	3.825598	-1.189481	2.934392
C	3.729592	-1.971650	0.886928
H	3.755038	-3.014600	0.542295
H	4.748381	-1.573172	0.801178
C	2.742298	-1.156068	0.018297
H	3.257726	-0.432109	-0.625004
C	1.852333	-2.038954	-0.841209
H	1.434713	-2.843523	-0.223398
C	2.578956	-2.587879	-2.093424
H	3.653631	-2.370663	-2.019878
H	2.466617	-3.676764	-2.167609
C	1.938926	-1.863795	-3.300574
H	2.684555	-1.509691	-4.024970
H	1.243916	-2.527727	-3.834415
C	1.187215	-0.689795	-2.675369
H	0.340825	-0.308642	-3.258888
H	1.875809	0.136935	-2.471145
N	0.698707	-1.218692	-1.366638
C	-0.487634	-2.095031	-1.559873
H	-0.212998	-3.030778	-2.064743
H	-1.206404	-1.562236	-2.199047
C	-1.120944	-2.369120	-0.234799
C	-1.868334	-3.508358	0.050384
H	-1.969368	-4.287067	-0.706503
C	-2.476575	-3.619404	1.300715
H	-3.069999	-4.502650	1.545842
C	-2.318279	-2.591409	2.233379
H	-2.779899	-2.640019	3.220220
C	-1.548424	-1.485749	1.892113
H	-1.377429	-0.651469	2.571386
N	-0.964512	-1.396449	0.686089
O	-1.125845	0.639602	-0.992484
O	-0.379597	1.052327	1.611475
C	-0.551596	2.347226	1.835734
C	-0.811439	2.621495	3.301419
H	-0.812888	3.703371	3.486181
H	-1.793383	2.202853	3.575287
H	-0.054817	2.126141	3.927761
O	-0.544983	3.213383	0.983055
C	-3.264640	1.604320	0.147005
H	-2.359701	1.107547	-0.441703

H	-3.425640	1.018057	1.061767
H	-2.939412	2.632056	0.343994
C	-4.412592	1.534470	-0.823818
O	-4.766140	2.555364	-1.378495
C	-5.127180	0.214905	-1.024102
H	-5.886177	0.175161	-0.220234
H	-5.676174	0.282496	-1.975035
C	-4.232552	-1.018940	-0.960047
H	-3.761275	-1.127951	0.025883
H	-4.834925	-1.922516	-1.138563
H	-3.441149	-0.986015	-1.723907

SCF Done: E(UB3LYP)= -2797.2337
Sum of electronic and zero-point Energies= -2794.753041
Sum of electronic and thermal Energies= -2794.719833
Sum of electronic and thermal Enthalpies= -2794.718889
Sum of electronic and thermal Free Energies= -2794.81656

24

Fe	-0.000046	-0.341669	-0.126304
N	-1.900135	-0.713302	-0.606430
C	-2.290921	-1.285602	-1.756089
H	-1.509174	-1.495535	-2.485636
C	-3.625133	-1.592500	-1.991017
H	-3.912400	-2.052113	-2.937526
C	-4.569082	-1.304270	-1.002140
H	-5.625240	-1.532159	-1.160604
C	-4.148311	-0.718337	0.191166
H	-4.851178	-0.474104	0.988630
C	-2.793870	-0.440584	0.362285
C	-2.210372	0.133033	1.613616
H	-2.929909	0.797255	2.111626
H	-1.961032	-0.678971	2.310118
N	-0.954904	0.854137	1.273857
C	-0.200040	1.204999	2.516677
H	0.814651	1.498034	2.229699
H	-0.141581	0.328589	3.172193
C	-0.950242	2.407040	3.093307
H	-0.280334	3.025908	3.705306
H	-1.777542	2.075823	3.737116
C	-1.485341	3.158111	1.850291
H	-0.929739	4.088319	1.667950
H	-2.542919	3.426740	1.966812
C	-1.291157	2.187236	0.661487
H	-2.209582	2.068498	0.073546
C	-0.157222	2.599017	-0.264136
H	0.728008	2.847502	0.334442
C	-0.546038	3.752013	-1.221822
H	-1.517056	4.170853	-0.922681
H	0.190164	4.564472	-1.177799
C	-0.615300	3.119372	-2.630605
H	-1.498961	3.443115	-3.196832
H	0.274257	3.379563	-3.222160
C	-0.659255	1.616629	-2.360390
H	-0.290105	0.981795	-3.174932
H	-1.678353	1.306246	-2.104804
N	0.195632	1.430233	-1.149837
C	1.640894	1.485245	-1.503116
H	1.944891	2.501210	-1.789077
H	1.805312	0.826534	-2.368421
C	2.454306	0.993274	-0.347613
C	3.773027	1.369657	-0.109328
H	4.248898	2.103214	-0.761019
C	4.458006	0.787071	0.958093
H	5.495213	1.062676	1.159371
C	3.804534	-0.147365	1.764836
H	4.306109	-0.622512	2.608555
C	2.483458	-0.470900	1.482331
H	1.910971	-1.184900	2.073436
N	1.837721	0.092398	0.446154
O	0.534012	-1.159696	-1.498937
O	-0.039923	-1.715543	1.136138
C	-0.525642	-2.936484	0.973487
C	-0.658780	-3.677812	2.283717
H	-0.959593	-4.717575	2.103241
H	0.292133	-3.648267	2.836641
H	-1.417617	-3.174754	2.904656
O	-0.817260	-3.421581	-0.104693
C	2.277687	-2.912176	-1.201706
H	2.088227	-3.199567	-0.161441
H	1.934535	-3.598602	-1.987024
H	1.278348	-1.991737	-1.423317
C	3.481492	-2.213561	-1.442480
N	4.454110	-1.598640	-1.622507

SCF Done: E(UB3LYP)= -2697.441396
Sum of electronic and zero-point Energies= -2695.145367
Sum of electronic and thermal Energies= -2695.114635
Sum of electronic and thermal Enthalpies= -2695.113691
Sum of electronic and thermal Free Energies= -2695.206453

25

Fe	-0.014815	0.216682	-0.045994
N	1.583634	1.325274	-0.485283
C	1.653658	2.132165	-1.555791
H	0.799200	2.124213	-2.232137
C	2.764673	2.936480	-1.773356
H	2.797987	3.577936	-2.654737
C	3.812530	2.905921	-0.849915
H	4.698656	3.526694	-0.997420
C	3.718475	2.071006	0.262982
H	4.514830	2.014561	1.006204
C	2.576172	1.290548	0.423580
C	2.327329	0.394592	1.593074
H	3.270553	-0.003848	1.990059
H	1.835543	0.963656	2.394030
N	1.411036	-0.700348	1.174489
C	0.925138	-1.461650	2.368748
H	0.069996	-2.073578	2.063854
H	0.598394	-0.761854	3.146055
C	2.104074	-2.358790	2.751524
H	1.752366	-3.254206	3.281226
H	2.794607	-1.825380	3.420018
C	2.789130	-2.693440	1.404977
H	2.602823	-3.732781	1.101676
H	3.876458	-2.558122	1.461314
C	2.168073	-1.725042	0.370829
H	2.933344	-1.198821	-0.213446
C	1.198739	-2.414636	-0.576279
H	0.506116	-3.039927	-0.000680
C	1.912313	-3.220173	-1.688853
H	2.986924	-3.279395	-1.467931
H	1.527578	-4.246453	-1.736707
C	1.648424	-2.449872	-3.002916
H	2.549095	-2.352032	-3.623496

H	0.879230	-2.952766	-3.606254
C	1.156092	-1.079596	-2.541762
H	0.522103	-0.543482	-3.258209
H	2.005062	-0.441890	-2.271990
N	0.379462	-1.369388	-1.296206
C	-0.967152	-1.919491	-1.619501
H	-0.890553	-2.933819	-2.033402
H	-1.427828	-1.274872	-2.382454
C	-1.815912	-1.906430	-0.389255
C	-2.886398	-2.767529	-0.169501
H	-3.110331	-3.542571	-0.903212
C	-3.652837	-2.609122	0.985175
H	-4.500939	-3.270125	1.174727
C	-3.325937	-1.600195	1.894240
H	-3.902092	-1.444893	2.806993
C	-2.239190	-0.778677	1.624877
H	-1.926697	0.023916	2.291955
N	-1.509787	-0.945626	0.507980
O	-0.891544	0.903127	-1.283244
O	-0.390810	1.353156	1.380747
C	-0.452260	2.678929	1.340810
C	-0.618118	3.268660	2.722712
H	-0.669291	4.362717	2.658387
H	-1.537122	2.876862	3.185400
H	0.228293	2.966000	3.358546
O	-0.407996	3.340965	0.322733
C	-3.216422	1.998836	-0.606959
H	-3.193169	2.163746	0.481144
H	-2.156889	1.590909	-0.854126
C	-4.110022	0.900904	-0.912149
N	-4.793323	-0.003752	-1.161489
C	-3.410737	3.272732	-1.410625
H	-2.620696	3.987574	-1.142956
H	-3.372935	3.075834	-2.492105
H	-4.388779	3.724574	-1.172801

SCF Done: E(UB3LYP)= -2736.787714
Sum of electronic and zero-point Energies= -2734.427078
Sum of electronic and thermal Energies= -2734.395054
Sum of electronic and thermal Enthalpies= -2734.39411
Sum of electronic and thermal Free Energies= -2734.490127

26

Fe	0.057267	0.179157	-0.015455
N	1.421021	1.555356	-0.497550
C	1.304836	2.372464	-1.556628
H	0.435764	2.223101	-2.196911
C	2.251932	3.356469	-1.807766
H	2.135821	4.002820	-2.678477
C	3.332566	3.494184	-0.933002
H	4.093208	4.257625	-1.108588
C	3.432766	2.644323	0.167813
H	4.260875	2.715808	0.874146
C	2.445756	1.681310	0.365749
C	2.404421	0.750960	1.533986
H	3.418977	0.514677	1.881564
H	1.864074	1.229770	2.362404
N	1.666216	-0.481680	1.148883
C	1.351468	-1.301082	2.362001
H	0.605364	-2.053225	2.085796
H	0.931222	-0.658693	3.144027
C	2.676092	-1.980700	2.711002
H	2.500808	-2.906964	3.274436
H	3.296575	-1.322589	3.335993
C	3.346343	-2.235191	1.340617
H	3.290052	-3.294587	1.054516
H	4.406646	-1.953381	1.349877
C	2.555575	-1.375419	0.324099
H	3.216699	-0.739602	-0.277101
C	1.685258	-2.209605	-0.600989
H	1.122927	-2.940415	-0.006918
C	2.485315	-2.882488	-1.741482
H	3.561615	-2.781332	-1.545266
H	2.258715	-3.954415	-1.798426
C	2.074808	-2.142995	-3.036450
H	2.935311	-1.892817	-3.671066
H	1.383179	-2.752928	-3.635063
C	1.380170	-0.876466	-2.539976
H	0.652805	-0.436437	-3.232507
H	2.120118	-0.114667	-2.270512
N	0.687190	-1.307295	-1.287630
C	-0.555009	-2.072151	-1.591001
H	-0.316058	-3.049453	-2.030642
H	-1.141779	-1.502046	-2.326442
C	-1.352771	-2.225640	-0.336752
C	-2.236029	-3.272181	-0.093105
H	-2.336078	-4.071800	-0.827794
C	-2.981103	-3.263767	1.086233
H	-3.683828	-4.072638	1.295983
C	-2.819747	-2.214728	1.994158
H	-3.385049	-2.173479	2.925736
C	-1.911817	-1.204873	1.700732
H	-1.726736	-0.365353	2.369580
N	-1.201743	-1.228647	0.560736
O	-0.949256	0.710498	-1.211238
O	-0.445486	1.220610	1.446137
C	-0.774933	2.503445	1.395417
C	-0.974534	3.085882	2.776062
H	-1.236391	4.148392	2.698977
H	-1.776472	2.539105	3.295072
H	-0.052886	2.964256	3.365641
O	-0.926731	3.135381	0.367632
C	-3.530894	1.328415	-0.762125
H	-2.388469	1.201776	-0.749017
C	-3.995718	-0.002994	-1.135383
N	-4.331826	-1.073518	-1.430796
C	-3.802577	2.372736	-1.842260
H	-3.305680	3.313582	-1.565469
H	-3.427052	2.045314	-2.822649
H	-4.886286	2.559242	-1.925977
C	-3.980130	1.730853	0.640208
H	-3.682342	0.986495	1.390778
H	-3.542456	2.703533	0.900227
H	-5.078612	1.827251	0.663220

SCF Done: E(UB3LYP)= -2776.139029
Sum of electronic and zero-point Energies= -2773.693991
Sum of electronic and thermal Energies= -2773.660718
Sum of electronic and thermal Enthalpies= -2773.659774
Sum of electronic and thermal Free Energies= -2773.758064

Dubois-Sigman Transition-state Structures

1

C	0.356732	0.251695	2.169307
C	-0.069354	1.879882	-1.449052
N	-0.500457	-0.060147	1.187238
N	0.710679	0.858923	-1.065441
C	-0.031824	0.918214	3.320956
C	0.433837	3.141407	-1.722361
N	-2.030796	-0.770386	-0.841954
N	2.068197	-1.260599	-0.262372
C	-1.383553	1.285677	3.457657
C	1.818789	3.355489	-1.587850
C	-2.279312	0.947055	2.424817
C	2.630839	2.274129	-1.191308
C	-1.811626	0.273670	1.307987
C	2.054441	1.041043	-0.940390
C	-2.672575	-0.144281	0.183468
C	2.817052	-0.148357	-0.511275
C	-4.041888	0.056801	0.150146
C	4.189774	-0.165094	-0.341478
C	-4.787342	-0.387499	-0.959047
C	4.823649	-1.345172	0.098966
C	-4.104241	-1.022018	-2.013263
C	4.029258	-2.477482	0.362198
C	-2.733567	-1.189230	-1.907164
C	2.661214	-2.385929	0.164734
Ru	0.030831	-1.099091	-0.644857
H	1.397289	-0.044810	2.029970
H	0.712940	1.138869	4.083049
H	-3.327660	1.221463	2.528079
H	-4.561621	0.549102	0.970139
H	-4.613912	-1.384906	-2.903829
H	-2.166380	-1.676587	-2.701208
H	-1.136716	1.676612	-1.543122
H	-0.251143	3.928516	-2.031304
H	3.703314	2.430502	-1.085926
H	4.795385	0.717205	-0.542131
H	4.452549	-3.417468	0.710839
H	1.999614	-3.232192	0.356864
O	-6.095288	-0.170151	-0.924359
O	-1.892691	1.933853	4.497595
O	6.140950	-1.294590	0.235542
O	2.431960	4.510102	-1.806780
C	1.668961	5.651903	-2.208429
H	1.158958	5.464464	-3.166312
H	0.930330	5.919224	-1.436620
H	2.390012	6.469321	-2.328046
C	6.853843	-2.456929	0.669779
H	7.911307	-2.168466	0.698902
H	6.526468	-2.764319	1.675211
H	6.715932	-3.287721	-0.039613
C	-1.041140	2.303471	5.585547
H	-0.242836	2.982017	5.246137
H	-1.682659	2.821717	6.308311
H	-0.598194	1.412170	6.057064
C	-6.913562	-0.610302	-2.012235
H	-6.622770	-0.109711	-2.949022
H	-6.847190	-1.702659	-2.135487
H	-7.940857	-0.330916	-1.749465
O	-0.211396	-2.645729	0.315431
O	0.156497	-1.470561	-2.303793
H	-1.312619	-2.928269	0.664891
C	-2.541156	-3.295759	1.094852
H	-2.343716	-4.322665	1.426402
H	-2.747113	-2.582364	1.901208
H	-3.192361	-3.210342	0.217945

SCF Done: E(UB3LYP)= -1735.323313
Sum of electronic and zero-point Energies= -1732.962759
Sum of electronic and thermal Energies= -1732.928109
Sum of electronic and thermal Enthalpies= -1732.927165
Sum of electronic and thermal Free Energies= -1733.029114

2

C	-0.929151	-0.787535	2.191276
C	-1.100055	-2.181715	-1.566459
N	-0.002065	-0.784349	1.223890
N	-1.412233	-0.965770	-1.095846
C	-0.860260	-1.624241	3.295024
C	-2.061634	-3.108696	-1.935717
N	1.734543	-0.613524	-0.763192
N	-1.819131	1.457693	-0.121615
C	0.232070	-2.505286	3.399174
C	-3.418144	-2.754940	-1.807039
C	1.204094	-2.492242	2.380478
C	-3.736217	-1.472725	-1.315905
C	1.061821	-1.623185	1.310715
C	-2.718205	-0.599395	-0.972368
C	2.036719	-1.522717	0.205329
C	-2.946535	0.762736	-0.446250
C	3.197160	-2.275623	0.137973
C	-4.198915	1.322770	-0.266414
C	4.085345	-2.097208	-0.940469
C	-4.310487	2.626282	0.259359
C	3.751284	-1.158908	-1.934295
C	-3.133075	3.322486	0.591451
C	2.569764	-0.448207	-1.801588
C	-1.914763	2.697806	0.380908
Ru	-0.014277	0.514530	-0.524382
H	-1.760147	-0.088901	2.083759
H	-1.644510	-1.575167	4.048311
H	2.056105	-3.165158	2.458995
H	3.445847	-3.002605	0.909178
H	4.385997	-0.973537	-2.798651
H	2.271896	0.286034	-2.550752
H	-0.039047	-2.419735	-1.651598
H	-1.744621	-4.078334	-2.314782
H	-4.783617	-1.192407	-1.215497
H	-5.107045	0.778949	-0.521531
H	-3.149348	4.329778	1.002904
H	-0.971427	3.190499	0.621538
O	5.184509	-2.840059	-0.937997
O	0.427299	-3.359525	4.396452
O	-5.538547	3.104253	0.404640
O	-4.439340	-3.542451	-2.115016
C	-4.191255	-4.863156	-2.605784
H	-3.628314	-4.830929	-3.551611
H	-3.640013	-5.459383	-1.861742
H	-5.177292	-5.310685	-2.779156
C	-5.725215	4.417083	0.941897
H	-6.808728	4.584689	0.959247
H	-5.324109	4.481132	1.965587
H	-5.243837	5.174013	0.303105
C	-0.512693	-3.415021	5.472349
H	-0.136300	-4.178921	6.163304

H	-0.573013	-2.445244	5.990950
H	-1.510433	-3.706436	5.108088
C	6.135634	-2.692338	-1.995946
H	5.684141	-2.947933	-2.967272
H	6.531608	-1.665252	-2.025621
H	6.948269	-3.393697	-1.772085
O	0.812134	1.741879	0.552611
O	0.065362	1.053498	-2.143719
C	3.326117	1.672302	0.973313
H	3.559110	0.599886	0.977028
H	2.021833	1.655528	0.768075
H	3.345577	2.101317	1.984965
C	3.996594	2.464803	-0.114577
H	5.076808	2.213720	-0.073150
H	3.664509	2.092221	-1.097959
C	3.857518	3.997839	-0.045741
H	4.411547	4.390792	-0.918117
C	2.405211	4.489482	-0.171277
H	2.407259	5.587966	-0.060038
H	1.817604	4.098988	0.677595
C	4.516284	4.571390	1.212882
H	3.975585	4.274563	2.126966
H	5.559419	4.229126	1.314144
H	4.524432	5.673026	1.183306
C	1.713985	4.120255	-1.481192
H	0.689587	4.525665	-1.517194
H	2.262460	4.523754	-2.349472
H	1.633293	3.031685	-1.613097

SCF Done: E(UB3LYP)= -1932.002516
Sum of electronic and zero-point Energies= -1929.286167
Sum of electronic and thermal Energies= -1929.245034
Sum of electronic and thermal Enthalpies= -1929.24409
Sum of electronic and thermal Free Energies= -1929.36242

3

C	-0.848031	-0.409060	2.196700
C	-1.030716	-2.244673	-1.377482
N	0.027963	-0.437722	1.183601
N	-1.455718	-1.022833	-1.025211
C	-0.646086	-1.098984	3.382616
C	-1.898892	-3.296574	-1.621134
N	1.640021	-0.340104	-0.905491
N	-2.087278	1.437435	-0.305533
C	0.527873	-1.862929	3.520467
C	-3.281636	-3.068550	-1.489642
C	1.445511	-1.881146	2.453006
C	-3.718422	-1.782374	-1.114509
C	1.171178	-1.158617	1.302977
C	-2.789073	-0.780888	-0.890398
C	2.078233	-1.097326	0.138724
C	-3.143720	0.595438	-0.488753
C	3.294262	-1.758170	0.079215
C	-4.440913	1.032971	-0.286133
C	4.091293	-1.654158	-1.076890
C	-4.674109	2.366331	0.108079
C	3.607552	-0.891685	-2.155854
C	-3.567996	3.216912	0.292655
C	2.384051	-0.257278	-2.020529
C	-2.298801	2.706026	0.074924
Ru	-0.200767	0.646164	-0.691094
H	-1.748555	0.190792	2.055785
H	-1.395238	-1.031488	4.169169
H	2.360448	-2.461264	2.556347
H	3.653960	-2.358258	0.913542
H	4.163241	-0.773905	-3.083893
H	1.975837	0.347937	-2.830277
H	0.046515	-2.384301	-1.472389
H	-1.490385	-4.263576	-1.908565
H	-4.786849	-1.600405	-1.011340
H	-5.293597	0.369858	-0.422773
H	-3.675796	4.255556	0.599227
H	-1.405057	3.316599	0.212864
O	5.252679	-2.296021	-1.061419
O	0.847949	-2.577727	4.592857
O	-5.940431	2.720007	0.279871
O	-4.223697	-3.979092	-1.692692
C	-3.855913	-5.306021	-2.081052
H	-3.325357	-5.298513	-3.045915
H	-3.226650	-5.779482	-1.311218
H	-4.795696	-5.862022	-2.181665
C	-6.255036	4.059980	0.670148
H	-7.348681	4.106261	0.735384
H	-5.816041	4.295274	1.652187
H	-5.898360	4.780796	-0.082029
C	-0.037287	-2.602315	5.715301
H	-1.015812	-3.022905	5.434917
H	0.439712	-3.248019	6.462422
H	-0.171050	-1.591724	6.132116
C	6.113197	-2.222973	-2.201522
H	5.626957	-2.658385	-3.088613
H	6.402671	-1.180538	-2.407734
H	7.004219	-2.808755	-1.945706
O	0.483186	2.060126	0.235779
O	-0.227676	1.001727	-2.363675
C	3.045542	1.520458	2.321377
H	3.354770	0.505043	2.035319
H	2.132047	1.453093	2.933308
H	3.835334	1.936694	2.974317
C	2.848521	2.409471	1.121942
H	1.694468	2.109229	0.622959
H	2.596508	3.445358	1.401455
C	3.849544	2.321438	-0.012848
H	3.971220	1.254760	-0.264532
C	3.378010	3.038832	-1.293338
H	2.460475	2.546126	-1.652741
H	4.140001	2.870626	-2.073741
C	5.226547	2.827853	0.460742
H	5.176425	3.868399	0.818503
H	5.616982	2.208620	1.282482
H	5.951049	2.786548	-0.369177
C	3.109903	4.537529	-1.160130
H	2.824247	4.966054	-2.134472
H	2.284554	4.744384	-0.460145
H	3.996713	5.087627	-0.806498

SCF Done: E(UB3LYP)= -1932.008733
Sum of electronic and zero-point Energies= -1929.291536
Sum of electronic and thermal Energies= -1929.250069
Sum of electronic and thermal Enthalpies= -1929.249125
Sum of electronic and thermal Free Energies= -1929.367164

4

C	0.565428	-0.116384	2.150632
C	0.785124	2.671438	-0.768922

N	-0.238434	0.134144	1.108915
N	1.309566	1.438221	-0.728615
C	0.179773	0.095250	3.465705
C	1.552992	3.814323	-0.613321
N	-1.700918	0.508778	-1.064206
N	2.139925	-1.067187	-0.656263
C	-1.113973	0.590889	3.710772
C	2.936994	3.668459	-0.402223
C	-1.946058	0.868238	2.609874
C	3.479665	2.368353	-0.366775
C	-1.482191	0.629794	1.325914
C	2.647447	1.274585	-0.534971
C	-2.282733	0.879437	0.110369
C	3.115352	-0.126437	-0.509632
C	-3.535895	1.468695	0.130076
C	4.436528	-0.497205	-0.331856
C	-4.218476	1.703890	-1.078572
C	4.779149	-1.864639	-0.302827
C	-3.596823	1.323314	-2.281973
C	3.753916	-2.818541	-0.446978
C	-2.347147	0.729207	-2.220777
C	2.454324	-2.370531	-0.620749
Ru	0.210066	-0.350729	-0.974110
H	1.556498	-0.512841	1.926669
H	0.878613	-0.136983	4.266757
H	-2.948183	1.253430	2.790998
H	-4.005370	1.765133	1.066349
H	-4.063974	1.472831	-3.253540
H	-1.831325	0.416353	-3.129442
H	-0.289640	2.746305	-0.937143
H	1.069521	4.788148	-0.659136
H	4.550268	2.249624	-0.207178
H	5.222940	0.246332	-0.212692
H	3.947634	-3.889375	-0.427625
H	1.619952	-3.065455	-0.727669
O	-5.410475	2.279653	-0.987160
O	-1.623847	0.819898	4.915494
O	6.063179	-2.149430	-0.134022
O	3.786828	4.671714	-0.231731
C	3.303535	6.018062	-0.252882
H	2.839061	6.252416	-1.223504
H	2.578606	6.185933	0.558979
H	4.182168	6.656265	-0.100768
C	6.486487	-3.515007	-0.083744
H	7.573227	-3.488401	0.060386
H	6.014183	-4.040443	0.760934
H	6.250381	-4.034058	-1.025883
C	-0.836015	0.545357	6.076325
H	0.077455	1.160420	6.085377
H	-1.463590	0.806225	6.936954
H	-0.567867	-0.521775	6.124598
C	-6.152557	2.559743	-2.177133
H	-5.598899	3.251638	-2.831101
H	-6.382202	1.631880	-2.724206
H	-7.085361	3.032635	-1.847036
O	-0.397198	-2.003912	-0.533969
O	0.376741	-0.231711	-2.673562
C	-2.171886	-2.830323	2.321389
H	-2.043568	-3.917054	2.442246
H	-2.503910	-2.427789	3.291185
H	-1.184265	-2.398407	2.099864
C	-3.180781	-2.487524	1.227715
H	-4.144099	-2.995740	1.437338
H	-3.406401	-1.410438	1.256991
C	-2.788303	-2.857169	-0.196429
H	-1.675965	-2.273429	-0.368890
C	-2.372145	-4.308058	-0.402378
H	-3.238301	-4.939196	-0.117180
H	-1.572149	-4.558059	0.311986
C	-3.729558	-2.300686	-1.243187
H	-4.056489	-1.283488	-0.989152
H	-3.281330	-2.282487	-2.247124
H	-4.634221	-2.935821	-1.299407
C	-1.918165	-4.663484	-1.816641
H	-1.553136	-5.702021	-1.857267
H	-2.734122	-4.571043	-2.549969
H	-1.095918	-4.004820	-2.140859

SCF Done: E(UB3LYP)= -1932.014076
Sum of electronic and zero-point Energies= -1929.297103
Sum of electronic and thermal Energies= -1929.255774
Sum of electronic and thermal Enthalpies= -1929.25483
Sum of electronic and thermal Free Energies= -1929.372242

5

C	0.871811	0.446494	2.180699
C	1.091634	2.191471	-1.409865
N	0.017030	0.417242	1.149521
N	1.540577	0.986607	-1.029379
C	0.607264	1.133252	3.355854
C	1.936116	3.267992	-1.626455
N	-1.539855	0.222367	-0.975565
N	2.213223	-1.439282	-0.239831
C	-0.612042	1.827913	3.464704
C	3.318458	3.085420	-1.432543
C	-1.504728	1.791348	2.376062
C	3.780660	1.814454	-1.035761
C	-1.164701	1.078831	1.237138
C	2.874801	0.785799	-0.842242
C	-2.037545	0.967532	0.051066
C	3.253727	-0.575239	-0.412568
C	-3.282905	1.564548	-0.040603
C	4.555556	-0.977096	-0.171435
C	-4.049259	1.407913	-1.211104
C	4.810319	-2.297227	0.253308
C	-3.502716	0.668725	-2.275356
C	3.720341	-3.170514	0.428961
C	-2.252936	0.094794	-2.106167
C	2.445083	-2.695013	0.170693
Ru	0.322576	-0.702553	-0.694663
H	1.805984	-0.105422	2.064789
H	1.343713	1.114678	4.157124
H	-2.451229	2.323173	2.454473
H	-3.691116	2.150133	0.781235
H	-4.031451	0.514515	-3.213859
H	-1.797878	-0.497698	-2.900360
H	0.015220	2.295628	-1.549205
H	1.510428	4.219429	-1.939315
H	4.849105	1.667380	-0.886664
H	5.395344	-0.296278	-0.301161
H	3.845141	-4.200129	0.758960
H	1.563622	-3.324650	0.300296
O	-5.252030	1.970078	-1.211717
O	-0.998611	2.524047	4.526831

O	6.079996	-2.616856	0.461182
O	4.237522	4.026842	-1.593439
C	3.842648	5.345183	-1.985348
H	3.364081	5.331771	-2.976910
H	3.157268	5.785240	-1.244238
H	4.765727	5.935374	-2.029735
C	6.417416	-3.941693	0.882931
H	7.510152	-3.960536	0.972510
H	5.962589	-4.169421	1.859565
H	6.093927	-4.684022	0.136731
C	-0.150877	2.590971	5.676272
H	0.813168	3.061542	5.426759
H	-0.683202	3.209557	6.408795
H	0.021233	1.587163	6.095489
C	-6.096036	1.832795	-2.358538
H	-5.629739	2.290320	-3.244931
H	-6.317481	0.772330	-2.555980
H	-7.023981	2.363970	-2.115147
O	-0.366879	-2.112508	0.248917
O	0.400578	-1.099422	-2.353269
C	-2.553621	-3.715730	-1.596054
H	-2.493993	-2.850201	-2.276218
H	-2.600202	-4.624779	-2.217396
H	-1.612866	-3.749925	-1.025974
C	-3.777013	-3.616248	-0.686569
H	-4.688742	-3.670834	-1.305692
H	-3.813812	-4.490137	-0.010587
C	-3.855703	-2.335946	0.159321
H	-3.812130	-1.468639	-0.519785
C	-5.221230	-2.251916	0.895535
H	-5.249204	-3.025153	1.683504
H	-6.002735	-2.526511	0.166104
C	-2.739480	-2.227429	1.165546
H	-2.552298	-3.138983	1.754241
H	-1.544163	-2.114335	0.605360
H	-2.738209	-1.324854	1.790552
C	-5.551582	-0.884290	1.487878
H	-6.528297	-0.906755	1.998006
H	-4.803209	-0.556427	2.226724
H	-5.606332	-0.112742	0.703675

SCF Done: E(UB3LYP)= -1932.003849
Sum of electronic and zero-point Energies= -1929.288033
Sum of electronic and thermal Energies= -1929.24663
Sum of electronic and thermal Enthalpies= -1929.245686
Sum of electronic and thermal Free Energies= -1929.364179

6

C	-0.761117	-0.224406	2.194376
C	-0.987082	-2.445052	-1.170211
N	0.103511	-0.377187	1.182727
N	-1.398924	-1.188489	-0.947380
C	-0.545774	-0.762427	3.454284
C	-1.864510	-3.513610	-1.257044
N	1.705674	-0.526549	-0.914229
N	-2.003047	1.341947	-0.504789
C	0.634041	-1.496764	3.675330
C	-3.241351	-3.265577	-1.100381
C	1.541071	-1.646021	2.608919
C	-3.665043	-1.940143	-0.876934
C	1.250064	-1.075783	1.379830
C	-2.727340	-0.924381	-0.806270
C	2.139255	-1.172224	0.204501
C	-3.067635	0.492848	-0.568400
C	3.336539	-1.868335	0.207065
C	-4.359144	0.960225	-0.400495
C	4.120472	-1.917380	-0.961549
C	-4.578266	2.333301	-0.166575
C	3.648586	-1.257223	-2.111344
C	-3.464057	3.191537	-0.105559
C	2.444080	-0.577292	-2.035148
C	-2.201085	2.649007	-0.278466
Ru	-0.127188	0.491976	-0.807449
H	-1.663968	0.353199	1.990460
H	-1.287243	-0.601900	4.234565
H	2.458640	-2.207618	2.775005
H	3.690923	-2.380979	1.099701
H	4.198663	-1.254733	-3.050370
H	2.044992	-0.048708	-2.901678
H	0.085832	-2.599981	-1.286834
H	-1.468686	-4.510055	-1.443710
H	-4.728444	-1.737343	-0.760921
H	-5.215733	0.288940	-0.444881
H	-3.561478	4.260456	0.074222
H	-1.303138	3.266714	-0.229456
O	5.260824	-2.591003	-0.886057
O	0.968423	-2.068631	4.825986
O	-5.839105	2.715372	-0.017314
O	-4.187804	-4.192696	-1.146471
C	-3.826577	-5.561226	-1.354837
H	-3.332022	-5.691434	-2.330070
H	-3.165325	-5.918077	-0.549772
H	-4.765614	-6.127186	-1.339323
C	-6.139199	4.094954	0.215166
H	-7.231039	4.156391	0.295754
H	-5.679121	4.443645	1.152861
H	-5.794498	4.717510	-0.625345
C	0.091146	-1.957583	5.949321
H	0.576374	-2.504300	6.766780
H	-0.044159	-0.903757	6.239483
H	-0.887341	-2.413304	5.729911
C	6.117316	-2.657803	-2.029423
H	6.992957	-3.239767	-1.717575
H	5.615226	-3.166764	-2.867019
H	6.434648	-1.650084	-2.340531
O	0.587380	1.982890	-0.036135
O	-0.153309	0.664856	-2.506793
C	2.926003	2.210483	0.961433
C	3.998256	2.044182	-0.087991
C	3.839917	3.046267	-1.236473
C	3.736766	4.481963	-0.710128
C	2.600814	4.629335	0.308287
C	2.734541	3.625469	1.461753
H	4.683899	2.950498	-1.938731
H	4.973054	2.218409	0.413217
H	4.033356	1.011693	-0.461126
H	1.781030	1.971049	0.401230
H	2.924861	1.438177	1.745710
H	4.693646	4.759010	-0.230740
H	3.588263	5.185002	-1.546587
H	2.570824	5.656467	0.706926
H	1.636352	4.456185	-0.200233
H	3.622749	3.884698	2.073928
H	1.866556	3.682660	2.138480

H	2.925328	2.795944	-1.803831

SCF Done: E(UB3LYP)= -1930.801107
Sum of electronic and zero-point Energies= -1928.109482
Sum of electronic and thermal Energies= -1928.070597
Sum of electronic and thermal Enthalpies= -1928.069653
Sum of electronic and thermal Free Energies= -1928.182782

7

C	-0.927656	-0.162284	2.179552
C	-1.439262	-2.303672	-1.162737
N	-0.077749	-0.382111	1.167691
N	-1.689345	-1.006722	-0.934471
C	-0.774292	-0.742974	3.429554
C	-2.446016	-3.249402	-1.271694
N	1.486500	-0.696864	-0.944072
N	-1.968246	1.578844	-0.463417
C	0.321137	-1.601321	3.638181
C	-3.781815	-2.825671	-1.138491
C	1.210867	-1.825351	2.570073
C	-4.034314	-1.459724	-0.899799
C	0.988940	-1.200554	1.353084
C	-2.973832	-0.575146	-0.800365
C	1.876085	-1.356394	0.182682
C	-3.130809	0.869110	-0.531447
C	3.044836	-2.098743	0.205271
C	-4.351450	1.488902	-0.331477
C	3.849644	-2.172175	-0.947874
C	-4.395056	2.871765	-0.059667
C	3.420445	-1.499738	-2.107057
C	-3.182870	3.584887	0.001671
C	2.237640	-0.780651	-2.054042
C	-1.999465	2.894910	-0.205589
Ru	-0.220162	0.510909	-0.815597
H	-1.765740	0.508576	1.986000
H	-1.498921	-0.520667	4.210509
H	2.060990	-2.487552	2.724639
H	3.367656	-2.618180	1.105982
H	3.986090	-1.519267	-3.036555
H	1.871144	-0.241839	-2.928690
H	-0.392658	-2.593277	-1.265170
H	-2.179344	-4.287623	-1.459250
H	-5.065623	-1.125082	-0.799689
H	-5.285512	0.931198	-0.373156
H	-3.144754	4.652900	0.207543
H	-1.031006	3.395918	-0.160124
O	4.966720	-2.880870	-0.849686
O	0.591530	-2.226244	4.777942
O	-5.596297	3.401686	0.124898
O	-4.840259	-3.620493	-1.218795
C	-4.657411	-5.020881	-1.448437
H	-4.153250	-5.197394	-2.411408
H	-4.076199	-5.478243	-0.632396
H	-5.663373	-5.456349	-1.473405
C	-5.715701	4.797540	0.414719
H	-6.789066	4.992148	0.526270
H	-5.194311	5.048288	1.351760
H	-5.313293	5.404513	-0.411239
C	-0.260782	-2.033469	5.909439
H	-1.283900	-2.380075	5.694676
H	0.169576	-2.636698	6.717879
H	-0.280993	-0.974195	6.209980
C	5.845519	-2.973959	-1.974268
H	5.345706	-3.465177	-2.823705
H	6.202379	-1.976638	-2.276035
H	6.694601	-3.584637	-1.644325
O	0.727334	1.899132	-0.098590
O	-0.278894	0.687416	-2.515061
C	3.266534	1.837373	0.070431
C	3.598347	2.621057	1.316247
C	5.123573	2.871224	1.364827
C	5.616406	3.543551	0.080201
C	5.229737	2.740278	-1.165057
C	3.705732	2.490929	-1.216538
H	5.364963	3.486810	2.247257
H	3.078932	3.595120	1.294537
H	3.268090	2.085682	2.220462
H	3.549588	0.776092	0.139655
H	1.972413	1.781636	0.023063
H	5.178426	4.555614	0.008914
H	6.710915	3.674826	0.119759
H	5.546587	3.262928	-2.082833
H	5.751456	1.766869	-1.152695
H	3.189540	3.459539	-1.336314
H	3.447646	1.866250	-2.085455
H	5.640941	1.904423	1.495717

SCF Done: E(UB3LYP)= -1930.800831
Sum of electronic and zero-point Energies= -1928.108171
Sum of electronic and thermal Energies= -1928.069221
Sum of electronic and thermal Enthalpies= -1928.068277
Sum of electronic and thermal Free Energies= -1928.181708

8

C	0.685739	-0.222531	2.108680
C	1.113962	2.570705	-0.844929
N	-0.061456	0.100503	1.044601
N	1.577898	1.315108	-0.763189
C	0.323331	0.104995	3.406472
C	1.928823	3.679513	-0.684421
N	-1.448571	0.543038	-1.157960
N	2.296211	-1.224024	-0.649087
C	-0.878524	0.809019	3.607834
C	3.297035	3.475228	-0.424516
C	-1.651551	1.153042	2.483813
C	3.776056	2.152152	-0.345865
C	-1.225034	0.776415	1.220719
C	2.899799	1.094614	-0.521345
C	-1.995239	1.034100	-0.010814
C	3.304031	-0.324952	-0.463759
C	-3.194105	1.725118	-0.031615
C	4.599124	-0.751213	-0.226832
C	-3.871090	1.915791	-1.249672
C	4.881326	-2.131858	-0.180435
C	-3.283667	1.416161	-2.426490
C	3.824904	-3.041768	-0.374748
C	-2.076168	0.744972	-2.327864
C	2.554303	-2.539503	-0.604210
Ru	0.406350	-0.426815	-1.017799
H	1.607680	-0.773217	1.916382
H	0.968278	-0.195977	4.229626
H	-2.590054	1.683007	2.632928
H	-3.638690	2.111176	0.883012
H	-3.741148	1.538332	-3.406496

H	-1.578624	0.357294	-3.216766
H	0.050529	2.693645	-1.052042
H	1.491935	4.672810	-0.766262
H	4.834579	1.985680	-0.151968
H	5.410860	-0.042329	-0.072454
H	3.972817	-4.119701	-0.350590
H	1.696630	-3.197929	-0.749699
O	-5.026662	2.567255	-1.193645
O	-1.359916	1.168228	4.792707
O	6.142054	-2.471600	0.049979
O	4.187434	4.441475	-0.248171
C	3.772517	5.809084	-0.321422
H	3.354145	6.038700	-1.313992
H	3.029621	6.034766	0.459493
H	4.676062	6.407539	-0.154568
C	6.500418	-3.854869	0.122599
H	7.578703	-3.876867	0.320523
H	5.963549	-4.355759	0.943338
H	6.288477	-4.365569	-0.829722
C	-0.649449	0.810939	5.980573
H	0.349034	1.275264	5.996399
H	-1.246292	1.194328	6.816867
H	-0.554099	-0.283036	6.065674
C	-5.770008	2.787832	-2.394406
H	-5.198468	3.409654	-3.101367
H	-6.038746	1.832064	-2.871266
H	-6.681576	3.317985	-2.093012
O	-0.262722	-2.064082	-0.583498
O	0.614309	-0.316263	-2.710593
C	-3.139208	-1.908137	3.486579
H	-3.600748	-2.850295	3.822388
H	-3.605464	-1.058307	3.997829
H	-2.068155	-1.958806	3.735124
C	-3.305358	-1.766359	2.003116
O	-3.893880	-0.883402	1.432060
O	-2.684810	-2.794330	1.360178
C	-2.595183	-2.909425	-0.027809
H	-2.254596	-3.938637	-0.215978
H	-1.487726	-2.314945	-0.353044
C	-3.727763	-2.469026	-0.927362
H	-3.736936	-1.376015	-1.048767
H	-4.675433	-2.725453	-0.420152
C	-3.671226	-3.171056	-2.289489
H	-4.579012	-2.891922	-2.850261
H	-3.731228	-4.262236	-2.131074
C	-2.438835	-2.842265	-3.130995
H	-1.501961	-3.122488	-2.623454
H	-2.467322	-3.378371	-4.093139
H	-2.384852	-1.765460	-3.351360

SCF Done: E(UB3LYP)= -2081.324199
Sum of electronic and zero-point Energies= -2078.444917
Sum of electronic and thermal Energies= -2078.402235
Sum of electronic and thermal Enthalpies= -2078.401291
Sum of electronic and thermal Free Energies= -2078.522085

9

C	0.575213	-0.174208	1.932660
C	0.258893	3.032683	-0.440743
N	-0.329153	0.104503	0.985241
N	0.932841	1.889256	-0.628987
C	0.281938	-0.125627	3.287083
C	0.888091	4.223793	-0.116141
N	-1.973301	0.580535	-1.023734
N	2.063379	-0.461431	-1.018562
C	-1.023901	0.217507	3.676575
C	2.289078	4.226749	0.021723
C	-1.972063	0.503207	2.674065
C	2.988085	3.020739	-0.184233
C	-1.596031	0.442402	1.342690
C	2.288479	1.871240	-0.509186
C	-2.515548	0.710405	0.218849
C	2.923254	0.555504	-0.725530
C	-3.845391	1.060947	0.382602
C	4.283265	0.324762	-0.619627
C	-4.655121	1.283915	-0.747575
C	4.786126	-0.978942	-0.810120
C	-4.077226	1.140774	-2.022202
C	3.879168	-2.013714	-1.107654
C	-2.739955	0.789605	-2.106054
C	2.532242	-1.704865	-1.201480
Ru	0.049323	0.036697	-1.151788
H	1.572402	-0.455930	1.598358
H	1.061746	-0.368728	4.005930
H	-2.985969	0.764279	2.972342
H	-4.284928	1.168935	1.372242
H	-4.641052	1.294639	-2.940195
H	-2.253611	0.672135	-3.074924
H	-0.824792	2.991597	-0.558653
H	0.287244	5.120832	0.020214
H	4.071795	3.014134	-0.081450
H	4.978690	1.129355	-0.385222
H	4.197924	-3.042295	-1.265430
H	1.786280	-2.468360	-1.422720
O	-5.918814	1.618107	-0.518971
O	-1.447225	0.295927	4.932915
O	6.097543	-1.131165	-0.687848
O	3.016631	5.289853	0.336068
C	2.369668	6.544436	0.568949
H	1.837114	6.883564	-0.333257
H	1.666497	6.471212	1.413383
H	3.168206	7.254659	0.814330
C	6.678125	-2.428399	-0.852217
H	7.754662	-2.300269	-0.687355
H	6.271695	-3.135622	-0.112374
H	6.502475	-2.809936	-1.870292
C	-0.538055	0.021228	6.001130
H	0.313478	0.719437	5.981391
H	-1.108155	0.162524	6.927314
H	-0.171246	-1.015937	5.947842
C	-6.793159	1.869387	-1.622789
H	-6.423863	2.709605	-2.231785
H	-6.900181	0.971278	-2.251278
H	-7.764391	2.130284	-1.185491
O	-0.317896	-1.747169	-1.026411
O	0.090499	0.516996	-2.789591
C	1.439429	-4.979293	0.211788
H	2.478224	-4.841009	0.534950
H	1.367017	-4.803076	-0.873858
H	1.109891	-6.011211	0.401630
C	0.547481	-3.999467	0.918715
O	0.929942	-3.054011	1.569781
O	-0.750776	-4.305474	0.727988
C	-1.758703	-3.388422	1.181226

H	-1.317758	-2.657451	1.872050
H	-2.501991	-3.989235	1.735483
C	-2.421961	-2.709579	0.012007
H	-1.413554	-2.098237	-0.554045
H	-3.089381	-1.898876	0.337761
C	-2.989103	-3.559336	-1.096864
H	-3.823806	-4.150305	-0.666734
H	-2.234542	-4.294644	-1.420784
C	-3.491174	-2.743544	-2.285510
H	-2.666548	-2.184385	-2.755915
H	-3.938764	-3.394094	-3.052936
H	-4.253491	-2.011395	-1.973773

SCF Done: E(UB3LYP)= -2081.331092
Sum of electronic and zero-point Energies= -2078.451962
Sum of electronic and thermal Energies= -2078.409053
Sum of electronic and thermal Enthalpies= -2078.408108
Sum of electronic and thermal Free Energies= -2078.530164

10

C	0.943759	-0.138719	2.144466
C	1.562977	2.469101	-0.842811
N	0.204253	0.129260	1.059998
N	1.953536	1.191557	-0.733256
C	0.561861	0.234609	3.424136
C	2.444450	3.531532	-0.724498
N	-1.127190	0.531344	-1.186963
N	2.511068	-1.382056	-0.511973
C	-0.654900	0.923184	3.585622
C	3.802036	3.252409	-0.477891
C	-1.426579	1.199528	2.440379
C	4.200993	1.906022	-0.356860
C	-0.972112	0.792496	1.196063
C	3.260903	0.898687	-0.491256
C	-1.719622	1.011755	-0.058076
C	3.576128	-0.540373	-0.378079
C	-2.960753	1.623632	-0.108666
C	4.844442	-1.037311	-0.135893
C	-3.646778	1.710100	-1.334839
C	5.039366	-2.429602	-0.026808
C	-3.017401	1.212531	-2.490447
C	3.924186	-3.278447	-0.159783
C	-1.758798	0.647872	-2.366742
C	2.685402	-2.707681	-0.402695
Ru	0.690297	-0.489612	-0.968142
H	1.878349	-0.678069	1.984682
H	1.206593	-0.016052	4.264273
H	-2.373428	1.723692	2.557992
H	-3.436201	2.010676	0.790220
H	-3.483802	1.254647	-3.472666
H	-1.232965	0.256696	-3.238464
H	0.504512	2.646624	-1.036872
H	2.066534	4.546790	-0.828038
H	5.248645	1.682605	-0.162271
H	5.703589	-0.377056	-0.028084
H	4.003038	-4.361119	-0.081375
H	1.786844	-3.317344	-0.512420
O	-4.852737	2.261854	-1.305456
O	-1.145203	1.337258	4.747617
O	6.280552	-2.836564	0.199610
O	4.753182	4.167139	-0.348787
C	4.426378	5.553991	-0.478818
H	4.006373	5.765661	-1.474708
H	3.713428	5.862957	0.301485
H	5.369492	6.099036	-0.352651
C	6.557776	-4.234678	0.323872
H	7.636856	-4.312970	0.502566
H	6.009539	-4.668424	1.174761
H	6.296232	-4.769909	-0.602402
C	-0.423370	1.074649	5.953647
H	0.564093	1.561779	5.934405
H	-1.026593	1.499042	6.765243
H	-0.302580	-0.008840	6.110538
C	-5.686588	2.194299	-2.466051
H	-5.241441	2.750250	-3.305382
H	-5.857408	1.144719	-2.748604
H	-6.637295	2.660536	-2.180886
O	-0.137552	-2.063203	-0.541950
O	0.967310	-0.440720	-2.653770
C	-6.040983	0.364621	1.226338
H	-5.357930	0.618022	2.049294
H	-7.019530	0.118132	1.671039
H	-6.154889	1.213658	0.543511
C	-5.541476	-0.836844	0.474285
O	-5.583385	-0.978261	-0.729210
O	-5.060783	-1.766040	1.318066
C	-4.613185	-3.031505	0.800693
H	-5.174913	-3.277680	-0.110892
H	-4.858562	-3.761700	1.584266
C	-3.101233	-3.039065	0.552658
H	-2.791936	-4.089911	0.424397
H	-2.610579	-2.660285	1.464901
C	-2.684450	-2.222691	-0.646986
H	-1.399498	-2.108349	-0.544605
H	-2.985940	-1.173204	-0.565450
C	-2.916371	-2.802026	-2.015377
H	-4.001562	-2.832659	-2.225010
H	-2.453217	-2.184595	-2.800087
H	-2.526012	-3.829325	-2.095552

SCF Done: E(UB3LYP)= -2081.332121
Sum of electronic and zero-point Energies= -2078.451668
Sum of electronic and thermal Energies= -2078.408962
Sum of electronic and thermal Enthalpies= -2078.408018
Sum of electronic and thermal Free Energies= -2078.529413

11

C	-0.552431	0.003494	2.175741
C	-1.131113	-2.758790	-0.798426
N	0.198651	-0.322321	1.115078
N	-1.521921	-1.477602	-0.723833
C	-0.178755	-0.286866	3.479095
C	-2.022510	-3.816682	-0.724259
N	1.549825	-0.893119	-1.096070
N	-2.068573	1.095409	-0.515669
C	1.045073	-0.947530	3.690614
C	-3.391531	-3.530090	-0.564923
C	1.818052	-1.304773	2.570928
C	-3.791239	-2.181240	-0.478257
C	1.372329	-0.980075	1.300049
C	-2.839375	-1.179626	-0.559086
C	2.118937	-1.306622	0.068469
C	-3.145830	0.259505	-0.437078
C	3.320016	-1.995773	0.065264

C	-4.416957	0.754008	-0.204322
C	3.973247	-2.259197	-1.151844
C	-4.607496	2.138968	-0.024408
C	3.372159	-1.815998	-2.344354
C	-3.479675	2.978942	-0.063728
C	2.166077	-1.138858	-2.262593
C	-2.240807	2.410306	-0.309896
Ru	-0.241222	0.182318	-0.955753
H	-1.488233	0.527062	1.976730
H	-0.829196	0.013423	4.298149
H	2.765835	-1.816148	2.728888
H	3.783056	-2.328265	0.992108
H	3.819859	-1.983047	-3.322326
H	1.662105	-0.779836	-3.161110
H	-0.064318	-2.943406	-0.927757
H	-1.643900	-4.834453	-0.795379
H	-4.847325	-1.952893	-0.346185
H	-5.280898	0.093714	-0.144873
H	-3.544565	4.053620	0.094889
H	-1.347077	3.029796	-0.331550
O	5.126498	-2.915258	-1.079932
O	1.542460	-1.262150	4.882310
O	-5.850942	2.544928	0.187668
O	-4.352167	-4.440043	-0.484773
C	-4.021014	-5.829122	-0.574606
H	-3.545429	-6.055767	-1.541645
H	-3.353783	-6.126342	0.249455
H	-4.970672	-6.371390	-0.493988
C	-6.117900	3.936027	0.391808
H	-7.201428	4.016206	0.539896
H	-5.593708	4.307814	1.286050
H	-5.819796	4.525114	-0.489556
C	0.811176	-0.923012	6.062294
H	-0.164714	-1.433410	6.079961
H	1.421063	-1.267741	6.906107
H	0.663743	0.166075	6.134472
C	5.846529	-3.207678	-2.279036
H	5.254436	-3.854470	-2.945750
H	6.123238	-2.281744	-2.807557
H	6.754496	-3.737235	-1.965647
O	0.779085	1.676206	-0.609316
O	-0.444404	0.153815	-2.661540
C	2.485675	2.260965	2.622439
H	2.850996	1.475458	3.294505
H	1.398754	2.140616	2.490740
H	2.661063	3.255191	3.057476
C	3.141778	2.141071	1.275657
O	3.708923	1.154810	0.857744
O	3.010361	3.268655	0.563533
C	3.437880	3.235076	-0.809154
H	3.008881	2.341434	-1.285307
H	4.535203	3.143798	-0.846177
C	2.974735	4.513364	-1.483785
H	3.299529	4.461182	-2.536850
H	3.499058	5.371905	-1.032460
C	1.465601	4.767438	-1.420732
H	1.249034	5.725670	-1.936409
H	1.147468	4.928950	-0.376565
C	0.597045	3.726587	-2.065059
H	0.988751	3.251852	-2.976255
H	0.569063	2.691989	-1.252532
H	-0.469248	3.976082	-2.143363

SCF Done: E(UB3LYP)= -2081.317521
Sum of electronic and zero-point Energies= -2078.437864
Sum of electronic and thermal Energies= -2078.395371
Sum of electronic and thermal Enthalpies= -2078.394427
Sum of electronic and thermal Free Energies= -2078.515334

12

C	0.851518	0.752376	2.099110
C	1.141473	2.190825	-1.592624
N	-0.025876	0.657628	1.091256
N	1.518708	0.986973	-1.140199
C	0.625850	1.535313	3.221042
C	2.050307	3.184824	-1.919827
N	-1.611786	0.381979	-1.010044
N	2.055271	-1.413556	-0.170636
C	-0.579945	2.255208	3.301419
C	3.423179	2.913076	-1.768802
C	-1.497238	2.149448	2.238889
C	3.809606	1.645548	-1.289505
C	-1.194188	1.345283	1.151806
C	2.840758	0.704940	-0.982580
C	-2.090921	1.172116	-0.009121
C	3.142689	-0.639537	-0.447837
C	-3.338389	1.765849	-0.108225
C	4.423106	-1.103185	-0.200800
C	-4.120919	1.563472	-1.261690
C	4.604994	-2.389284	0.347425
C	-3.592273	0.772092	-2.298550
C	3.467280	-3.166993	0.633664
C	-2.340457	0.205705	-2.123704
C	2.217846	-2.635982	0.356260
Ru	0.200959	-0.608623	-0.669375
H	1.770774	0.172073	2.012114
H	1.377209	1.563985	4.007899
H	-2.433641	2.701158	2.297579
H	-3.732586	2.390968	0.691170
H	-4.133456	0.581638	-3.223304
H	-1.898138	-0.425192	-2.895062
H	0.069444	2.363081	-1.699188
H	1.681108	4.140883	-2.285678
H	4.869732	1.429674	-1.167728
H	5.300040	-0.494003	-0.414680
H	3.536646	-4.165076	1.061863
H	1.300878	-3.190944	0.562916
O	-5.310311	2.151058	-1.284428
O	-0.932522	3.036000	4.316282
O	5.857356	-2.770408	0.560116
O	4.400400	3.767115	-2.042519
C	4.083166	5.076259	-2.523767
H	3.543277	5.021979	-3.482002
H	3.480925	5.629323	-1.785997
H	5.043728	5.584546	-2.670834
C	6.118188	-4.055574	1.131591
H	7.208811	-4.132025	1.216732
H	5.662466	-4.139616	2.130642
H	5.741247	-4.858639	0.479237
C	-0.046919	3.190267	5.427725
H	0.910242	3.632240	5.108986
H	-0.551729	3.870067	6.124619
H	0.135212	2.223119	5.922319
C	-6.156415	1.991642	-2.426447

H	-5.676314	2.398938	-3.330081
H	-6.408209	0.930898	-2.582641
H	-7.069234	2.558392	-2.207144
O	-0.590021	-1.896093	0.329193
O	0.259869	-1.131375	-2.302053
C	-3.199018	-4.577800	-2.388064
H	-2.479172	-5.302499	-1.976018
H	-3.018422	-4.487351	-3.470418
H	-4.216982	-4.970776	-2.237713
C	-3.038727	-3.227479	-1.728988
H	-3.746614	-2.487626	-2.143729
H	-2.018330	-2.831038	-1.880575
O	-3.277307	-3.365395	-0.326872
C	-3.163120	-2.223361	0.414302
H	-3.567141	-1.330839	-0.100148
H	-1.948391	-1.957019	0.457025
C	-3.692002	-2.400491	1.819096
H	-3.296319	-3.342856	2.234824
H	-4.785511	-2.535533	1.725738
C	-3.388495	-1.227665	2.758891
H	-4.134827	-1.228041	3.570243
H	-3.533977	-0.278747	2.213192
C	-1.988303	-1.269865	3.369322
H	-1.861826	-2.171981	3.991418
H	-1.206799	-1.291247	2.596654
H	-1.806035	-0.393045	4.009799

SCF Done: E(UB3LYP)= -2007.261651
Sum of electronic and zero-point Energies= -2004.447722
Sum of electronic and thermal Energies= -2004.405616
Sum of electronic and thermal Enthalpies= -2004.404672
Sum of electronic and thermal Free Energies= -2004.523917

13

C	0.528055	-0.372476	2.151321
C	0.284696	2.345163	-0.859589
N	-0.325455	-0.264269	1.124282
N	0.977291	1.200064	-0.783417
C	0.168118	-0.086207	3.459620
C	0.885615	3.590933	-0.771942
N	-1.878189	-0.188668	-1.011358
N	2.164919	-1.158732	-0.655457
C	-1.150964	0.333139	3.714461
C	2.281004	3.650377	-0.597328
C	-2.041872	0.442746	2.629367
C	3.001982	2.441736	-0.529254
C	-1.602818	0.135313	1.351320
C	2.328178	1.235788	-0.621993
C	-2.463629	0.200971	0.154034
C	2.992186	-0.081036	-0.544840
C	-3.784552	0.613661	0.183542
C	4.352352	-0.247758	-0.351877
C	-4.541410	0.623763	-1.003863
C	4.892211	-1.547793	-0.277767
C	-3.917463	0.222605	-2.198762
C	4.019673	-2.645843	-0.396191
C	-2.591998	-0.174181	-2.149577
C	2.668985	-2.399783	-0.581049
Ru	0.140572	-0.749330	-0.947307
H	1.540729	-0.706660	1.920765
H	0.908290	-0.197273	4.249546
H	-3.065755	0.760077	2.819062
H	-4.261680	0.919071	1.112751
H	-4.440355	0.205392	-3.152841
H	-2.067956	-0.488867	-3.052898
H	-0.793659	2.262391	-1.000305
H	0.266735	4.483396	-0.842452
H	4.082800	2.480970	-0.404373
H	5.021284	0.605505	-0.251828
H	4.369223	-3.675221	-0.345599
H	1.947102	-3.213732	-0.664423
O	-5.807246	1.006162	-0.899510
O	-1.634028	0.635161	4.913622
O	6.202502	-1.636883	-0.095068
O	2.986158	4.768321	-0.490535
C	2.319034	6.032975	-0.532777
H	3.102546	6.791582	-0.418000
H	1.806273	6.174294	-1.496958
H	1.594841	6.120694	0.292300
C	6.818130	-2.925532	-0.010480
H	6.416766	-3.496016	0.841622
H	6.669576	-3.491790	-0.943014
H	7.888094	-2.739450	0.141372
C	-0.786933	0.536420	6.061290
H	0.067982	1.225786	5.978665
H	-1.406788	0.820993	6.920023
H	-0.423735	-0.494825	6.193669
C	-6.641856	1.002088	-2.061452
H	-6.253801	1.693690	-2.825361
H	-6.721519	-0.013087	-2.480867
H	-7.629072	1.340787	-1.725133
O	-0.200023	-2.460042	-0.472312
O	0.251395	-0.627725	-2.649642
C	-4.618975	-2.390292	0.200734
H	-4.534613	-2.129544	1.260309
H	-5.530915	-2.086556	-0.319445
C	-3.646092	-3.091863	-0.428630
H	-3.773923	-3.333370	-1.490623
C	-2.427655	-3.547707	0.210907
H	-1.422871	-2.877701	-0.174589
H	-2.388917	-3.426160	1.302848
H	-2.055900	-4.525807	-0.128894

SCF Done: E(UB3LYP)= -1812.770644
Sum of electronic and zero-point Energies= -1810.291559
Sum of electronic and thermal Energies= -1810.254848
Sum of electronic and thermal Enthalpies= -1810.253904
Sum of electronic and thermal Free Energies= -1810.361865

14

C	0.595778	0.178556	2.160408
C	0.593784	2.300922	-1.239969
N	-0.276593	0.170671	1.143347
N	1.146988	1.107237	-0.983376
C	0.310758	0.753127	3.389661
C	1.341839	3.460653	-1.368404
N	-1.871558	0.015639	-0.957148
N	2.045326	-1.322056	-0.449879
C	-0.947955	1.355943	3.570455
C	2.739352	3.375991	-1.222544
C	-1.861267	1.336821	2.498771
C	3.311931	2.116558	-0.954806
C	-1.500796	0.735323	1.303625
C	2.496341	1.003476	-0.840678

C	-2.399135	0.633416	0.136237
C	2.999989	-0.353781	-0.546103
C	-3.703031	1.099945	0.130037
C	4.336198	-0.654106	-0.348849
C	-4.502558	0.926484	-1.016481
C	4.716747	-1.977242	-0.045719
C	-3.939467	0.282575	-2.134247
C	3.714025	-2.960676	0.049322
C	-2.625937	-0.149736	-2.055581
C	2.397616	-2.583974	-0.160432
Ru	0.079995	-0.729113	-0.805583
H	1.562315	-0.296840	1.986729
H	1.062111	0.722762	4.176443
H	-2.840677	1.791889	2.634767
H	-4.132571	1.592809	1.000809
H	-4.497292	0.113007	-3.053299
H	-2.149421	-0.650360	-2.899329
H	-0.490899	2.328778	-1.351517
H	0.830389	4.397711	-1.580652
H	4.392291	2.042991	-0.842108
H	5.106442	0.112541	-0.417032
H	3.937114	-4.000526	0.280662
H	1.580892	-3.304330	-0.089979
O	-5.743068	1.391085	-0.953130
O	-1.353469	1.947966	4.687178
O	6.012094	-2.195216	0.133487
O	3.576732	4.399935	-1.318161
C	3.067832	5.708568	-1.591182
H	2.557278	5.734281	-2.566532
H	2.376442	6.033275	-0.797886
H	3.940197	6.372591	-1.614302
C	6.470586	-3.512390	0.452118
H	7.559881	-3.436273	0.552898
H	6.034173	-3.859256	1.401658
H	6.221584	-4.219304	-0.354624
C	-0.479373	1.997201	5.817829
H	0.446540	2.542064	5.575152
H	-1.027869	2.534483	6.600798
H	-0.234510	0.982353	6.168872
C	-6.608720	1.252348	-2.083348
H	-6.198464	1.781257	-2.957764
H	-6.766456	0.190342	-2.327959
H	-7.562080	1.708513	-1.790882
O	-0.473687	-2.267962	-0.052297
O	0.172292	-0.916635	-2.503583
C	-3.921457	-4.041499	-1.257084
H	-4.294120	-3.145447	-1.765597
H	-4.106040	-5.006374	-1.738164
C	-3.266673	-3.954499	-0.080205
H	-2.895174	-4.871643	0.394628
C	-2.964248	-2.692207	0.600501
H	-1.816375	-2.443215	0.230926
H	-3.548480	-1.849789	0.203748
C	-2.855275	-2.700901	2.111412
H	-2.188320	-3.505329	2.461063
H	-2.469133	-1.741541	2.487545
H	-3.847139	-2.865606	2.569538

SCF Done: E(UB3LYP)= -1852.109036
Sum of electronic and zero-point Energies= -1849.557399
Sum of electronic and thermal Energies= -1849.519028
Sum of electronic and thermal Enthalpies= -1849.518084
Sum of electronic and thermal Free Energies= -1849.631009

15

C	0.014375	1.161745	2.227599
C	-0.705170	1.956467	-1.722311
N	-0.746130	0.507235	1.339545
N	0.260477	1.227577	-1.145875
C	-0.517785	1.940772	3.243757
C	-0.449327	3.148687	-2.382054
N	-2.087344	-0.811921	-0.529072
N	1.994254	-0.302694	0.127139
C	-1.917330	2.047136	3.342056
C	0.880546	3.604627	-2.449874
C	-2.710367	1.352474	2.408216
C	1.887953	2.835955	-1.833268
C	-2.099744	0.593838	1.422020
C	1.549504	1.657668	-1.189680
C	-2.847127	-0.163920	0.396299
C	2.518610	0.809025	-0.466895
C	-4.230346	-0.222959	0.345388
C	3.857485	1.126232	-0.324325
C	-4.862781	-0.966483	-0.669666
C	4.688605	0.311863	0.471994
C	-4.057843	-1.627257	-1.615441
C	4.112849	-0.788811	1.132136
C	-2.681117	-1.520745	-1.501295
C	2.769129	-1.052590	0.925965
Ru	-0.009275	-0.711442	-0.298264
H	1.094873	1.057205	2.122323
H	0.156207	2.444898	3.933568
H	-3.794260	1.427500	2.480136
H	-4.844897	0.293273	1.080980
H	-4.476663	-2.217249	-2.428468
H	-2.018476	-2.015361	-2.212599
H	-1.722341	1.568289	-1.656476
H	-1.276575	3.695021	-2.831028
H	2.916772	3.189747	-1.869952
H	4.286560	2.005128	-0.802833
H	4.684179	-1.439420	1.791464
H	2.284240	-1.883083	1.434904
O	-6.189915	-0.987056	-0.655568
O	-2.562324	2.760335	4.257689
O	5.963004	0.665853	0.555600
O	1.270871	4.719849	-3.052960
C	0.301985	5.553435	-3.694599
H	-0.209316	5.008941	-4.503612
H	-0.437410	5.925388	-2.968056
H	0.861585	6.397257	-4.115664
C	6.860739	-0.107813	1.357446
H	7.842478	0.370258	1.257679
H	6.549600	-0.097470	2.413650
H	6.915173	-1.145469	0.993166
C	-1.818389	3.500355	5.228831
H	-1.179046	4.254167	4.742595
H	-2.561441	4.001253	5.860998
H	-1.200903	2.829149	5.846083
C	-6.893726	-1.732769	-1.652213
H	-6.674285	-1.345790	-2.659754
H	-6.634698	-2.801926	-1.597951
H	-7.959834	-1.600859	-1.431586
O	-0.101829	-2.121561	0.828571

O	0.222925	-1.379427	-1.869998
C	2.846491	-3.531341	-1.618797
H	2.081997	-3.412076	-2.390907
H	3.878378	-3.305520	-1.902266
C	2.549875	-3.923733	-0.364792
H	3.364562	-3.980633	0.366302
C	1.207048	-4.246435	0.159235
H	0.770707	-3.155275	0.550382
C	1.213876	-5.072360	1.434512
H	0.214783	-5.101283	1.894941
H	1.507730	-6.113222	1.205482
H	1.930549	-4.675845	2.170417
C	0.144495	-4.664123	-0.844402
H	-0.843089	-4.712789	-0.362452
H	0.076420	-3.970829	-1.693079
H	0.378827	-5.668915	-1.238643

SCF Done: E(UB3LYP)= -1891.434988
Sum of electronic and zero-point Energies= -1888.814252
Sum of electronic and thermal Energies= -1888.774376
Sum of electronic and thermal Enthalpies= -1888.773432
Sum of electronic and thermal Free Energies= -1888.888753

16

C	-0.692147	1.191655	2.215396
C	-1.378252	1.660891	-1.800388
N	-1.247221	0.342048	1.340325
N	-0.305010	1.176712	-1.160332
C	-1.421701	1.843801	3.197876
C	-1.348806	2.845718	-2.520069
N	-2.187110	-1.309275	-0.511775
N	1.645799	0.118852	0.257766
C	-2.805721	1.602617	3.274519
C	-0.138276	3.560950	-2.583121
C	-3.384098	0.714457	2.347612
C	0.983566	3.048164	-1.901351
C	-2.583956	0.102379	1.395639
C	0.870365	1.861158	-1.197773
C	-3.104196	-0.830576	0.373918
C	1.963349	1.271899	-0.397455
C	-4.437062	-1.198418	0.283706
C	3.206939	1.857996	-0.239840
C	-4.854374	-2.076621	-0.734442
C	4.145496	1.278011	0.637946
C	-3.890724	-2.557363	-1.639591
C	3.762315	0.143082	1.374118
C	-2.575922	-2.147804	-1.484302
C	2.512426	-0.402250	1.141153
Ru	-0.195304	-0.732151	-0.223284
H	0.382083	1.358606	2.127989
H	-0.909383	2.519499	3.879968
H	-4.455274	0.526214	2.398321
H	-5.176512	-0.819449	0.987075
H	-4.140472	-3.237291	-2.451790
H	-1.795183	-2.495819	-2.162336
H	-2.295337	1.073522	-1.741788
H	-2.253928	3.185912	-3.019421
H	1.920121	3.602537	-1.936364
H	3.473704	2.771054	-0.769832
H	4.418622	-0.333443	2.097791
H	2.178841	-1.282622	1.686683
O	-6.145325	-2.385822	-0.762619
O	-3.625053	2.155414	4.161478
O	5.329579	1.869129	0.719815
O	0.036438	4.700586	-3.239545
C	-1.059174	5.280285	-3.952810
H	-1.417907	4.600082	-4.741134
H	-1.885457	5.527947	-3.268305
H	-0.670613	6.199045	-4.408238
C	6.322897	1.341166	1.604747
H	7.206348	1.978755	1.480834
H	5.978650	1.385489	2.649854
H	6.573617	0.303614	1.336135
C	-3.102889	3.068016	5.130209
H	-2.649662	3.944313	4.640710
H	-3.958894	3.387570	5.736821
H	-2.358540	2.573699	5.774337
C	-6.637179	-3.266169	-1.776395
H	-6.467334	-2.843362	-2.779197
H	-6.159770	-4.255939	-1.702954
H	-7.714496	-3.363476	-1.595693
O	0.006888	-2.113017	0.955928
O	0.265543	-1.426334	-1.733453
C	5.634332	-2.032987	-0.519025
C	4.615192	-1.861553	-1.467068
C	3.365930	-2.434395	-1.257725
C	3.105983	-3.197960	-0.092340
C	4.145725	-3.355432	0.856845
C	5.396232	-2.786806	0.639293
H	6.613158	-1.575670	-0.681227
H	4.800680	-1.270969	-2.367106
H	2.561834	-2.287248	-1.981776
H	3.952974	-3.933774	1.763739
H	6.191658	-2.919100	1.376302
C	1.787662	-3.760258	0.148463
H	1.017105	-2.867395	0.668216
H	1.193200	-3.989566	-0.744762
H	1.726166	-4.528000	0.930469

SCF Done: E(UB3LYP)= -1966.497357
Sum of electronic and zero-point Energies= -1963.809415
Sum of electronic and thermal Energies= -1963.770655
Sum of electronic and thermal Enthalpies= -1963.769711
Sum of electronic and thermal Free Energies= -1963.882167

17

C	-0.707967	1.195823	2.326610
C	-1.544322	1.589952	-1.870791
N	-1.224019	0.349636	1.425593
N	-0.436340	1.235872	-1.204900
C	-1.473091	1.807962	3.309169
C	-1.652869	2.782910	-2.570330
N	-2.080344	-1.301308	-0.470277
N	1.634984	0.401767	0.207426
C	-2.850322	1.525687	3.356978
C	-0.549489	3.655111	-2.582651
C	-3.386695	0.634528	2.406946
C	0.613096	3.276051	-1.883335
C	-2.552816	0.066881	1.457338
C	0.639130	2.068631	-1.205355
C	-3.027351	-0.864401	0.410651
C	1.798533	1.600629	-0.418378
C	-4.343870	-1.272381	0.289301
C	2.969763	2.322674	-0.267851

C	-4.714607	-2.148279	-0.751073
C	3.998935	1.823821	0.555736
C	-3.720948	-2.586943	-1.647212
C	3.790748	0.604998	1.225871
C	-2.424853	-2.137185	-1.465378
C	2.599733	-0.067708	1.016153
Ru	-0.136823	-0.630492	-0.174049
H	0.363265	1.392492	2.261229
H	-0.992167	2.485290	4.012308
H	-4.451915	0.412122	2.437719
H	-5.108698	-0.928645	0.983953
H	-3.936282	-3.262840	-2.472561
H	-1.619904	-2.446614	-2.133788
H	-2.380273	0.890045	-1.850343
H	-2.582155	3.010524	-3.089273
H	1.471387	3.946340	-1.885323
H	3.112157	3.279314	-0.767504
H	4.533056	0.166208	1.888322
H	2.398422	-1.016109	1.511609
O	-5.992226	-2.494340	-0.806864
O	-3.702306	2.040425	4.236221
O	5.098216	2.560488	0.646110
O	-0.513182	4.825905	-3.207008
C	-1.661221	5.274953	-3.931311
H	-1.904885	4.580423	-4.750585
H	-2.529342	5.383503	-3.262320
H	-1.392330	6.253550	-4.347016
C	6.176719	2.116861	1.474668
H	6.962525	2.875781	1.380041
H	5.857815	2.043477	2.526144
H	6.558880	1.143209	1.130988
C	-3.227843	2.958547	5.223785
H	-2.795389	3.854583	4.751588
H	-4.104612	3.243137	5.817982
H	-2.478984	2.482067	5.875998
C	-6.444781	-3.374559	-1.840684
H	-6.272757	-2.931442	-2.834006
H	-5.939278	-4.350360	-1.772742
H	-7.521021	-3.504598	-1.675794
O	0.318384	-1.971520	0.929877
O	0.445400	-1.374012	-1.665042
C	5.643336	-1.758005	-0.470702
C	4.699107	-1.588026	-1.491702
C	3.468375	-2.233265	-1.417439
C	3.151468	-3.075151	-0.325246
C	4.111841	-3.228107	0.699497
C	5.344198	-2.581101	0.622351
H	6.607333	-1.246444	-0.523997
H	4.924960	-0.942551	-2.343810
H	2.722668	-2.086900	-2.201025
H	3.892583	-3.863381	1.559068
H	6.077736	-2.715383	1.420986
C	1.829440	-3.724115	-0.266221
H	1.081557	-2.860810	0.255117
H	1.378985	-3.839925	-1.259496
C	1.606657	-4.916075	0.638226
H	1.851402	-4.700119	1.689087
H	0.556582	-5.241142	0.593484
H	2.236454	-5.764806	0.315119

SCF Done: E(UB3LYP)= -2005.838584
Sum of electronic and zero-point Energies= -2003.079537
Sum of electronic and thermal Energies= -2003.039254
Sum of electronic and thermal Enthalpies= -2003.038309
Sum of electronic and thermal Free Energies= -2003.15443

18

C	-0.829225	1.218289	2.269884
C	-1.593759	1.874603	-1.690745
N	-1.329388	0.383724	1.348241
N	-0.479973	1.433178	-1.091251
C	-1.597583	1.763976	3.287161
C	-1.659130	3.097694	-2.340565
N	-2.160228	-1.232143	-0.585831
N	1.561872	0.436834	0.241343
C	-2.961561	1.424407	3.350732
C	-0.503931	3.900741	-2.374255
C	-3.481691	0.552254	2.375264
C	0.662712	3.429496	-1.739308
C	-2.646577	0.051105	1.389450
C	0.644282	2.198993	-1.104281
C	-3.106331	-0.859259	0.319747
C	1.788975	1.642992	-0.353617
C	-4.412430	-1.307819	0.207193
C	2.993913	2.301729	-0.182619
C	-4.769276	-2.166079	-0.850455
C	3.984888	1.739155	0.647824
C	-3.774122	-2.545021	-1.769967
C	3.689047	0.547040	1.331819
C	-2.490312	-2.053532	-1.594042
C	2.474708	-0.068488	1.086823
Ru	-0.214076	-0.521090	-0.275175
H	0.231413	1.459981	2.192609
H	-1.128845	2.434898	4.004657
H	-4.536735	0.287751	2.416384
H	-5.176899	-1.010841	0.923273
H	-3.976557	-3.207188	-2.609634
H	-1.688388	-2.317676	-2.284647
H	-2.465295	1.219530	-1.656090
H	-2.593495	3.401100	-2.808810
H	1.557915	4.049351	-1.755653
H	3.190577	3.258122	-0.664573
H	4.386183	0.080942	2.023315
H	2.210104	-0.994893	1.592466
O	-6.037348	-2.555781	-0.898523
O	-3.813546	1.866911	4.267948
O	5.130904	2.399302	0.740597
O	-0.423133	5.088008	-2.961026
C	-1.571955	5.629835	-3.618752
H	-1.893699	4.978323	-4.446335
H	-2.401649	5.768370	-2.907925
H	-1.261069	6.603321	-4.016558
C	6.170312	1.890497	1.582518
H	7.013204	2.583267	1.473393
H	5.844410	1.867184	2.634177
H	6.474123	0.882270	1.262363
C	-3.350577	2.744123	5.297479
H	-2.962162	3.681833	4.870025
H	-4.223457	2.960783	5.924948
H	-2.570194	2.259013	5.904775
C	-6.470828	-3.418481	-1.953130
H	-6.326922	-2.940551	-2.935028
H	-5.931198	-4.378064	-1.922511
H	-7.539967	-3.592177	-1.781367
O	0.094689	-1.937787	0.812379

O	0.264279	-1.050485	-1.847506
C	5.595887	-1.337554	-0.859221
C	4.459740	-1.280718	-1.675072
C	3.317813	-2.001869	-1.336669
C	3.273634	-2.800096	-0.170657
C	4.428110	-2.841079	0.641416
C	5.575054	-2.127268	0.295396
H	6.489833	-0.765781	-1.119269
H	4.460392	-0.659819	-2.574037
H	2.431337	-1.917682	-1.965752
H	4.436215	-3.443277	1.549753
H	6.457977	-2.181273	0.936841
C	2.028821	-3.528796	0.204789
H	1.222928	-2.629399	0.535040
C	2.072890	-4.366400	1.469232
H	2.429678	-3.797367	2.339516
H	1.070468	-4.755242	1.700960
H	2.743837	-5.233479	1.332692
C	1.276574	-4.211395	-0.929384
H	0.273068	-4.516952	-0.598308
H	1.166765	-3.574253	-1.815497
H	1.824286	-5.123104	-1.229894

SCF Done: E(UB3LYP)= -2045.171845
Sum of electronic and zero-point Energies= -2042.341868
Sum of electronic and thermal Energies= -2042.300117
Sum of electronic and thermal Enthalpies= -2042.299173
Sum of electronic and thermal Free Energies= -2042.417665

19

C	-1.074647	-0.919222	2.160134
C	-1.371988	-2.125751	-1.638604
N	-0.154963	-0.929654	1.186543
N	-1.601263	-0.911378	-1.118769
C	-1.037579	-1.792560	3.237030
C	-2.394586	-2.969850	-2.041368
N	1.564558	-0.786768	-0.817710
N	-1.838992	1.488470	-0.039518
C	0.014112	-2.725202	3.305492
C	-3.723887	-2.531245	-1.890764
C	0.981181	-2.722643	2.282120
C	-3.953979	-1.254228	-1.340669
C	0.871127	-1.815673	1.240103
C	-2.878883	-0.465493	-0.968508
C	1.836031	-1.732876	0.124293
C	-3.012453	0.884079	-0.381086
C	2.949680	-2.548351	0.013566
C	-4.223927	1.515115	-0.159535
C	3.816564	-2.403986	-1.086902
C	-4.245966	2.797889	0.425408
C	3.511551	-1.430200	-2.055764
C	-3.022209	3.399373	0.775033
C	2.379166	-0.653084	-1.876897
C	-1.849605	2.706331	0.522232
Ru	-0.099708	0.448362	-0.502826
H	-1.873246	-0.180284	2.078761
H	-1.815211	-1.733221	3.996554
H	1.801873	-3.436089	2.332948
H	3.173301	-3.305637	0.762987
H	4.131973	-1.266113	-2.934745
H	2.105305	0.111183	-2.604375
H	-0.329164	-2.429992	-1.739262
H	-2.144254	-3.941938	-2.462011
H	-4.980179	-0.910935	-1.220261
H	-5.167361	1.042282	-0.427865
H	-2.966105	4.385203	1.232485
H	-0.874123	3.122414	0.779056
O	4.866501	-3.213957	-1.129534
O	0.174354	-3.621122	4.272397
O	-5.439691	3.346044	0.606545
O	-4.797050	-3.232407	-2.229403
C	-4.641503	-4.533613	-2.802840
H	-4.075884	-4.480632	-3.746134
H	-4.134559	-5.213180	-2.100116
H	-5.656270	-4.898989	-3.001095
C	-5.539684	4.644653	1.198537
H	-6.610708	4.876321	1.238275
H	-5.122992	4.642792	2.217961
H	-5.020553	5.396228	0.583272
C	-0.769331	-3.678473	5.344565
H	-1.778003	-3.911343	4.968269
H	-0.428445	-4.485394	6.004358
H	-0.788624	-2.728990	5.902392
C	5.783324	-3.120719	-2.223245
H	5.276234	-3.330025	-3.178140
H	6.250514	-2.124049	-2.258514
H	6.551543	-3.881365	-2.039580
O	0.798257	1.534890	0.637063
O	0.004658	1.057903	-2.097382
C	3.238376	1.051840	1.347456
H	3.686529	0.778560	0.385133
H	2.031181	1.216451	1.003089
H	3.226351	0.221222	2.064080
C	3.606576	2.349631	1.897226
C	3.782988	2.488967	3.240770
H	3.661761	1.638086	3.917827
H	4.064115	3.450390	3.681081
C	3.682516	3.555802	0.983705
H	2.646892	3.895040	0.818767
H	4.178782	4.368084	1.536298
C	4.378782	3.358310	-0.377169
H	4.774400	4.335510	-0.703504
H	5.264669	2.718470	-0.223012
C	3.527974	2.779230	-1.522119
H	4.211714	2.304894	-2.246474
H	2.885556	1.970019	-1.147532
C	2.651403	3.774567	-2.294575
H	3.289331	4.582950	-2.696610
H	2.244258	3.246194	-3.174488
C	1.484015	4.384262	-1.516848
H	0.818698	4.951994	-2.188173
H	0.882292	3.599520	-1.030297
H	1.823107	5.079653	-0.733036

SCF Done: E(UB3LYP)= -2009.4433
Sum of electronic and zero-point Energies= -2006.607026
Sum of electronic and thermal Energies= -2006.563993
Sum of electronic and thermal Enthalpies= -2006.563049
Sum of electronic and thermal Free Energies= -2006.685245

20

C	0.791046	0.534711	2.189441
C	0.567119	2.029219	-1.561700

N	-0.117774	0.372879	1.217471
N	1.167009	0.915188	-1.115810
C	0.560566	1.323662	3.305704
C	1.274177	3.166869	-1.913812
N	-1.792248	-0.133223	-0.757379
N	2.149933	-1.353575	-0.190636
C	-0.679980	1.979672	3.417878
C	2.676427	3.150730	-1.790006
C	-1.633649	1.792186	2.398378
C	3.297743	1.972989	-1.328332
C	-1.325705	0.985840	1.314760
C	2.523779	0.872026	-1.004683
C	-2.256233	0.719823	0.200244
C	3.076263	-0.405820	-0.513272
C	-3.518902	1.274761	0.106170
C	4.428273	-0.657944	-0.363764
C	-4.349165	0.944875	-0.982164
C	4.854817	-1.907631	0.131358
C	-3.846507	0.077659	-1.969459
C	3.880588	-2.867243	0.466302
C	-2.569912	-0.431322	-1.812726
C	2.545997	-2.543974	0.286092
Ru	0.161941	-0.856312	-0.549470
H	1.740860	0.011265	2.070709
H	1.338640	1.412349	4.061633
H	-2.599987	2.285950	2.485275
H	-3.899287	1.948876	0.871329
H	-4.427891	-0.217002	-2.840794
H	-2.141976	-1.106082	-2.554354
H	-0.520465	2.009028	-1.640307
H	0.730636	4.038923	-2.272335
H	4.382030	1.953056	-1.232097
H	5.178212	0.087669	-0.622255
H	4.139711	-3.849260	0.857498
H	1.751574	-3.249948	0.532418
O	-5.558066	1.487289	-0.992426
O	-1.032576	2.770620	4.423169
O	6.163128	-2.083070	0.246410
O	3.473991	4.169386	-2.076580
C	2.912720	5.396933	-2.551753
H	2.381945	5.241208	-3.504056
H	2.226489	5.828032	-1.806164
H	3.760095	6.074793	-2.708879
C	6.672238	-3.325101	0.742151
H	7.764341	-3.227279	0.734241
H	6.324415	-3.507337	1.770950
H	6.370388	-4.160005	0.090822
C	-0.110389	3.017015	5.488004
H	0.802583	3.503911	5.110856
H	-0.625796	3.690065	6.183631
H	0.151241	2.080844	6.005565
C	-6.471164	1.158707	-2.043098
H	-6.076531	1.476216	-3.020966
H	-6.676479	0.076790	-2.055103
H	-7.394794	1.707520	-1.823428
O	-0.303954	-2.250034	0.529021
O	0.167002	-1.363662	-2.179080
C	-2.580300	-2.507677	1.621173
H	-1.438588	-2.315404	0.966994
H	-2.345261	-3.498269	2.034722
H	-2.588460	-1.695118	2.357953
C	-3.709642	-2.465760	0.659719
O	-4.519621	-1.550220	0.719726
C	-3.870335	-3.599362	-0.333012
H	-4.346662	-4.423838	0.230196
H	-4.601702	-3.266662	-1.084808
C	-2.586106	-4.108750	-0.987434
H	-1.866279	-4.489852	-0.247631
H	-2.820857	-4.936230	-1.674637
H	-2.087810	-3.320373	-1.570682

SCF Done: E(UB3LYP)= -1927.385318
Sum of electronic and zero-point Energies= -1924.741771
Sum of electronic and thermal Energies= -1924.702751
Sum of electronic and thermal Enthalpies= -1924.701807
Sum of electronic and thermal Free Energies= -1924.815018

21

C	-0.115843	-1.303633	2.145587
C	0.623224	-1.829537	-1.831327
N	0.677094	-0.623185	1.305872
N	-0.325399	-1.114299	-1.208732
C	0.378702	-2.157553	3.119211
C	0.343695	-2.993099	-2.529157
N	2.083422	0.768748	-0.458775
N	-2.024809	0.390086	0.144393
C	1.773115	-2.313365	3.227756
C	-0.991412	-3.435924	-2.587565
C	2.599907	-1.593721	2.343068
C	-1.980906	-2.677025	-1.931105
C	2.026405	-0.761790	1.395027
C	-1.620730	-1.526484	-1.250692
C	2.810458	0.022321	0.417902
C	-2.570406	-0.688758	-0.493902
C	4.194155	0.008452	0.358757
C	-3.915201	-0.984650	-0.370670
C	4.862001	0.784702	-0.608180
C	-4.738349	-0.179932	0.443492
C	4.090615	1.553790	-1.498796
C	-4.148701	0.893111	1.134600
C	2.710377	1.511598	-1.383562
C	-2.797558	1.134674	0.950774
Ru	-0.000145	0.739921	-0.237247
H	-1.191464	-1.159279	2.037079
H	-0.319199	-2.678894	3.771325
H	3.679925	-1.707419	2.422902
H	4.782896	-0.591202	1.050961
H	4.537465	2.175862	-2.272206
H	2.073589	2.087033	-2.056971
H	1.644097	-1.451490	-1.774535
H	1.157761	-3.527721	-3.014564
H	-3.014571	-3.016338	-1.965816
H	-4.356469	-1.838795	-0.881795
H	-4.713831	1.539850	1.803011
H	-2.312116	1.944736	1.487268
O	6.187628	0.728990	-0.603924
O	2.383118	-3.096391	4.108656
O	-6.017809	-0.517127	0.510199
O	-1.400657	-4.527960	-3.217769
C	-0.448299	-5.350121	-3.899010
H	0.049423	-4.787139	-4.703736
H	0.302787	-5.743403	-3.196095
H	-1.020460	-6.180249	-4.330107
C	-6.908179	0.243324	1.332832

H	-7.894550	-0.222068	1.219592
H	-6.597477	0.200452	2.388345
H	-6.952194	1.290946	0.997061
C	1.604238	-3.865445	5.029084
H	0.947908	-4.569904	4.494126
H	2.323460	-4.424220	5.639762
H	1.000335	-3.209958	5.675970
C	6.930285	1.511093	-1.542781
H	6.689172	1.218050	-2.576518
H	6.730033	2.584904	-1.402238
H	7.987714	1.304096	-1.338869
O	0.211654	2.064020	1.014620
O	-0.206874	1.533190	-1.740773
C	-0.687232	4.696070	-1.581538
H	0.313689	4.247700	-1.484511
H	-0.566569	5.784654	-1.453282
H	-1.101455	4.485354	-2.575497
C	-1.608395	4.159479	-0.517258
O	-2.703280	3.683934	-0.776766
C	-1.142653	4.209820	0.907705
H	-1.983873	4.109474	1.607979
H	-0.576368	3.033494	0.998158
C	-0.063611	5.161621	1.333922
H	-0.428511	6.204028	1.262222
H	0.217313	4.986562	2.383465
H	0.837336	5.081540	0.708106

SCF Done: E(UB3LYP)= -1927.378382
Sum of electronic and zero-point Energies= -1924.735461
Sum of electronic and thermal Energies= -1924.69596
Sum of electronic and thermal Enthalpies= -1924.695016
Sum of electronic and thermal Free Energies= -1924.80968

22

C	0.242963	0.045748	1.918831
C	-2.176626	2.380637	-0.308690
N	-0.610571	-0.281977	0.939527
N	-0.904365	2.004296	-0.507256
C	0.007244	-0.249133	3.252129
C	-2.523549	3.664946	0.077122
N	-2.219787	-0.775267	-1.113968
N	1.527964	1.047647	-0.890713
C	-1.180609	-0.922979	3.587559
C	-1.496829	4.609789	0.265014
C	-2.081382	-1.250587	2.554911
C	-0.164074	4.204874	0.051236
C	-1.771395	-0.920123	1.245633
C	0.102974	2.901455	-0.329902
C	-2.657617	-1.212475	0.099009
C	1.462306	2.367604	-0.538219
C	-3.871544	-1.868698	0.218063
C	2.611968	3.112987	-0.348377
C	-4.665194	-2.088238	-0.924581
C	3.875905	2.508807	-0.507449
C	-4.193029	-1.626226	-2.166535
C	3.923763	1.144869	-0.844568
C	-2.967043	-0.981496	-2.208733
C	2.730351	0.466834	-1.020636
Ru	-0.308670	0.089115	-1.177876
H	1.161008	0.555405	1.627745
H	0.747098	0.036114	3.997175
H	-3.007283	-1.763554	2.810403
H	-4.231539	-2.223144	1.182124
H	-4.751765	-1.761017	-3.090755
H	-2.561807	-0.612002	-3.151792
H	-2.946880	1.625825	-0.467916
H	-3.574669	3.907016	0.221797
H	0.636529	4.928085	0.196431
H	2.563804	4.163949	-0.067555
H	4.856744	0.599629	-0.970561
H	2.754607	-0.586748	-1.268279
O	-5.814816	-2.723369	-0.736831
O	-1.528294	-1.279561	4.817475
O	4.934541	3.280379	-0.313700
O	-1.681803	5.868492	0.635373
C	-3.006828	6.348295	0.884128
H	-3.624350	6.280879	-0.024900
H	-3.479997	5.782951	1.702062
H	-2.896429	7.399027	1.177486
C	6.245864	2.722090	-0.449871
H	6.945145	3.541730	-0.246788
H	6.402357	1.911296	0.278408
H	6.404104	2.343269	-1.471500
C	-0.645302	-0.999145	5.907161
H	-0.490941	0.085593	6.018399
H	-1.136853	-1.394940	6.803917
H	0.324191	-1.501558	5.763927
C	-6.667464	-2.988248	-1.854170
H	-6.990253	-2.050410	-2.332878
H	-6.159357	-3.629105	-2.591693
H	-7.540533	-3.514045	-1.449223
O	0.272663	-1.654219	-1.252694
O	-0.527149	0.611051	-2.789458
C	2.231803	-2.573575	-2.562583
H	1.615081	-3.337616	-3.051637
H	2.550088	-1.747584	-3.210121
H	1.291080	-2.019032	-1.787538
C	3.248143	-3.053423	-1.594240
O	4.229212	-2.364833	-1.339072
C	3.640887	-4.608009	0.415890
H	4.611135	-4.087001	0.451007
H	3.859939	-5.678198	0.557507
C	2.732002	-4.149769	1.564757
H	3.224389	-4.403846	2.520836
H	1.805284	-4.750254	1.530627
C	2.348345	-2.665373	1.589666
H	1.598280	-2.521916	2.385565
H	1.825485	-2.394216	0.655918
C	3.514378	-1.708664	1.828771
H	4.252508	-1.756664	1.014384
H	3.166282	-0.665588	1.897536
H	4.034707	-1.948287	2.772152
C	3.029406	-4.417521	-0.975187
H	1.951628	-4.649103	-0.980341
H	3.486235	-5.123916	-1.694073

SCF Done: E(UB3LYP)= -2045.378041
Sum of electronic and zero-point Energies= -2042.520715
Sum of electronic and thermal Energies= -2042.478084
Sum of electronic and thermal Enthalpies= -2042.47714
Sum of electronic and thermal Free Energies= -2042.597406

23

C	0.325813	-0.068008	1.875025
C	-2.224268	2.351397	-0.198012

N	-0.560476	-0.347595	0.909419
N	-0.949106	2.001025	-0.425923
C	0.148999	-0.455551	3.193601
C	-2.584127	3.614955	0.240318
N	-2.234825	-0.758062	-1.112447
N	1.488545	1.107032	-0.909479
C	-1.009197	-1.179830	3.527777
C	-1.568554	4.566741	0.452123
C	-1.941711	-1.461725	2.509958
C	-0.232489	4.188373	0.211021
C	-1.695574	-1.029886	1.216997
C	0.047812	2.904938	-0.223804
C	-2.628886	-1.254208	0.092842
C	1.411235	2.401426	-0.475301
C	-3.847927	-1.897558	0.228490
C	2.553938	3.148634	-0.253547
C	-4.687847	-2.051722	-0.891557
C	3.823097	2.571745	-0.465246
C	-4.257809	-1.534451	-2.127019
C	3.883343	1.233217	-0.892179
C	-3.026885	-0.900792	-2.185835
C	2.695976	0.553352	-1.097403
Ru	-0.337168	0.131012	-1.196436
H	1.222542	0.478983	1.583706
H	0.912732	-0.204329	3.926496
H	-2.842834	-2.017688	2.763280
H	-4.177158	-2.288646	1.189479
H	-4.854400	-1.615575	-3.033652
H	-2.655711	-0.486377	-3.124215
H	-2.986431	1.593660	-0.379695
H	-3.636830	3.837040	0.404622
H	0.559563	4.917551	0.372348
H	2.496560	4.179294	0.093209
H	4.821192	0.709832	-1.065790
H	2.725548	-0.480085	-1.416981
O	-5.838164	-2.681270	-0.690566
O	-1.300886	-1.625250	4.743188
O	4.874325	3.342631	-0.234178
O	-1.767140	5.808887	0.867607
C	-3.097120	6.264593	1.135247
H	-3.717522	6.215684	0.226986
H	-3.559740	5.670209	1.938517
H	-2.998520	7.307710	1.458452
C	6.191797	2.815346	-0.425909
H	6.881255	3.632922	-0.184595
H	6.373348	1.964794	0.249392
H	6.338152	2.501764	-1.471199
C	-0.389955	-1.383068	5.818944
H	-0.260491	-0.302468	5.987696
H	-0.841238	-1.842890	6.706259
H	0.587090	-1.849546	5.616966
C	-6.740539	-2.871460	-1.783954
H	-7.068127	-1.903563	-2.194689
H	-6.273550	-3.475607	-2.577391
H	-7.603909	-3.408201	-1.372745
O	0.265396	-1.602444	-1.362613
O	-0.606625	0.716454	-2.777193
C	2.218876	-2.494763	-2.698751
H	1.612634	-3.300800	-3.126908
H	2.518123	-1.699100	-3.388454
H	1.261227	-1.925178	-1.931674
C	3.250088	-2.896990	-1.716391
O	4.258095	-2.250725	-1.492038
O	2.906326	-4.018287	-1.076010
C	3.666899	-4.432612	0.082062
H	4.610357	-3.872808	0.109454
H	3.891923	-5.497921	-0.069490
C	2.832912	-4.231196	1.339080
H	3.430269	-4.616921	2.184291
H	1.936378	-4.870306	1.270374
C	2.405363	-2.785676	1.617703
H	1.744129	-2.791718	2.499818
H	1.776427	-2.423231	0.785517
C	3.559040	-1.813200	1.857805
H	4.193359	-1.703598	0.965085
H	3.184783	-0.811039	2.120056
H	4.200891	-2.155278	2.687611

SCF Done: E(UB3LYP)= -2081.311928
Sum of electronic and zero-point Energies= -2078.430783
Sum of electronic and thermal Energies= -2078.388523
Sum of electronic and thermal Enthalpies= -2078.387579
Sum of electronic and thermal Free Energies= -2078.507603

24

C	0.362710	-0.816270	1.965047
C	0.221092	2.490281	-0.333692
N	-0.446277	-0.495127	0.944909
N	0.930198	1.362868	-0.491757
C	-0.065136	-0.834582	3.283026
C	0.800565	3.684734	0.061572
N	-1.885960	0.060813	-1.192593
N	2.137660	-0.957506	-0.844318
C	-1.404259	-0.499530	3.558315
C	2.186942	3.710529	0.306178
C	-2.247604	-0.165918	2.480984
C	2.922397	2.520143	0.136759
C	-1.742995	-0.173322	1.192084
C	2.273260	1.365945	-0.265082
C	-2.551719	0.126950	-0.004313
C	2.952189	0.072359	-0.473700
C	-3.898810	0.439241	0.040192
C	4.309643	-0.126025	-0.299189
C	-4.598622	0.694172	-1.155392
C	4.859486	-1.408720	-0.503100
C	-3.892022	0.627122	-2.371599
C	3.998302	-2.458833	-0.875198
C	-2.544557	0.311211	-2.337321
C	2.650731	-2.183422	-1.034390
Ru	0.135022	-0.483996	-1.144011
H	1.393623	-1.072953	1.718210
H	0.640212	-1.108762	4.065157
H	-3.288238	0.081505	2.683280
H	-4.435536	0.488830	0.985652
H	-4.366455	0.815297	-3.332935
H	-1.960798	0.252485	-3.256714
H	-0.848975	2.435355	-0.535269
H	0.172528	4.567121	0.168306
H	3.995138	2.531063	0.322496
H	4.968850	0.689920	-0.006613
H	4.354410	-3.473425	-1.043703
H	1.942242	-2.962300	-1.320217
O	-5.886335	0.983551	-1.040082
O	-1.947128	-0.474770	4.767904

O	6.166251	-1.528471	-0.322718
O	2.869253	4.780846	0.685830
C	2.189257	6.026499	0.870520
H	1.711472	6.353873	-0.065966
H	1.434422	5.945304	1.668180
H	2.959554	6.749460	1.164000
C	6.795989	-2.799008	-0.518138
H	7.860768	-2.642794	-0.308061
H	6.387101	-3.548878	0.176714
H	6.669337	-3.141724	-1.556871
C	-1.151955	-0.811544	5.908207
H	-0.307097	-0.113531	6.016398
H	-1.816354	-0.722376	6.776022
H	-0.777441	-1.844455	5.833820
C	-6.661237	1.251485	-2.213189
H	-6.273296	2.134771	-2.744288
H	-6.664724	0.380279	-2.886878
H	-7.680740	1.450233	-1.861902
O	-0.224294	-2.272131	-1.143754
O	0.339656	0.041004	-2.752874
H	-1.354743	-2.663010	-1.056465
C	-2.601356	-3.175122	-1.004433
C	-2.931622	-3.280399	0.373999
N	-3.154777	-3.321247	1.516486
H	-3.219652	-2.467223	-1.570172
H	-2.425725	-4.134933	-1.508143

SCF Done: E(UB3LYP)= -1827.614507
Sum of electronic and zero-point Energies= -1825.148437
Sum of electronic and thermal Energies= -1825.112401
Sum of electronic and thermal Enthalpies= -1825.111457
Sum of electronic and thermal Free Energies= -1825.218356

25

C	0.436130	-0.422053	2.055815
C	0.428263	2.522362	-0.740607
N	-0.381903	-0.191397	1.018849
N	1.056004	1.336949	-0.718471
C	0.063248	-0.189549	3.370247
C	1.092332	3.721320	-0.540228
N	-1.865359	0.117862	-1.138905
N	2.101197	-1.086535	-0.732250
C	-1.225484	0.317563	3.621685
C	2.479904	3.688774	-0.305285
C	-2.079063	0.554559	2.527093
C	3.131349	2.439113	-0.289950
C	-1.635831	0.281382	1.244788
C	2.399495	1.283224	-0.500898
C	-2.475931	0.426782	0.040120
C	2.985350	-0.072120	-0.507548
C	-3.804959	0.812232	0.073833
C	4.325557	-0.337395	-0.292065
C	-4.542314	0.886343	-1.124162
C	4.786882	-1.669869	-0.315522
C	-3.891359	0.570784	-2.331774
C	3.856627	-2.700391	-0.549149
C	-2.559347	0.196282	-2.287122
C	2.529774	-2.358875	-0.748760
Ru	0.124444	-0.535179	-1.063116
H	1.427363	-0.814798	1.826229
H	0.771369	-0.406134	4.167492
H	-3.083298	0.930366	2.714152
H	-4.302338	1.050848	1.012394
H	-4.397794	0.610065	-3.294146
H	-2.018160	-0.053089	-3.200696
H	-0.645123	2.510726	-0.932895
H	0.528506	4.651419	-0.573701
H	4.205513	2.410318	-0.114000
H	5.042076	0.460568	-0.106387
H	4.142712	-3.750103	-0.578103
H	1.768519	-3.120901	-0.922324
O	-5.811729	1.252293	-1.021174
O	-1.712682	0.588390	4.825133
O	6.082884	-1.850428	-0.109565
O	3.237410	4.755620	-0.095667
C	2.642648	6.057121	-0.101652
H	2.186656	6.273638	-1.080186
H	1.885139	6.144725	0.692814
H	3.459978	6.762786	0.088742
C	6.626120	-3.174441	-0.126276
H	7.699798	-3.062136	0.066069
H	6.170923	-3.793469	0.662460
H	6.472563	-3.646830	-1.109020
C	-0.908120	0.347880	5.983024
H	0.007081	0.959698	5.958580
H	-1.522452	0.638711	6.843528
H	-0.643972	-0.718324	6.060758
C	-6.619349	1.338260	-2.199501
H	-6.211029	2.083607	-2.899708
H	-6.691430	0.358056	-2.696118
H	-7.613237	1.654815	-1.861481
O	-0.344672	-2.270454	-0.776966
O	0.301081	-0.274661	-2.739265
H	-1.529239	-2.550376	-0.548206
C	-2.738386	-3.003247	-0.306561
C	-2.819115	-2.919010	1.121821
N	-2.823886	-2.817702	2.281007
C	-2.743799	-4.380994	-0.930338
H	-3.737658	-4.848171	-0.810879
H	-2.531902	-4.304425	-2.006632
H	-1.997821	-5.039522	-0.461122
H	-3.382700	-2.260725	-0.798255

SCF Done: E(UB3LYP)= -1866.953369
Sum of electronic and zero-point Energies= -1864.415956
Sum of electronic and thermal Energies= -1864.37827
Sum of electronic and thermal Enthalpies= -1864.377326
Sum of electronic and thermal Free Energies= -1864.48744

26

C	0.487921	-0.506940	2.039180
C	0.479167	2.599049	-0.631326
N	-0.322917	-0.195090	1.018532
N	1.106597	1.413652	-0.657264
C	0.117823	-0.347022	3.365365
C	1.140468	3.787868	-0.370559
N	-1.804962	0.247842	-1.116540
N	2.159248	-1.004577	-0.782884
C	-1.160454	0.170274	3.646229
C	2.524881	3.745275	-0.119681
C	-2.006445	0.492563	2.568085
C	3.176286	2.496093	-0.155534
C	-1.565770	0.291099	1.271661
C	2.448283	1.351759	-0.433252
C	-2.393576	0.542911	0.077059

C	3.039480	0.001671	-0.512959
C	-3.684387	1.039861	0.130868
C	4.383527	-0.264625	-0.324927
C	-4.406876	1.242486	-1.060929
C	4.852156	-1.591360	-0.415208
C	-3.780338	0.935425	-2.283441
C	3.925578	-2.614551	-0.691920
C	-2.486040	0.443884	-2.258078
C	2.595305	-2.271453	-0.866156
Ru	0.175458	-0.444611	-1.078297
H	1.470814	-0.905573	1.785687
H	0.820028	-0.627796	4.147881
H	-3.005305	0.870888	2.778255
H	-4.158503	1.276109	1.081852
H	-4.276730	1.067265	-3.242836
H	-1.963952	0.197384	-3.183396
H	-0.592575	2.598265	-0.832357
H	0.575738	4.718005	-0.369584
H	4.248273	2.457090	0.030838
H	5.095663	0.529515	-0.108139
H	4.217403	-3.659896	-0.774253
H	1.836814	-3.027787	-1.072992
O	-5.639607	1.714185	-0.936795
O	-1.645742	0.375292	4.863785
O	6.150763	-1.774102	-0.226495
O	3.278781	4.801730	0.148150
C	2.683991	6.102713	0.190600
H	2.236047	6.359662	-0.781941
H	1.919625	6.157806	0.981460
H	3.499634	6.799633	0.416863
C	6.700347	-3.093075	-0.306107
H	7.773924	-2.984514	-0.110921
H	6.250068	-3.750630	0.453791
H	6.547057	-3.520071	-1.309524
C	-0.848130	0.051846	6.005678
H	0.081209	0.642575	6.015598
H	-1.456273	0.307860	6.881530
H	-0.608273	-1.022844	6.023482
C	-6.432084	1.935926	-2.107038
H	-5.958083	2.680198	-2.765616
H	-6.589251	0.994867	-2.657248
H	-7.395633	2.319352	-1.750718
O	-0.262348	-2.189935	-0.846363
O	0.339167	-0.114512	-2.745011
H	-1.441123	-2.567945	-0.567352
C	-2.505610	-3.247670	-0.275679
C	-2.640713	-2.957367	1.130351
N	-2.704749	-2.692901	2.260980
C	-3.634282	-2.730499	-1.147474
H	-3.955111	-1.722445	-0.857357
H	-3.321307	-2.723223	-2.201772
H	-4.504266	-3.405110	-1.057323
C	-2.028689	-4.659774	-0.574637
H	-2.832243	-5.382549	-0.348239
H	-1.780144	-4.748362	-1.642630
H	-1.145220	-4.926793	0.023058

SCF Done: E(UB3LYP)= -1906.292439
Sum of electronic and zero-point Energies= -1903.683942
Sum of electronic and thermal Energies= -1903.644846
Sum of electronic and thermal Enthalpies= -1903.643902
Sum of electronic and thermal Free Energies= -1903.756463

Tert-butoxy Transition-state Structures

Transition-state energies and structures are given in Liu et al[24].

Cumyloxy Transition-state Structures

1

C	-1.600111	2.472343	0.821993
H	-0.637962	2.257143	1.284548
H	-2.445270	2.449220	1.508800
H	-1.587047	3.339968	0.163149
H	-1.810145	1.474710	-0.010443
C	3.020959	0.214392	0.036901
C	2.217603	0.911255	-0.861475
C	0.849730	0.664740	-0.914855
C	0.257777	-0.277441	-0.070402
C	1.073209	-0.974766	0.823675
C	2.443112	-0.731153	0.878115
H	4.088928	0.406581	0.081147
H	2.657128	1.651340	-1.524304
H	0.219263	1.208986	-1.610397
H	0.644578	-1.717567	1.489896
H	3.058891	-1.281857	1.583554
C	-1.246049	-0.550994	-0.183637
C	-1.887292	-0.923686	1.160113
H	-1.658908	-0.173871	1.924842
H	-2.971968	-0.968964	1.027784
H	-1.547296	-1.897633	1.524896
C	-1.471388	-1.682313	-1.203977
H	-2.541462	-1.885881	-1.308195
H	-1.068063	-1.394259	-2.178406
H	-0.962726	-2.591878	-0.869417
O	-1.922904	0.548712	-0.750772

SCF Done: E(UwB97X-D)= -465.219537806
Sum of electronic and zero-point Energies= -464.86219
Sum of electronic and thermal Energies= -464.850087
Sum of electronic and thermal Enthalpies= -464.849143
Sum of electronic and thermal Free Energies= -464.901306

2

C	-3.452323	1.231511	-0.309994
H	-2.898953	1.459828	-1.228278
H	-3.694656	2.182063	0.176741
H	-4.396727	0.755856	-0.594861
C	-2.618652	0.346412	0.614183
H	-1.768266	0.929367	0.987703
H	-3.217226	0.064596	1.493312
C	-2.071748	-0.926114	-0.046275
H	-1.434099	-0.615642	-0.885318
C	-3.189295	-1.819392	-0.592236
H	-3.747981	-1.321536	-1.390729
H	-2.797385	-2.753978	-1.007706
H	-3.899168	-2.079173	0.203992
C	-1.183444	-1.686954	0.949900
H	-0.579400	-0.967546	1.518380
H	-1.825176	-2.192539	1.690766
C	-0.268019	-2.708217	0.321104
H	-0.722236	-3.350436	-0.438028

H	0.623224	-2.095300	-0.372511
H	0.326552	-3.292056	1.027266
C	-0.087941	3.033458	0.076822
C	0.621719	2.586309	1.185525
C	1.348572	1.397719	1.122581
C	1.373102	0.635724	-0.046072
C	0.647783	1.091756	-1.151013
C	-0.071649	2.278980	-1.094697
H	-0.654225	3.958799	0.124526
H	0.613206	3.161888	2.106732
H	1.899188	1.072947	2.000096
H	0.648866	0.492758	-2.056691
H	-0.625636	2.615891	-1.966330
C	2.211325	-0.639354	-0.197608
C	2.620281	-1.262986	1.143107
H	1.754948	-1.419690	1.794959
H	3.087857	-2.231903	0.947097
H	3.341174	-0.636638	1.677784
C	3.482323	-0.296048	-1.000713
H	4.102436	-1.189916	-1.117215
H	3.214864	0.078769	-1.992333
H	4.055637	0.477113	-0.479271
O	1.552621	-1.585045	-1.008469

SCF Done: E(UwB97X-D)= -661.794907426
Sum of electronic and zero-point Energies= -661.240751
Sum of electronic and thermal Energies= -661.222911
Sum of electronic and thermal Enthalpies= -661.221966
Sum of electronic and thermal Free Energies= -661.286604

3

C	4.097308	0.930829	0.235648
H	3.310922	1.628614	0.540102
H	4.836777	1.500966	-0.335841
H	4.592211	0.552947	1.138937
C	3.525460	-0.207048	-0.608372
H	2.932254	0.218618	-1.426493
H	4.346929	-0.767408	-1.072945
C	2.646918	-1.210864	0.160053
H	3.296871	-1.743279	0.877003
C	2.059767	-2.241080	-0.808132
H	2.847223	-2.669282	-1.437733
H	1.566343	-3.065594	-0.284597
H	1.322002	-1.765732	-1.464996
C	1.572971	-0.522562	0.993136
H	2.006492	0.180488	1.711672
H	1.028630	0.265161	0.171860
C	0.511896	-1.393209	1.629654
H	-0.168963	-0.803005	2.249677
H	-0.094782	-1.917065	0.886193
H	0.985656	-2.147869	2.274071
C	-3.478301	-1.656826	-0.132076
C	-2.490707	-1.586274	-1.112629
C	-1.588648	-0.529347	-1.118857
C	-1.651229	0.475569	-0.149447
C	-2.651589	0.402679	0.819647
C	-3.556953	-0.657029	0.830774
H	-4.180960	-2.484814	-0.120267
H	-2.419925	-2.360358	-1.871580
H	-0.805409	-0.480274	-1.868660
H	-2.728053	1.167568	1.586350
H	-4.322844	-0.700540	1.599933
C	-0.622416	1.609967	-0.204448
C	-0.429174	2.320674	1.141164
H	-0.193091	1.604686	1.935336
H	0.406934	3.019215	1.046138
H	-1.316237	2.887444	1.441427
C	-1.055947	2.633381	-1.271702
H	-0.319143	3.439639	-1.338592
H	-1.139280	2.149103	-2.248353
H	-2.030185	3.057056	-1.007447
O	0.612937	1.127569	-0.675960

SCF Done: E(UwB97X-D)= -661.796078898
Sum of electronic and zero-point Energies= -661.243729
Sum of electronic and thermal Energies= -661.22555
Sum of electronic and thermal Enthalpies= -661.224606
Sum of electronic and thermal Free Energies= -661.290953

4

C	1.944276	-2.052291	1.750627
H	3.029059	-1.978285	1.877160
H	1.621257	-2.979422	2.235150
H	1.485131	-1.208800	2.275791
C	1.535678	-2.049782	0.277352
H	2.086372	-2.836669	-0.262848
H	0.474491	-2.311394	0.196235
C	1.755355	-0.733738	-0.463238
H	1.156737	0.112179	0.237661
C	1.107896	-0.745530	-1.836336
H	0.056278	-1.041237	-1.774134
H	1.157977	0.226695	-2.334006
H	1.626633	-1.471300	-2.479746
C	3.193004	-0.226804	-0.433929
H	3.550063	-0.235859	0.601278
H	3.818022	-0.948827	-0.983947
C	3.395161	1.176390	-1.003472
H	4.437045	1.491554	-0.887760
H	3.151626	1.229805	-2.069473
H	2.762214	1.891654	-0.469164
C	-3.276010	-1.555963	-0.609567
C	-2.495600	-1.696501	0.536301
C	-1.611430	-0.690277	0.906236
C	-1.485512	0.474380	0.143211
C	-2.279095	0.609313	-0.995996
C	-3.166030	-0.398523	-1.371542
H	-3.963912	-2.342920	-0.904258
H	-2.572122	-2.595692	1.141205
H	-0.987739	-0.808301	1.787098
H	-2.205316	1.498582	-1.613511
H	-3.768362	-0.276370	-2.267243
C	-0.489885	1.546854	0.598767
C	-1.087622	2.306328	1.800962
H	-1.310878	1.612848	2.615923
H	-0.375637	3.055446	2.160623
H	-2.014354	2.806860	1.502316
C	-0.128450	2.549112	-0.503876
H	0.646401	3.219658	-0.121809
H	0.263621	2.039453	-1.389027
H	-0.986109	3.158988	-0.806024
O	0.673886	0.951693	1.119939

SCF Done: E(UwB97X-D)= -661.799855377
Sum of electronic and zero-point Energies= -661.248262
Sum of electronic and thermal Energies= -661.229997
Sum of electronic and thermal Enthalpies= -661.229053
Sum of electronic and thermal Free Energies= -661.29473

5

C	3.058192	-1.873898	-0.135329
C	2.268674	-1.503075	-1.222590
C	1.542678	-0.320143	-1.184834
C	1.590716	0.522117	-0.069017
C	2.384714	0.141685	1.012484
C	3.111462	-1.048922	0.981407
H	3.622997	-2.801096	-0.159116
H	2.212838	-2.142609	-2.098882
H	0.910003	-0.042676	-2.022820
H	2.445313	0.769454	1.895847
H	3.719675	-1.328206	1.837020
C	0.775870	1.820185	-0.102049
C	1.391343	2.780947	-1.137338
H	1.399230	2.324588	-2.130519
H	0.806368	3.704460	-1.181229
H	2.421611	3.020898	-0.856023
C	0.698479	2.531109	1.254331
H	0.020753	3.383922	1.159922
H	0.307250	1.867714	2.032332
H	1.676824	2.901922	1.577082
O	-0.521781	1.568960	-0.596848
C	-4.419252	0.664931	0.010083
H	-4.938058	0.202368	0.858579
H	-5.178071	0.979655	-0.713494
H	-3.919433	1.569657	0.370759
C	-3.430874	-0.307747	-0.631666
H	-3.987259	-1.112892	-1.128506
H	-2.863912	0.211295	-1.415097
C	-2.432172	-0.951323	0.345062
H	-3.014483	-1.513142	1.098456
C	-1.634883	0.084294	1.107425
H	-2.228140	0.791282	1.691460
H	-0.799176	-0.308257	1.690031
H	-1.081677	0.832175	0.225983
C	-1.535606	-1.955296	-0.395126
H	-2.186395	-2.657622	-0.932319
H	-0.963060	-1.413500	-1.157755
C	-0.575599	-2.741499	0.495785
H	-0.058627	-3.513677	-0.082714
H	0.198977	-2.100896	0.929215
H	-1.111746	-3.236678	1.314811

SCF Done: E(UwB97X-D)= -661.794095408
Sum of electronic and zero-point Energies= -661.240004
Sum of electronic and thermal Energies= -661.221964
Sum of electronic and thermal Enthalpies= -661.22102
Sum of electronic and thermal Free Energies= -661.286916

6

C	1.763634	-1.691520	0.214591
C	1.414288	-0.404107	0.934527
C	2.609961	0.396566	1.412838
C	3.607023	0.632859	0.272549
C	3.998893	-0.683268	-0.407702
C	2.766406	-1.438812	-0.916472
H	2.281254	1.350579	1.840635
H	0.894026	0.315698	0.052519
H	0.620741	-0.519572	1.679292
H	2.202867	-2.389582	0.945824
H	0.852818	-2.165584	-0.166594
H	3.138993	1.296826	-0.465321
H	4.497726	1.146119	0.652503
H	4.688506	-0.486529	-1.236660
H	4.540327	-1.315918	0.310868
H	2.273432	-0.843080	-1.695683
H	3.063553	-2.388839	-1.375100
H	3.103363	-0.162304	2.224531
C	-3.429769	-1.939470	0.263929
C	-3.590928	-0.802050	1.047468
C	-2.765726	0.304655	0.857994
C	-1.765977	0.291368	-0.115464
C	-1.617106	-0.854914	-0.901345
C	-2.438414	-1.960869	-0.714384
H	-4.070892	-2.803132	0.413880
H	-4.359999	-0.773061	1.814157
H	-2.908330	1.180290	1.483909
H	-0.836202	-0.870647	-1.655165
H	-2.303133	-2.843188	-1.333769
C	-0.851283	1.493087	-0.377557
C	-0.656146	2.382833	0.857548
H	-0.324485	1.792341	1.718120
H	0.113077	3.126108	0.629643
H	-1.571873	2.913178	1.137292
C	-1.436205	2.327214	-1.533586
H	-0.784727	3.180069	-1.747434
H	-1.523769	1.713693	-2.434230
H	-2.431067	2.694221	-1.261746
O	0.398985	1.066359	-0.862635

SCF Done: E(UwB97X-D)= -660.592580535
Sum of electronic and zero-point Energies= -660.062124
Sum of electronic and thermal Energies= -660.046245
Sum of electronic and thermal Enthalpies= -660.045301
Sum of electronic and thermal Free Energies= -660.106916

7

C	1.493215	-1.240656	0.167755
C	1.491872	-0.093463	1.158114
C	2.938927	0.364305	1.420810
C	3.644096	0.734956	0.112959
C	3.615979	-0.427323	-0.884164
C	2.174016	-0.897468	-1.142130
H	2.934779	1.217181	2.109340
H	0.922707	0.749205	0.748077
H	1.011088	-0.382456	2.099043
H	1.867600	-2.174446	0.605504
H	0.318200	-1.575420	-0.169977
H	3.139505	1.603960	-0.332230
H	4.678940	1.036180	0.313603
H	4.085689	-0.133636	-1.830168
H	4.203840	-1.264617	-0.483075
H	1.616164	-0.086806	-1.629023
H	2.160674	-1.756331	-1.820997
H	3.493560	-0.444389	1.916884
C	-1.262597	2.991042	-0.314994
C	-0.935509	2.138845	-1.368226
C	-1.134317	0.769167	-1.244519
C	-1.656566	0.221335	-0.069045
C	-1.995617	1.084109	0.972753
C	-1.798075	2.458738	0.852487
H	-1.102497	4.061365	-0.405803
H	-0.519693	2.542956	-2.287039
H	-0.858751	0.098304	-2.052201
H	-2.402013	0.690878	1.899276

H	-2.058485	3.112685	1.679909
C	-1.819691	-1.300037	0.018369
C	-3.096323	-1.715181	-0.738072
H	-3.039744	-1.394292	-1.781659
H	-3.211376	-2.803000	-0.708989
H	-3.972122	-1.248975	-0.275222
C	-1.882323	-1.822373	1.459024
H	-1.880416	-2.915394	1.429768
H	-1.011818	-1.491368	2.034508
H	-2.786908	-1.495085	1.981769
O	-0.781431	-1.942809	-0.681002

SCF Done: E(UwB97X-D)= -660.592759858
Sum of electronic and zero-point Energies= -660.060724
Sum of electronic and thermal Energies= -660.044839
Sum of electronic and thermal Enthalpies= -660.043895
Sum of electronic and thermal Free Energies= -660.104859

8

C	0.002661	-2.868673	0.738599
H	0.814769	-3.465362	0.314992
H	-0.741574	-2.704927	-0.047183
H	-0.458056	-3.389526	1.577444
C	0.514787	-1.536069	1.198028
O	0.314109	-1.029255	2.273753
O	1.251090	-0.947272	0.221469
C	1.745023	0.339458	0.458676
H	1.908525	0.521472	1.523903
H	0.866526	1.171863	0.120198
C	2.909436	0.634292	-0.449774
H	3.159184	1.696180	-0.338813
H	2.591989	0.488849	-1.489434
C	4.138931	-0.232034	-0.149789
H	3.862269	-1.288104	-0.247164
H	4.441263	-0.081368	0.894619
C	5.309383	0.086406	-1.077688
H	5.617511	1.133460	-0.979013
H	6.176655	-0.541627	-0.850381
H	5.036855	-0.083156	-2.125488
C	-2.942133	-1.831304	-1.313256
C	-3.318309	-1.352030	-0.061973
C	-2.741363	-0.190966	0.448012
C	-1.782652	0.512305	-0.284379
C	-1.397341	0.010452	-1.530123
C	-1.971406	-1.147901	-2.043039
H	-3.395579	-2.733590	-1.713360
H	-4.063958	-1.882331	0.523413
H	-3.047649	0.162885	1.427163
H	-0.635873	0.542627	-2.090732
H	-1.660351	-1.517878	-3.015973
C	-1.195684	1.845908	0.196036
C	-1.155493	1.980183	1.723285
H	-0.644045	1.127160	2.178997
H	-0.612159	2.896003	1.973662
H	-2.159013	2.054247	2.154253
C	-2.036902	2.991160	-0.405908
H	-1.632990	3.957261	-0.088584
H	-2.020464	2.939634	-1.497923
H	-3.073926	2.905514	-0.066140
O	0.084362	2.056977	-0.347559

SCF Done: E(UwB97X-D)= -811.051074949
Sum of electronic and zero-point Energies= -810.463796
Sum of electronic and thermal Energies= -810.443858
Sum of electronic and thermal Enthalpies= -810.442913
Sum of electronic and thermal Free Energies= -810.513806

9

C	-1.998372	2.076707	1.452000
H	-2.899328	2.629945	1.188864
H	-1.688358	2.323915	2.471613
H	-2.196492	1.001631	1.409908
C	-0.901274	2.415599	0.482564
O	-0.988485	3.161513	-0.462272
O	0.234425	1.761426	0.803175
C	1.330218	1.931096	-0.094670
H	1.763385	2.930944	0.050429
H	0.973154	1.878070	-1.127628
C	2.341635	0.859816	0.201499
H	1.793082	-0.252587	-0.085060
H	2.559132	0.770554	1.270971
C	3.580455	0.868690	-0.667790
H	4.087017	1.839927	-0.558509
H	3.280604	0.794190	-1.720768
C	4.545372	-0.263989	-0.319496
H	4.044419	-1.230995	-0.420199
H	5.418499	-0.253498	-0.978739
H	4.900701	-0.169926	0.712973
C	-3.434165	-0.224795	-0.996284
C	-2.260995	0.127192	-1.655714
C	-1.042418	-0.417154	-1.257265
C	-0.969406	-1.298594	-0.180604
C	-2.155112	-1.649216	0.473509
C	-3.377724	-1.123376	0.066642
H	-4.385257	0.196986	-1.306995
H	-2.289161	0.833026	-2.480062
H	-0.128790	-0.161613	-1.782461
H	-2.131125	-2.344667	1.308843
H	-4.287216	-1.411115	0.586450
C	0.376738	-1.886087	0.256282
C	0.404104	-3.397060	-0.044889
H	0.284856	-3.566489	-1.118398
H	1.358701	-3.822290	0.278438
H	-0.410610	-3.905283	0.480267
C	0.624543	-1.637466	1.752136
H	1.634312	-1.971144	2.011614
H	0.528009	-0.571126	1.977521
H	-0.091199	-2.185077	2.372561
O	1.441570	-1.378131	-0.509547

SCF Done: E(UwB97X-D)= -811.051845769
Sum of electronic and zero-point Energies= -810.46273
Sum of electronic and thermal Energies= -810.442874
Sum of electronic and thermal Enthalpies= -810.44193
Sum of electronic and thermal Free Energies= -810.512076

10

C	-2.377388	0.942275	-2.297985
H	-3.372235	1.366784	-2.453705
H	-1.953567	0.604763	-3.244071
H	-1.739603	1.713768	-1.856965
C	-2.431928	-0.207519	-1.331598
O	-1.891407	-1.278914	-1.491202
O	-3.163314	0.116600	-0.252021
C	-3.262281	-0.835140	0.812437
H	-2.947025	-1.816953	0.453590
H	-4.323821	-0.874682	1.070611

C	-2.456129	-0.376266	2.021345
H	-2.760455	-1.006424	2.871933
H	-2.750458	0.649637	2.269243
C	-0.943796	-0.458089	1.896477
H	-0.465732	-0.025929	2.781672
H	-0.636559	0.385018	1.005870
C	-0.350518	-1.794420	1.509831
H	-0.651274	-2.088897	0.500628
H	0.741658	-1.764386	1.539592
H	-0.691299	-2.569823	2.211747
C	3.317261	-1.930233	-0.735722
C	2.109947	-1.669299	-1.379957
C	1.379165	-0.531404	-1.062479
C	1.836149	0.366532	-0.093759
C	3.048983	0.100253	0.542659
C	3.784301	-1.040932	0.225698
H	3.887194	-2.822302	-0.978723
H	1.725502	-2.360784	-2.123945
H	0.418747	-0.362161	-1.536884
H	3.431282	0.776816	1.300692
H	4.723112	-1.233618	0.737303
C	0.992548	1.605763	0.218788
C	1.181409	2.640256	-0.908334
H	0.898416	2.206114	-1.871389
H	0.561104	3.521854	-0.718056
H	2.231363	2.945209	-0.960554
C	1.332195	2.250520	1.568125
H	0.598716	3.035422	1.772052
H	1.289407	1.516151	2.378924
H	2.328892	2.703120	1.568972
O	-0.383139	1.303254	0.164261

SCF Done: E(UwB97X-D)= -811.050304466
Sum of electronic and zero-point Energies= -810.462498
Sum of electronic and thermal Energies= -810.443061
Sum of electronic and thermal Enthalpies= -810.442117
Sum of electronic and thermal Free Energies= -810.511267

11

C	2.668607	-1.859477	-1.573964
H	3.398871	-1.701242	-2.370424
H	1.697133	-1.482290	-1.909374
H	2.579564	-2.920493	-1.338255
C	3.041691	-1.096367	-0.333717
O	2.890894	-1.486550	0.801605
O	3.560506	0.104226	-0.649577
C	3.826677	1.003799	0.435512
H	4.527916	1.731198	0.018379
H	4.310835	0.457328	1.248839
C	2.544746	1.668862	0.916168
H	2.790876	2.345812	1.742960
H	1.904513	0.885741	1.329765
C	1.796190	2.417254	-0.199048
H	2.078692	2.001538	-1.172935
H	2.094584	3.475616	-0.217615
C	0.296495	2.314227	-0.057064
H	-0.099554	2.516075	0.941301
H	-0.289276	2.807355	-0.835658
H	0.083000	1.071451	-0.262258
C	-4.863380	0.576391	-0.432505
C	-3.850656	0.798860	-1.360266
C	-2.554730	0.362345	-1.101711
C	-2.244750	-0.298229	0.088615
C	-3.271109	-0.524003	1.009598
C	-4.568258	-0.090389	0.753078
H	-5.875037	0.917583	-0.631571
H	-4.068831	1.313998	-2.291635
H	-1.764167	0.530796	-1.825247
H	-3.065214	-1.044350	1.940383
H	-5.350230	-0.273077	1.484693
C	-0.816873	-0.796239	0.334130
C	-0.709245	-2.276682	-0.080986
H	-0.945283	-2.389188	-1.143022
H	0.306167	-2.637173	0.109319
H	-1.417537	-2.876419	0.499233
C	-0.376274	-0.646662	1.796059
H	-0.966859	-1.277543	2.466953
H	0.670934	-0.950863	1.877477
H	-0.478960	0.391195	2.129943
O	0.093985	-0.144571	-0.521359

SCF Done: E(UwB97X-D)= -811.044722064
Sum of electronic and zero-point Energies= -810.456639
Sum of electronic and thermal Energies= -810.437385
Sum of electronic and thermal Enthalpies= -810.436441
Sum of electronic and thermal Free Energies= -810.505753

12

C	-4.117672	-0.735754	-0.180399
H	-3.318518	-1.070166	-0.848127
H	-5.086064	-0.939102	-0.650164
H	-4.056836	-1.314800	0.745892
C	-3.992832	0.750790	0.118199
H	-4.735495	1.059687	0.859432
H	-4.158745	1.343404	-0.793442
O	-2.735348	1.100557	0.679531
C	-1.710164	1.287912	-0.219977
H	-2.063296	1.747957	-1.158621
H	-1.287926	0.202796	-0.618791
C	-0.547580	2.028377	0.404919
H	-0.033984	1.373701	1.119804
H	-0.948199	2.874235	0.979684
C	0.442418	2.525563	-0.647856
H	-0.049060	3.280076	-1.276691
H	0.714431	1.693507	-1.306421
C	1.706588	3.109655	-0.024127
H	2.225245	2.351727	0.572045
H	2.401191	3.462121	-0.793523
H	1.469777	3.956782	0.630638
C	3.845087	0.018572	0.179211
C	3.202481	-0.106400	-1.051221
C	1.917048	-0.629202	-1.116625
C	1.244987	-1.041193	0.038545
C	1.895088	-0.904226	1.265349
C	3.184748	-0.377822	1.336315
H	4.849307	0.428325	0.234077
H	3.703959	0.208515	-1.961954
H	1.406872	-0.711934	-2.071845
H	1.401497	-1.205819	2.183663
H	3.670828	-0.278437	2.302723
C	-0.146498	-1.670734	-0.112870
C	-0.925934	-1.755046	1.205085
H	-1.087714	-0.766587	1.644932
H	-1.904109	-2.197959	1.003616
H	-0.414422	-2.387966	1.936900
C	0.025000	-3.095581	-0.683580

H	-0.955306	-3.563818	-0.813842
H	0.531355	-3.061903	-1.651936
H	0.625835	-3.700773	0.003137
O	-0.894305	-1.002187	-1.096657

SCF Done: E(UwB97X-D)= -737.008664863
Sum of electronic and zero-point Energies= -736.426702
Sum of electronic and thermal Energies= -736.407852
Sum of electronic and thermal Enthalpies= -736.406908
Sum of electronic and thermal Free Energies= -736.474316

13

C	-0.327790	2.633973	0.755992
H	-1.143611	2.248083	0.149024
H	-0.582395	3.014934	1.740348
C	0.937621	2.626633	0.313032
H	1.729427	2.994249	0.964499
C	1.344684	2.098782	-0.993300
H	0.537525	2.042579	-1.726139
H	2.249211	2.545690	-1.412649
H	1.684522	0.907084	-0.893326
C	-3.014541	-0.209453	-0.173094
C	-2.223080	-0.231144	-1.319485
C	-0.861610	-0.498043	-1.223696
C	-0.263165	-0.741124	0.014685
C	-1.066524	-0.729834	1.155390
C	-2.430963	-0.464910	1.063612
H	-4.077423	0.002082	-0.244218
H	-2.667542	-0.038165	-2.291890
H	-0.237079	-0.501423	-2.111504
H	-0.631227	-0.913071	2.132623
H	-3.037105	-0.451906	1.965015
C	1.242495	-1.030198	0.070156
C	1.469877	-2.530281	-0.213308
H	1.064472	-2.795531	-1.193255
H	2.540239	-2.756999	-0.197479
H	0.964064	-3.129429	0.550765
C	1.880929	-0.654403	1.414777
H	1.539898	-1.300676	2.229919
H	2.965063	-0.764652	1.323454
H	1.653264	0.382538	1.678596
O	1.915137	-0.388172	-0.981543

SCF Done: E(UwB97X-D)= -542.61567838
Sum of electronic and zero-point Energies= -542.202826
Sum of electronic and thermal Energies= -542.189316
Sum of electronic and thermal Enthalpies= -542.188372
Sum of electronic and thermal Free Energies= -542.242923

14

C	-2.502516	-1.881755	-0.180921
C	-2.363013	-1.214225	1.031038
C	-1.590402	-0.057253	1.112243
C	-0.942501	0.447409	-0.014712
C	-1.101379	-0.222896	-1.230967
C	-1.870957	-1.377199	-1.316226
H	-3.099705	-2.786781	-0.242313
H	-2.850714	-1.597375	1.922933
H	-1.481374	0.435676	2.072819
H	-0.587526	0.160351	-2.107117
H	-1.975250	-1.887214	-2.269864
C	-0.054398	1.697490	0.021804
C	0.462207	2.038027	1.425564
H	0.976910	1.180097	1.869194
H	1.171773	2.865595	1.339203
H	-0.343520	2.347374	2.099306
C	-0.845006	2.894221	-0.546969
H	-1.727337	3.079902	0.073965
H	-0.215913	3.789406	-0.554075
H	-1.173214	2.683397	-1.568233
O	1.024372	1.551659	-0.864897
C	2.047445	-1.491452	1.974560
H	1.503566	-2.096638	2.693415
H	2.929441	-0.968165	2.337833
C	1.653878	-1.397613	0.699326
H	0.761449	-1.932686	0.375269
C	2.335078	-0.583478	-0.324523
H	1.691246	0.453626	-0.490246
H	3.300824	-0.196978	0.018703
C	2.390641	-1.176419	-1.720902
H	1.394579	-1.500033	-2.040115
H	2.760715	-0.442847	-2.442597
H	3.054615	-2.049138	-1.744793

SCF Done: E(UwB97X-D)= -581.932475628
Sum of electronic and zero-point Energies= -581.481112
Sum of electronic and thermal Energies= -581.466031
Sum of electronic and thermal Enthalpies= -581.465086
Sum of electronic and thermal Free Energies= -581.523664

15

C	-1.789696	-1.618468	1.905764
H	-2.689544	-1.170677	2.318688
H	-1.212314	-2.252936	2.571336
C	-1.403242	-1.418335	0.642253
H	-0.490697	-1.900123	0.292350
C	-2.098013	-0.575137	-0.364404
H	-1.392815	0.401872	-0.540934
C	-2.119487	-1.202935	-1.752464
H	-2.811096	-2.055059	-1.775752
H	-2.446045	-0.475118	-2.501639
H	-1.124884	-1.563954	-2.033216
C	-3.427266	0.027114	0.055992
H	-3.802374	0.694918	-0.724905
H	-4.174653	-0.759060	0.223687
H	-3.330618	0.610463	0.976933
C	2.828503	-1.843442	-0.168350
C	2.197427	-1.346540	-1.307147
C	1.405704	-0.206961	-1.224672
C	1.224801	0.455643	-0.007377
C	1.871337	-0.041554	1.123710
C	2.665806	-1.183651	1.045000
H	3.442707	-2.737137	-0.227784
H	2.319033	-1.851227	-2.261564
H	0.891519	0.169762	-2.103366
H	1.744946	0.445975	2.085001
H	3.152341	-1.561516	1.939767
C	0.314699	1.689604	0.028277
C	1.100319	2.912252	-0.491128
H	1.462159	2.728555	-1.506244
H	0.456185	3.796684	-0.497814
H	1.960455	3.098931	0.159841
C	-0.250815	1.988619	1.423014
H	-0.981404	2.797262	1.331340
H	-0.751552	1.107121	1.835801
H	0.526049	2.307492	2.125551
O	-0.733484	1.543814	-0.892236

SCF Done: E(UwB97X-D)= -621.249622261
Sum of electronic and zero-point Energies= -620.759865
Sum of electronic and thermal Energies= -620.743424
Sum of electronic and thermal Enthalpies= -620.74248
Sum of electronic and thermal Free Energies= -620.803993

16

C	3.425443	0.292797	0.114457
C	3.263038	-0.680362	-0.869047
C	2.234899	-1.608858	-0.766737
C	1.354667	-1.587169	0.323946
C	1.531213	-0.601360	1.305212
C	2.554507	0.329879	1.201634
H	4.224998	1.022995	0.031954
H	3.939163	-0.714202	-1.718389
H	2.104228	-2.362255	-1.539463
H	0.844135	-0.558649	2.146103
H	2.667252	1.094144	1.964237
C	0.229035	-2.532794	0.401286
H	-0.757498	-2.040901	-0.187612
H	0.365263	-3.459242	-0.161724
H	-0.142382	-2.727455	1.409392
C	0.524176	2.782109	-0.317198
C	0.485798	1.802268	-1.305782
C	-0.425903	0.757811	-1.219577
C	-1.311273	0.666364	-0.143455
C	-1.268331	1.654966	0.840445
C	-0.357427	2.705665	0.755097
H	1.240677	3.595977	-0.380110
H	1.180135	1.842149	-2.139821
H	-0.442733	-0.020285	-1.975321
H	-1.945039	1.613473	1.688811
H	-0.337330	3.463703	1.533253
C	-2.315762	-0.491384	-0.099953
C	-3.570949	-0.093201	-0.904681
H	-4.300704	-0.908533	-0.892911
H	-4.021644	0.801886	-0.464022
H	-3.298277	0.125859	-1.940326
C	-2.722337	-0.878533	1.329249
H	-3.307219	-1.801550	1.286984
H	-1.840663	-1.051643	1.955076
H	-3.333425	-0.107320	1.808197
O	-1.827962	-1.614666	-0.786711

SCF Done: E(UwB97X-D)= -696.264365591
Sum of electronic and zero-point Energies= -695.764267
Sum of electronic and thermal Energies= -695.748512
Sum of electronic and thermal Enthalpies= -695.747568
Sum of electronic and thermal Free Energies= -695.808083

17

C	-3.573872	-0.187333	-0.999609
C	-2.835808	-1.033076	-0.181122
C	-1.817213	-0.535450	0.645086
C	-1.559218	0.841594	0.622038
C	-2.295288	1.688323	-0.197776
C	-3.304650	1.179835	-1.011109
H	-4.359983	-0.594291	-1.628872
H	-3.044639	-2.100242	-0.179757
H	-0.757199	1.255631	1.225061
H	-2.067595	2.750059	-0.208403
H	-3.877193	1.843652	-1.652205
C	-1.013123	-1.475060	1.466694
H	0.025424	-1.750988	0.850242
H	-1.479105	-2.464941	1.514403
C	-0.527481	-1.013906	2.827481
H	0.099661	-1.783888	3.285546
H	0.065127	-0.097804	2.758347
H	-1.377853	-0.818996	3.492342
C	1.757540	2.832587	0.422695
C	2.135744	1.815269	1.297170
C	2.049854	0.485703	0.899190
C	1.580262	0.144617	-0.371986
C	1.218175	1.170625	-1.244253
C	1.304415	2.504205	-0.850529
H	1.819647	3.872029	0.731423
H	2.496868	2.058426	2.292680
H	2.325285	-0.311925	1.582013
H	0.839742	0.938843	-2.234488
H	1.005797	3.287470	-1.541523
C	1.500103	-1.338005	-0.753867
C	2.905264	-1.819786	-1.174319
H	3.616710	-1.676147	-0.356717
H	2.874103	-2.881782	-1.435772
H	3.246542	-1.245395	-2.041615
C	0.501002	-1.620877	-1.883833
H	0.408923	-2.704719	-1.997329
H	-0.485751	-1.208219	-1.654475
H	0.835450	-1.205237	-2.839908
O	1.204474	-2.124641	0.370912

SCF Done: E(UwB97X-D)= -735.579693087
Sum of electronic and zero-point Energies= -735.042481
Sum of electronic and thermal Energies= -735.025329
Sum of electronic and thermal Enthalpies= -735.024385
Sum of electronic and thermal Free Energies= -735.087986

18

C	-1.600553	2.358302	-0.050709
C	-1.185490	1.192834	0.579995
C	-1.856452	-0.022775	0.376796
C	-2.965536	-0.017409	-0.480983
C	-3.387622	1.150985	-1.107222
C	-2.705185	2.345186	-0.897897
H	-1.047262	3.277765	0.115952
H	-0.305733	1.230807	1.213428
H	-3.516017	-0.933989	-0.663311
H	-4.253689	1.124958	-1.762273
H	-3.029988	3.256334	-1.391616
C	-1.364229	-1.285653	1.022680
H	-0.321080	-1.594438	0.459547
C	-0.945838	-1.145778	2.481304
H	-0.478260	-2.072542	2.827793
H	-0.231072	-0.333901	2.634378
H	-1.825078	-0.947763	3.107948
C	-2.202944	-2.532372	0.784705
H	-2.322644	-2.743619	-0.281808
H	-1.712321	-3.398388	1.237509
H	-3.199303	-2.430892	1.234604
C	2.556873	2.314927	1.001457
C	2.554450	1.097932	1.680609
C	2.174282	-0.067157	1.023419
C	1.784762	-0.040089	-0.318246
C	1.807554	1.179783	-0.993827
C	2.188296	2.349072	-0.339425
H	2.847124	3.227697	1.513456

H	2.845151	1.057138	2.726698
H	2.146696	-1.014129	1.552998
H	1.501891	1.235015	-2.033619
H	2.186562	3.291266	-0.880201
C	1.352617	-1.349918	-0.986875
C	2.610967	-2.112124	-1.454681
H	3.268468	-2.315766	-0.605265
H	2.323733	-3.060859	-1.917919
H	3.157628	-1.506294	-2.184539
C	0.402941	-1.139900	-2.174366
H	0.041747	-2.118936	-2.502127
H	-0.457236	-0.527019	-1.888765
H	0.903175	-0.660311	-3.021889
O	0.770519	-2.212151	-0.046422

SCF Done: E(UwB97X-D)= -774.894517913
Sum of electronic and zero-point Energies= -774.31934
Sum of electronic and thermal Energies= -774.300771
Sum of electronic and thermal Enthalpies= -774.299827
Sum of electronic and thermal Free Energies= -774.366378

19

C	-1.605913	-2.530620	1.784481
H	-2.537257	-2.724273	2.309502
H	-0.259324	-0.795119	-0.449291
H	-0.695494	-2.542022	2.378596
C	-1.579307	-2.303358	0.460967
C	-0.310860	-2.015645	-0.230608
H	0.593202	-2.225102	0.344486
H	-0.240907	-2.406286	-1.250086
C	-2.839285	-2.281462	-0.374398
H	-2.758129	-3.050155	-1.155250
H	-3.697521	-2.553775	0.251669
C	-3.098634	-0.920513	-1.041338
H	-2.254187	-0.664272	-1.693062
H	-3.977280	-1.009303	-1.692979
C	-3.311688	0.211133	-0.037513
H	-4.242369	0.036122	0.522052
H	-2.499921	0.192344	0.699209
C	-3.346348	1.589820	-0.693314
H	-2.400502	1.737188	-1.228412
H	-4.146087	1.622196	-1.445852
C	-3.545252	2.719463	0.315189
H	-3.559922	3.698417	-0.175707
H	-4.488856	2.603682	0.861345
H	-2.735693	2.729594	1.055417
C	4.760058	-0.608357	-0.354298
C	3.791946	-0.770162	-1.340714
C	2.517918	-0.238450	-1.166512
C	2.185063	0.457932	-0.003060
C	3.166902	0.622523	0.977157
C	4.442779	0.093678	0.804688
H	5.754454	-1.024092	-0.487574
H	4.028162	-1.312613	-2.251876
H	1.761146	-0.360525	-1.934083
H	2.944212	1.169500	1.888668
H	5.190243	0.230134	1.581056
C	0.781368	1.057636	0.147493
C	0.817314	2.539839	-0.280797
H	1.153875	2.623561	-1.317406
H	-0.181605	2.978378	-0.191509
H	1.511514	3.093051	0.359868
C	0.240507	0.943215	1.579258
H	-0.776951	1.343359	1.606409
H	0.207931	-0.102011	1.901367
H	0.845336	1.506442	2.295834
O	-0.117185	0.475692	-0.757808

SCF Done: E(UwB97X-D)= -739.190212335
Sum of electronic and zero-point Energies= -738.583417
Sum of electronic and thermal Energies= -738.563367
Sum of electronic and thermal Enthalpies= -738.562423
Sum of electronic and thermal Free Energies= -738.63362

20

C	-0.309375	-2.394737	-1.009216
H	-0.559092	-2.437929	-2.071292
H	0.082183	-3.331056	-0.611770
H	0.744507	-1.653679	-1.036607
C	-1.334199	-1.765639	-0.121417
O	-1.370677	-2.034592	1.066555
C	-2.298502	-0.785837	-0.757928
H	-1.696316	0.045349	-1.149838
H	-2.750208	-1.265885	-1.636604
C	-3.363304	-0.277693	0.203100
H	-2.898447	0.186986	1.075397
H	-3.997565	0.465571	-0.289030
H	-3.996616	-1.095981	0.558052
C	-1.051549	2.809412	0.002532
C	-0.810571	2.129237	1.190521
C	0.150430	1.120378	1.243192
C	0.885138	0.778935	0.108472
C	0.631660	1.466881	-1.083453
C	-0.323797	2.474467	-1.138361
H	-1.802825	3.592469	-0.037186
H	-1.378114	2.374570	2.083507
H	0.305915	0.589772	2.176324
H	1.179922	1.187033	-1.978147
H	-0.505947	2.995800	-2.073814
C	1.958224	-0.314294	0.103212
C	1.948492	-1.209350	1.347011
H	0.968358	-1.669523	1.504861
H	2.687754	-2.002900	1.206228
H	2.218226	-0.647653	2.247117
C	3.348998	0.337978	-0.045104
H	4.122144	-0.434897	-0.079600
H	3.402840	0.933848	-0.959768
H	3.533600	0.994010	0.811101
O	1.839404	-1.095951	-1.065842

SCF Done: E(UwB97X-D)= -657.184238936
Sum of electronic and zero-point Energies= -656.701866
Sum of electronic and thermal Energies= -656.685865
Sum of electronic and thermal Enthalpies= -656.684921
Sum of electronic and thermal Free Energies= -656.74567

21

C	-0.399761	-2.544446	-0.508834
H	0.144926	-3.061603	0.281736
H	0.299144	-1.957274	-1.113762
H	-0.876587	-3.278636	-1.169549
C	-1.450889	-1.645803	0.096249
O	-1.712928	-1.664099	1.285148
C	-2.170689	-0.714348	-0.839392
H	-1.460669	0.325128	-0.911898
H	-2.129646	-1.043609	-1.882633
C	-3.527248	-0.228283	-0.390909

H	-3.867136	0.598268	-1.020437
H	-4.265745	-1.036704	-0.455982
H	-3.490890	0.105090	0.648547
C	3.129675	-1.196029	-0.051608
C	2.723792	-0.508491	-1.194630
C	1.680914	0.406718	-1.122532
C	1.030077	0.663093	0.089690
C	1.442702	-0.031178	1.226030
C	2.483832	-0.956317	1.155253
H	3.940720	-1.916219	-0.105223
H	3.217253	-0.691477	-2.144971
H	1.344601	0.920632	-2.018243
H	0.943853	0.126884	2.176066
H	2.783474	-1.493570	2.050285
C	-0.108172	1.688982	0.101933
C	0.471809	3.099706	-0.137501
H	-0.336248	3.836636	-0.157045
H	1.165453	3.347809	0.671809
H	1.012162	3.142256	-1.086495
C	-0.928557	1.694782	1.396360
H	-0.332032	2.037354	2.248108
H	-1.769302	2.382558	1.268666
H	-1.323269	0.701197	1.627841
O	-0.945192	1.487218	-1.013583

SCF Done: E(UwB97X-D)= -657.187894863
Sum of electronic and zero-point Energies= -656.705344
Sum of electronic and thermal Energies= -656.689196
Sum of electronic and thermal Enthalpies= -656.688252
Sum of electronic and thermal Free Energies= -656.748844

22

C	1.611607	2.583218	-0.656885
H	1.407400	2.964159	-1.659897
H	2.181841	1.462811	-0.931260
H	2.384600	3.134174	-0.121818
C	0.417037	2.261338	0.176398
O	0.487558	2.272435	1.392638
C	-0.853578	1.895246	-0.561487
H	-1.233658	2.804391	-1.051739
H	-0.580843	1.209663	-1.374982
C	-1.910743	1.267459	0.337227
H	-1.447928	0.444973	0.892980
H	-2.236346	1.998486	1.086564
C	-3.111326	0.738992	-0.443381
H	-2.758792	0.037061	-1.212181
H	-3.606942	1.561883	-0.979011
C	-4.126119	0.027203	0.450478
H	-3.610992	-0.770013	1.002840
H	-4.501946	0.730015	1.205777
C	-5.296779	-0.564177	-0.331870
H	-4.945094	-1.299219	-1.065707
H	-6.009973	-1.066306	0.330130
H	-5.839181	0.215548	-0.879152
C	-1.126236	-2.316392	0.127944
C	-0.403460	-2.087853	1.294410
C	0.837186	-1.455503	1.240855
C	1.376738	-1.045930	0.020524
C	0.638263	-1.273747	-1.144303
C	-0.601454	-1.901576	-1.093791
H	-2.094242	-2.807189	0.169700
H	-0.807335	-2.395406	2.254539
H	1.378363	-1.279734	2.164759
H	1.049452	-0.946553	-2.094598
H	-1.158801	-2.069924	-2.011069
C	2.775796	-0.431953	-0.100178
C	3.766309	-1.546260	-0.503955
H	3.468986	-1.994452	-1.455698
H	4.774449	-1.133501	-0.602483
H	3.767350	-2.325545	0.264331
C	3.267738	0.250760	1.182007
H	4.210344	0.760173	0.961942
H	2.543562	0.985243	1.547461
H	3.454434	-0.476856	1.977711
O	2.843119	0.458962	-1.190525

SCF Done: E(UwB97X-D)= -775.126929544
Sum of electronic and zero-point Energies= -774.526691
Sum of electronic and thermal Energies= -774.506856
Sum of electronic and thermal Enthalpies= -774.505912
Sum of electronic and thermal Free Energies= -774.576185

23

C	1.363379	2.593547	-0.650400
H	1.013227	2.966310	-1.612184
H	1.993876	1.515627	-1.005118
H	2.140011	3.193705	-0.181188
C	0.299034	2.167309	0.293698
O	0.436824	2.106480	1.497734
O	-0.817216	1.813588	-0.350091
C	-1.837543	1.217941	0.465649
H	-2.176540	1.949312	1.207230
H	-1.400062	0.369673	1.001164
C	-2.961288	0.775663	-0.448891
H	-2.538723	0.137237	-1.233075
H	-3.399667	1.649822	-0.946602
C	-4.039115	0.007561	0.315810
H	-4.465439	0.649507	1.097991
H	-3.572671	-0.841463	0.832403
C	-5.153736	-0.498793	-0.597093
H	-4.754523	-1.174304	-1.362570
H	-5.915721	-1.044600	-0.031597
H	-5.648697	0.331784	-1.112999
C	-1.059583	-2.395844	0.326328
C	-0.692509	-1.905027	-0.924443
C	0.503699	-1.213261	-1.081416
C	1.361584	-1.009816	0.002501
C	0.977295	-1.490623	1.255740
C	-0.223605	-2.178122	1.417409
H	-1.991118	-2.940887	0.449155
H	-1.339633	-2.063632	-1.782683
H	0.787861	-0.822053	-2.052962
H	1.612689	-1.330921	2.120719
H	-0.503788	-2.544270	2.400811
C	2.723689	-0.349674	-0.240306
C	3.702624	-1.428235	-0.752823
H	3.328324	-1.872261	-1.678996
H	4.684774	-0.984419	-0.939934
H	3.799337	-2.216981	-0.000458
C	3.312958	0.332078	1.000771
H	4.210165	0.880857	0.700158
H	2.598626	1.029664	1.448199
H	3.603623	-0.399144	1.761195
O	2.664488	0.556585	-1.319375

SCF Done: E(UwB97X-D)= -811.046872515
Sum of electronic and zero-point Energies= -810.458108

Sum of electronic and thermal Energies= -810.43871
Sum of electronic and thermal Enthalpies= -810.437766
Sum of electronic and thermal Free Energies= -810.507112

24

C	1.893019	-1.419059	-0.809005
H	0.989662	-1.844519	-0.371216
H	2.083844	-1.763465	-1.825909
H	1.586568	-0.174834	-0.997584
C	3.038136	-1.466482	0.048716
N	3.958364	-1.462473	0.757066
C	-3.094932	-1.333288	0.156420
C	-2.510204	-1.021815	-1.068870
C	-1.402524	-0.183411	-1.121225
C	-0.856050	0.356225	0.047054
C	-1.450493	0.040263	1.269554
C	-2.561778	-0.798418	1.324020
H	-3.959169	-1.989237	0.199856
H	-2.917903	-1.433810	-1.987530
H	-0.939219	0.053665	-2.074058
H	-1.048583	0.441852	2.194378
H	-3.007369	-1.036069	2.285548
C	0.350742	1.293706	-0.058837
C	1.199420	1.347666	1.216595
H	1.486133	0.345377	1.550714
H	2.111544	1.912389	1.006939
H	0.670734	1.843220	2.036288
C	-0.141352	2.711562	-0.420287
H	-0.694438	2.693276	-1.362745
H	-0.805313	3.074763	0.369964
H	0.709987	3.391297	-0.517254
O	1.155134	0.945215	-1.163958

SCF Done: E(UwB97X-D)= -557.457793886
Sum of electronic and zero-point Energies= -557.071379
Sum of electronic and thermal Energies= -557.057953
Sum of electronic and thermal Enthalpies= -557.057009
Sum of electronic and thermal Free Energies= -557.113631

25

C	1.919396	-1.209140	-0.928737
H	1.588518	0.026584	-0.938228
H	2.871096	-1.145704	-1.463397
C	2.112878	-1.605597	0.442411
N	2.244944	-1.903984	1.556617
C	0.829294	-1.955842	-1.674916
H	1.146586	-2.985068	-1.878720
H	-0.095267	-1.982937	-1.094382
H	0.629079	-1.458759	-2.627311
C	-2.857696	-1.193799	0.307169
C	-2.608650	-0.493896	-0.872703
C	-1.549715	0.401863	-0.939391
C	-0.726179	0.629951	0.169176
C	-0.983536	-0.076381	1.343298
C	-2.040050	-0.984419	1.410934
H	-3.680892	-1.899971	0.361429
H	-3.235427	-0.654955	-1.745116
H	-1.337051	0.912815	-1.873828
H	-0.352270	0.057611	2.214808
H	-2.215792	-1.531472	2.332300
C	0.453560	1.597332	0.021924
C	1.325879	1.718547	1.275545
H	2.158979	2.391717	1.055598
H	0.760230	2.132808	2.116450
H	1.739346	0.754410	1.582008
C	-0.053637	3.001916	-0.365658
H	-0.634559	2.974408	-1.290164
H	-0.689739	3.388012	0.436753
H	0.794681	3.677844	-0.505674
O	1.238575	1.210916	-1.089145

SCF Done: E(UwB97X-D)= -596.774799098
Sum of electronic and zero-point Energies= -596.349785
Sum of electronic and thermal Energies= -596.335173
Sum of electronic and thermal Enthalpies= -596.334229
Sum of electronic and thermal Free Energies= -596.392801

26

C	2.025486	-0.739471	-0.408933
H	1.394042	0.337689	-0.550629
C	2.028840	-1.021589	1.011924
N	2.014766	-1.230174	2.153595
C	1.253659	-1.769061	-1.220321
H	0.280864	-1.983485	-0.772584
H	1.095642	-1.389539	-2.233746
H	1.826913	-2.702199	-1.283188
C	3.396418	-0.370092	-0.958054
H	3.291972	-0.030696	-1.992386
H	3.854609	0.430798	-0.372875
H	4.063340	-1.240218	-0.942793
C	-2.805146	-1.787513	-0.025395
C	-2.498514	-1.095798	-1.196518
C	-1.674030	0.020397	-1.149059
C	-1.149747	0.479537	0.064797
C	-1.461585	-0.220482	1.229359
C	-2.281225	-1.348192	1.184264
H	-3.443929	-2.665069	-0.059161
H	-2.894578	-1.434500	-2.149577
H	-1.405671	0.529346	-2.070132
H	-1.054182	0.092151	2.184454
H	-2.502494	-1.884552	2.102120
C	-0.205417	1.687108	0.047202
C	0.366556	2.055728	1.420017
H	1.056768	2.894588	1.294665
H	-0.423484	2.359969	2.114379
H	0.918103	1.225689	1.869012
C	-0.925443	2.919922	-0.537693
H	-0.234115	3.766141	-0.585398
H	-1.303046	2.720521	-1.543004
H	-1.768910	3.183937	0.107662
O	0.840712	1.442211	-0.870191

SCF Done: E(UwB97X-D)= -636.092108969
Sum of electronic and zero-point Energies= -635.629672
Sum of electronic and thermal Energies= -635.613456
Sum of electronic and thermal Enthalpies= -635.612511
Sum of electronic and thermal Free Energies= -635.674374

Hydroxy Transition-state Structures

1

O	-1.284880	0.109069	0.000027
H	-1.423431	-0.853220	0.000025
C	1.207288	-0.009835	0.000302
H	1.409118	-0.937507	-0.535028
H	1.570054	0.870552	-0.530275

H	-0.038698	0.147587	0.019076
H	1.518270	-0.040951	1.044176

SCF Done: E(UwB97X-D)= -116.251581012
Sum of electronic and zero-point Energies= -116.139675
Sum of electronic and thermal Energies= -116.134977
Sum of electronic and thermal Enthalpies= -116.134033
Sum of electronic and thermal Free Energies= -116.165744

2

O	-3.321031	0.275365	0.158637
H	-3.248375	0.391246	1.122146
C	-1.404204	-1.366610	0.030048
H	-1.842601	-2.201018	-0.523671
H	-2.299173	-0.532843	-0.015847
H	-1.304498	-1.622769	1.089683
C	-0.125782	-0.830189	-0.580072
H	0.581396	-1.672121	-0.610351
H	-0.299825	-0.544734	-1.626036
C	0.511391	0.352039	0.169848
H	0.445051	0.140352	1.248940
C	-0.239853	1.656840	-0.114780
H	-1.316044	1.556601	0.051437
H	0.137498	2.469858	0.515637
H	-0.096164	1.954043	-1.161483
C	2.000076	0.511282	-0.180564
H	2.102445	0.568008	-1.273685
H	2.344433	1.478935	0.206422
C	2.910344	-0.586775	0.369321
H	3.957499	-0.387292	0.119610
H	2.832952	-0.647082	1.461207
H	2.661821	-1.573624	-0.035915

SCF Done: E(UwB97X-D)= -312.820218045
Sum of electronic and zero-point Energies= -312.512034
Sum of electronic and thermal Energies= -312.501794
Sum of electronic and thermal Enthalpies= -312.500849
Sum of electronic and thermal Free Energies= -312.548176

3

C	-1.143970	1.952057	-0.092032
H	-1.076337	2.028855	-1.182424
H	-0.409398	2.640322	0.343075
H	-2.137874	2.294343	0.211113
C	-0.901171	0.525838	0.366316
H	-0.945766	0.439194	1.460607
H	-1.839141	-0.096698	-0.020872
C	0.328784	-0.187145	-0.189243
H	0.280607	-0.123750	-1.286471
C	0.306823	-1.666791	0.204297
H	0.424396	-1.781149	1.290100
H	-0.646023	-2.117032	-0.090095
H	1.110118	-2.228762	-0.280837
C	1.619188	0.520259	0.266252
H	1.577841	1.571329	-0.043327
H	1.654448	0.521087	1.365183
C	2.901700	-0.101273	-0.286961
H	2.861323	-0.175014	-1.380072
H	3.772165	0.508891	-0.024905
H	3.072488	-1.106604	0.110327
O	-2.916149	-0.916495	-0.329942
H	-3.037783	-1.300721	0.556353

SCF Done: E(UwB97X-D)= -312.824143179
Sum of electronic and zero-point Energies= -312.51557
Sum of electronic and thermal Energies= -312.505246
Sum of electronic and thermal Enthalpies= -312.504302
Sum of electronic and thermal Free Energies= -312.551557

4

C	2.228211	0.285297	-0.819985
H	2.867309	-0.446475	-0.316468
H	2.202794	1.188937	-0.200686
H	2.701538	0.534084	-1.775056
C	0.811860	-0.249678	-1.036968
H	0.275483	0.430419	-1.709846
H	0.852640	-1.218979	-1.556132
C	0.001192	-0.427058	0.248148
H	-0.030301	0.629808	0.757776
C	0.672013	-1.340800	1.265669
H	0.063446	-1.430891	2.170785
H	0.801635	-2.346820	0.843185
H	1.656879	-0.968612	1.560448
C	-1.460954	-0.807194	0.007015
H	-1.484979	-1.767743	-0.529716
H	-1.934422	-0.986891	0.979639
C	-2.280759	0.235539	-0.752887
H	-3.333906	-0.058493	-0.799434
H	-2.222072	1.202987	-0.242195
H	-1.932681	0.366461	-1.782773
O	-0.033270	2.039322	1.116308
H	-0.046588	2.380992	0.204050

SCF Done: E(UwB97X-D)= -312.825905315
Sum of electronic and zero-point Energies= -312.517661
Sum of electronic and thermal Energies= -312.507431
Sum of electronic and thermal Enthalpies= -312.506487
Sum of electronic and thermal Free Energies= -312.553217

5

C	-2.709298	-0.440345	0.112839
H	-2.807463	-1.301969	0.784086
H	-3.551800	-0.464217	-0.585696
H	-2.814685	0.468191	0.714610
C	-1.381259	-0.478455	-0.642599
H	-1.388262	-1.335240	-1.328662
H	-1.279775	0.420566	-1.263773
C	-0.135000	-0.589476	0.250149
H	-0.262363	-1.467060	0.908174
C	0.021185	0.619000	1.154188
H	-0.870055	0.877234	1.731289
H	0.896445	0.589164	1.807668
H	0.176836	1.593533	0.432176
C	1.113688	-0.828195	-0.614170
H	0.929747	-1.705087	-1.247401
H	1.225004	0.027201	-1.293204
C	2.408856	-1.044640	0.168188
H	3.226892	-1.323318	-0.503801
H	2.723136	-0.142878	0.705356
H	2.295275	-1.847217	0.906542
O	0.514233	2.479497	-0.484701
H	1.478178	2.347787	-0.461327

SCF Done: E(UwB97X-D)= -312.821803049
Sum of electronic and zero-point Energies= -312.513275
Sum of electronic and thermal Energies= -312.503018
Sum of electronic and thermal Enthalpies= -312.502074
Sum of electronic and thermal Free Energies= -312.549497

6

O	-2.321631	0.114654	-1.019609
H	-2.467097	-0.847311	-0.981576
C	0.940811	1.158565	-0.574710
C	0.175963	1.352581	0.738749
C	-0.759061	0.184675	1.014293
C	-0.070876	-1.170882	0.949151
C	0.696463	-1.348769	-0.365635
C	1.669270	-0.189027	-0.601366
H	-1.351279	0.317097	1.926003
H	0.890909	1.426091	1.573519
H	-0.387864	2.291410	0.721438
H	0.223979	1.197179	-1.404184
H	1.652240	1.979540	-0.719061
H	0.632628	-1.241384	1.792964
H	-0.800197	-1.978543	1.086409
H	1.230974	-2.305479	-0.363720
H	-0.023796	-1.379078	-1.193625
H	2.443858	-0.201396	0.179261
H	2.184841	-0.320332	-1.559547
H	-1.571566	0.222109	0.136097

SCF Done: E(UwB97X-D)= -311.620827713
Sum of electronic and zero-point Energies= -311.334294
Sum of electronic and thermal Energies= -311.326434
Sum of electronic and thermal Enthalpies= -311.32549
Sum of electronic and thermal Free Energies= -311.367122

7

C	0.766882	0.090982	0.550369
C	0.243140	-1.217362	-0.020119
C	-1.280179	-1.310437	0.157338
C	-1.983074	-0.093060	-0.451372
C	-1.438254	1.214898	0.130731
C	0.085395	1.311102	-0.047073
H	-1.653081	-2.235564	-0.297068
H	0.485888	-1.260161	-1.090562
H	0.733445	-2.073310	0.458611
H	0.737610	0.098894	1.647401
H	1.929038	0.188488	0.280321
H	-1.829280	-0.095023	-1.539673
H	-3.064403	-0.159851	-0.284717
H	-1.922846	2.076035	-0.343561
H	-1.681171	1.263633	1.201420
H	0.324319	1.361942	-1.117504
H	0.469536	2.228033	0.411670
H	-1.515184	-1.365728	1.229434
O	3.168124	0.106698	-0.283078
H	3.277674	-0.857713	-0.210389

SCF Done: E(UwB97X-D)= -311.620914892
Sum of electronic and zero-point Energies= -311.332613
Sum of electronic and thermal Energies= -311.324449
Sum of electronic and thermal Enthalpies= -311.323505
Sum of electronic and thermal Free Energies= -311.366581

8

C	-3.323132	-0.681277	-0.408900
H	-3.390665	-1.729119	-0.104123
H	-3.285297	-0.656790	-1.502087
H	-4.194201	-0.129335	-0.057215
C	-2.075361	-0.056511	0.150498
O	-2.031336	0.948217	0.822334
O	-0.982456	-0.762496	-0.198258
C	0.261347	-0.290939	0.273992
H	0.235145	-0.137213	1.358086
H	0.425530	0.823844	-0.183986
C	1.363445	-1.205854	-0.202850
H	1.383187	-1.202176	-1.299354
H	1.104536	-2.227646	0.106710
C	2.739288	-0.828436	0.356112
H	3.440620	-1.631223	0.100633
H	2.688338	-0.805817	1.452998
C	3.281013	0.503564	-0.165365
H	2.635680	1.344652	0.104744
H	4.280397	0.696966	0.237435
H	3.356556	0.489363	-1.258656
O	0.302547	2.095114	-0.504226
H	-0.469469	2.274536	0.065102

SCF Done: E(UwB97X-D)= -462.078146354
Sum of electronic and zero-point Energies= -461.734615
Sum of electronic and thermal Energies= -461.722989
Sum of electronic and thermal Enthalpies= -461.722045
Sum of electronic and thermal Free Energies= -461.773409

9

C	-2.673126	-0.350604	-1.288327
H	-3.596600	0.226587	-1.242726
H	-2.886099	-1.416051	-1.395978
H	-2.097256	-0.030145	-2.162978
C	-1.854055	-0.084130	-0.056049
O	-1.994128	0.872224	0.675449
O	-0.925696	-1.034313	0.123306
C	-0.016332	-0.870046	1.222189
H	0.207183	-1.890616	1.550387
H	-0.518744	-0.333684	2.030244
C	1.253002	-0.167271	0.795579
H	1.910810	-0.024145	1.661103
H	0.973856	0.978798	0.464794
C	1.976037	-0.760091	-0.398603
H	1.280454	-0.813570	-1.242813
H	2.259159	-1.796806	-0.160893
C	3.212225	0.045831	-0.791313
H	3.933557	0.089754	0.032668
H	3.714421	-0.401573	-1.654596
H	2.931514	1.071278	-1.050474
O	0.528396	2.087869	-0.056393
H	-0.367339	2.051808	0.331514

SCF Done: E(UwB97X-D)= -462.079213957
Sum of electronic and zero-point Energies= -461.735028
Sum of electronic and thermal Energies= -461.723417
Sum of electronic and thermal Enthalpies= -461.722473
Sum of electronic and thermal Free Energies= -461.774567

10

C	2.762789	0.308456	-0.318060
H	3.287727	-0.517558	-0.800663
H	3.405388	0.807773	0.407910
H	2.461708	1.030317	-1.084657
C	1.503552	-0.155512	0.356622
O	1.024855	0.351025	1.350133
O	0.946959	-1.177045	-0.306464
C	-0.319979	-1.671631	0.149069
H	-0.445825	-1.428885	1.206120
H	-0.252674	-2.756176	0.037481
C	-1.458745	-1.134323	-0.710002

H	-2.341964	-1.756509	-0.498267
H	-1.204981	-1.301139	-1.762635
C	-1.855637	0.319738	-0.496970
H	-2.591505	0.624609	-1.248748
H	-0.925230	1.039426	-0.792763
C	-2.295114	0.703161	0.902903
H	-2.596075	1.754103	0.935758
H	-3.154029	0.095377	1.216824
H	-1.488625	0.558631	1.627835
O	-0.022074	2.027482	-0.870891
H	0.226964	2.019007	0.072206

SCF Done: E(UwB97X-D)= -462.078252438
Sum of electronic and zero-point Energies= -461.735898
Sum of electronic and thermal Energies= -461.724825
Sum of electronic and thermal Enthalpies= -461.723881
Sum of electronic and thermal Free Energies= -461.772807

11

C	-3.077699	0.130336	0.612586
H	-3.766912	-0.033774	-0.220807
H	-3.366809	1.025118	1.162907
H	-3.133788	-0.746990	1.262901
C	-1.674923	0.292725	0.087740
O	-1.008819	1.296584	0.230407
O	-1.276179	-0.810220	-0.547863
C	0.034944	-0.850995	-1.151996
H	0.384150	0.160044	-1.367602
H	-0.118697	-1.388593	-2.090180
C	1.007918	-1.612371	-0.260910
H	1.884328	-1.869621	-0.870102
H	0.534692	-2.559247	0.024247
C	1.468043	-0.862132	0.995752
H	1.906790	-1.592322	1.691035
H	0.606274	-0.431859	1.517999
C	2.507679	0.210399	0.743987
H	3.395405	-0.154822	0.218067
H	2.097052	1.090994	-0.029158
H	2.788093	0.768998	1.639717
O	1.596801	1.999414	-0.772586
H	0.699221	1.998080	-0.381650

SCF Done: E(UwB97X-D)= -462.078568981
Sum of electronic and zero-point Energies= -461.734417
Sum of electronic and thermal Energies= -461.723378
Sum of electronic and thermal Enthalpies= -461.722434
Sum of electronic and thermal Free Energies= -461.772332

12

C	3.049957	-0.572593	-0.195906
H	3.139574	-0.385328	-1.271294
H	3.944842	-1.112237	0.131441
H	3.019925	0.391210	0.320334
C	1.804350	-1.402942	0.088808
H	1.739458	-1.645760	1.160400
H	1.843796	-2.346147	-0.464390
O	0.611107	-0.766144	-0.330535
C	0.097740	0.179301	0.559974
H	0.755992	1.101768	0.591217
H	0.093028	-0.214043	1.591301
C	-1.290394	0.597158	0.115913
H	-1.223546	1.004760	-0.900662
H	-1.621494	1.418976	0.763009
C	-2.304186	-0.547513	0.152903
H	-2.361217	-0.944753	1.175467
H	-1.938873	-1.364359	-0.478812
C	-3.693988	-0.111626	-0.306300
H	-3.667270	0.263019	-1.336020
H	-4.403799	-0.944449	-0.271628
H	-4.086841	0.690957	0.328716
O	1.536201	2.421673	-0.034902
H	1.607095	1.991451	-0.907932

SCF Done: E(UwB97X-D)= -388.031135206
Sum of electronic and zero-point Energies= -387.692846
Sum of electronic and thermal Energies= -387.68153
Sum of electronic and thermal Enthalpies= -387.680586
Sum of electronic and thermal Free Energies= -387.731275

13

C	-1.839242	-0.559995	-0.208160
H	-1.857675	-0.586598	-1.295544
H	-2.598230	-1.138649	0.309474
C	-0.934758	0.164021	0.456638
H	-0.950014	0.162924	1.545489
C	0.134828	0.957314	-0.186103
H	0.326440	1.918504	0.299347
H	1.177098	0.394475	-0.049474
H	0.007779	1.079241	-1.264423
O	2.248643	-0.487002	0.026983
H	1.740491	-1.301922	-0.134981

SCF Done: E(UwB97X-D)= -193.643503177
Sum of electronic and zero-point Energies= -193.474121
Sum of electronic and thermal Energies= -193.467895
Sum of electronic and thermal Enthalpies= -193.46695
Sum of electronic and thermal Free Energies= -193.504417

14

C	-2.138539	-0.576609	0.118668
H	-2.955957	-0.918758	-0.509023
H	-2.273535	-0.670627	1.194059
C	-1.026410	-0.055725	-0.401084
H	-0.928946	0.024387	-1.484273
C	0.137635	0.421657	0.392253
H	-0.081950	0.427173	1.465530
H	0.993555	-0.370706	0.274697
C	0.741848	1.736736	-0.080905
H	0.018707	2.553455	0.027689
H	1.634175	1.988144	0.498864
H	1.029088	1.675332	-1.135647
O	1.885959	-1.465003	-0.049988
H	1.189991	-2.144725	-0.105581

SCF Done: E(UwB97X-D)= -232.958194752
Sum of electronic and zero-point Energies= -232.74949
Sum of electronic and thermal Energies= -232.741912
Sum of electronic and thermal Enthalpies= -232.740968
Sum of electronic and thermal Free Energies= -232.782234

15

C	2.070661	-0.832316	-0.066979
H	2.230097	-0.743006	1.004081
H	2.846120	-1.341410	-0.631595
C	0.992157	-0.335429	-0.672033
H	0.897228	-0.453294	-1.752164
C	-0.148077	0.383266	-0.017643
H	-1.062359	-0.317254	-0.136874
C	0.001791	0.617315	1.478496

H	0.855149	1.275202	1.684017
H	-0.898788	1.091396	1.879187
H	0.153712	-0.321891	2.019221
C	-0.531124	1.652478	-0.779253
H	-1.446626	2.089890	-0.369468
H	0.270800	2.396962	-0.700093
H	-0.697853	1.444859	-1.841120
O	-2.017919	-1.484344	-0.097023
H	-1.316577	-2.158594	-0.034538

SCF Done: E(UwB97X-D)= -272.273482632
Sum of electronic and zero-point Energies= -272.025853
Sum of electronic and thermal Energies= -272.017136
Sum of electronic and thermal Enthalpies= -272.016192
Sum of electronic and thermal Free Energies= -272.060072

16

C	2.315949	0.000969	0.444651
C	1.660946	1.204983	0.195977
C	0.360671	1.202956	-0.295880
C	-0.307378	-0.000931	-0.552739
C	0.361602	-1.203839	-0.293748
C	1.661884	-1.203988	0.198105
H	3.332052	0.001703	0.827465
H	2.165426	2.148083	0.384239
H	-0.147471	2.144729	-0.487742
H	-0.145802	-2.146346	-0.483945
H	2.167095	-2.146362	0.388031
C	-1.712461	-0.001882	-1.034909
H	-1.990121	-0.903365	-1.586173
H	-2.459373	-0.000746	-0.100986
H	-1.990515	0.897998	-1.588589
O	-3.087631	0.001574	1.126477
H	-2.277525	0.002102	1.667143

SCF Done: E(UwB97X-D)= -347.289422842
Sum of electronic and zero-point Energies= -347.033672
Sum of electronic and thermal Energies= -347.025389
Sum of electronic and thermal Enthalpies= -347.024445
Sum of electronic and thermal Free Energies= -347.068762

17

C	1.631846	1.217648	0.659217
C	0.297961	0.846550	0.540068
C	-0.058246	-0.344508	-0.104596
C	0.954452	-1.144947	-0.638904
C	2.291702	-0.777346	-0.516494
C	2.634170	0.404073	0.133999
H	1.891144	2.146178	1.159471
H	-0.486164	1.491192	0.929500
H	0.692396	-2.068344	-1.149668
H	3.066445	-1.414440	-0.933006
H	3.676612	0.693577	0.227012
C	-1.497092	-0.747223	-0.207714
H	-1.638340	-1.559662	-0.928381
H	-2.100597	0.168093	-0.667297
C	-2.189034	-1.038213	1.116232
H	-3.245279	-1.274723	0.959554
H	-1.711630	-1.890310	1.614374
H	-2.127784	-0.176631	1.787503
O	-2.579820	1.451923	-0.938769
H	-1.772799	1.773479	-1.379754

SCF Done: E(UwB97X-D)= -386.602637198
Sum of electronic and zero-point Energies= -386.309402
Sum of electronic and thermal Energies= -386.300032
Sum of electronic and thermal Enthalpies= -386.299087
Sum of electronic and thermal Free Energies= -386.345091

18

C	-2.059511	1.274956	0.266203
C	-0.682811	1.088080	0.292438
C	-0.120668	-0.167374	0.030154
C	-0.978159	-1.229466	-0.266123
C	-2.358741	-1.045254	-0.289623
C	-2.904569	0.205864	-0.023463
H	-2.474125	2.258403	0.468062
H	-0.021234	1.925598	0.500918
H	-0.571705	-2.213826	-0.478015
H	-3.008373	-1.884937	-0.519414
H	-3.980760	0.349201	-0.045462
C	1.379219	-0.338564	0.111105
H	1.840778	0.624275	-0.353592
C	1.881273	-0.327756	1.554858
H	2.975075	-0.359404	1.585296
H	1.546303	0.569249	2.083210
H	1.493482	-1.202616	2.091695
C	1.950585	-1.499117	-0.692393
H	1.577528	-1.500575	-1.721236
H	3.042295	-1.433390	-0.721644
H	1.691959	-2.461494	-0.232794
O	2.219771	1.945719	-0.878936
H	1.490897	1.995557	-1.524479

SCF Done: E(UwB97X-D)= -425.91729206
Sum of electronic and zero-point Energies= -425.585646
Sum of electronic and thermal Energies= -425.574991
Sum of electronic and thermal Enthalpies= -425.574047
Sum of electronic and thermal Free Energies= -425.623031

19

C	2.218761	1.079500	0.274175
H	2.927355	1.574390	-0.393508
H	2.517640	1.201018	1.320379
H	1.238297	1.743489	0.223433
C	1.924068	-0.328460	-0.097557
C	2.315249	-0.824673	-1.278790
H	2.867020	-0.223582	-1.997008
H	2.105176	-1.853563	-1.558922
C	1.138827	-1.152979	0.896388
H	1.213811	-2.214709	0.631243
H	1.592594	-1.039741	1.889661
C	-0.346872	-0.757882	0.982479
H	-0.800347	-1.297791	1.823637
H	-0.426771	0.310094	1.213635
C	-1.125415	-1.086925	-0.293366
H	-0.667631	-0.573721	-1.151755
H	-1.018600	-2.161127	-0.498143
C	-2.615368	-0.733358	-0.224877
H	-3.136790	-1.225679	-1.055012
H	-3.041935	-1.152674	0.696189
C	-2.901820	0.767533	-0.284519
H	-3.975139	0.968016	-0.204587
H	-2.399324	1.316231	0.518412
H	-2.563679	1.187114	-1.241193
O	0.032906	2.467998	0.072894
H	-0.339507	1.921720	-0.643214

SCF Done: E(UwB97X-D)= -390.215159797

Sum of electronic and zero-point Energies= -389.852564
Sum of electronic and thermal Energies= -389.84065
Sum of electronic and thermal Enthalpies= -389.839706
Sum of electronic and thermal Free Energies= -389.891191

20

C	-0.786810	-0.441727	1.096753
H	-0.406765	0.076468	1.979760
H	-1.479642	-1.249930	1.332549
H	-1.463407	0.405905	0.529649
C	0.235821	-0.837583	0.068883
O	-0.022415	-1.701465	-0.746142
C	1.546517	-0.077107	0.059306
H	2.067298	-0.272048	1.006607
H	2.155761	-0.487539	-0.750119
C	1.347798	1.435046	-0.113893
H	0.794137	1.871015	0.723362
H	2.318292	1.935860	-0.172230
H	0.787331	1.656244	-1.026145
O	-2.056454	1.102517	-0.408722
H	-2.202006	0.383838	-1.050810

SCF Done: E(UwB97X-D)= -308.208256195
Sum of electronic and zero-point Energies= -307.969288
Sum of electronic and thermal Energies= -307.960935
Sum of electronic and thermal Enthalpies= -307.959991
Sum of electronic and thermal Free Energies= -308.003379

21

C	-1.828913	0.672954	0.463243
H	-1.423288	1.684054	0.345937
H	-2.029969	0.522086	1.529920
H	-2.755643	0.569940	-0.103106
C	-0.808297	-0.327416	-0.027917
O	-1.041953	-1.123113	-0.914002
C	0.560153	-0.254200	0.612275
H	0.974109	0.811140	0.262514
H	0.492008	-0.102576	1.695938
C	1.534824	-1.335065	0.205320
H	1.202780	-2.307599	0.585221
H	1.594534	-1.417111	-0.882835
H	2.531525	-1.131910	0.605900
O	1.217656	2.016698	-0.369924
H	1.261717	1.685661	-1.285613

SCF Done: E(UwB97X-D)= -308.21298007
Sum of electronic and zero-point Energies= -307.97482
Sum of electronic and thermal Energies= -307.966167
Sum of electronic and thermal Enthalpies= -307.965223
Sum of electronic and thermal Free Energies= -308.009221

22

C	2.311306	0.877372	-0.423751
H	2.543629	0.725570	-1.480698
H	3.065082	1.466561	0.099013
H	1.320661	1.580178	-0.469139
C	1.924478	-0.362823	0.336316
O	2.135616	-0.438827	1.530397
C	1.224853	-1.459811	-0.441453
H	1.864721	-1.760194	-1.281293
H	1.108800	-2.318587	0.226346
C	-0.142240	-0.999770	-0.977438
H	-0.014048	-0.121443	-1.622336
H	-0.551218	-1.794567	-1.612857
C	-1.139316	-0.666138	0.131702
H	-0.690886	0.058351	0.823722
H	-1.342831	-1.569215	0.723694
C	-2.445987	-0.085301	-0.405159
H	-2.216419	0.834216	-0.957747
H	-2.888699	-0.785329	-1.126622
C	-3.455400	0.217938	0.700257
H	-3.045480	0.938508	1.417668
H	-4.379187	0.641329	0.292825
H	-3.718017	-0.689690	1.255922
O	0.247345	2.347602	-0.336358
H	0.214045	2.395306	0.636337

SCF Done: E(UwB97X-D)= -426.150033367
Sum of electronic and zero-point Energies= -425.793696
Sum of electronic and thermal Energies= -425.781643
Sum of electronic and thermal Enthalpies= -425.780698
Sum of electronic and thermal Free Energies= -425.833604

23

C	-2.085450	-0.473507	1.013016
H	-2.051543	0.185153	1.881690
H	-2.210946	-1.523138	1.274455
H	-3.134148	-0.108862	0.416615
C	-0.977584	-0.191340	0.048069
O	-0.902966	0.835716	-0.594892
O	-0.104506	-1.198976	-0.013110
C	1.037459	-1.060742	-0.881971
H	0.869709	-0.220317	-1.557618
H	1.070477	-1.986762	-1.461010
C	2.304920	-0.896892	-0.055996
H	3.152340	-0.917006	-0.754506
H	2.410175	-1.773420	0.594254
C	2.365014	0.381137	0.786712
H	3.266024	0.333360	1.409774
H	1.516993	0.395657	1.483336
C	2.380809	1.670564	-0.034213
H	1.441941	1.810179	-0.578156
H	2.518159	2.540885	0.615384
H	3.203007	1.663291	-0.759891
O	-3.870528	0.594985	-0.286368
H	-3.179201	1.171860	-0.663070

SCF Done: E(UwB97X-D)= -462.069935763
Sum of electronic and zero-point Energies= -461.725901
Sum of electronic and thermal Energies= -461.714531
Sum of electronic and thermal Enthalpies= -461.713587
Sum of electronic and thermal Free Energies= -461.765287

24

C	0.000000	0.994577	0.000000
H	-0.024797	1.599297	0.907619
H	-1.083168	0.402501	0.000000
H	-0.024797	1.599297	-0.907619
C	1.065250	0.025541	0.000000
N	1.892889	-0.786665	0.000000
O	-2.104862	-0.371464	0.000000
H	-1.670060	-1.243439	0.000000

SCF Done: E(UwB97X-D)= -208.486103761
Sum of electronic and zero-point Energies= -208.345102
Sum of electronic and thermal Energies= -208.339277
Sum of electronic and thermal Enthalpies= -208.338333
Sum of electronic and thermal Free Energies= -208.374748

25

C	0.049498	0.427105	0.525577
H	0.058331	0.584117	1.607902
H	0.977177	-0.327485	0.349948
C	-1.150576	-0.278361	0.121267
N	-2.089175	-0.864600	-0.224281
C	0.359323	1.680333	-0.279243
H	0.430669	1.448337	-1.344347
H	-0.423628	2.432539	-0.137928
H	1.311960	2.101403	0.050089
O	1.920458	-1.161278	-0.089196
H	1.356582	-1.870947	-0.447733

SCF Done: E(UwB97X-D)= -247.801850585
Sum of electronic and zero-point Energies= -247.621782
Sum of electronic and thermal Energies= -247.61478
Sum of electronic and thermal Enthalpies= -247.613836
Sum of electronic and thermal Free Energies= -247.653467

C	1.159573	-0.469608	0.000036
N	2.095426	-1.153508	0.000048
C	-0.188669	1.170977	-1.284589
H	-1.153138	1.685957	-1.279625
H	0.606800	1.921146	-1.355926
H	-0.140575	0.527896	-2.166477
C	-0.188429	1.171464	1.284301
H	-0.140120	0.528719	2.166422
H	0.607028	1.921690	1.355179
H	-1.152917	1.686410	1.279345
O	-1.931019	-1.379055	0.000341
H	-1.357290	-2.167422	-0.000675

SCF Done: E(UwB97X-D)= -287.118226969
Sum of electronic and zero-point Energies= -286.899883
Sum of electronic and thermal Energies= -286.891486
Sum of electronic and thermal Enthalpies= -286.890542
Sum of electronic and thermal Free Energies= -286.9338

26

C	-0.039238	0.361123	-0.000005
H	-0.949037	-0.401131	0.000236

5 References

[1]Stateman, L.; Nakafuku, K.; Nagib, D. Remote C–H Functionalization via Selective Hydrogen Atom Transfer. *Synthesis* **2018**, *50* (08), 1569–1586. https://doi.org/10.1055/s-0036-1591930.

[2]Zhang, J.; Li, Y.; Zhang, F.; Hu, C.; Chen, Y. Generation of Alkoxyl Radicals by Photoredox Catalysis Enables Selective C(Sp ^{3})−H Functionalization under Mild Reaction Conditions. *Angew. Chem.* **2016**, *128* (5), 1904–1907. https://doi.org/10.1002/ange.201510014.

[3]Chang, L.; An, Q.; Duan, L.; Feng, K.; Zuo, Z. Alkoxy Radicals See the Light: New Paradigms of Photochemical Synthesis. *Chem. Rev.* **2022**, *122* (2), 2429–2486. https://doi.org/10.1021/acs.chemrev.1c00256.

[4]Bovicelli, P.; Lupattelli, P.; Mincione, E.; Prencipe, T.; Curci, R. Oxidation of Natural Targets by Dioxiranes. 2. Direct Hydroxylation at the Side Chain C-25 of Cholestane Derivatives and of Vitamin D3 Windaus-Grundmann Ketone. *J. Org. Chem.* **1992**, *57* (19), 5052–5054. https://doi.org/10.1021/jo00045a004.

[5]DesMarteau, D. D.; Donadelli, A.; Montanari, V.; Petrov, V. A.; Resnati, G. Mild and Selective Oxyfunctionalization of Hydrocarbons by Perfluorodialkyloxaziridines. *J. Am. Chem. Soc.* **1993**, *115* (11), 4897–4898. https://doi.org/10.1021/ja00064a063.

[6]Murray, R. W.; Jeyaraman, Ramasubbu.; Mohan, Lily. Chemistry of Dioxiranes. 4. Oxygen Atom Insertion into Carbon-Hydrogen Bonds by Dimethyldioxirane. *J. Am. Chem. Soc.* **1986**, *108* (9), 2470–2472. https://doi.org/10.1021/ja00269a069.

[7]Chen, M. S.; White, M. C. A Predictably Selective Aliphatic C–H Oxidation Reaction for Complex Molecule Synthesis. *Science* **2007**, *318* (5851), 783–787. https://doi.org/10.1126/science.1148597.

[8]Mack, J. B. C.; Gipson, J. D.; Du Bois, J.; Sigman, M. S. Ruthenium-Catalyzed C–H Hydroxylation in Aqueous Acid Enables Selective Functionalization of Amine Derivatives. *J. Am. Chem. Soc.* **2017**, *139* (28), 9503–9506. https://doi.org/10.1021/jacs.7b05469.

[9]Yamazaki, S. Chromium(VI) Oxide-Catalyzed Benzylic Oxidation with Periodic Acid. *Org. Lett.* **1999**, *1* (13), 2129–2132. https://doi.org/10.1021/ol991175k.

[10]Bigi, M.; Liu, P.; Zou, L.; Houk, K.; White, M. Cafestol to Tricalysiolide B and Oxidized Analogues: Biosynthetic and Derivatization Studies Using Non-Heme Iron Catalyst Fe(PDP). *Synlett* **2012**, *23* (19), 2768–2772. https://doi.org/10.1055/s-0032-1317708.

[11]Wender, P. A.; Hilinski, M. K.; Mayweg, A. V. W. Late-Stage Intermolecular CH Activation for Lead Diversification: A Highly Chemoselective Oxyfunctionalization of the C-9 Position of Potent Bryostatin Analogues. *Org. Lett.* **2005**, *7* (1), 79–82. https://doi.org/10.1021/ol047859w.

[12]Chen, K.; Baran, P. S. Total Synthesis of Eudesmane Terpenes by Site-Selective C–H Oxidations. *Nature* **2009**, *459* (7248), 824–828. https://doi.org/10.1038/nature08043.

[13]Liu, F.; Yang, Z.; Yu, Y.; Mei, Y.; Houk, K. N. Bimodal Evans–Polanyi Relationships in Dioxirane Oxidations of Sp ^{3} C–H: Non-Perfect Synchronization in Generation of Delocalized Radical Intermediates. *J. Am. Chem. Soc.* **2017**, *139* (46), 16650–16656. https://doi.org/10.1021/jacs.7b07988.

[14]White, M. C.; Zhao, J. Aliphatic C–H Oxidations for Late-Stage Functionalization. *J. Am. Chem. Soc.* **2018**, *140* (43), 13988–14009. https://doi.org/10.1021/jacs.8b05195.

[15]Groves, J. T. Key Elements of the Chemistry of Cytochrome P-450: The Oxygen Rebound Mechanism. *J. Chem. Educ.* **1985**, *62* (11), 928. https://doi.org/10.1021/ed062p928.

[16]Evans, M. G.; Polanyi, M. Further Considerations on the Thermodynamics of Chemical Equilibria and Reaction Rates. *Trans. Faraday Soc.* **1936**, *32*, 1333. https://doi.org/10.1039/tf9363201333.

[17]The Theory of Reactions Involving Proton Transfers. *Proc. R. Soc. Lond. A* **1936**, *154* (882), 414–429. https://doi.org/10.1098/rspa.1936.0060.

[18]Evans, M. G.; Polanyi, M. Inertia and Driving Force of Chemical Reactions. *Trans. Faraday Soc.* **1938**, *34*, 11. https://doi.org/10.1039/tf9383400011.

[19]Salamone, M.; Galeotti, M.; Romero-Montalvo, E.; Van Santen, J. A.; Groff, B. D.; Mayer, J. M.; DiLabio, G. A.; Bietti, M. Bimodal Evans–Polanyi Relationships in Hydrogen Atom Transfer from C(Sp^3)–H Bonds to the Cumyloxyl Radical. A Combined Time-Resolved Kinetic and Computational Study. *J. Am. Chem. Soc.* **2021**, *143* (30), 11759–11776. https://doi.org/10.1021/jacs.1c05566.

[20]Bernasconi, C. F. The Principle of Imperfect Synchronization. *Tetrahedron* **1985**, *41* (16), 3219–3234. https://doi.org/10.1016/S0040-4020(01)96673-6.

[21]Bernasconi, C. F. The Principle of Nonperfect Synchronization: More than a Qualitative Concept? *Acc. Chem. Res.* **1992**, *25* (1), 9–16. https://doi.org/10.1021/ar00013a002.

[22]Bernasconi, C. F. Intrinsic Barriers of Reactions and the Principle of Nonperfect Synchronization. *Acc. Chem. Res.* **1987**, *20* (8), 301–308. https://doi.org/10.1021/ar00140a006.

[23]Roberts, B. P.; Steel, A. J. An Extended Form of the Evans–Polanyi Equation: A Simple Empirical Relationship for the Prediction of Activation Energies for Hydrogen-Atom Transfer Reactions. *J. Chem. Soc., Perkin Trans. 2* **1994**, No. 10, 2155–2162. https://doi.org/10.1039/P29940002155.

[24]Liu, F.; Ma, S.; Lu, Z.; Nangia, A.; Duan, M.; Yu, Y.; Xu, G.; Mei, Y.; Bietti, M.; Houk, K. N. Hydrogen Abstraction by Alkoxyl Radicals: Computational Studies of Thermodynamic and Polarity Effects on Reactivities and Selectivities. *J. Am. Chem. Soc.* **2022**, *144* (15), 6802–6812. https://doi.org/10.1021/jacs.2c00389.

[25]Salamone, M.; Bietti, M. Tuning Reactivity and Selectivity in Hydrogen Atom Transfer from Aliphatic C–H Bonds to Alkoxyl Radicals: Role of Structural and Medium Effects. *Acc. Chem. Res.* **2015**, *48* (11), 2895–2903. https://doi.org/10.1021/acs.accounts.5b00348.

[26]Wang, Y.; Janardanan, D.; Usharani, D.; Han, K.; Que, L.; Shaik, S. Nonheme Iron Oxidant Formed in the Presence of H_2O_2 and Acetic Acid Is the Cyclic Ferric Peracetate Complex, Not a Perferryloxo Complex. *ACS Catal.* **2013**, *3* (6), 1334–1341. https://doi.org/10.1021/cs400134g.

[27]Griffin, J. D.; Vogt, D. B.; Du Bois, J.; Sigman, M. S. Mechanistic Guidance Leads to Enhanced Site-Selectivity in C–H Oxidation Reactions Catalyzed by Ruthenium Bis(Bipyridine) Complexes. *ACS Catal.* **2021**, *11* (16), 10479–10486. https://doi.org/10.1021/acscatal.1c02593.

[28]Mack, J. B. C.; Walker, K. L.; Robinson, S. G.; Zare, R. N.; Sigman, M. S.; Waymouth, R. M.; Du Bois, J. Mechanistic Study of Ruthenium-Catalyzed C–H Hydroxylation Reveals an Unexpected Pathway for Catalyst Arrest. *J. Am. Chem. Soc.* **2019**, *141* (2), 972–980. https://doi.org/10.1021/jacs.8b10950.

[29]*PyMOL | pymol.org*. https://pymol.org/2/ (accessed 2023-03-06).

[30]Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe,

V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[31]Eggleston, D. S.; Goldsby, K. A.; Hodgson, D. J.; Meyer, T. J. Structural Variations Induced by Changes in Oxidation State and Their Role in Electron Transfer. Crystal and Molecular Structures of Cis-[Ru(Bpy)2Cl2].3.5H2O and Cis-[Ru(Bpy)2Cl2]Cl.2H2O. *Inorg. Chem.* **1985**, *24* (26), 4573–4580. https://doi.org/10.1021/ic00220a029.

[32]Bannwarth, C.; Ehlert, S.; Grimme, S. GFN2-XTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* **2019**, *15* (3), 1652–1671. https://doi.org/10.1021/acs.jctc.8b01176.

[33]Pracht, P.; Bohle, F.; Grimme, S. Automated Exploration of the Low-Energy Chemical Space with Fast Quantum Chemical Methods. *Phys. Chem. Chem. Phys.* **2020**, *22* (14), 7169–7192. https://doi.org/10.1039/C9CP06869D.

[34]Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113* (18), 6378–6396. https://doi.org/10.1021/jp810292n.

[35]Chai, J.-D.; Head-Gordon, M. Systematic Optimization of Long-Range Corrected Hybrid Density Functionals. *The Journal of Chemical Physics* **2008**, *128* (8), 084106. https://doi.org/10.1063/1.2834918.

[36]Chai, J.-D.; Head-Gordon, M. Long-Range Corrected Hybrid Density Functionals with Damped Atom–Atom Dispersion Corrections. *Phys. Chem. Chem. Phys.* **2008**, *10* (44), 6615. https://doi.org/10.1039/b810189b.

[37]Shaik, S.; Cohen, S.; Wang, Y.; Chen, H.; Kumar, D.; Thiel, W. P450 Enzymes: Their Structure, Reactivity, and Selectivity—Modeled by QM/MM Calculations. *Chem. Rev.* **2010**, *110* (2), 949–1017. https://doi.org/10.1021/cr900121s.

[38]Hirao, H.; Thellamurege, N.; Zhang, X. Applications of Density Functional Theory to Iron-Containing Molecules of Bioinorganic Interest. *Front. Chem.* **2014**, *2*. https://doi.org/10.3389/fchem.2014.00014.

[39]*CYLview Visualization Software*. https://www.cylview.org/ (accessed 2023-03-06).