FORCE FIELD DEVELOPMENT FOR FERROCENE AND THE
PREDICTION OF ENANTIOSELECTIVITY

A Thesis

Submitted to the Graduate School
of the University of Notre Dame
in Partial Fulfillment of the Requirements
for the Degree of

Master of Science

by

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February 2017
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Abstract

By

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Experimentalists commonly explore the use of ferrocene-based chiral ligands in enantioselective catalysis. Being able to computationally predict enantioselectivity for the rhodium-catalyzed hydrogenation of enamides would accelerate experimentalist’s work significantly. To accomplish this feat, force field parameters for ferrocene were optimized using Q2MM. Once the force field was developed, it was combined with a previously developed rhodium force field. Together, the two force fields were tested to predict enantioselectivity in the hydrogenation of enamides.

The force field was tested on several ferrocene derivatives. The energies predicted by the force field and the energies calculated quantum mechanically have shown an R^2 of 0.910. This displays the performance of the force field for ferrocene alone. The ferrocene and rhodium force fields were combined and compared to experimental data. The resulting predictions showed initial agreement, however, there could be further
improvements toward predicting the enantioselectivity of the rhodium-catalyzed hydrogenation of enamides.
For Merrilee:

Thank you for your love and commitment, especially throughout my time at Notre Dame.

The long-distance relationship is now over.

For my parents and siblings:

Thank you for your love, support, prayers, and guidance you have given me.
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ACKNOWLEDGMENTS

I would like to acknowledge all those who have helped and guided me throughout my research on this thesis. I thank all the members of the Wiest/Helquist research group for their support and input toward my project. Specifically, I would like to thank Eric Hansen and Anthony Rosales for their expertise and advise on Q2MM, Python, etc. Also, Aaron Forbes helped this get started and was very informative with previous work, and I thank him for that.

I wish to thank my unofficial advisor Prof. Per-Ola Norrby for his guidance, specifically with Q2MM. My co-advisors Prof. Olaf Wiest and Prof. Paul Helquist have really helped and guided me during my time in graduate school. They have helped me through tough decisions and have supported me throughout.
CHAPTER 1:
INTRODUCTION

1.1 Computational Approaches to Enantioselectivity

1.1.1 Prediction of Enantioselectivity

In organic chemistry, asymmetric catalysis is an intriguing and current topic. Many weeks have been spent toward experimental discovery of enantioselective catalysts. Since bench work toward this achievement is often performed on a trial and error basis, computational advancements toward predicting such chiral ligands could be critical. A method to screen through a library of ligands computationally should be quick and cheap. It could allow synthetic chemists to purchase or synthesize only a select number of ligands within the library rather than the whole library. This screening method should not be limited to existing libraries either.

By having a large virtual library, one could screen through the library without having to dedicate a large amount of their time. The results from the virtual screening would give synthetic chemists a much smaller library to focus their efforts on. The virtual screening method is unlikely to be perfect and could lead to some inaccurate results, but the purpose of the method is to lead the synthetic chemists in the right direction.¹
Predicting the enantioselectivity of a reaction depends on the energies of the diastereomeric transition states (TSs) which yield the enantiomeric products. Calculating the difference in these TS energies gives the $\Delta\Delta G^\ddagger$ of the reaction. Significant errors are cancelled by choosing this calculation if the structures are similar (e.g., bond enthalpies would cancel as a part of the force field calculation). As described in Figure 1.1, only the $\Delta\Delta G^\ddagger$ is needed for the prediction of selectivity. With that said, there is still the problem of using inaccurate TSs since there are many TSs (e.g., different conformations) that lead to the same enantiomer. Thus, the entire conformational space needs to be taken into account. By performing a conformational search and then using a Boltzmann distribution to find the enantioselectivity, the error can decrease.

Figure 1.1: Representation of diastereomeric transition states that define enantioselectivity in a reaction
The enantioselectivity is then defined as

\[
%{ee} = \frac{er - 1}{er + 1} \times 100 \text{ with } er = \frac{\sum \exp(-\Delta G_i/RT)}{\sum \exp(-\Delta G_j/RT)}
\]  

(1.1)

where \(i\) and \(j\) are summed over all the conformations for each diastereomeric TS. Other approaches toward predicting enantioselectivity include the quantitative structure-activity/selectivity relationships (QSAR or QSSR) methods.\(^3,4\) Both methods are usually applied to biological systems, although they have been applied to asymmetric catalysis,\(^5\) and they correlate quantitative relationships between TS structures with activity or selectivity.\(^6\) Similarly, Lipkowitz and Darden as well as Sigman have developed techniques in predicting enantioselectivity.\(^7-9\)

The number of conformations that need to be sampled can be impractical for large and flexible molecules. Conformational sampling using a Monte Carlo (MC) search would be very expensive and time consuming using quantum mechanical (QM) methods. With MC sampling, the system jumps abruptly to different conformations and overcomes energetic barriers, which can allow the global minimum to be achieved. One alternative that has shown to be advantageous in speed is using molecular mechanics (MM) methods instead of QM methods. However, MC sampling of transition states are not a common characteristic with MM. Additionally, MM methods do not typically offer sufficient parameters for most transition metals. Another alternative is using QM/MM hybrid methods. This involves using QM at the reaction center and MM on the rest of the molecule. Similar to the QM method, this method is unfeasible due to expense and time requirements. Therefore, in order to take advantage of the computational speed, MM models are commonly used to screen a large virtual library.
1.1.2 Transition State Force Fields

Molecular mechanics has a long history with modeling transition states. One of the first examples of applying empirical force fields to reactions was when Westheimer studied the rotational barrier of biphenyls in the 1940s. Garbisch and coworkers took force field modeling a step forward by applying their diimide reduction of alkenes force field to model reaction rates. Many studies have been performed using ground state parameters considering TSs have more torsional and nonbonded strain than energy minima. Because bonds are known to form and break, unmodified ground state parameters are not suitable. One way to correct this is by using information from *ab initio* methods at the transition states. Houk et al. used a technique called the rigid TS model. In this model, the *ab initio* TS is located at the QM level and then the atoms involved at the reaction center are held fixed while the other atoms’ geometries are optimized. Later, Dorigo and Houk took on a flexible TS model where new parameters are developed as an energy minimum. The transition state force field (TSFF) that they developed involved fixing the bond and angle parameters to the QM values and optimizing the force constants to fit the appropriate MP2 energies. However, Menger and Sherrod have pointed out this approach used parameters that were under-defined, and not enough data were used to create the TS force fields.

Some techniques involve finding the potential energy surface (PES) to accurately describe the transition state of a reaction. In 1980, Warshel and Weiss developed the empirical valence bond (EVB) technique which uses ground state force fields to depict the PES. This method is used for comparing the free energies of enzymatic reactions with solution reactions. Rappé et al. more recently proposed the reaction force field (RFF)
method,\textsuperscript{19} and Kim et al. came up with the term multiconfigurational molecular mechanics (MCMM)\textsuperscript{20} as a general term for obtaining the PES. The MCMM method mixes empirical force fields to describe the PES through the use of an experimental correction.

There are also other approaches to modeling TSs more directly. Jensen developed the SEAM method\textsuperscript{21–24} for locating the minimum on the intersection of the reactant and product PES. There are some advantages in using the SEAM method, especially when it comes to performing geometry optimizations,\textsuperscript{12} but SEAM has also been known to provide differing geometries when comparing to the \textit{ab initio} results in some cases.\textsuperscript{21} Although there has been some improvement in the geometries,\textsuperscript{23} SEAM generally overestimates energies. More recent TS methods include asymmetric catalyst evaluation

\begin{figure}[h]
  \centering
  \includegraphics[width=\textwidth]{figure1.png}
  \caption{Relationship between different force field methods for TS modeling}
\end{figure}
(ACE)\textsuperscript{25} and true transition state force field (TTSFF).\textsuperscript{26} A comparison of the force field methods for TS modeling is given in Figure 1.2.

1.1.3 Transition State Force Fields and Q2MM

The quantum-guided molecular mechanics (Q2MM) method relies on QM reference data to begin the process. The training set is designed for a given reaction. Continuing down the flowchart in Figure 1.3, analysis of the initial force field is essential. The appropriate atom types and their respective parameters need to be defined in the working force field. For studies involving small organometallic molecules, the
MM3* force field\textsuperscript{27–29} is used. Although this force field has proven to be suitable, the parameters can in principle be fitted for the functional form of any force field.

Next, the force field parameters are fitted to the QM reference data by using a penalty function that is the weighted sum of squared differences between the QM and the MM calculated data points. The penalty function is

\[ \chi^2 = \sum_i w_i^2 (y_{QM} - y_{MM})^2 \]  

(1.2)

where \( w_i \) is the weight. Since each data type (e.g., bond lengths, bond angles) has different significant error, these data types need to be weighted differently.\textsuperscript{30} This penalty function is then minimized using a combination of Newton-Raphson and Simplex optimizations.\textsuperscript{31} Ideally, the objective function value should equal the number of data points used in the calculation. Following these steps, the results for each data point \( y_{MM} \) from the force field is compared to the QM reference data points \( y_{QM} \). Further adjustments can be made to the parameters to ensure the force field is accurate. Next, a test set of additional structures not incorporated in the training set are tested with their QM and MM parameters compared, with further adjusting if necessary. Then the force field is tested on experimental data. The enantiomeric excess (e.e.) is calculated using Equation 1.1 for a variety of experimental reactions in attempts to replicate the e.e. Assuming the data are reproduced well, the force field is then ready for use in predicting other important experimental reactions.

The Q2MM method has developed into a highly accurate predictive tool. This automated parameterization tool\textsuperscript{31} uses QM data to generate new MM parameters that are designed for a specific reaction.\textsuperscript{32} Therefore, each reaction requires its compatible force
field. TSFF’s from the Q2MM method work by replacing the negative Hessian eigenvalue depicting the reaction coordinate with a positive.\textsuperscript{2} The force field treats the transition state structure as a minimum. This is contrary to Paton’s TTSFF where he describes the TS structures as saddle points with the inclusion of the negative Hessian eigenvalue.\textsuperscript{26}

A unique quality that Q2MM has when compared to other methods\textsuperscript{33-36} is the use of the Hessian Matrix for the fitting of the parameters. This is significant because of the fact that the Hessian matrix is very large and contains $3N \times 3N$ data points, where $N$ is the number of atoms. Having so many data points allows Q2MM’s parameters to be fitted and defined properly\textsuperscript{30} in contrast to Houk’s TS model.\textsuperscript{13,16} More recently, the vibrational $\nu_{4}$ modes that describe the energy surface have been used as reference for parameterization. Limé and Norrby also noted how the reaction coordinate’s eigenvalue should be treated with the rest of the Hessian matrix (e.g., not holding the value fixed until the other parameters are well defined). Some reviews have also discussed this process.\textsuperscript{37-39}

1.2 Molecular Mechanics Parameter Development

In general, when using the Q2MM method, MM parameters in a substructure are developed. The more critical parameters for substructure development within the MM3* force field\textsuperscript{27} define stretching, bending, and dihedral interactions. Other parameters included define stretch-bend, improper torsion, van der Waals, and hydrogen bonding interactions. The functional form of the MM3 force field uses a quadratic function that describes a Morse potential.\textsuperscript{27} Although the MM3* force field is based on the MM3 force
field, it is not identical to it. MM3* uses point charges instead of bond dipoles to evaluate the electrostatics, and it uses a non-directional 10-12 potential instead of the MM3 Buckingham potential for hydrogen bonding.\(^{31}\) The general form of the MM3 total energy is

\[ E_{\text{Total}} = E_{\text{Stretch}} + E_{\text{Bend}} + E_{\text{Stretch-Bend}} + E_{\text{Torsion}} + E_{\text{Improper Torsion}} + E_{\text{Van der Waals}} + E_{\text{Coulombic}} + E_{\text{Hydrogen Bonding}} + E_{\text{1-4 Interactions}} \]  

(1.3)

Within this equation the bond stretch energy \((E_s)\) is defined as

\[ E_s = 71.94k_s(l-l_0)^2[1-2.55(l-l_0) + (7/12)2.55(l-l_0)^2] \]  

(1.4)

where \(k_s\) is the force constant, \(l\) is the bond length, and \(l_0\) is the equilibrium bond length.

The bending parameter is based on a sixth power function and was determined to fit experimental and \textit{ab initio} data.\(^{27}\) The bending energy \((E_\theta)\) is defined as

\[ E_\theta = 0.021914(k_\theta)(\theta-\theta_0)^2[1-0.014(\theta-\theta_0) + 5.6(10^{-5})\times(\theta-\theta_0)^2 - 7.0(10^{-7})(\theta-\theta_0)^3 + 9.0(10^{-10})(\theta-\theta_0)^4] \]  

(1.5)

where \(k_\theta\) is the force constant, \(\theta\) is the angle, and \(\theta_0\) is the equilibrium angle. The dihedral torsion parameter is based on a three-term Fourier series expansion and consists of three torsional constants, \(V_1\), \(V_2\), and \(V_3\).\(^{27}\) The torsional energy \((E_\omega)\) is defined as

\[ E_\omega = (V_1/2)(1+\cos \omega) + (V_2/2)(1-\cos 2\omega) + (V_3/2)(1+\cos 3\omega) \]  

(1.6)

where \(\omega\) is the dihedral angle.

An example substructure is represented in Figure 1.4. This example is part of the ferrocene substructure discussed in Section 2.4.1. When adding a substructure to the
force field, it is added to the bottom. Parameters at the bottom of the MM3* force field take priority over the parameters near the top in the version of the force field this thesis.\textsuperscript{40}

A typical substructure begins with a comment line followed by a line to describe atoms and their interactions. The line describing interactions, beginning with ‘9’, is how MacroModel\textsuperscript{41} defines a substructure. The symbols used are taken from the atom.typ file discussed later within this section. The characters in between the atom types describe the bonding pattern. The period (.), dash (-), equals sign (=), percent sign (%), and asterisk (*) represent a zeroth order bond, single bond, double bond, triple bond, and wildcard, respectively. The wildcard could be a single, double, or triple bond. Also, within this interaction line, numbers can be used. If a ‘5’ is used, then it is in reference to the 5\textsuperscript{th} atom presented (e.g., the ‘5’ used in Figure 1.4 corresponds to the second ‘D1’ atom type mentioned).

Atom types are defined by MacroModel\textsuperscript{41} and follow a specific format. Each atom type is depicted by two characters such as ‘C3’ (sp\textsuperscript{3} carbon), ‘O2’ (double bonded oxygen), ‘H1’ (electroneutral hydrogen), etc. There is also special atom type ‘00’ that is a wildcard. It can be used to define any atom type. In addition to the name of the atom type, there are also columns for atom weight, van der Waals radius, electronegativity, charge, valence, and more.
Continuing through to the next part of the substructure, there is a spacer line, indicated by a ‘-2’. Then the next set of lines define the parameters until the line ‘-3’ is reached, which signals the end of the substructure. These parameter lines commonly start with a ‘1’, ‘2’, or ‘4’ which indicate stretching, bending, and dihedral interactions. The other interactions mentioned earlier as well as these can be indicated with the digits 1-7. The parameters are described by three constants which are referenced in Table 1.1. A line can also begin with a ‘5’ preceding the digits just mentioned. This is an indication to continue from the previous line. For example, the ‘54’ in Figure 1.4 continues to describe the dihedral on the previous line with $V_4$, $V_5$, and $V_6$ terms all with units of kcal/mol.

<table>
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<tr>
<th></th>
<th>1</th>
<th>3</th>
<th>4</th>
<th>1.6781</th>
<th>4.0016</th>
<th>0.3026</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>6</td>
<td>7</td>
<td>1.4281</td>
<td>4.7290</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1</td>
<td>3</td>
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<td>87.0688</td>
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<tr>
<td></td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>180.0000</td>
<td>0.4436</td>
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<tr>
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<td></td>
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<td></td>
<td>5</td>
<td>0.0000</td>
<td>-0.1190</td>
<td>0.0000</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>6</td>
<td>7</td>
<td>8</td>
<td>CR</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Figure 1.4: Example substructure
TABLE 1.1

MM3* FORCE FIELD PARAMETER DESCRIPTIONS

<table>
<thead>
<tr>
<th>Interaction</th>
<th>First Constant</th>
<th>Second Constant</th>
<th>Third Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stretch</td>
<td>Bond Length (Å)</td>
<td>Force Constant (mdyn/Å)</td>
<td>Bond Moment (Debye)</td>
</tr>
<tr>
<td>Bend</td>
<td>Angle (°)</td>
<td>Force Constant (mdyn/rad²)</td>
<td>Bend-Bend FC</td>
</tr>
<tr>
<td>Dihedral</td>
<td>V₁ (kcal/mol)</td>
<td>V₂ (kcal/mol)</td>
<td>V₃ (kcal/mol)</td>
</tr>
</tbody>
</table>

Additionally, these parameters can also end with more columns. These indicate other interactions not described by the substructure. They describe two branched atoms per atom in the interaction. A bending parameter could have two additional columns that describe two branched atoms for each atom in the parameter. They can be written like ‘0000’, ‘C2C2’, another two atom type pair. An example is in Figure 1.5.

```
2  CR  C3  C0  109.6674  0.0666  0000 0000 C2C2
2  CR  C3  H1  105.2081  0.1056  0000 C200 0000
```

Figure 1.5: Optional parameters with indication of branching atoms

1.3 Rhodium-Catalyzed Hydrogenation of Enamides

Catalytic hydrogenation of alkenes has long been a hot topic in research. Many industries, including the pharmaceutical industry, have adopted these reactions into their manufacturing processes.⁴²⁻⁴⁴ The asymmetric hydrogenation of enamides reaction is frequently used in the synthesis of chiral, non-racemic derivatives of natural and
unnatural α-amino acids. These asymmetric reactions require chiral catalysts, an increasingly large number of which employ chiral ferrocene derivatives as ligands.

A generalized form of this type of hydrogenation using a rhodium catalyst is represented in Figure 1.6. The R groups determine the amino acid produced. Selecting a ligand that gives a specific enantiomer in high e.e. is not an easy task, and this is where Q2MM can make an impact. The development of the Q2MM force field for a virtual screening of a library of ligands used in this reaction would significantly advance experimentalist’s methods. So far, there have been many published parameters optimized by Q2MM for the Rh-catalyzed asymmetric hydrogenation of enamides and other asymmetric catalysis reactions.

![Figure 1.6: Rhodium-catalyzed hydrogenation of enamides](image)

Mechanistically, the rhodium-catalyzed hydrogenation of enamides is a multi-step process. There has already been a significant amount of work determining this mechanism. As described in Figure 1.7, the substrate initially binds to the Rh-complex to form a square planar substrate-catalyst complex. Following, the oxidative addition of H₂ to the complex presumably forms an octahedral dihydride species, although this complex has not been experimentally observed. Transfer of one hydrogen to the substrate forms the alkyl hydride complex which has been observed at low temperatures. Lastly, the other hydrogen transfers to the substrate creating the product.
A distinctive feature of the mechanism is the “anti-lock-and-key” principle, which means that the more stable square planar complex actually favors the formation of the minor product enantiomer.\(^{53,57,58}\) It is in fact the two substrate-catalyst complexes with hydrogen that the observed enantioselectivity is based on. Also, it has been determined that the formation of the alkyl hydride complex is irreversible.\(^{59}\) It is worth noting that Gridnev et al. has suggested an alternative mechanism that involves the dissociation of the carbon – carbon double bond from the metal as the rate determining step. Therefore, the stereoselection does not necessarily take place once the hydrogen chelates via oxidative addition.\(^{60}\)

![Diagram of mechanism](image)

**Figure 1.7**: Overall mechanism of rhodium-catalyzed hydrogenation of enamides

Formerly, the Wiest/Helquist group published a set of parameters to define the Rh-catalyzed reaction.\(^{48,49}\) The parameter set for this reaction will be referred to as Force
Field 08. The parameters were used to predict enantioselectivity, where it performed well. According to this publication,\textsuperscript{49} the prediction of enantioselectivity agrees with experimental data showing an R\textsuperscript{2} of 0.92. However, there is still room for improvement. There were three false positives which lowered the R\textsuperscript{2} value. One possibility is that the error comes from steric bulk as the false positives presented are some of the most sterically demanding in the data set. To improve on the results, the Wiest/Helquist Group is working on refining and improving Force Field 08. This working force field will be presented as Force Field 16 for the remainder of this thesis. The potential new set of parameters has displayed some significant improvement thus far.
CHAPTER 2:
DEVELOPMENT OF FERROCENE FORCE FIELD PARAMETERS

2.1 Introduction

A ligand class that is commonly used in industry and academia and has performed well in asymmetric hydrogenation are ferrocene-based ligands.\textsuperscript{46,47,61–63} However, the MM3* force field\textsuperscript{27–29} does not include metallocene structures, nor do the Rh-catalysis parameters developed by the Wiest/Helquist group cover ferrocene-based ligands. In order to use ferrocene-based ligands, new parameters must be developed to account for the various interactions. By placing these parameters within the MM3* force field along with the existing hydrogenation force fields, a working TSFF can be generated that will accurately account for these common ligands.

There are a number of ways in which the metallocene can be represented: rigid body,\textsuperscript{64,65} electrostatic and van der Waals interactions,\textsuperscript{66–68} σ-bonding,\textsuperscript{68–70} and dummy-bonding.\textsuperscript{71–75} Fey’s review\textsuperscript{76} suggests that the dummy-bonding approach is more accurate and produces less errors in comparison to the other approaches. This method involves a dummy atom at each of the centers of the cyclopentadienyl (Cp) rings that make up ferrocene. In the study presented here, the dummy atom has a zeroth order bond to each of the carbons within the Cp ring. The connectivity of the Cp ring to the Fe atom is simply a σ bond which allows for free rotation of the Cp rings.
Previously, an earlier member of the Wiest/Helquist group had done some initial work on the project. Ferrocene was modeled with the same dummy-bonding approach previously mentioned. Building upon the initial studies became the basis of the research described in this thesis. In this further work, many steps were taken differently along the process. All work done using Q2MM has been updated and replaced with the latest version of Q2MM. All other changes are addressed throughout the chapter. This older version of the ferrocene force field will be referred to as Force Field 13.

2.2 Computational Methodology

The QM calculations were performed using Gaussian 09, Revision D.01.\textsuperscript{77} Optimizations were done at the B3LYP level of theory using LANL2DZ ECP (effective core potential)\textsuperscript{78} on the Fe and Rh metals and 6-31G** on all remaining atoms. This level of theory is identical to that used in Donoghue’s work.\textsuperscript{48} Dummy atoms were placed at the center of the Cp rings after the QM optimizations were finished. Partial charges were calculated by electrostatic potential fitting.\textsuperscript{79} All partial charges on atoms not involved within the parameterization were held fixed at the MM3* force field’s values.\textsuperscript{27} Molecular mechanics level calculations were performed using MacroModel 10.3.\textsuperscript{41} All Gaussian calculations were considered complete after inspecting the convergence criteria and vibrational frequencies.

Generally, the force field was parameterized in the following order. Details are discussed in Section 2.4. First the partial charges were parameterized. Then the bond distances and angles followed. The force constants for those bonds distances and angles were parameterized next. Then the dihedral V terms were parameterized. Lastly, any
inaccurate parameters were reparameterized accordingly. Each substructure developed was also treated separately, i.e. the ferrocene core substructure was parameterized first, then the various ligands in the order presented.

Scans that are mentioned in Section 2.3 were parameterized initially to fit the energy curve. These scans contained approximately 16-26 structures depending on type of parameter and how the parameter can stretch, bend, or rotate. Building the structure included the use of another dummy atom which better defined the scan within Gaussian.

2.3 Quantum Mechanical Reference Data

Five common classes of ferrocene diphosphine ligands, three other types of substituted ferrocene derivatives, the unsubstituted ferrocene, and two non-ferrocene aminophosphines were used as reference structures for the parameterization (Figure 2.1). The five common classes of diphosphine ligands consist of Josiphos,\textsuperscript{80} Walphos,\textsuperscript{81} Taniaphos,\textsuperscript{82} Mandyphos,\textsuperscript{83} and Bophoz\textsuperscript{84} ligands. The three other types of ferrocene derivatives are modified structures based on the Walphos and Bophoz ligand classes. The two aminophosphines are structures designed to aid in the parameterization of the aminophosphine substructure referenced in Section 2.4.3. The five diphosphine classes were selected based upon the previous work done for Force Field 13. The reference structures used here, however, differ slightly from this previous work. The large training set selected for this study is to account for the large number of parameters needed for optimization. Because some of the parameters were pre-defined by the MM3* force field, the number of parameters that needed to be optimized was limited.
Figure 2.1: The reference structures that were used for parameterization of the MM3* force field

The ligands J1-J3, T1-T3, M1-M3, W1-W3, and B1-B3 from Figure 2.1 were complexed to Rh based on Donoghue’s publication. The resulting complexes will be referenced with the suffix Rh (e.g., J1Rh). The ligands J1, T1, M1, W1, and B1 were also optimized according to Figure 2.1. Ligands in black were used for parameterization whereas the ligands in red were used for internal validation.

2.3.1 Scans

Some parameters needed to be defined with higher accuracy, and therefore, needed additional reference data. Five different scans were included to better define several parameters. For example, a bond angle parameter could be scanned 15° above and below the predicted equilibrium angle with a step size of 2°. Figure 2.2 depicts which
parameters were scanned. Four of the scans consisted of the (1) angle bending of the Cp rings at the Fe center, (2) angle bending of the Cp rings at the dummy center, (3) bond stretching between the dummy and Fe, and (4) dihedral rotation of the Cp rings. These scans were performed on MB, MW, and UF from Figure 2.1. The remaining scan was performed on MF to describe the rotation of the ferrocene ligand with the ferrocene core. Scan 5 in Figure 2.2 shows one example. The scan used structure MF from Figure 2.1, and described the energy surface for both a phosphorus and sp^{3} carbon ligand.

![Figure 2.2: Depiction of the five scans performed](image)

2.4 Ferrocene Force Field

2.4.1 Ferrocene Core

The parameterization must begin with creating a substructure. Atom types and molecular mechanics parameters must be implemented into the existing MM3* force
field from MacroModel\textsuperscript{41} in order to accurately describe ferrocene. The substructure must be general but specific to ferrocene. By using the dummy approach, the substructure created is shown in Figure 2.3.

![Ferrocene substructure and MacroModel\textsuperscript{41} atom types](image)

Figure 2.3: Ferrocene substructure and MacroModel\textsuperscript{41} atom types

The carbon atom type $C_R$ was chosen because it is rarely used in the force field and is $sp^2$ hybridized. This atom type is unique because it is defined as an $sp^2$-type with 3 single bonds and no double bonds which allows the $Cp$ ring to become symmetric. The dummy atoms $D_1$ are a custom atom type with 0 amu, van der Waals radius of 0 Å, and electronegativity of 0. Another custom atom type created was $z_1$. This is the iron atom with 55.85 amu,\textsuperscript{85} 1.75 Å estimated van der Waals radius, 1.83 electronegativity on the Pauling scale,\textsuperscript{86,87} and 0 formal charge. The ‘00’ is a place holder that indicates any atom bonded to a $C_R$ atom.

Because of the symmetry of ferrocene, the substructure can be written with an emphasis on one $Cp$ ring. The first $C_R$ atom in the substructure is to account for the rotation between the $Cp$ rings and is only used in one parameter. Likewise, the ‘00’ is only used in one parameter. It helps define the angle of the ligand and whether it is toward or away from the Fe atom. The parameters of this ferrocene core substructure

21
consist of 4 bonds, 9 angles, and 7 dihedral torsions (Figure 2.4). Equilibrium bond angles indicated by an asterisk are considered ideal and were not parameterized. Many parameters that involve the dummy atom were not parameterized. This is due to the symmetry and orbital alignment of ferrocene.\textsuperscript{88–90} Many pentagon-related parameters remained unoptimized.

The parameters for this substructure were created by first averaging the equilibrium bonds and angles from the training set and estimating the remaining parameters. Then the charges were fitted to the training set, followed by both of the bond and angle force constants. These force constants were fit to the Hessian eigenvalues. Then the equilibrium bonds and angles were fitted together. Once more, both the bond and angle force constants were fitted to the Hessian eigenvalues. Next, scans were incorporated to more accurately define the four indicated parameters in Figure 2.4. The torsions were developed by first fitting to the torsions, and then to both the torsions and the Hessian eigenvalues. The weight for each of the data types varied. The Hessian eigenvalues were weighted to 0.10 per eigenvalue except the first eigenvalue, which was 0.00 due to the negative eigenvalue on the TS models. The bonds are weighted as 100.00, angles as 2.00, torsions as 1.00, charges as 10.00, and averaged energies as 20.00. The objective function (Equation 1.2) for this substructure with the inclusions of the scans is 32,699,902.75 (703,076 data points). A large contribution to this value is due to the scans. The minimum of the energy curves is defined well, but outside the minimum the MM calculated energies can be significantly different from the QM. Further information can be found in Appendix A.4. The objective function excluding the scans is 402,633.19 (702,827 data points).
The initial parameters for the ferrocene substructure in Force Field 13 were nearly finished. The C\textsubscript{R} atom type was kept along with the dummy atoms and Fe atom. However, there were a few issues that needed to be resolved. One issue was the torsions. Many of the MM calculated torsions deviated from the QM calculated reference structures. It has been mentioned that because of this fact is why the diastereomeric TSs’ energies differ so much from experimental results. A dihedral parameter not included in Force field 13 was the parameter that defines the rotation of Cp rings. By including it here, the appropriate eclipsed or staggered conformation is modeled accurately. Going beyond the typical V1, V2, and V3 terms to the V5 term was needed to describe the rotation of the 5-membered rings. Another new parameter introduced was the z\textsubscript{1}-D\textsubscript{1}-00 angle where 00 represents any atom adjacent to the Cp ring. In the unsubstituted ferrocene, each of those atoms would be hydrogens. Additionally, the parameterizations involving scans was a new addition to the project. The ferrocene core has shown significant improvement when comparing the MM data to the QM data which is discussed in Section 2.5.
Figure 2.4: MM3* bond, angle, and torsional parameters for the ferrocene substructure. Values in red were determined by fitting to the energies from several scans.

2.4.2 Ferrocene Ligands

Initially, the core parameters were finished using only reference structures MW and UF. When testing those parameters, it became clear that several parameters were missing because of the uniqueness of the C_R atom type. Essentially, every parameter that includes one of the carbons from a Cp ring of ferrocene needed to be optimized. To resolve this issue, a larger training set was required.

Because the C_R atom type is so specific, each ligand needed to be carefully checked for missing parameters within the MM3* file. An additional three substructures
were created for ferrocene to account for these parameters. Each ligand, depending on atom type, has its own substructure to organize the ferrocene parameters in a convenient method. The substructures created (Figure 2.5) are unique to ferrocene because of the inclusion of the $C_R$ atom type.

![Chemical structure diagram](image)

Figure 2.5: Three ferrocene ligands substructures and MacroModel atom types

The atom types $C_2$ and $C_3$ are the standard $sp^2$ and $sp^3$ carbons, and the $P_X$ signifies any phosphorus atom type. The parameters for the three substructures are shown in Figures 2.6, 2.7, and 2.8.

The parameters for these three substructures were created similarly to the ferrocene core substructure. First, the equilibrium bonds and angles were averaged from the training set, and the remaining parameters were estimated. The charges were then fitted to the training set. The bond and angle force constants were fitted to the Hessian eigenvalues, the equilibrium bonds and angles were fitted to the training set’s bonds and angles, and the bond and angle force constants were again fitted to the Hessian eigenvalues. Next, the torsions were fitted to the training set’s torsions, and then to both the torsions and the Hessian eigenvalues. Then the scans were included to further define the parameters indicated in Figures 2.7 and 2.8. The weights for the different data types
were the same as those mentioned in Section 2.4.1. The objective function for the C₂ substructure is 77,134.09 (131,679 data points). The objective function for the C₃ substructure is 701,704.86 (698,088 data points), and it is 423,139.97 (697,980 data points) excluding the scans. For the Pₓ substructure, the objective function is 667,011.80 (566,280 data points), and it is 356,273.49 (566,208 data points) excluding the scans.

C  Ferrocene_C2_Ligands
9  CR-CR-C2*C2
-2
1  2  3     1.4818     4.4006     0.0416
2  1  2  3     127.5207     0.7638
2  D1  2  3     180.0000     0.0000
2  2  3  4     120.9351     0.1868
4  H1  1  2  3     0.0000     0.0164     0.0000
4  CR  1  2  3     0.0000     6.2370     0.0000
4  1  2  3  4     0.0000     0.0095     0.0000
4  2  3  4  00     0.0000    11.0467     0.0000
4  4  PX  C3  00     0.0000     0.0000     5.1050
-3

Figure 2.6: Ferrocene C2 ligand’s force field parameters

C  Ferrocene_C3_Ligands
9  CR-CR-C3
-2
1  2  3     1.4942     4.9992     0.3048
2  1  2  3     127.7934     0.6321
2  D1  2  3     180.0000     0.0000
2  2  3  00     108.6564     0.1652
2  2  3  C0     109.7558     0.3648
2  2  3  H1     111.0907     0.4379
2  2  3  00     108.7430     0.4477     0.0000 C200 0000
2  2  3  C0     109.6674     0.0666     0.0000 0000 C2C2
2  2  3  H1     105.2081     0.1056     0.0000 C200 0000
4  H1  1  2  3     0.0000    7.4660     0.0000
4  C2  1  2  3     0.0000     6.9446     0.0000
4  CR  1  2  3     0.0000     1.6282     0.0000
4  1  2  3  00     0.0000     0.0000     1.3513
4  2  3  00  00     0.0000     0.0000     1.0195
-3

Figure 2.7: Ferrocene C3 ligand’s force field parameters. Values in red were determined by fitting to the energies from several scans.
C Ferrocene_PX_Ligands
9 CR-CR-PX
-2
  1 2 3 1.8152 2.9094 -0.2916
  2 1 2 3 127.6534 0.7646
  2 D1 2 3 180.0000 0.0000
  2 2 3 00 104.3945 1.4235
  2 2 3 H1 99.5890 0.9354
  4 H1 1 2 3 0.0000 1.0879 0.0000
  4 C3 1 2 3 0.0000 2.0940 0.0000
  4 CR 1 2 3 0.0000 1.9346 0.0000
  4 1 2 3 00 -7.2055 -0.8095 1.0684
  4 2 3 00 00 0.0000 0.0000 1.4752
-3

Figure 2.8: Ferrocene PX ligand’s force field parameters. Values in red were determined by fitting to the energies from several scans.

2.4.3 Aminophosphine Ligands

With the majority of the parameters optimized, there were still certain ligands that did not contain enough parameters. Specifically, the Bophoz ligands lacked a predefined phosphorus-nitrogen bond in the MM3* force field. This was advantageous to selecting its substructure recognition. The small PX-N3 substructure was selected and was specific enough in order to implement this into the force field.

The parameters for these three substructures were created similarly to the ferrocene ligands’ substructures. The only difference is the lack of any scans used in this substructure. The weights for the different data types were the same as those mentioned in Section 2.4.1. The objective function for the substructure is 139,950.01 (117,564 data points).
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<tr>
<td></td>
<td>4</td>
<td>1</td>
<td>2</td>
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</table>

Figure 2.9: Aminophosphine force field parameters

2.4.4 Combining with the Rhodium Force Field

Ultimately, the ferrocene force field was designed to work with the previously developed rhodium force field. Combining these force fields is critical for its use. When attempting to join these force fields together, there was a minor issue that needed to be addressed. Some parameters were not defined within Force Field 08. Parameters were developed on the basis of having hydrogens on the phosphorus atoms. By adding angle and torsional parameters that account for the variety of atoms bonded to phosphorus, the issue was resolved.

Once the modified version of the rhodium force field, Force Field 16, is finished, the ferrocene force field needs to work with this version as well. Similar parameters will need to be added along with other more rhodium-based parameters depending on the tested structure.

The parameters for these two substructures were created similarly to the others. The differences here were that there were no scans used in parameterization as well as no bonds or charges. The weights for the different data types were the same as those mentioned in Section 2.4.1. The objective function when combining with Force Field 08
is 4,559,869.52 (636,630 data points), and it is 345,106.28 (636,593 data points) when combining with Force Field 16.

<table>
<thead>
<tr>
<th>C</th>
<th>Ferrocene_Rhodium</th>
<th>9</th>
<th>PX=z2</th>
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<tr>
<td>-2</td>
<td></td>
<td>2</td>
<td>00 1 2</td>
</tr>
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<td>00 00 1 2</td>
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</table>

<table>
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<tr>
<th>C</th>
<th>Force_Field_16_Rhodium</th>
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<th>HX-z2(-PX)-HX.C2=C2(.2)-N2-C2=O2.2</th>
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<td>-2</td>
<td></td>
<td>2</td>
<td>4 5 O3</td>
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<td>4</td>
<td>O3 5 6 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>2 6 C2 C2</td>
</tr>
</tbody>
</table>

Figure 2.10: Ferrocene-rhodium combined force field parameters. Parameters highlighted in red should also be added to Force Field 16

2.5 Internal Validation

The parameters developed were used to calculate MM data such as bond lengths, bond angles, Hessian eigenvalues, dihedral torsions, etc. The comparable QM data were previously calculated when creating the reference structures in Figure 2.1. The MM data were fitted to the QM reference data when creating the parameters in Section 2.4. The penalty function from Equation 1.2 is used to optimize those parameters. Ideally, the MM data should fit exactly to the QM reference data with an $R^2$ of 1.0. The data were compared and tested to determine the accuracy of the parameters. Figures 2.11 and 2.12 display the comparison of the MM bond lengths and angles to the QM reference bond
lengths and angles, respectively. The plots show good reproducibility overall with an $R^2$ of 0.999 for the bond lengths and an $R^2$ of 0.998 for the bond angles.

Similarly, Figure 2.13 shows the comparison of Hessian eigenvalues calculated by MM compared to the Hessian eigenvalues calculated by QM. The eigenvalues agree well with an $R^2$ of 0.996. The data for this figure were generated using only the structures from the training set that excluded Rh. This is to show how the new ferrocene force field performs in comparison to QM data.

![Figure 2.11: Internal validation of bonds for the test set](image)

Figure 2.11: Internal validation of bonds for the test set
Figure 2.12: Internal validation of angles for the test set

Figure 2.13: Internal validation of Hessian eigenvalues for the test set
The MM calculated torsions were validated just as the previous data types. The MM calculations correlated well with the QM calculated torsions. The $R^2$ was 0.998 as seen in Figure 2.14. This validation was compared to a similar validation with Force Field 13. The same reference structures and calculations were used in Figures 2.14 and 2.15. As Figure 2.15 shows, the calculated $R^2$ is 0.450. Comparing the two figures, it is apparent that the newly developed ferrocene force field outperforms Force Field 13 for the calculation of torsions. The correlation coefficient improves by 0.548, and the slope increases from 0.450 to 1.007. If both the slope and the correlation coefficient were 1.0, then the MM data points would agree perfectly with QM data. Additionally, the new dihedral torsion agreement has not caused a disruption in the performance of the other parameters. A representative overlay of the QM structure and the MM structure is displayed in Figure 2.16.

![Figure 2.14: Internal validation of torsions with the new force field](image)

Figure 2.14: Internal validation of torsions with the new force field
Figure 2.15: Internal validation of torsions with Force Field 13

Figure 2.16: Overlay of structure J2Rh. QM structure is colored blue and MM structure is colored orange
Another noteworthy example displaying the differences in the force field presented in this thesis and Force Field 13 is a newly implemented torsion. This torsional parameter describes the eclipsed and staggered conformations of the Cp rings. The parameter was also developed through the use of the scan technique as mentioned previously. By scanning the parameter, in this case, from 0° (eclipsed) to 36° (staggered) to 72° (eclipsed), the rotation is described and compared to Force Field 13 in Figures 2.17 and 2.18. The MM energies in the new force field agree well with the QM energies, and agree better than that for Force Field 13. In fact, Force Field 13 calculates the wrong conformation (staggered) as being the minimum energy structure according to the QM calculations. Additional parameters treated by the scan technique showed similar agreement and are presented in Appendix A.4.

![Figure 2.17: Example dihedral torsion scan with new force field](image)
The new force field developed for ferrocene has shown improvement and better agreement with the QM data than Force Field 13. This updated version has applied a new technique with a variety of scans. It has also been created to be a more general force field with fewer parameters overall. With that said, this is an area where there could be more improvement in the future. There are many different kinds of metal-coordinating groups that could potentially be incorporated into ferrocene. This force field was designed to be generic for the most common types of coordinating groups associated with ferrocene.

2.6 Comparison of Diastereomers

Before testing the ferrocene force field on experimental data, the force field was tested prior to combination with the rhodium force field. Various diastereomers from Figure 2.1 were selected to compare energy differences at the QM and MM levels.

Figure 2.18: Example dihedral torsion scan with Force Field 13
Structures highlighted in red (except for the Mandyphos-type ligands due to their symmetry) were subjected to a conformational search to find the lowest energy structure. This was done for four different stereoisomers per structure. The energetic differences between the central (R/S<sub>c</sub>) and planar (R/S<sub>p</sub>) absolute configurations were compared. Following, a single point QM calculation was performed for each lowest-energy conformation. A set of four different diastereomers that were tested is represented in Figure 2.19.
Figure 2.19: Example of the four diastereomers tested for T4Rh
The energy difference in diastereomers produced from QM calculations were compared to the MM results. Each structure contributed to four data points in Figure 2.20. The energies are in agreement with each other with an $R^2$ of 0.910.

Figure 2.20: Representation of diastereomeric energy differences for various ferrocene-based ligands
CHAPTER 3:
EXTERNAL VALIDATION

3.1 Introduction

The newly generated ferrocene force field, Force Field 17, was to be further investigated on its reproducibility of experimental data. The rhodium-catalyzed hydrogenation of enamides is a well-studied reaction, and ferrocene ligands are frequently used. The experiments provided the data to test Force Field 17. However, finding a variety of ferrocene derivatives used in published work was more difficult since it is common to use one general type of ligand in a study.

Testing experimental data helps ensure that the parameters accurately define the energy differences, particularly those energy differences in the lowest energy conformation for each enantiomer. By analyzing these data, small adjustments can be made to correct any errors.

3.2 Computational Methodology

Molecular mechanics calculations were performed with MacroModel 10.3. Conformational searches were sampled with Monte Carlo for a minimum of 15,000 conformations per structure. Rings were broken and opened prior to any torsional motion. The structures were considered converged when no new energy structures were generated.
within the last 5000 steps. Implicit solvent conformational searches were performed using parameters for CHCl₃.

QM calculations were performed using Gaussian 09, Revision D.01. The level of theory used was B3LYP with LANL2DZ ECP on the Fe and Rh metals and 6-31G** on all remaining atoms.

The enantiomeric excess calculation uses a Boltzmann distribution to find the enantioselectivity of the reaction. The enantioselectivity is defined by Equation 1.1. Further discussion of enantioselectivity is discussed in Chapter 1.

3.3 Reference Structures

The test set consists of a variety of ferrocene-based ligands and substrates. Common ferrocene derivatives such as Bophoz-, Josiphos-, Taniaphos-, and Walphos-type compounds are included in Figure 3.1. The test set was designed to be different from the training set, however, it was also created to use similar ferrocene derivatives. Since the training set consisted of the more common ferrocene-based ligands, finding experimental data for these ligands came with ease.
Figure 3.1: Ferrocene-based ligands and substrates used in experimental test set. Ligands are denoted with letters and substrates with numbers.

3.4 Test of Computational Parameters

A few questions still remained that needed to be addressed. Could Force Field 08 or Force Field 16’s current rhodium force field be used to determine enantiomeric excess? In other words, which force field yields better predictions for the Rh-catalyzed hydrogenation of enamides? Also, should solvent be used to give better agreement with experimental data? To answer these questions a series of tests were run for ligand b and substrate 2 in Table 3.1. The idea behind this test was to validate the computational parameters that could be carried out to the rest of the test set. This ligand and substrate
### TABLE 3.1
DEVELOPMENT OF CONFORMATIONAL SEARCH PARAMETERS

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<tr>
<th>Entry</th>
<th>Ligand</th>
<th>Substrate</th>
<th>Solvent</th>
<th>Rh FF</th>
<th>R (kJ/mol)(^a)</th>
<th>S (kJ/mol)(^a)</th>
<th>ΔG (kJ/mol)</th>
<th>% e.e. (Config)</th>
<th>Exp. % e.e. (Config.)</th>
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<td>98.8 (R)</td>
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<td>98.8 (R)</td>
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\(^a\) Lowest energy structures of R and S configurations
pair was chosen to test due to the lack of agreement between the MM and experimental predictions as seen in entry 1 of Table 3.1.

The initial test run with no solvent and Force Field 08 predicted an enantiomeric excess of 71.6% favoring the S configuration. This was different from the experimental data showing 98.8% preference for the R configuration. It was found that by introducing solvent into the system, the agreement improved slightly; the enantiomeric excess was predicted to be 45.5% favoring the S configuration. When exchanging Force Field 08 for a revised edition, Force Field 16, the agreement of the enantiomeric excess improved to 21.3% favoring the R configuration. It was not until the addition of Force Field 16’s updated rhodium force field that the experimentally favored configuration was predicted. A combination of solvent with Force Field 16 produced the best result of 73.4% e.e. whereas the experimental % e.e. was 98.8%.

Using the best conditions from Table 3.1, the three lowest energy structures for both configurations were taken and tested further. Each of these structures underwent a single point QM calculation to see if the QM energies resulted in better enantiomeric excess prediction. When comparing the predicted energies produced by QM to MM, the QM energies showed even further improvement from the MM energies. The MM energies resulted in 73.5% e.e., and the QM energies predicted the enantiomeric excess of 95.9%. This was much closer to the experimental e.e. of 98.8%. This indicates that the MM likely produces the correct minimum structures, but QM more accurately defines the energies.
### TABLE 3.2

**QUANTUM MECHANICAL CALCULATIONS OF MOLECULAR MECHANICS MINIMUM ENERGY STRUCTURES**

<table>
<thead>
<tr>
<th>Entry</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Configuration/Structure</strong></td>
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<tr>
<td><strong>MM Energy (kJ/mol)</strong></td>
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<tr>
<td><strong>QM Energy (kJ/mol)</strong></td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
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</tr>
<tr>
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<td>5</td>
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<tr>
<td>6</td>
</tr>
</tbody>
</table>

Predicted % e.e. (Config.): 73.5 (R) 95.9 (R)

Experimental % e.e. (Config.): 98.8 (R) 98.8 (R)

---

a) Optimized conditions (CHCl\textsubscript{3} Solvent, Force Field 16’s Rh FF)
b) Single point, gas phase calculations with Gaussian 09, Revision D.01: Fe and Rh – LANL2DZ ECP
All other atoms – B3LYP/6-31G**
3.5 Initial Testing

The method outlined in the previous section applied to ligand $b$ and substrate $2$ improved the agreement of e.e. and the experimental e.e. The experimental e.e. was 98.8% in favor of the R configuration. Initially, the e.e. prediction was 71.6% favoring the S configuration. By following the procedure described in Section 3.4, the e.e. prediction improved to 95.9% in favor of the R configuration, in close agreement with experiment.

This method was then applied to the remainder of the test set. Table 3.3 displays the performance of Force Field 17. It can be seen that entry 2 shows good agreement to the experimental e.e. The predicted e.e. was 96.3% (R), and the experimental e.e. was 99.6 (R). Entry 2 uses the same ligand as entry 6, the ligand-substrate pair used for optimization purposes. Other entries that have resulted in good agreement to the experimental data were 7 and 13. These entries predicted e.e. that were 8.9% and 6.0% above the experimental e.e., respectively. Many other entries show differing % e.e., and some display differing major enantiomers. For example, entries 1, 3, 4, 5, and 10 all predict the incorrect major configuration according to the experimental results. Entries 1 and 3 were initially expected to perform well because to the only difference to the ligands were changes in chirality when compared to entries 2 and 6 (ligand $b$). However, the chirality significantly effects the outcome of the predictions. Ligand $a$ predicted 100.0% e.e. favoring R (experimental e.e. 10.6% favoring the S configuration), and ligand $c$ predicted 100.0% favoring R (experimental e.e. 99.6% favoring the S configuration). Ligand $b$’s results were discussed earlier. Thus, Table 3.3’s results are inconclusive as the successful attempts appear to be random.
A new method to initialize conformational sampling was developed at this point. This method initializes and sets up conformational searches in an automated fashion. The automation requires a library of ligands and substrates to be created to work with the reaction template, Rh core. The conformational searches were initialized with this new development for the same test set as Table 3.3. The new results are shown in Table 3.4. Similarly, the results from this test do not show agreement of calculated to experimental results. However, the M.M. % e.e.’s in Table 3.4 agree consistently better than that in Table 3.3. For example, entry 5 predicted 3.4% - R in Table 3.3 and 14.4% - R in Table 3.4. The experimental result was 61.8% - R. Also, entry 7 predicted 34.1% - R,S in Table 3.3 and 96.5% - S,R in Table 3.4. The experimental result was 91% - S,R. Differences between the two tables occur because Table 3.4’s data were produced without implicit solvent conformational searches whereas Table 3.3’s data involved solvent. Only entry 8’s predictions worsened by a significant margin. In Table 3.3, the predicted e.e. was 96.5% - R,S, and in Table 3.4, the prediction changed to 97.8% - S,R. The experimental e.e. was 46% - R,S. The same lowest energy structures were obtained in each method, but there is a significant solvent contribution. The lowest energy structure in the R configuration is stabilized by the solvent more than the S configuration. However, neither predict the experimental e.e. The present version of the force field will, therefore, have to be modified before it can be used in real-life applications.
### TABLE 3.3

**INITIAL ENANTIOMERIC EXCESS PREDICTIONS**

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<th>QM Predicted % e.e. (Config.)</th>
<th>Exp. % e.e. (Config.)</th>
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<tr>
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## TABLE 3.4
SECOND ENANTIOMERIC EXCESS PREDICTIONS

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3.6 Conclusion

Overall, Force Field 17 reproduces QM energies and data types (bonds, angles, etc.) very well. The various parameters are reproduced with an $R^2 > 0.996$ as shown in Section 2.5. Also, the relative energies of diastereomers from the validation set are accurately predicted by the given force field and gave an $R^2$ of 0.910 relative to QM data. After the Force Field 17 underwent internal validation, it was then tested for the prediction of experimentally observed enantiomeric excess. By testing one ligand-substrate pair, conditions were developed that improved the e.e. agreement. Ligand $b$ and substrate 2 from Figure 3.1 initially predicted an e.e. of 71.6% S. After applying Force Field 16 and solvent, the predicted e.e. improved to 95.9% R. The experimental e.e. was 98.8% R. By applying the procedure from Section 3.3 to the rest of the test set, initial results were gathered. The predictions often were very different from the experimental values as described in Section 3.5. Some predictions were accurate, however. Entries 7 and 13 overpredicted the e.e. by 8.9% and 6.0%, respectively, in Table 3.3. Unfortunately, the results were inconclusive.

Notably, the rhodium force fields, Force Field 08 and Force Field 16, significantly affect the outcome of the predictions. According to Table 3.1, Force Field 08 predicted at best an e.e. of 45.5% S compared to the experimental 98.8% R. Force Field 16 predicted an e.e. of 74.4% R for the same ligand-substrate pair. In this case, the version of the rhodium force field affects the prediction of e.e. by a large margin. Finding the best parameters for the rhodium force field, although difficult, is necessary for testing the ferrocene force field with the Rh-catalyzed hydrogenation of enamides reaction. One possibility is that the rhodium force field needs to be parameterized with the inclusion of
the ferrocene ligand class. Additionally, the version of Force Field 16 that was used to generate this data is currently being modified further. Once those parameters are in their final condition, it could positively impact the ferrocene force field’s e.e. predictions.

It would be ideal to create a method for testing the ferrocene force field without the combination with Force Field 08 or Force Field 16. The test on the various diastereomers in Section 2.6 tried to do just that. The energy differences predicted from QM single point calculations were reproduced by Force Field 17 with a correlation coefficient of 0.910. Comparing the calculated energy differences with experimental data would further enhance the force field. By testing just the ferrocene force field and not the rhodium force field, the source of error in the e.e. predictions would become apparent.
### A.1 Additional Force Fields

The two versions of the rhodium force fields are represented below for reference. Since the version of the force field alters the predicted outcome, it is important to know the parameters involved in each.

**Force Field 08’s Rhodium Substructure**

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**Force Field 16’s Current Rhodium Substructures**

C Rhodium Force Field 16

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53
A.2 Quantum Mechanical Training Set

Structures follow the naming scheme in Figure 2.1. All Cartesian coordinates shown are optimized with B3LYP/LANL2DZ ECP for metals and B3LYP/6-31G** for nonmetals. Coordinates are listed in ångströms. Energies are in Hartrees and negative frequencies are in cm⁻¹.

**TABLE A.1**

ENERGIES AND NEGATIVE FREQUENCIES OF QM TRAINING SET

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C   -2.992034756    -0.8042375787   0.7283496857
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C   0.8990061510  0.8313061313  2.2652176041
C   1.1724407307  1.9622407831  1.8133228567
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Structure 22, MB

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C   0.9827796329 -0.7140266771  1.6869073094
C  -0.3753612969 -1.1552590427  1.6862085532
H  -0.7098975812  2.1831732070  1.6590727589
H   1.8573928753  1.3495291846  1.6614044428
H   1.8573928755 -1.3495291842  1.6580252432
H   1.8573928755  1.3495291848  1.6614044383
H   1.8573928755 -1.3495291840  1.6580252432
H  -0.7098975807 -2.1831732072  1.6590727596
C   0.9827796329 -0.7140266771  1.6869073108
H  -0.3753612971  1.1552590426  1.6862085522
H  -1.2146568370  0.0000000000  -1.6857491366
C  -0.3753612969 -1.1552590425 -1.6862085534
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C   0.9827796328  0.7140266775  1.6869073107
C  -0.3753612971  1.1552590426 -1.6862085522
H  -0.7098975807 -2.1831732074  1.6590727599
H   1.8573928755 -1.3495291840  1.6614044427
H   1.8573928755  1.3495291848  1.6614044427
H  -0.7098975812  2.1831732072 -1.6590727587
H  -2.2956751261  0.0000000000 -1.6580252432

Structure 24, A1

C   -1.6386922844  0.4689028795  0.5952015105
H   -2.6679465933  0.7263766929  0.8843573224
N   -0.8785229159  1.7142689856  0.4531619086
C   -1.4027494724  2.6895930205  -0.4978997220
H   -1.3212584215  2.3617700041  -1.5436323224
H   -2.4609200957  2.8880694163  -0.2866206385
H   -0.8550272377  3.6282234128  -0.3843631698
P   0.7567777446  1.6991360517   0.9453873686
C  -1.6613865209  0.4284577990  -0.6482501376
H   -2.2377826349  1.3383015777  -0.4487018258
H   -2.1230865972  0.0735255902  -1.5040995890
H   -0.6460279210  0.7202882740  -0.9342513647
O   0.9531131298  3.3383519503   1.2887172311
O   1.6870946836  1.7907521220  -0.4251860287
H   0.4458751317  3.5778707835   2.0766743823
H   1.6919522807  2.6904174502  -0.7909887460
H  -1.2045322754  0.0857086851  1.4348159290

Structure 25, A2

C   -1.2099258176  0.2516414235  0.2667998146
H   -2.2525107138  0.1568844762  0.6023871038
A.3 Quantum Mechanical Validation Set

Structures follow the naming scheme in Figure 2.1. All Cartesian coordinates shown are optimized with B3LYP/LANL2DZ ECP for metals and B3LYP/6-31G** for nonmetals. Coordinates are listed in ångströms, and energies are in Hartrees. Many of the structures in Table A.2 contain diastereomers that were mentioned previously. All of the energies are listed, but only the (a) diastereomer’s coordinates are listed.

**TABLE A.2**
ENERGIES OF QM VALIDATION SET

<table>
<thead>
<tr>
<th>Structure (Diastereomer) – Name</th>
<th>SCF Energy</th>
<th>Zero Point Energy</th>
<th>Total Energy</th>
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<tr>
<td>3 (b) – T4</td>
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### TABLE A.2 (contd.)

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TABLE A.2 (contd.)

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C 3.948745 2.113094 -1.543486
C 4.349020 2.728182 -2.776695
C 3.775660 1.997230 -3.854842
H 3.850500 2.248089 -4.905668
H 2.425117 0.219510 -3.869871
C 5.843273 -1.082994 -2.024746
C 6.684987 0.004185 -1.630366
C 7.133856 0.669222 -2.815563
C 6.569813 -0.009173 -3.942942
C 5.771741 -1.092072 -3.453328
H 6.976308 0.244021 -0.615369
H 7.823538 1.503266 -2.853989
H 6.758115 0.221842 -4.984064
H 5.247415 -1.821791 -4.057979
H 5.383693 -1.803997 -1.360490
C 4.166294 2.688557 -0.156548
H 4.125495 1.835275 0.562199
P 2.689805 3.766042 0.274468
C 5.529702 3.375072 0.038532
H 6.366337 2.674109 -0.176056
H 5.664545 4.251093 -0.631822
H 5.675459 3.730128 1.081783
H 4.911891 3.647379 -2.872122
P 2.022105 0.070390 -0.709893
C 0.991694 -4.011717 -2.643601
C 0.294069 -2.871933 -3.045034
C 0.583670 -1.635874 -2.464031
C 1.562791 -1.536765 -1.472691
C 2.268085 -2.678089 -1.084676
C 1.981244 -3.914989 -1.664754
H 0.764390 -4.988335 -3.103599
H -0.483736 -2.946609 -3.823918
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**Structure 2, J5**

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A.4 Scan Information

Scans are presented in the same order as Figure 2.2. Structures follow the same naming scheme in Figure 2.1. All Cartesian coordinates shown are optimized with B3LYP/LANL2DZ ECP for metals and B3LYP/6-31G** for nonmetals. Coordinates are listed in ångström, and energies are in Hartrees. Within each scan, only the starting structure’s coordinates are listed. Force Field 17 was used to calculate MM energies for each scan. Energies for each scan will be presented in the following format.

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**Scan 1 – D1-z1-D1 Bend**

*Structure 1, UF*

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| 169.9000° | -510.52231 | -100.4093 | -86.8885 |
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**Scan 2 – z1-D1-CR Bend**

**Structure 4, UF**

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Structure 5, MW

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\text{H} & 4.248533 & -0.477847 & 2.951287 \\
\text{C} & 3.117351 & 0.889785 & 3.957110 \\
\text{H} & 3.619368 & 0.656258 & 4.898755 \\
\text{H} & 3.528161 & 1.838690 & 3.570079 \\
\text{H} & 2.058832 & 1.049091 & 4.175357 \\
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**Scan 4 – C\(_R\)-D\(_1\)-D\(_1\)-C\(_R\) Dihedral Torsion**

**Structure 10, UF**

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15.0000 & -510.52722 & -0.2584 & -0.2471 \\
18.0000 & -510.52709 & 0.0803 & 0.0449 \\
21.0000 & -510.52697 & 0.3951 & 0.3369 \\
24.0000 & -510.52686 & 0.6891 & 0.6092 \\
27.0000 & -510.52676 & 0.9532 & 0.8429 \\
30.0000 & -510.52668 & 1.1677 & 1.0224 \\
33.0000 & -510.52662 & 1.3219 & 1.1352 \\
36.0000 & -510.52659 & 1.3817 & 1.1736 \\
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42.0000 & -510.52667 & 1.1719 & 1.0222 \\
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H    0.709744 -2.182533 -1.661673
H    2.293241 -0.002525 -1.663833
C    0.374993 -1.154047  1.685836
C   -0.981677  0.713292  1.685917
C   -0.981746  0.713251  1.685985
C    0.374973 -1.154101  1.685985
H   -1.854222 -1.347922  1.665326
H   -1.854766  1.347429  1.666665
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Structure 11, MW

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| C  | -0.997938 | 0.745535 | -1.652925 |
| C  | -1.039503 | -0.684282 | -1.673192 |
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| H  | -1.861689 | 1.391749 | -1.602651 |
| H  | 2.254599 | -0.021763 | -1.694595 |
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| C  | 0.375585 | -1.153534 | 1.691706 |
| C  | -0.981372 | -0.713599 | 1.691009 |
| C  | -0.982092 | 0.713189 | 1.689687 |
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| H  | -1.856024 | -1.346185 | 1.678811 |
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| C  | 1.775787 | -2.852499 | -2.799609 |
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| C  | -4.367122 | -2.766479 | -3.244878 |
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**Structure 12, MB**

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129
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Scan 5 – C_R-C_R-00-00 Dihedral Torsion

Structure 13, F1 (R=PH₂)

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Structure 14, F1 ($R=P(CH_3)_2$)

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Structure 15, F2 (R=CH₃)

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Structure 16, F2 (R=C(CH3)3)

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Initial Coordinates:
Structure 17, F2 (R=C(CH\textsubscript{3})(NH\textsubscript{2})PH\textsubscript{2})

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REFERENCES


