2018

Catalyst Design and Mechanism Study with Computational Method for Small Molecule Activation

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CATALYST DESIGN AND MECHANISM STUDY WITH COMPUTATIONAL METHOD FOR SMALL MOLECULE ACTIVATION

by

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A dissertation submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy
in the Department of Chemistry
in the College of Science
at the University of Central Florida
Orlando, Florida

Fall Term
2018

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ABSTRACT

Computational chemistry is a branch of modern chemistry that utilizes the computers to solve chemical problems. The fundamental of computational chemistry is Schrödinger equation. To solve the equation, researchers developed many methods based on Born-Oppenheimer Approximation, such as Hartree-Fock method and DFT method, etc. Computational chemistry is now widely used on reaction mechanism study and new chemical designing.

In the first project described in Chapter 3, we designed phosphine oxide modified Ag_3, Au_3 and Cu_3 nanocluster catalysts with DFT method. We found that these catalysts were able to catalyze the activation of H_2 by cleaving the H-H bond asymmetrically. The activated catalyst-2H complex can be further used as reducing agent to hydrogenate CO molecule to afford HCHO. The mechanism study of these catalysts showed that the electron transfer from electron-rich metal clusters to O atom on the phosphine oxide ligand is the major driving force for H_2 activation. In addition, different substituent groups on phosphine oxide ligand were tested. Both H affinity of metal and the substituent groups on ligand can both affect the activation energy.

Another project described in Chapter 4 is the modelling of catalyst with DFT. We chose borane/NHC frustrated Lewis pair (FLP) catalyzed methane activation reaction as example to establish a relationship between activation energy and catalysts' physical properties. After performing simulation, we further proved the well-accepted theory that the electron transfer is the main driving force of catalysis. Furthermore, we were able to establish a linear

relationship for each borane between activation energy and the geometrical mean value of HOMO/LUMO energy gap (ΔE_{MO}). Based on that, we introduced the formation energy of borane/NHC complex (ΔE_F) and successfully established a generalized relationship between E_a and geometrical mean value of ΔE_{MO} and ΔE_F. This model can be used to predict reactivity of catalysts.

Key Words: Computational chemistry, DFT, catalyst design, nanocluster, frustrated Lewis pair (FLP), modelling

ACKNOWLEDGMENTS

First of all, I would like to thank my advisor in University of Central Florida, Dr. Shengli Zou, for all the support and help during my Ph.D. study and research. Besides solving specific questions with his knowledge, Dr. Zou guided me in my research with his patience and wisdom.

In addition, I would like to thank the rest of my committee member, Dr. Gang Chen, Dr. James Harper, Dr. Donovan Dixon and Dr. Xiaofeng Feng, for their valuable time and generous help.

I am very thankful to all of my lab mates and visiting scholars during my study and research. They are: Yadong Zhou, Ilia Toli, Dr. Yan Tian, Dr. Yan Zhao and Dr. Qiao Wang. I have learned a lot from them.

At last, I would like to thank my families, including my wife Xiao Wang and my parents, Hongxia Wang and Hansong Liu, for their love and tolerance in the past years. I cannot finish my study without all the support and accompany.

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CHAPTER 1: THEORIES OF COMPUTATIONAL CHEMISTRY

1.1 Introduction to computational chemistry

As a burgeoning branch of chemistry, computational chemistry uses computer software to simulate chemical reactions and study chemical processes using theoretical methods[1-2]. Compared with traditional chemistry research, computational chemistry methods are able to reduce the cost of research significantly, and can make predictions before conducting actual experiments so as to reduce possible attempt and human error. Although computational chemistry could provide relatively accurate results for some chemical problems, the accuracy of computational chemistry is still limited by computing resource and theoretical methods[3]. Since an exact description of chemical process can never be computed, approximation must be made in all theoretical methods in order to provide a quantitative result. By applying more computing resources, the accuracy of computational chemistry can always be improved. Thanks to rapid development of computer, the accuracy of computational chemistry has been significantly improved recently.

Nowadays, computational chemists are contributing in many different fields, including catalyst design, drug design, reaction mechanism study, etc[4-6]. Recent development of theoretical methods even allow chemist to simulate biomacromolecule, which further expanded the practical use of computational chemistry[1].

1.2 Theoretical Methods

Generally, there're three types of methods that are widely used in computational chemistry: molecular mechanics method, semi-empirical method, *ab initio* method and density functional theory (DFT) method. Different method provides different accuracy and computing cost, and is supported by different computational chemistry software. Choosing the correct method is critical for computation chemistry research. In this introduction, these methods will be briefly introduced.

1.2.1 Schrödinger Equation

The foundation of theoretical chemistry is Schrödinger Equation[2, 7-9]:

$$\hat{H}\Psi = E\Psi \tag{1.1}$$

$\hat{H}$ – Hamiltonian operator

Ψ – Wave function. For a given Hamiltonian, Ψ is the eigenfunction

E – Energy of the system

In a system containing *N* electrons and *M* nuclei, we can use wavefunction Ψ to describe the positions of each electron and nucleus. Therefore, the Schrödinger equation can be written as:

$$\hat{\mathrm{H}}\Psi_i(\overrightarrow{x_1}, \overrightarrow{x_2}, \ldots \overrightarrow{x_N}, \overrightarrow{R_1}, \overrightarrow{R_2}, \ldots, \overrightarrow{R_M}) = E\Psi_i(\overrightarrow{x_1}, \overrightarrow{x_2}, \ldots \overrightarrow{x_N}, \overrightarrow{R_1}, \overrightarrow{R_2}, \ldots, \overrightarrow{R_M}) \quad (1.2)$$

In equation (1.2), $\overrightarrow{x_N}$ and $\overrightarrow{R_M}$ describe the positions of electrons and nuclei, respectively.

So far, the Schrödinger equation can only be solved analytically for a very simple system, such as one hydrogen atom[9]. To simplify the equation, all wavefunctions are set to be orthogonal:

$$\int \Psi_i^* \Psi_j d\tau = <\Psi_i|\Psi_j> = \delta_{ij} = 0 \ (i \neq j) \quad (1.3)$$

$$\int \Psi_i^* \Psi_j d\tau = <\Psi_i|\Psi_j> = \delta_{ij} = 1 \ (i = j) \quad (1.4)$$

Where i and j represent different quantum numbers and dτ represents the integration over the whole space.

Another key step to solve Schrödinger equation is to determine $\hat{\mathrm{H}}$, the Hamiltonian. In a given system containing electrons and nuclei, the Hamiltonian operator is the sum total of all particles' kinetic energies and potential energies related to the system. Hence, the H can be written as:

$$H = T + V = T_e + T_n + V_{ee} + V_{nn} + V_{en} \quad (1.5)$$

Where T_e is the kinetic energy of electrons, T_n is the kinetic energy of nuclei, V_{ee} is the potential between two electrons, V_{nn} is the potential between two nucleus and V_{en} is the retraction potential between electron and nucleus. These energies can be expressed as following:

$$T_e = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 \tag{1.6}$$

$$T_n = -\frac{1}{2}\sum_{A=1}^{M}\frac{1}{m_A}\nabla_A^2 \tag{1.7}$$

$$V_{ee} = \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} \tag{1.8}$$

$$V_{nn} = \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} \tag{1.9}$$

$$V_{en} = -\sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} \tag{1.10}$$

In these equations, A and B denote the nuclei, i and j denote the electrons. r and R represent the distance between particles. m is the mass of the particle and Z is the charge of the particle.

By combining equation (1.5) to (1.10), the H can be written as:

$$H = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \frac{1}{2}\sum_{A=1}^{M}\frac{1}{m_A}\nabla_A^2 + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} \quad (1.11)$$

According to equation (1.11), the H is extremely complicated. Approximation must be employed if we want to apply the equation to a real system, even for a small system containing several particles.

One of the most important approximation method is the Born-Oppenheimer approximation[10]. Due to the huge difference in mass between electron and nuclei, the movement of nuclei can be ignored. Therefore, the kinetic energies of nuclei can be considered as zero, though the potential energies are still being considered. In addition, the V_{nn} can also be reduced to a constant. After approximation, the Hamiltonian becomes electronic Hamiltonian, and can be written as following:

$$H_e = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} \quad (1.12)$$

After the approximation, the wavefunction of the system only depends on the geometry of electrons. Equation (1.2) can be simplied as:

$$H_e\Psi_i(\overrightarrow{x_1}, \overrightarrow{x_2}, \ldots \overrightarrow{x_N}) = E_e\Psi_i(\overrightarrow{x_1}, \overrightarrow{x_2}, \ldots \overrightarrow{x_N}) \quad (1.13)$$

Where E_e is the total energy of electrons. In most cases, Born-Oppenheimer approximation can give trusted result. The approximate error introduced by such approximation can be estimated as:

$$error = (m_e \times \Delta E_{vibrational})/(m_n \times \Delta E_{electronic}) \approx 10^{-7} \quad (1.14)$$

Where m_e and m_n are the mass of electron and nuclei, respectively. $\Delta E_{vibrational}$ and $\Delta E_{electronic}$ are the difference of vibrational and electronic energy levels, respectively.

1.2.2 Slater Determinant and Hartree-Fock Method

One biggest obstacle in solving the Schrödinger Equation is that wavefunction is not observable. As a kind of fermion, two electrons cannot occupy the same state according to Pauli Exclusion Principle, or the antisymmetry principle[11]. This principle can be reflected in quantum chemistry as well: the sign of wavefunction has to change if two electrons exchanged. To express the wavefunction for a system contains N electrons, a Slater Determinant can be applied:

$$\Psi = \frac{1}{\sqrt{N!}}\begin{bmatrix} \chi_1(\overrightarrow{x_1}) & \cdots & \chi_N(\overrightarrow{x_1}) \\ \vdots & \ddots & \vdots \\ \chi_1(\overrightarrow{x_N}) & \cdots & \chi_N(\overrightarrow{x_N}) \end{bmatrix} \quad (1.15)$$

Where $\chi_i(\overrightarrow{x_i})$ indicates the one-electron wavefunctions.

Slater Determinant (1.15) is the basis of Hartree-Fock method in solving the time-independent Schrödinger Equation. In Hartree-Fock method, the wavefunction of the system is first treated by variational method[2, 12-13]:

$$E = < \Psi | H_e | \Psi > \tag{1.16}$$

And

$$H_e = \frac{1}{2}\sum_{i=1}^{N} \nabla_i^2 + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}} - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} \tag{1.17}$$

With the Born-Oppenheimer approximation, the Hamiltonian of an N-electron system can be divided into two parts, O_1 and O_2. O_1 represents the kinetic energy and the electron-nuclei interaction, and O_2 represents the repulsion potential between electrons. So the electron Hamiltonian can be written as:

$$H_e = O_1 + O_2 \tag{1.18}$$

$$O_1 = \frac{1}{2}\sum_{i=1}^{N} \nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} \tag{1.19}$$

$$O_2 = \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}} \tag{1.20}$$

To obtain the energy of the ground state, E_0, a corresponding wavefunction at the ground state, Ψ_0, must be obtained. By applying the variational method, the Hatree-Fock equation can be obtained:

$$\hat{f}(i)\chi_i = \epsilon_i \chi_i \tag{1.21}$$

In equation (1.21), $\hat{f}$ is the Fock operator (one-electron Hamiltonian) and ϵ_i is the *i*th orbital's energy. The Fock operator has a form as:

$$\hat{f}(i) = -\frac{1}{2}\nabla_i^2 - \sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + V_{HF} \tag{1.22}$$

Where V_{HF} is called Hartree-Fock potential. This value reflects the repulsion felt by one electron from all other electrons. Similarly, V_{HF} can be expressed by two terms: Coulomb operator $\widehat{J}_\iota(i)$ and exchange operator $\widehat{K}_\iota(i)$. These operators are defined as following:

$$\widehat{J}_J(i) = \int \left|\chi_j(j)\right|^2 r_{ij}^{-1} d\boldsymbol{r}_j \tag{1.23}$$

$$\widehat{K}_J(i)\chi_i(i) = \int [\chi_j^*(j)\chi_{ij}^{-1}\chi_i(j)]\chi_j(i) d\boldsymbol{r}_j \tag{1.24}$$

According to equation (1.23) and (1.24), the Coulomb operator indicates the repulsion potential between two electrons *i* and *j*, while the exchange operator indicates no classical meaning. The exchange operator is necessary due to the antisymmetry of the wavefunction as mentioned above.

By composing equation (1.23) and (1.24), the V_{HF} can be expressed as:

$$V_{HF} = \sum_{j}^{N} [\widehat{J}_J(i) - \widehat{K}_J(i)] \tag{1.25}$$

In practical cases, Hartree-Fock equations cannot be solved analytically. An iterative method, Self-Consistent Field (SCF) method must be applied in order to obtain solution[2]. For a SCF calculation, an initial guess of V_{HF} is mandatory. For a given V_{HF}, a corresponding χ can be easily calculated. This χ can be plugged back to equation (1.25) to calculate a new V_{HF}. These steps will be repeated until certain criteria are met, or converged. Once SCF is done, other properties of the system can be easily identified. Following flowchart shows how SCF works:

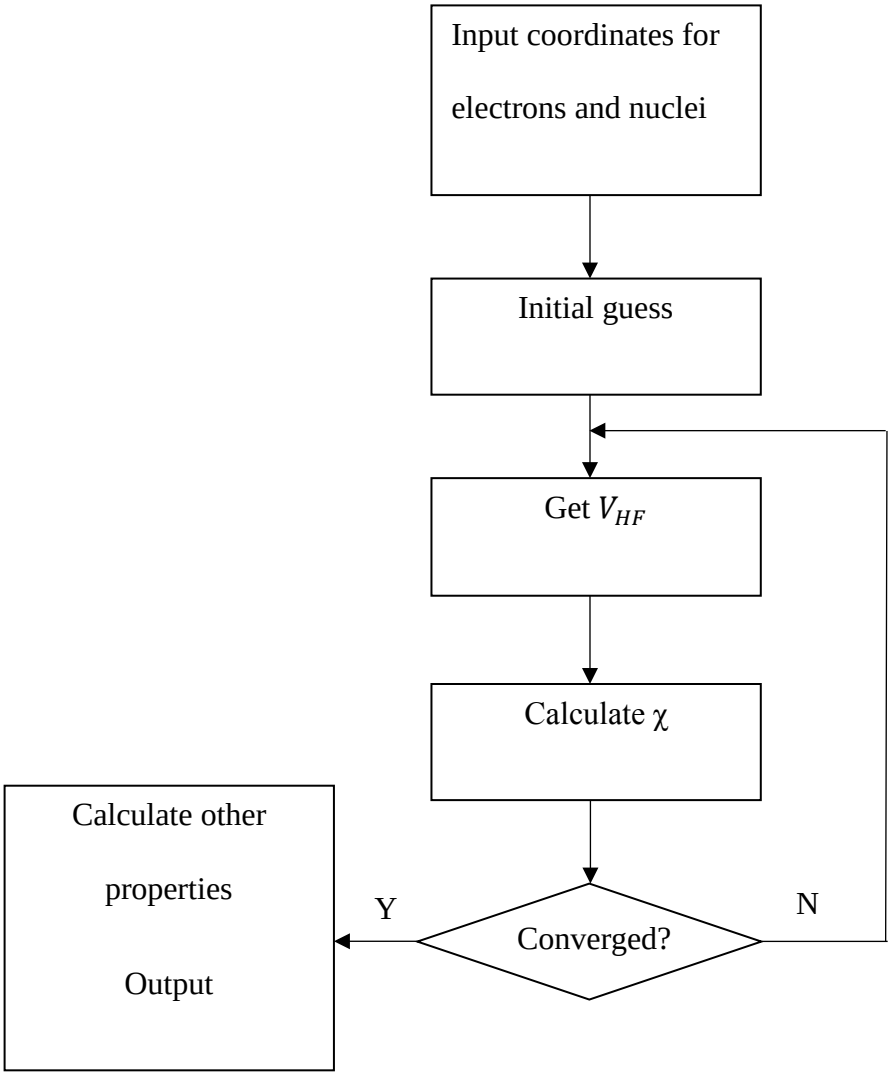


Figure 1. Illustration of SCF method.

1.2.3 Basis Set

Basis set is an approximation for the electron Hamiltonian showed in equation (1.12)[1-2]. Basis set is critical for *ab initio* methods. According to molecular orbital (MO) theory, molecular orbitals can be approximated by linearly combining atomic orbitals (LCAO)[11]. As the result, the wavefunction of molecular or atomic orbitals are treated as linear combination

of a series of basis functions. After the approximation was employed, the partial differential equations are converted into algebraic equations, which are much easier to be solved by computers.

The basis set can be expressed as the following form:

$$\Psi_i = \sum_{\mu=1}^{M} c_{\mu i}\, \phi_\mu \tag{1.26}$$

In equation (1.26), Ψ_i is the wavefunction of the *i*th molecular orbital, M is the number of basis functions, ϕ_μ is the basis function of the μth molecular orbital and *c* is the coefficient when these basis functions are linearly combined.

The accuracy of basis set is depending on the number of basis functions are used to describe the molecular orbitals. The more basis functions are used, the more accurate will it be. On the other hand, less basis functions can significantly reduce the cost of computing. To choose a proper basis set for a specific system is critical for research in computational chemistry. Lot of studies have been conducted in order to provide guidance in basis set selection.

There're two main categories of basis set in computational chemistry research[2, 8]: Slater basis set and Gaussian basis set. Gaussian basis set are the most commonly used in recent studies in quantum chemistry.

1.2.3.1 Slater Basis Function

Slater basis function was developed since 1930s by John C. Slater[14], which relatively primitive and is not widely used in modern research. In this basis set, the functions used are called Slater-type orbitals (STOs). The STO can be expressed as:

$$\phi_{STO} = Nr^{n-1}\exp(-\zeta r) \qquad n = 1,2,\ldots. \tag{1.27}$$

And

$$N = (2\zeta)^n \sqrt{\frac{2\zeta}{(2n)!}} \tag{1.28}$$

In equation (1.27), r is the distance between electron and nuclei, ζ is a constant that related to the charge of nucleus.

STO has a simple expression but has difficulty in calculating two-electron integrals, the most frequently calculated in computational chemistry. Hence, this basis set is soon deprecated in practical use.

1.2.3.2 Gaussian Basis Function

Gaussian basis functions are the most commonly used basis functions. A typical Gaussian function has the following image:

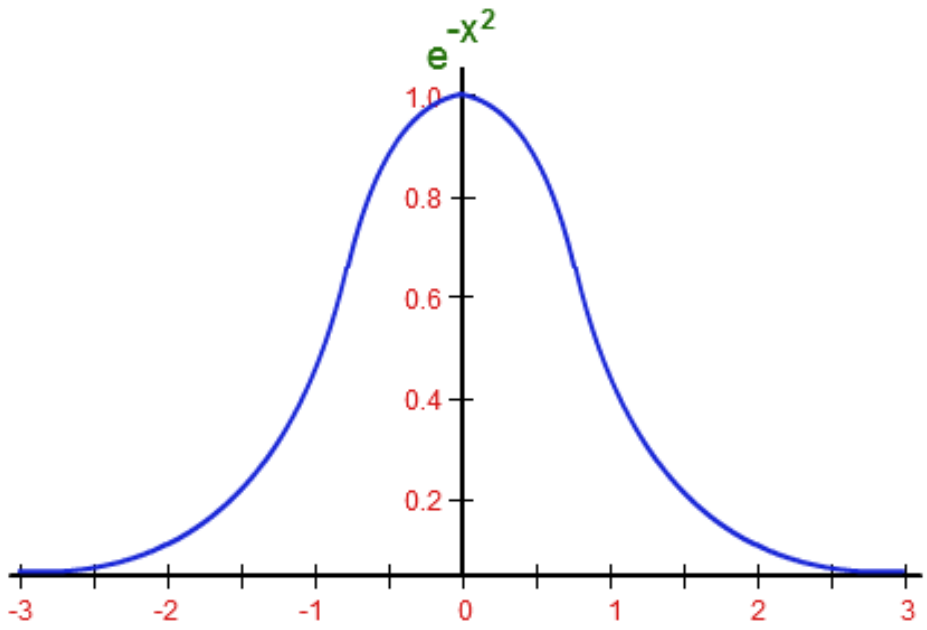


Figure 2. A typical Gaussian function image

In this function, Gaussian-type orbitals, or GTOs, are used instead of STOs. The general expression of GTO is[2]:

$$\phi_{GTO} = Nx^l y^m z^n \exp(-\alpha r^2) \tag{1.29}$$

In equation (1.29), x, y and z are the Cartesian coordinates, l, m and n are angular momentum, magnetic and principal quantum numbers, respectively. α is a coefficient that describes the shape of the orbital.

GTOs can significantly reduce the computing resource consumption during the two-electron integral calculation. Therefore, researchers often linearly combine several GTOs to

simulate STO, in order to achieve both accuracy and efficiency. In this case, the combined GTOs are called STO-NG basis sets. N represents the number of GTOs are used. For example, STO-3G means three GTOs are combined to simulate STO. These basis sets, including STO-3G, STO-4G, STO-6G, etc., are the primary part of minimal basis sets. They cannot provide sufficient accuracy, yet the cost is much cheaper than other basis sets.

To further enhance the accuracy of Gaussian basis set, many improvement were made after the invention of GTO.

1.2.3.3 Pople Basis Sets

John Pople's group focused on the valence electrons, which contribute the most during chemical reaction, to develop a series basis set *X*-*YZ*G[15-16]. In these basis sets, the electrons in the inner shell are described by *X* primitive GTOs while each of the valence electrons, are described by two basis functions: linear combination of *Y* primitive GTOs and *Z* primitive GTOs. For example, 6-31G basis set means that 6 primitive GTOs are employed to describe each core electron, and a combination of three and one GTOs are used to describe each valence electron.

Although the most commonly used Pople basis sets have two functions to describe valence electrons ("double-zeta"), more functions, such as triple-zeta or quadruple-zeta, can be used to achieve even better results[17].

Since core and valence electrons are treated separately, these basis sets are called split-valence basis sets.

1.2.3.4 Polarization Functions and Diffuse Functions

For split-valance basis sets, additional functions can be employed to further enhance their performance in describing the electrons. Take H atom for example, even though there is only one electron on the 1s orbital, additional functions that describe *p* orbitals (*px*, *py* and *pz*) can be added to the basis sets, in order to better describe the electron density in molecule[2, 18]. Although the polarization functions have no electron, they still can affect the electrons in the inner shell. Hence, polarization functions can significantly improve the accuracy, and employment of them are almost mandatory for research[18].

Diffuse functions are another kind of expansion for split-valence basis sets[19-20]. According to equation (1.29), the coefficient α plays an important role in determining the shape of the function. When the value α is small, the shape of the function will "diffuse" away from the original point. This kind of function is diffuse function. By applying diffuse function to split-valence basis set, the accuracy of calculation can be promoted, especially for systems containing non-bonded interactions, such as hydrogen bond and van der Waals force[21].

1.2.4 Molecular Mechanics Method

Except for Hartree-Fock method, another way to simulate a molecule is using molecular mechanics[2]. Molecular mechanics method use classic mechanics theory to simulate a multi-atom system. In the simulation, every atom is treated as a "ball". Each "ball" has a given

radius, charge and polarizability[22-23]. Every covalence bond is considered as a "spring", with a given bond length. Following image shows the molecular mechanics:

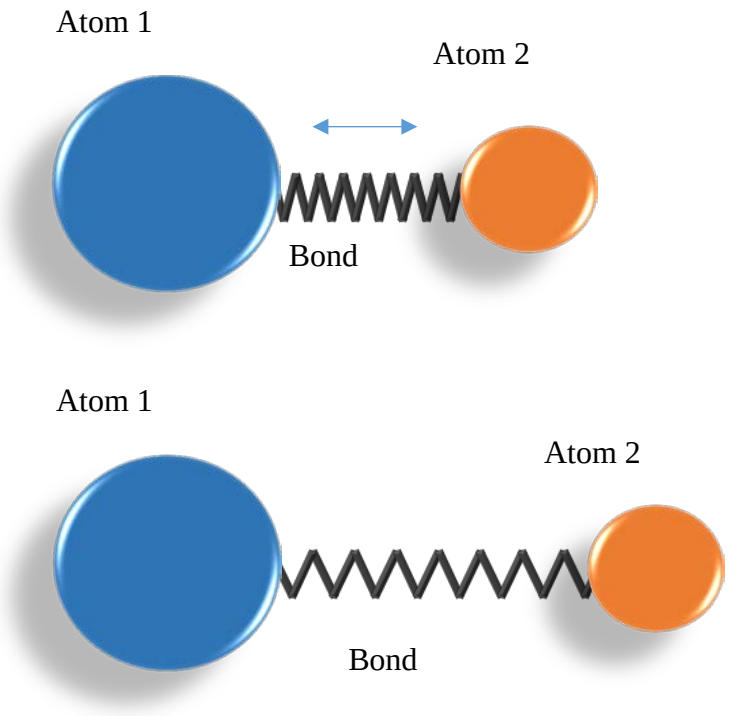


Figure 3. Illustration of molecular mechanics

Compare to HF method, molecular mechanics method is much simpler. For a given system, the potential energy E can be easily calculated:

$$E = E_{covalent} + E_{noncovalent} + E_{cross} \tag{1.30}$$

Where $E_{covalent}$ is the bonding interactions, including stretching, bending and torsion. $E_{noncovalent}$ describes the non-bonding interactions, including electrostatic interaction and van der Waals force. E_{cross} is the correction term. It includes the energy changes due to the coupling of all interactions. Although equation (1.30) has a simple express, a set of parameters, including atom mass and radius, bond length, etc., must be chosen before performing calculation with molecular mechanics method.

To solve the equation (1.30), a molecular dynamic method can be applied. This method utilizes Newton's classic equation:

$$F = -\frac{dE}{dr} = ma = m\frac{d^2r}{dt^2} \tag{1.31}$$

Compare with HF method, molecular mechanics method requires much less computational resources[22]. For researches on biochemistry, molecular mechanics plays an important role since molecules being studied in biochemistry are huge, such as proteins and DNAs[24]. In these studies, building units in proteins or DNAs, such as amino acids, can be considered together as one "ball", which could further reduce the computational power needed for simulation.

1.2.5 Semi-empirical Methods

Generally, the cost and accuracy of semi-empirical methods are between HF method and molecular mechanics method. Although semi-empirical method also based on HF function, more empirical approximation reduces its cost while make it less creditable at the same time.

To simplify the calculation of Hartree-Fock function, corrections derived from experimental data and analysis are made so as to reduce the computational cost. Generally speaking, there're several differences from HF method[2, 25]:

1. Only valence electrons or π electrons are considered.

In semi-empirical method, not all electrons are considered in calculation. Since valence electrons contribute most for chemical reaction, only these electrons are considered. For ab initio methods, each electron, no matter valence or non-valence electron, needs a wavefunction to simulate. But in semi-empirical methods, the "nuclei" is composed by atomic nuclei and non-valence electrons. By reducing the electrons considered during simulation, semi-empirical method is able to significantly reduce the total number of basis functions involved in calculation, especially for large systems. Take methane (CH_4) for example, there'll be 9 basis functions needed in ab initio method (5 for carbon atom and 1 for each hydrogen atom). When the atom gets heavier, for example, nickel(II) oxide (NiO) there'll be 15+5=20 basis functions. But with semi-empirical method, the number of basis functions can be reduced to 8 and 11, respectively.

2. Use minimal basis set

In ab initio method, each electron can be expressed by two (double-zeta) Slater functions, three (triple-zeta) functions, or even more. These functions will be represented by 1-6 Gaussian functions. But in semi-empirical method, each valence electron is described by only one Slater function and represented by three Gaussian functions. This is the minimal basis set STO-3G as mentioned above. Less functions could reduce cost for simulation as well.

3. Multi-electron integrals

Another approximation made in semi-empirical methods is to neglect the overlap of atomic orbitals. In this approximation, all atomic orbitals are assumed to be “frozen”, there is no interaction between each orbitals. If diatomic orbital overlap is neglect, the method is called “Neglect of Differential Diatomic Overlap”, or NDDO; if all overlaps are neglected, the method is “Complete Neglect of Diatomic Overlap”, or CNDO. In addition, many different modifications to these methods are developed, so as to increase the accuracy to fit different molecular systems.

1.3 Density Functional Theory (DFT)

DFT was first developed since 1960s[26]. In order to reduce the complexity of calculation or simulation, DFT uses electron density, instead of wave functions in HF method, to describe the properties of a system.

In HF method, the wave functions are very complex. For an N-electron system, there’re 3N variables in wave functions. But in DFT, there’re only 3 variables[26-27]. In addition,

electron density (ρ) can be obtained easily, either from experimental data or theory. Therefore, by applying DFT method, the cost of computation can be reduced significantly. At the same time, to simulate bigger system become more realistic.

1.3.1 Functional

Before talking about DFT, we need to talk about functional, a mathematical concept. Functional is different from function. A function describes a relationship between a set of quantities and another quantities. But for functional, the domain is a function and its range is a quantity. Hence, the functional is a map from space of functions to real numbers.

1.3.2 Hohenberg-Kohn Theorems

In 1964, Hohenberg and Kohn developed a series theories to describe the relationship between electron density and system's properties[28]. In their theory, the electron density is a function:

$$\rho = \rho_0(x, y, z) = \rho(\boldsymbol{r}) \tag{1.32}$$

And the energy of ground state (E_0) is a functional of ground state electron density:

$$E_0 = E[\rho_0(x, y, z)] \tag{1.33}$$

Equation (1.33) is the expression of the first Hohenburg-Kohn theorem. This theorem provides a connection between electron density and the energy.

Besides the first theorem, Hohenburg and Kohn proposed their second theorem on DFT. This second theorem gives the connection with HF method. This theorem refers that for any electron density functional ρ_t, the corresponding energy E_t is greater than the ground state. (Or equals to ground state, if ρ_t is exact the electron density of ground state). This theorem can be expressed as:

$$E_t[\rho_t] \geq E_0[\rho_0] \tag{1.34}$$

According to equation (1.34), for a given ρ_t, a corresponding energy values can be calculated. With SCF method, the lowest energy value, or the ground state energy, can be easily calculated by multiple steps of iteration.

After the establishment of Hohenburg-Kohn theorems, to solve the wave functions in HF method can be successfully transferred to finding the solution of electron density functional, which is much less complicated to deal with[2, 26]. Therefore, DFT method has been widely used in simulate multi-electron systems and has achieved numerous productive progress in many different fields, especially in chemistry, solid state physics and materials. Nowadays, many researchers are still focusing on improving the accuracy and further reduce the computation cost.

1.3.3 Kohn-Sham Approach

According to Hohenburg-Kohn Theorems, the properties of a system, including wavefunction Ψ, energy E, etc., are function of electron densityρ. According to chapter 1.2.1, the Schrödinger Equation after Born-Oppenheimer Approximation can be expressed as:

$$H\Psi = [T + U + V]\Psi \tag{1.35}$$

And according to Hohenburg-Kohn Theorems, the ground state of system can be expressed as:

$$E[\rho] = T[\rho] + U[\rho] + V[\rho] \tag{1.36}$$

In equation (1.35) and (1.36), T indicates the kinetic energy, U indicates the electron-electron interaction potential and V indicates the electron-nuclei interaction potential. Among these three operators, T and U are universally valid since they are independent of the number of electrons (N), distance between electron and nucleus (R), and charge (Z). Hence, we can define a new functional, Hohenberg-Kohn functional (F_{HK}), shown as following:

$$F_{HK}[\rho] = T[\rho] + U[\rho] \tag{1.37}$$

The last term in equation (1.35) and (1.36) is V, which is dependent to N, R and Z of the system:

$$V[\rho] = \int \rho\,(\boldsymbol{r})V d\boldsymbol{r} \tag{1.38}$$

By finding the minimum of equation (1.38), the minimum of E, or the energy of ground state, can be obtained. By combining equation (1.36) to (1.38), the energy of ground state can be written as:

$$E_0[\rho_0] = T[\rho_0] + U[\rho_0] + \int \rho_0\,(\boldsymbol{r})V d\boldsymbol{r} \tag{1.39}$$

To solve equation (1.39), Kohn and Sham proposed a series of fictitious systems that has exact same electron density as the real system but there's no electron-electron interaction. And there're deviation between the reference system and real system. Kohn and Sham defined an exchange-correlation energy, E_{xc}, to describe the deviation[29]:

$$E_{XC}[\rho_0] = \Delta T[\rho_0] + \Delta U[\rho_0] \tag{1.40}$$

$$\Delta T[\rho_0] = T_{REAL}[\rho_0] - T_{REF}[\rho_0] \tag{1.41}$$

$$\Delta U[\rho_0] = U_{REAL}[\rho_0] - U_{REF}[\rho_0] \tag{1.42}$$

Since the reference system has only Coulomb repulsion interaction, the electron-electron potential can be written as:

$$U_{REF}[\rho_0] = \frac{1}{2}\iint \frac{\rho_0(\boldsymbol{r}_1)\rho_0(\boldsymbol{r}_2)}{\boldsymbol{r}_{12}} d\boldsymbol{r}_1 d\boldsymbol{r}_2 \tag{1.43}$$

Therefore, the equation (1.39) can be written as:

$$E_0[\rho_0] = \int \rho_0(\boldsymbol{r}) V d\boldsymbol{r} + T_{REF}[\rho_0] + \frac{1}{2}\iint \frac{\rho_0(\boldsymbol{r}_1)\rho_0(\boldsymbol{r}_2)}{\boldsymbol{r}_{12}} d\boldsymbol{r}_1 d\boldsymbol{r}_2 + E_{XC}[\rho_0] \tag{1.44}$$

Since in equation (1.44), the only unknown is E_{xc}, which needs approximation to calculate. So many researchers have developed different methods to model this functional.

1.3.4 Approximation of E_{XC}

1.3.4.1 Local Density Approximation (LDA)

Most successful LDA is based on homogeneous electron gas (HEG) model[26]. In this approximation, the exchange-correlation energy E_{xc} is only related to the electron density at each point in HEG's space:

$$\rho = \frac{N}{V} \tag{1.45}$$

Where N is the number of electrons and V is the volume.

And for a spin-unpolarized system, the E_{xc} can be written as:

$$E_{XC}^{LDA}(\rho) = E_X^{LDA}(\rho) + E_C^{LDA}(\rho) \tag{1.46}$$

In equation, E_{XC} was separated in two parts: exchange term E_X and correlation term E_C. For HEG, the E_X can be calculated:

$$E_X^{LDA}(\rho) = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int \rho(\boldsymbol{r})^{\frac{4}{3}} d\boldsymbol{r} \tag{1.47}$$

E_C can be simulated and calculated by performing Monte Carlo simulation. After obtaining both exchange and correlation terms, the E_{XC} can be used in solving Kohn-Sham equation and obtain the properties of a system[26].

There're many famous functionals using LDA, including VWN (developed by Vosko, Wilk and Nusair)[30], PW92 (developed by Perdew and Wang)[31], etc.

1.3.4.2 Generalized Gradient Approximation (GGA)

In real molecules, the homogeneous electron gas is not a good way to describe the electron distribution since the electron density can change significantly even in a very small space. Therefore, to include the gradient of electron that may describe the change of electron

density is necessary for obtaining more accurate approximation of E_{XC}. Better than LDA, GGA functionals have considered the gradient of electron density and could provide better simulation results in DFT method[2].

Similarly, E_{XC} can be separated into two terms as well[26]:

$$E_{XC}^{GGA}(\rho) = E_X^{GGA}(\rho) + E_C^{GGA}(\rho) \tag{1.48}$$

There're many exchange, correlation and exchange-correlation functionals developed in decades. Some successful examples include exchange functional B (or B88) developed by Becke[32], and LYP, a correlation functional developed by Lee, Yang and Parr[33].

1.3.4.3 Hybrid Functionals

Although DFT method shows advantages over HF method, the exchange term in E_{XC} is hard to approximate while in HF method, this term can be defined exactly. In 1993 Axel Becke first introduced a hybrid functional that combines both DFT (including LDA and GGA) and HF in the functional to overcome this problem[34].

One of the most successful example is B3LYP functional[35]. In this functional, term "B3" is the exchange functional developed by Axel Becke. It contains both LDA and GGA part to approximate the exchange functional. The E_{XC} can be written as:

$$E_{XC}^{B3LYP} = E_{XC}^{LDA} + a(E_X^{HF} - (E_X^{LDA}) + b(E_X^B - E_X^{LDA}) + c(E_C^{LYP} - E_C^{LDA}) \tag{1.49}$$

In equation (1.49), a, b and c are 0.20, 0.72 and 0.81, respectively.

B3LYP was first used by Stephens, et al. in 1994[35]. Soon it became one of the most widely used hybrid functional in DFT study for organic reactions. It can provide relatively both good result and satisfying time consumption.

Besides B3LYP, there're many other hybrid functionals, such as B3P86, HSE, BP86, etc[36]. For different system or reaction, choosing appropriate functional can minimize the cost of computational and improve accuracy.

1.3.5 Advantages and Limitations of DFT Method

Unlike HF method, with which electron correlations are not well considered, DFT method can provide better results without consuming more computational resource[2]. In HF method, the approximation algorithm neglected the Coulomb repulsion between electrons, which could raise the energy. Therefore, the calculated energy is usually higher than real system.

DFT method contains the electron correlation, which makes it more comprehensive than HF method. In researches on transition metals, DFT is one of the best choices for geometry optimization and energy calculation. Meanwhile, HF method usually gives poor result.

Although DFT method is widely used in both chemistry and solid state physics, there are many weakness and limitations. First, the exchange-correlation energy in DFT theory cannot be well explained and is extremely difficult to improve its accuracy. Improvements on

exchange-correlation energy term cannot be based on theoretical approach, but based on experimental data and repeated attempts. As one of the most widely accepted functional, B3LYP showed its value in numerous study, but its accuracy may be very low in some studies, such as hydrogen bonding or van der Waals force calculation[37]. In addition, applying DFT method to study new or rare molecules may be risky, since there's no experimental result as support to its accuracy. In this case, high level HF method may be more suitable. Another problem with DFT is in organic area. DFT may over-consider the delocalization of electrons, which may cause error in simulating aromaticity[38].

1.4 Software

There're many software package developed for different system. Examples including Gaussian, Dalton, VASP, etc. These software supports different methods in simulation and has their own range of application.

CHAPTER 2 INTRODUCTION TO CATALYSIS

Catalyst is a chemical that can increase the rate of reaction but does not change its properties during the reaction. For a catalyzed reaction, the thermodynamic equilibrium can be achieved with a shorter time than un-catalyzed reaction, the equilibrium cannot be changed by catalysis, since catalyst can only change the kinetics, not thermodynamics.

Catalyst is widely used in industries. Nowadays, over 90% chemical process need catalyst for efficient production but there are still many opportunities to improve. To further enhance the activity of catalyst and lower the cost could further lower the cost in production and benefits the whole human being community.

2.1 Rate of reaction

As mentioned above, the purpose of catalysis is to increase the rate of reaction. The rate of reaction r is defined as below:

$$r = \frac{d[A]}{dt} \tag{2.1}$$

Where [A] is the concentration of reactant/product of reaction and t is time. Rate of reaction can be affected by many factors other than catalyst, including temperature, contacting surface area, concentration, et al. As mentioned above, the purpose of catalysis is to increase the rate of reaction.

2.2 Transition State (TS) Theory and Activation Energy

In 1889, Arrenhius first systematically studied the relationship between rate of reaction and temperature. After analyzing his data, he proposed Arrenhius equation that describes the relationship quantitively[39]:

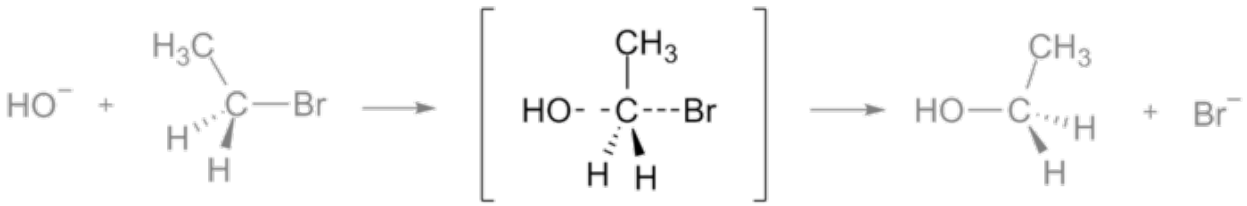
$$r = Ae^{(-\frac{E_a}{RT})} \tag{2.2}$$

In equation (2.2), A is a constant, E_a is activation energy, which indicates the energy barrier for reactant to overcome in order to proceed; R is the ideal gas constant and T is temperature.

Arrenhius equation gives a positive correlation between temperature and rate of reaction. In practical experiments, researchers are able to plot ln(r) versus T with experimental data, in order to obtain activation energy and A.

Although Arrenhius successfully demonstrated the factors that affect rate of reaction, the mechanism and explanation of activation energy E_a was not clear, until a well accepted theory, transition state theory (TST), was established in 1930s[40].

The most important concept in TST is transition state (TS). TS is a highly-reactive complex that formed by reactant and its energy is the highest along reaction coordinates. For example, the TS of a simple S_N2 reaction is shown below:



Reactants TS Products

Figure 4. TS in S_N2 reaction

In research, energy profiles are often used to demonstrate both reactants, TS and products. A typical energy profile for an elementary reaction is shown as following:

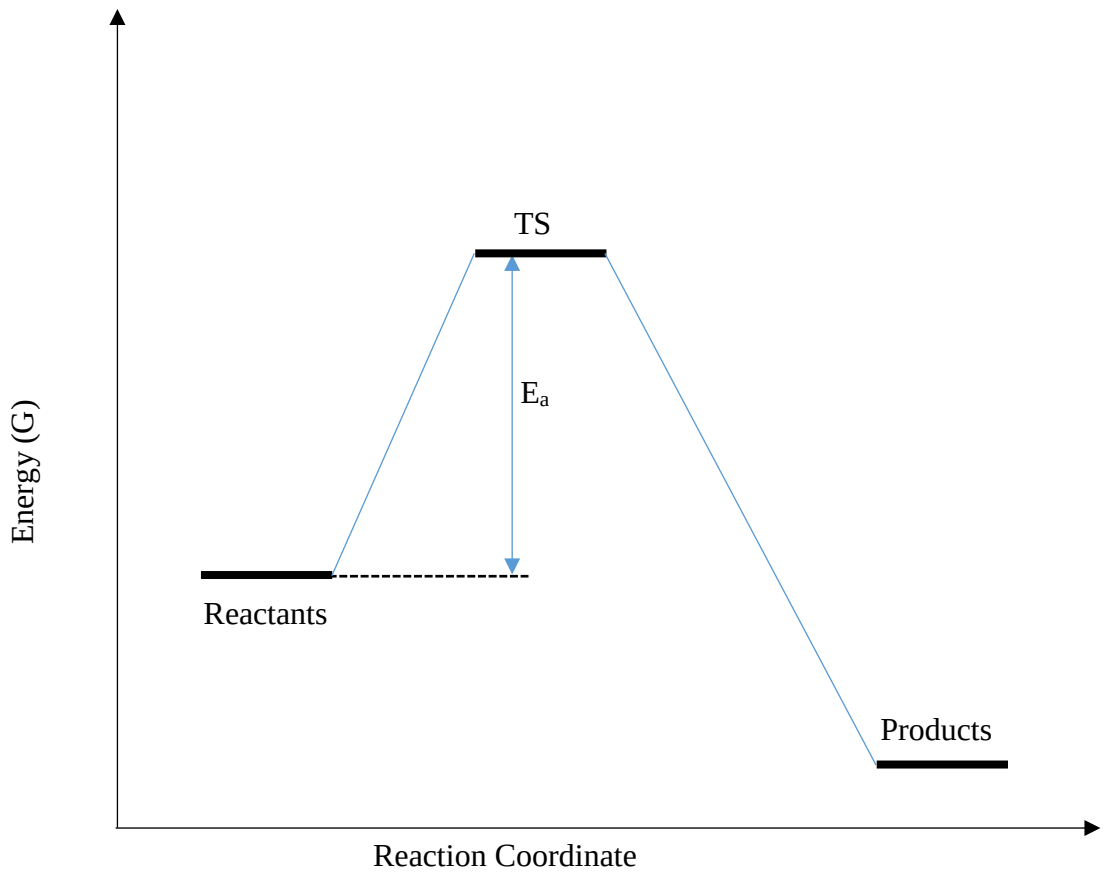


Figure 5. Energy profile for an elementary reaction

According to TST, there is an equilibrium (quasi-equilibrium) between reactants and TS. By combining TST and computation chemistry method, activation energy can be calculated using following equation[40]:

$$E_a = G_{TS} - \sum G_{Reatcant} \tag{2.3}$$

After optimization and energy calculation, computation chemistry method will be able to give the energy values of TS and reactants. By applying equation (2.3), the activation energy can be easily calculated.

2.3 Catalyst and Activation energy

As mentioned above, catalyst cannot change the thermodynamic of the reaction, in other word, the energy difference between reactants and products cannot be changed. The reason why catalysts can accelerate reaction is that activation energy can be lowered with the presence of catalyst.

A typical catalyzed reaction may have an energy profile looks like following:

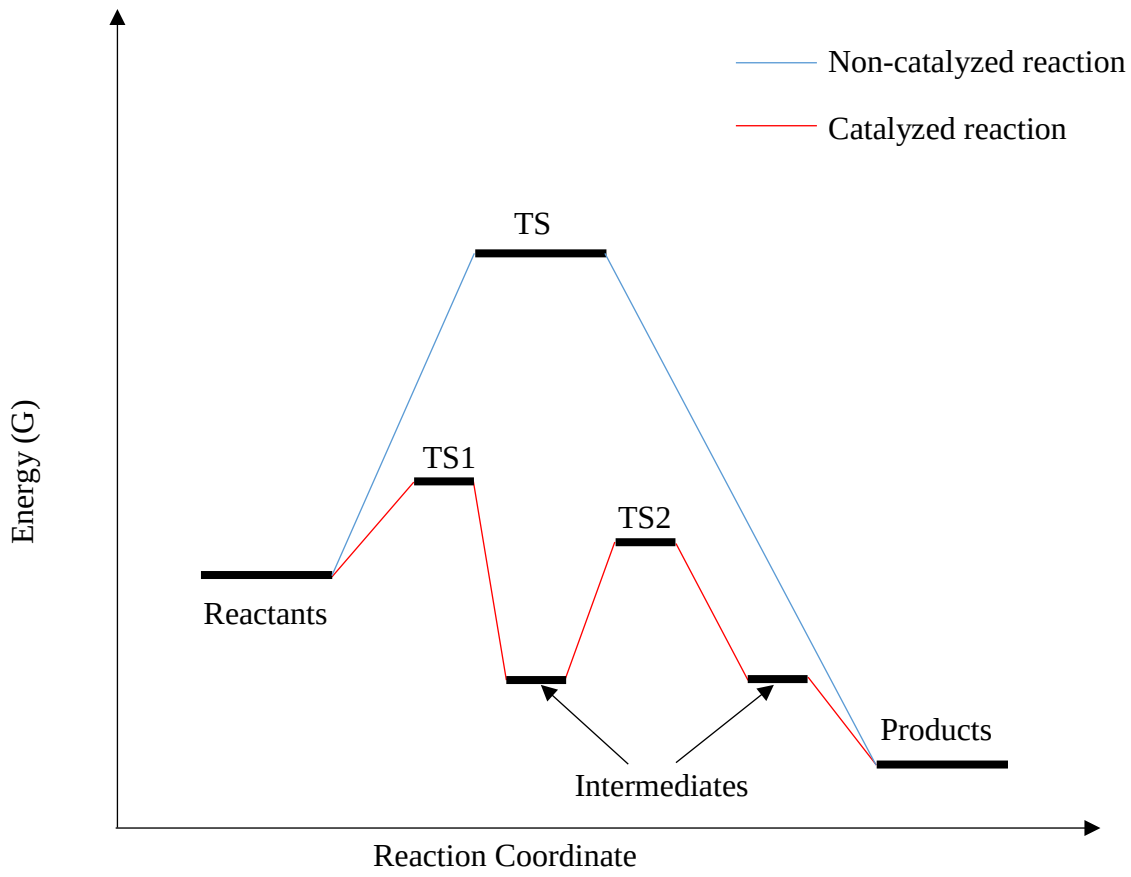


Figure 6. Typical energy profile of catalyzed reaction

As shown in the figure above, catalyst can reduce the energy level of TS, so as to reduce the energy barrier for the reactants to overcome and increase the rate of reaction eventually. In a catalyzed reaction, it is possible to have multiple TSs and intermediates. Among all steps, the step with the highest energy barrier is called rate determining step. This step determines the rate of conversion for the whole reaction.

Catalysts can be divided into homogeneous catalysts and heterogeneous catalysts[39, 41]. Homogeneous catalysis happens when catalyst and reactants are in the same phase. In most

cases, it refers to liquid phase. Many organocatalysis are homogeneous, since the catalysts can be dissolved in the solvent with the substrates. By dissolving catalyst with reactant in a same phase may enhance the catalysis reactivity since there's no absorption process, but separation of catalysts and reactants/products may be more difficult.

Heterogeneous catalysts are usually solid. The catalyzed reaction will occur on the active sites on the surface of catalysts. The first step in heterogeneous catalysis is usually adsorption. The reactant molecule will form bond to the active site and get activated, in order to proceed further reaction. Heterogeneous catalysis is very common in industry. For example, in the Haber-Bosch process to synthesize ammonia, solid catalyst pellets are used in the production[42-43].

Unlike the homogeneous catalysts, heterogeneous catalysts can be separated from reactants/products very easily. Meanwhile, supporting materials are usually very important for heterogeneous catalysts, since the reactivity of catalysts are usually rather high, which need to be stabilized by supporting material. Nowadays, porous materials, such as zeolite, and many different metal oxide materials are widely used as supporting material for heterogeneous catalysts[44-45]. They can not only provide huge surface area to promote dispersion of active site, but also get involved in catalysis: they may promote the adsorption process or help electron transfer between active sites and reactants.

2.4 Poisoning of Catalyst

Since the key to catalysis is the reversible binding before catalyst and reactants/products, once the active sites of the catalyst are permanently bonded with some chemicals, the catalyst will permanently lose its reactivity. This process is called poisoning of catalyst[39].

Following figure shows the poisoning process:

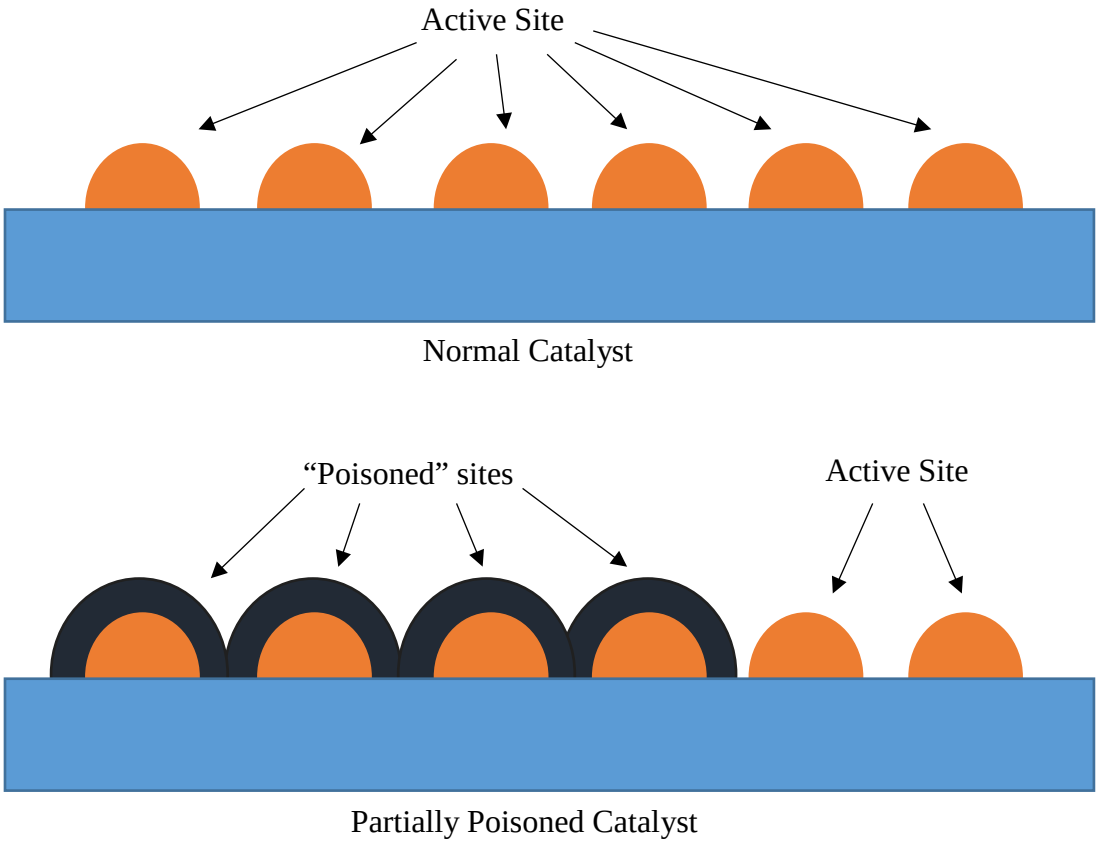


Figure 7. Normal and Partially poisoned catalyst

After poisoning, the number of active site on the surface of catalyst will be significantly reduced, eventually slow down or stop the catalysis. In order to protect the catalyst,

impurities in the reactants feeding, especially CO, SO_2, must be completely removed before the contact with catalyst.

2.5 Development of Catalyst with Computational Method

Traditionally, the development of catalyst is purely based on experiments. The process of development contains numerous of attempts, failure and waste. The cost for the development is extremely high and is still increasing. By introducing computational method into development of catalyst can significantly reduce the time of cost for development[46-47]. In addition, the reaction mechanism can be studied during the simulation process, which could provide evidence and guidance to chemists and accelerate the development process as well. With the rapid improvement of computer system, more and more complicated catalysts can be designed and tested by computation chemistry methods.

One recent example is the computational design of an enzyme. In 2010, Siegel and co-workers published their pioneering work on designing an enzyme to catalyze stereoselective Diels-Alder reaction[48]. The reaction is shown as following[48]:

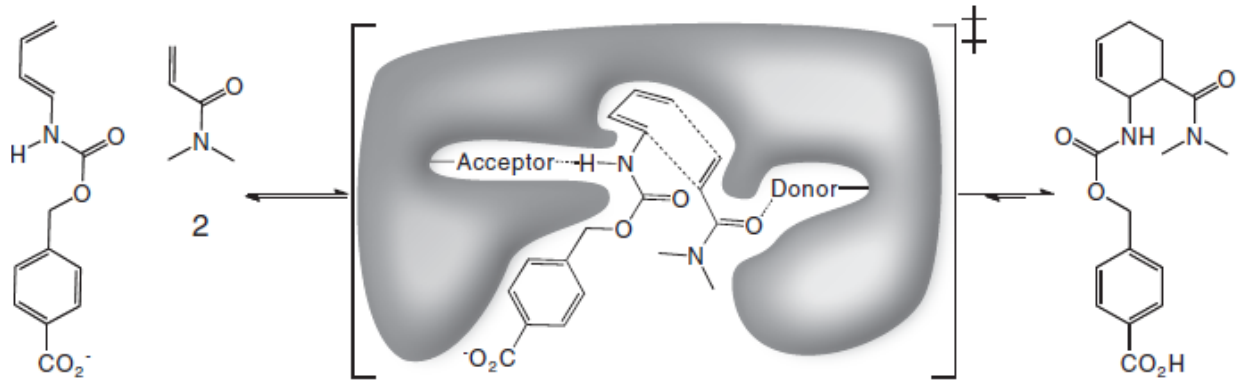


Figure 8. Computation-designed enzyme catalyzed Diels-Alder reaction. Gray structure illustrates the enzyme.

Under the guidance of computational method, researchers were able to prepare the enzyme and successfully used it as catalyst for stereoselective Diels-Alder reaction. In consideration of the importance of Diels-Alder reaction in organic synthesis field, their work provided a powerful tool for all synthesis chemists.

In this work, DFT method was chosen to perform all computational research because of its high accuracy and relatively low cost.

CHAPTER 3: COMPUTATIONAL STUDY OF MODIFIED Au_3, Ag_3 and Cu_3 NANOCLUSTER CATALYST FOR H_2 ACTIVATION AND CO HYDROGENATION

3.1 General Introduction

Syngas, short for synthesis gas, is a gaseous mixture widely used as intermediates in many synthesis productions, such as methanol, ammonia, etc[49]. Although the exact composition of syngas is different based on sources or processes, H_2, CO and CO_2 are three major components. One way to produce syngas is Steam Reforming Reaction (SRR)[50-52]:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad (3.1)$$

The composition of hydrogen in syngas can be controlled as well. With higher feeding of steam, carbon monoxide can be convert to hydrogen and carbon dioxide via following equation:

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (3.2)$$

As the raw material, the syngas need to be carefully purified before feeding in to reactors, since the impurities, such as SO_2, may poison the catalyst. Most important products from

syngas are alkanes and alcohols via Fischer-Tropsch (FT) process. The reaction equations of FT process are shown below:

$$nCO + (2n + 1)H_2 \rightarrow C_nH_{2n+2} + nH_2O \quad (3.3)$$

$$nCO + 2nH_2 \rightarrow CH_{2n+1}OH + (n - 1)H_2O \quad (3.4)$$

In industries, many different catalysts are used to promote the rate of FT reactions. Fe and Co based catalysts are commercially available[52-53].

Although the research on utilizing syngas has been well conducted for over one hundred years, there are still many problems for researchers to solve, such as low efficiency, low selectivity and harsh reaction conditions. Recently, Liu and et al. reported their progress in combining urea/NaOH treated carbon nanotubes (CNTs) and Fe-based catalyst for FT process[54]. They developed a one-step synthesis to treat CNTs and equip them with pyrrolic nitrogen atoms. Afterwards, they used the functionalized CNTs as the supporting material to support traditional Fe-based catalysts.

After test, Fe/CNT catalyst showed its catalytic performance in FT process to convert syngas to alkanes (>5C). Interestingly, this catalysts showed higher catalytic performance and higher selectivity towards alkanes with 5+ carbons. Researchers believe the pyrrolic nitrogen may work as an “electron reservoir”, which can increase the conductivity of supporting CNTs and enhance CNTs’ electron donating tendency. In addition, they believe

the urea/NaOH treatment may also suppress the destruction of CNT network, which protects the reactivity of catalyst.

Benefit from advancement of nano technology, more and more nano-sized materials have been produced. Due to the small size and large surface area, they show extraordinary physical and chemical properties. In 2015, Israel Cano et al. reported their work using a surface-modified gold nano-particle catalyst to reduce unsaturated aldehydes and nitro groups with high yield and selectivity[55]. In the research, H_2 gas was activated on the surface of phosphine oxides ligated gold nanoparticles and works as the reducing agent to selectively reduce the double bond in the substrate. The reaction is shown below:

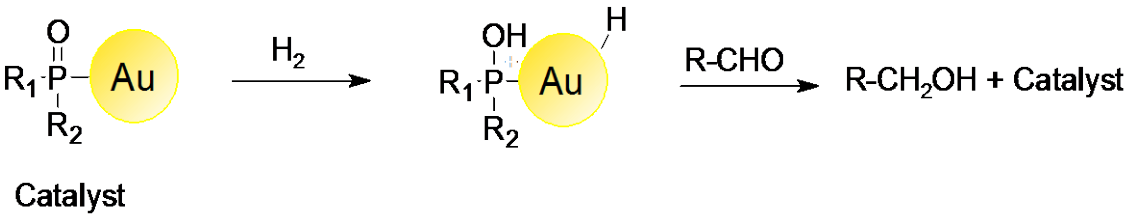


Figure 9. Surface-modified Au nanoparticle catalyzed aldehyde hydrogenation reaction

After examine the reaction mechanism, they found that the H-H bond was cleaved by both AuNP and phosphine oxide ligand. This catalyst also showed good chemoselectivity on substrate.

Although nanoparticles with hundreds of nanometers particle size are much smaller than traditional materials, scientists still making effort to synthesis even smaller particles, such as nanoclusters or even single-atom catalyst[56-59]. In 2015, Yan and et al. reported a single-atom Pd catalyst that has high performance on catalyzing hydrogenation reaction of 1,3-

butadiene[60]. In the experiment, they utilized atomic layer deposition (ALD) technique to deposit single Pd atoms on the supporting graphene.

In the experimental part, researchers investigated the catalytic performance of Pd single atom catalyst and compared to commercial Pd/C nano particle catalyst. The results showed that the Pd single atom showed both higher catalytic reactivity and superior selectivity on hydrogenation of 1,3-butadiene. With Pd single atom catalyst, 1,3-butadiene can be selectively converted to butane, especially 1-butene, while Pd/C will eventually produce butane. The illustration is shown below[60]:

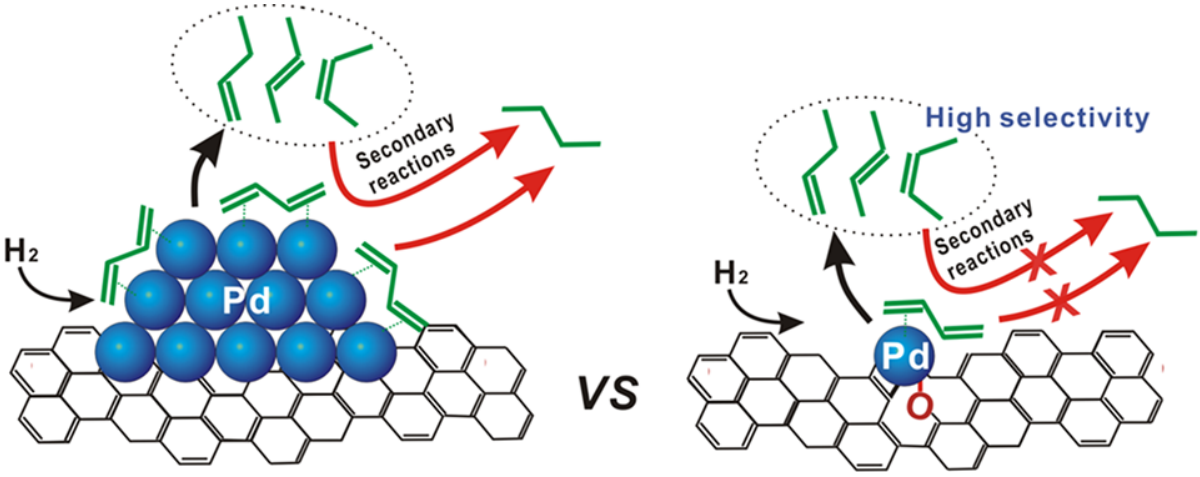


Figure 10. Comparison of Pd nanoparticles and Pd single atom catalyst on 1,3-butadiene hydrogenation

Another remarkable technique developed recently in small molecule activation is the frustrated Lewis pairs (FLPs). This method was first reported by Stephan in 2008[61]. He synthesized a pair sterically hindered Lewis acid and base in order to activate H_2 molecules. The reaction is shown below:

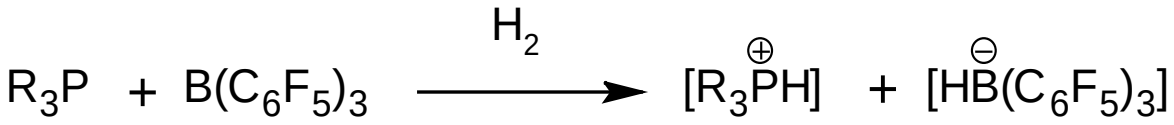


Figure 11. Hydrogen activation by FLP

Although there are strong electron withdrawing groups (EWGs) around boron atom and strong electron donating groups (EDGs) around phosphorous atom give them acidity and alkalinity, the two center atoms cannot approach each other so as to form an acid-base adduct, stopped by all the bulky substituent groups. As the result, there are high potential energy between Lewis and base. Many bonds, such as H-H and C-H, will be asymmetrically cleaved between them via an electron transfer process.

Followed by the invention of FLPs, scientists expanded the range of substrate of FLP catalyzed reaction other small molecules, such as carbon oxides, nitrogen oxides and sulfur oxides[62-64]. Different combinations of Lewis acids and bases could convert these stable small molecules to their more reactive forms.

Inspired by these researches, we used computational approach to design a series of phosphine oxide modified Cu_3, Ag_3 and Au_3 nanoclusters for H_2 activation and illustrate their potential use as CO hydrogenation.

3.2 Experimental Methods

In this project, all DFT calculations were performed using Gaussian 09 software package with B3LYP functional[65]. In order to achieve both satisfactory accuracy and efficiency at the same time, we combined LANL2DZ basis set for all metals and 6-31G** basis set for all

non-metal atoms. When performing optimizations and frequencies calculations, an "ultrafine" integration grid were applied for all molecules as well. To verify the TSs, Intrinsic reaction coordinate (IRC) calculations were performed. Unless specified, Gibbs free energies were discussed in this chapter.

3.3 Results and Discussion

3.3.1 Optimization of Catalysts

As the first stage of research, a series of catalysts were first designed and optimized using Gaussian software. $–PO(Me)_2$ phosphine oxide modified Ag_3, Au_3 and Cu_3 catalyst ("**CAgMe**", "**CAuMe**" and "**CCuMe**", respectively) were first optimized as the example. The optimized structures are shown below:

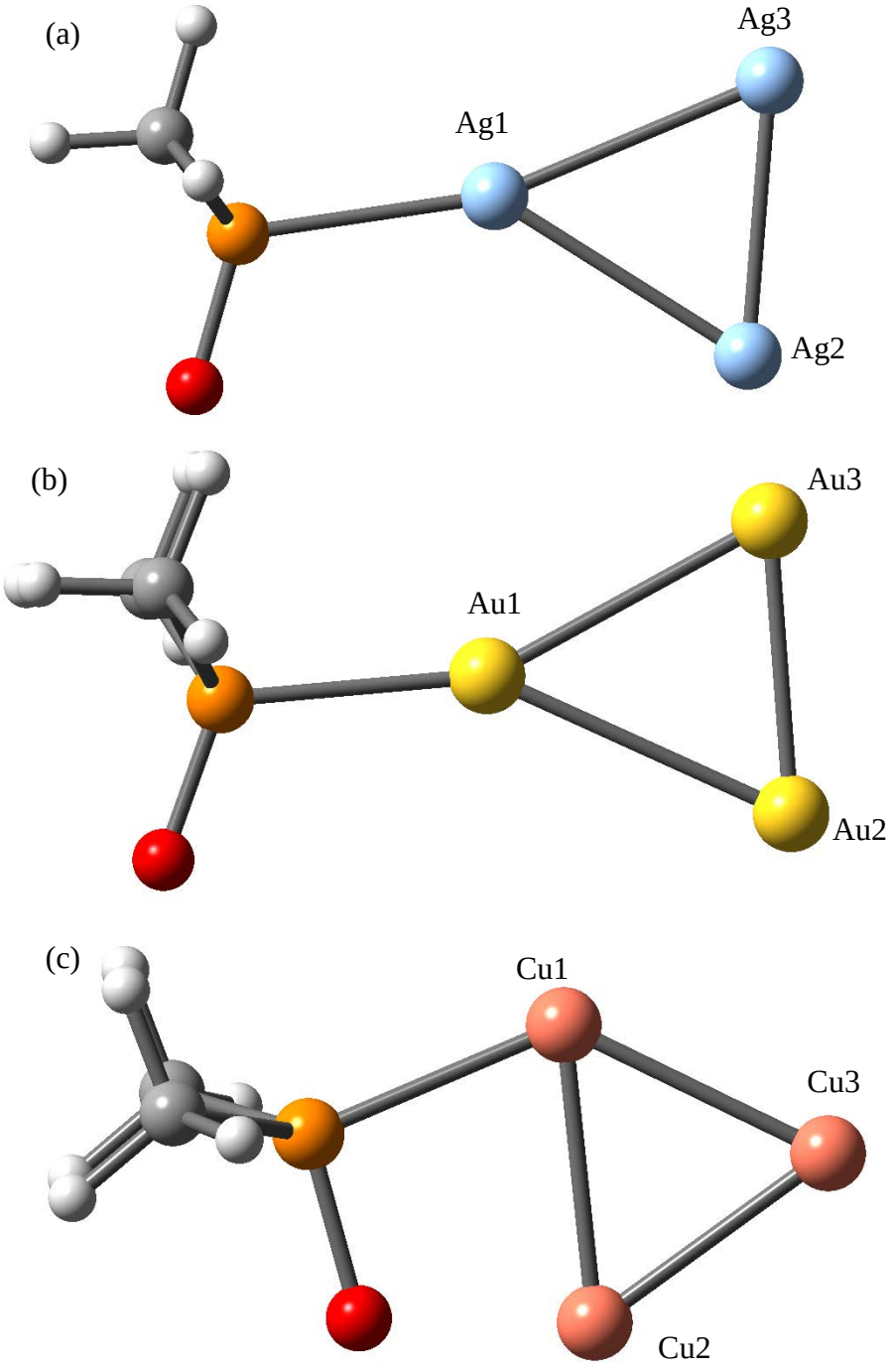
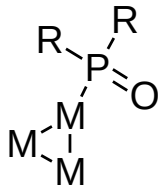


Figure 12. Optimized structure of (a)CAgMe, (b)CAuMe and (c)CCuMe. (Color scheme: light blue, Ag; yellow, Au; bronze, Cu; gray, C; white, H; red, O; orange, P)

As shown in Figure 12, both phosphine oxide modified Ag, Au and Cu catalysts are successfully designed and optimized. Among all these three catalysts, **CAgMe** and **CAuMe** have similar geometry though there's difference on bond lengths: triangle-shaped metal cluster, with phosphine ligand attached. On the other hand, the bond angle of P-Ag1-Ag2 and P-Au1-Au2 are much greater than **CCuMe**. As the result, the distance between O and Cu2 is much shorter than **CAgMe** and **CAuMe**.

After optimization of **CAgMe**, **CAuMe** and **CCuMe**, a series of catalyst with different ligands were designed and optimized as well. Following table showed the structures of all catalysts designed in this research.

Table 1. All catalysts designed in this research



-R = -Me, -*i*Pr, -Ph, -Cl, –Br

M = Cu, Ag, Au

Entry	Name	Metal (M)	-R
1	**CAgMe**	Ag	-Me
2	**CAgiPr**	Ag	-*i*Pr
3	**CAgPh**	Ag	-Ph
4	**CAgCl**	Ag	-Cl
5	**CAgBr**	Ag	-Br
6	**CAuMe**	Au	-Me
7	**CAuiPr**	Au	-*i*Pr
8	**CAuPh**	Au	-Ph
9	**CAuCl**	Au	-Cl
10	**CAuBr**	Au	-Br
11	**CCuMe**	Cu	-Me
12	**CCuiPr**	Cu	-*i*Pr
13	**CCuPh**	Cu	-Ph
14	**CCuCl**	Cu	-Cl
15	**CCuBr**	Cu	-Br
16	**Ag_3**	Ag	/
17	**Au_3**	Au	/
18	**Cu_3**	Cu	/

Entry 16-18 in Table 1 are the Ag_3, Au_3 and Cu_3 catalysts without any modification. These catalysts were examined for comparison purposes.

3.3.2 Hydrogen Activation

In this part of study, **CAgMe** was chosen as the example to study the mechanism and reaction pathway. As mentioned above, Ag_3 nanocluster catalyst without any modification was chosen to compare.

First, an unmodified Ag3 catalyst was first tested in hydrogen activation reaction. After TS optimization, one TS, **TSH_{Ag3}** was found. The optimized geometry is shown below.

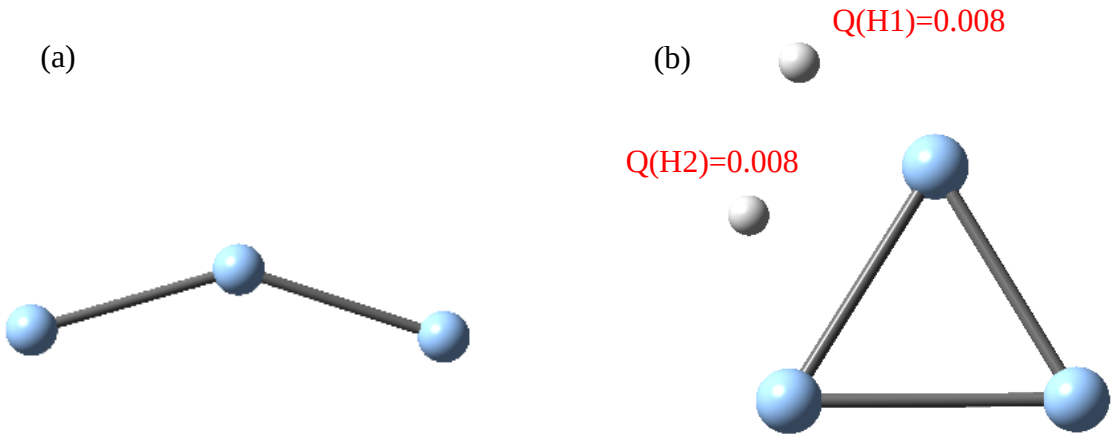


Figure 13. Optimized structure of (a)Ag_3 and (b)**TSH_{Ag3}**. The net Mulliken charge (a.u.) are given in red.

According to calculation, the unmodified Ag3 nanocluster can catalyze the hydrogenation activation reaction. In the TS, the net charge on both H atoms are 0.008 a.u., which indicates that the H-H bond was cleaved symmetrically. To evaluate the reactivity, activation energy of this reaction (E_aH) was calculated using equation (2.3) as 41.71 kcal/mol. Similarly, Au_3

and Cu_3 were examined with same methods. E_a for Au_3 and Cu_3 were calculated as 23.25 kcal/mol and 24.26 kcal/mol.

According to the calculation, all three unmodified nanoclusters can catalyze the hydrogen activation reaction. In addition, these three catalysts can significantly reduce the energy barrier to break H-H bonds, compare to H-H bonding energy (about 103 kcal/mol)[66].

After performing the calculation with unmodified nanoclusters, **CAgMe** was examined in hydrogen activation reaction. One TS, **TSHCAgMe**, was found. The optimized structure is shown below:

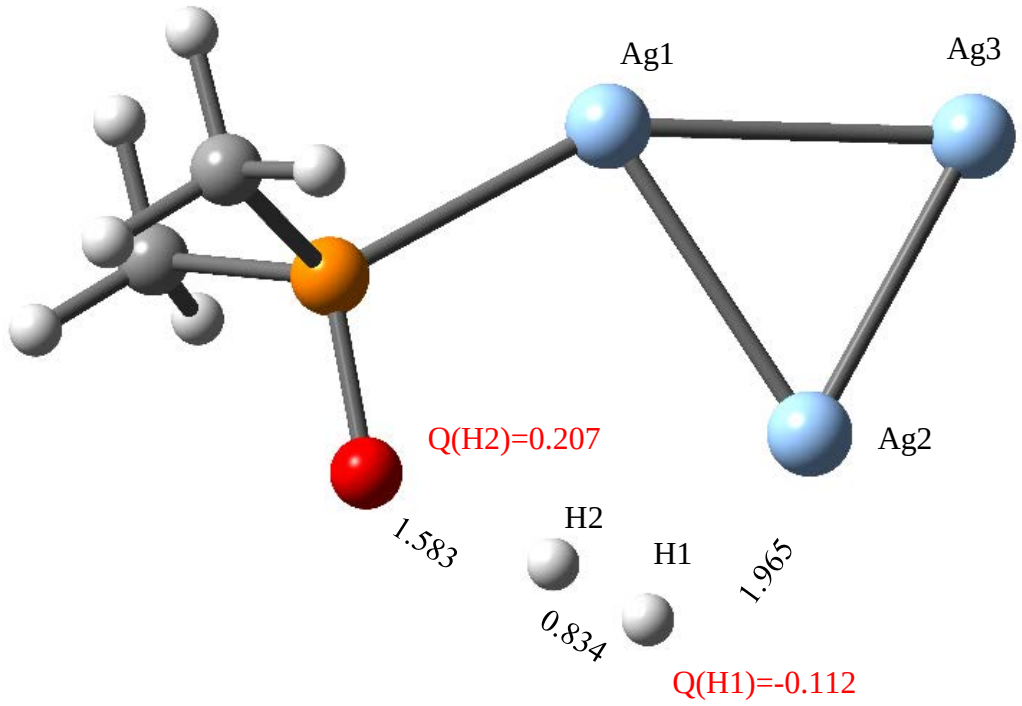


Figure 14. Optimized structure of **TSH$_{CAgMe}$**. The net Mulliken charge (a.u.) are given in red. The distances (Å) are given in black.

The reaction mechanism for **CAgMe** has shown many differences with Ag3 though they both are capable to catalyze the hydrogen activation reaction. First, the net charge on two H atoms are quite different. H1 atom has a negative charge of -0.112 a.u. while H2 atom has a positive 0.207 a.u., which indicates that the H-H bond was cleaved asymmetrically since the charges were not separated equally. During the reaction, electrons may flow from the electron-rich metal cluster to the σ* orbital of H_2, then flow from σ orbital to electron negative O atom:

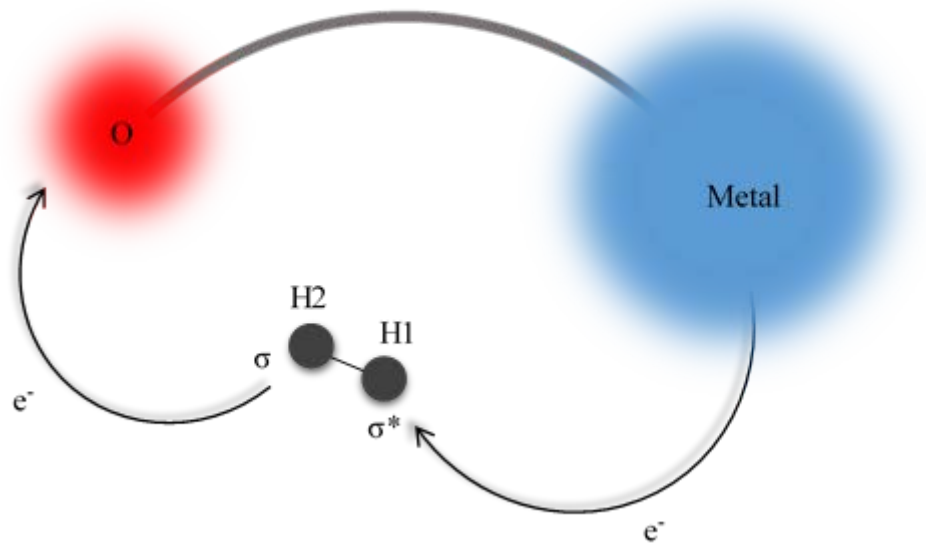


Figure 15. Illustration of electron transfer during **CAgMe** catalyzed hydrogen activation.

The catalyst can be considered as a frustrated Lewis pair (FLP) in hydrogen activation. The electron-rich metal cluster is the electron donor and the phosphine oxide ligand play a role of electron acceptor. By introducing the separation of electron density, the H-H bond can be cleaved with much lower energy. E_aH for **CAgMe** is remarkably as low as 4.92 kcal/mol according to calculation, which implies that the modification can increase the reactivity of the catalyst by altering the reaction mechanism.

Another change to note is the geometry alteration of catalyst. After forming the TS, the bond angle between P-Ag1-Ag2 has reduced from 139.5° in **CAgMe** to 93.1° in **TSH$_{CAgMe}$**. The alteration is necessary for the formation of cyclic TS and promote the occurrence of electron transfer process. Since the alteration may consume certain amount of energy, the energy barrier may be further reduced if the initial geometry of catalyst is more “fit” the cyclic TS to avoid huge alteration.

Furthermore, all designed catalysts listed in Table 1 were tested. Similar mechanisms were established for all catalysts. In Table 2, E_aHs for all catalysts were listed.

Table 2. List of catayts and their E_aHs

Entry	Catalyst Name	Transition State (H_2 activation)	EaH (kcal/mol)
1	**CAgMe**	**TSH_{CAgMe}**	4.92
2	**CAgiPr**	**TSH_{CAgiPr}**	4.05
3	**CAgPh**	**TSH_{CAgPh}**	5.43
4	**CAgCl**	**TSH_{CAgCl}**	13.12
5	**CAgBr**	**TSH_{CAgBr}**	20.03
6	**CAuMe**	**TSH_{CAuMe}**	3.54
7	**CAuiPr**	**TSH_{CAuiPr}**	2.89
8	**CAuPh**	**TSH_{CAuPh}**	3.59
9	**CAuCl**	**TSH_{CAuCl}**	8.26
10	**CAuBr**	**TSH_{CAuBr}**	4.36
11	**CCuMe**	**TSH_{CCuMe}**	21.55
12	**CCuiPr**	**TSH_{CCuiPr}**	21.22
13	**CCuPh**	**TSH_{CCuPh}**	20.29
14	**CCuCl**	**TSH_{CCuCl}**	21.23

Among all catalysts, Au based catalysts have the lowest activation energies. The reason that causes difference on E_aHs from metal to metal may be the H affinity. For example, Ag-H bonding energy (55.0±3 kcal/mol) is lower than Au-H bonding energy (68.1±3 kcal/mol), which indicates that TSH of Au based catalysts is more stable than Ag based catalysts. As the result, Ag based catalysts (**Entry 1-6**) have higher E_aHs than Au based catalysts (**Entry 6-10**) as shown in Table 2. One exception is Cu based catalysts. Even though the interaction between Cu and H is relatively strong (bonding energy is 66.0±2 kcal/mol[66], higher than Ag-H), the E_aHs are much higher than both Au and Ag based catalysts. Possible explanation for this phenomenon may be the geometry of catalyst. Following figures demonstrated the difference between **CCuMe** and **CAgMe**.

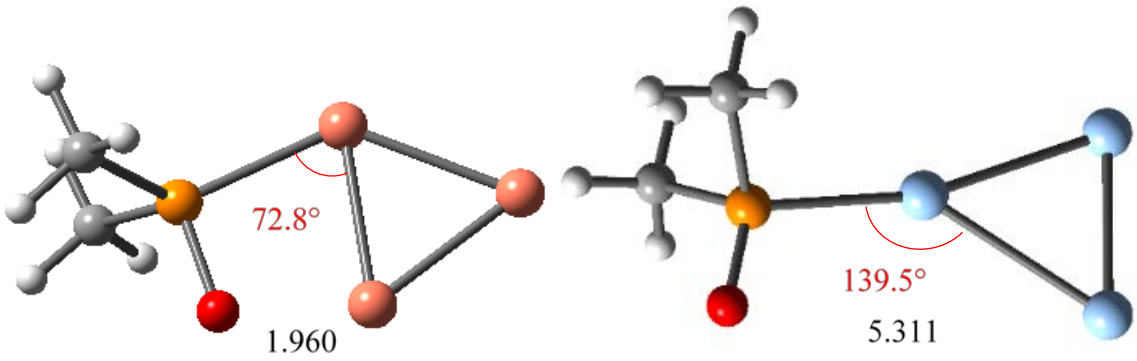


Figure 16. Different geometries of **CCuMe** (left) and **CAgMe** (right). Distance (Å) between two reaction center atoms are given by black, the bond angles are given in red.

According to calculation, the P-Cu1-Cu2 bond angle are much smaller than P-Ag1-Ag2, which shortens the distance between O and Cu2, two atoms interact directly with H. In order to form a TS, more energy is need to overcome the Cu-O interaction first. Meanwhile, the

interaction between Ag2 and O atom is much weaker, due to the long distance between them. Au based catalysts have similar geometries with Ag catalysts. Therefore, the activation energy of Cu based catalysts are much higher the other two categories.

Another factor that affects E_aHs is the –R groups in the phosphine oxide ligand. According to Table 2, electron withdrawing groups (EWGs), such as –Cl and –Br, are able to increase the E_aH but electron donating groups (EDGs) tend to decrease it. This substituent effect may be attributed to the electron density distribution difference. EWGs may decrease the electron density on the metal cluster through the induction significantly, thus decrease the ability for the donor to donate electrons to H_2. In the other hand, EDGs show opposite effect against EWGs. The level of effect EWGs/EDGs is affected by their intensity as well. For example, **CAgiPr** has even lower E_aH than **CAgMe**, since –*i*Pr is a stronger EDG than –Me.

In order to further understand the mechanism, HOMO-LUMO gap (ΔE_{MO}) of each catalyst molecules were obtained from calculation output files and plotted against E_aHs. Following figure is the plot.

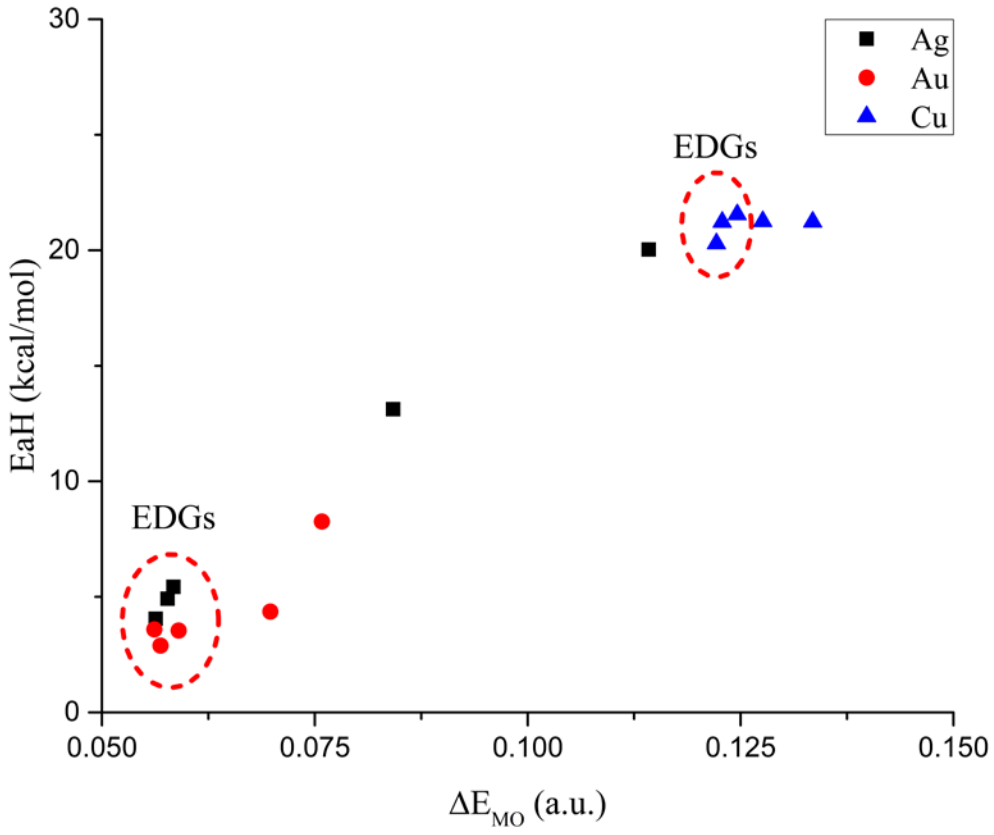


Figure 17. ΔE_{MO} (in a.u.) vs. E_aH (kcal/mol). Red dashed circles are catalysts with EDGs as their –R groups.

ΔE_{MO} is a good parameter to evaluate the difficulty for electron to transfer. It can be found from the plot that the energy barrier is positively correlated to ΔE_{MO}, and EDGs are able to lower them. But for Cu based catalysts, even those with EDGs have similar E_aH with the rest, which indicates that the bottleneck for Cu based catalysts in hydrogen activation is Cu-O breaking and geometry alteration before electron transfer could occur.

3.3.3 CO Hydrogenation

The product of hydrogen activation is a catalyst-2H complex. This complex also works as the reduce agent for CO. One optimized catalyst-2H complex, **CAgMe-2H**, is shown in the following figure:

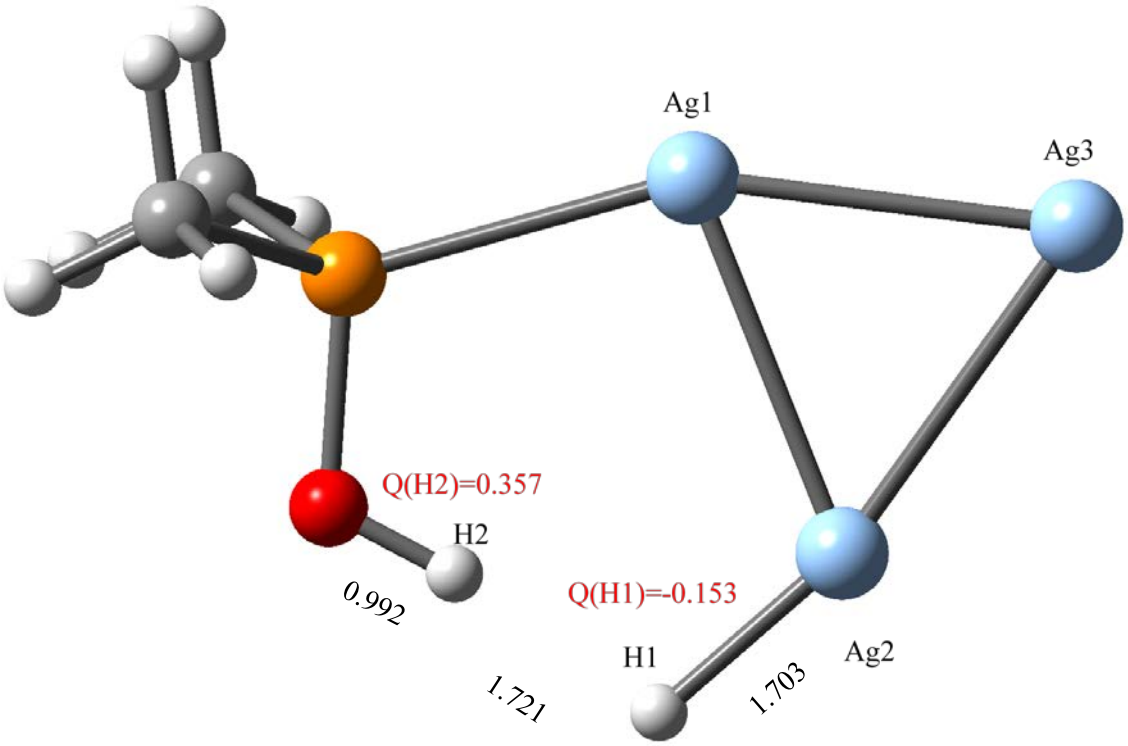


Figure 18. Optimized structure of **CAgMe-2H**. Distances (Å) are marked by black and net charges (a.u.) are given by red.

The asymmetry of two H atoms remained after the formation of **CAgMe-2H** intermediate complex. H1 atom that bonded with electron-rich Ag cluster has negative -0.153 net charge

while H2 atom bonded with O atom has positive charge of 0.357. The net charge is the evidence of electron transfer process during the reaction: electron flows from metal cluster to O. Distance between H1 and H2 has been extended from 0.74Å to 1.721Å as well, which proves the cleavage of H-H bond.

Start from **CAgMe-2H**, we initiated calculations to find out how this complex works as the reducing agent to hydrogenate CO to form HCHO as the product. After performing simulations, **TSCO$_{AgMe}$**, was found as the TS during the catalyzed CO hydrogenation reaction. The structure is shown below:

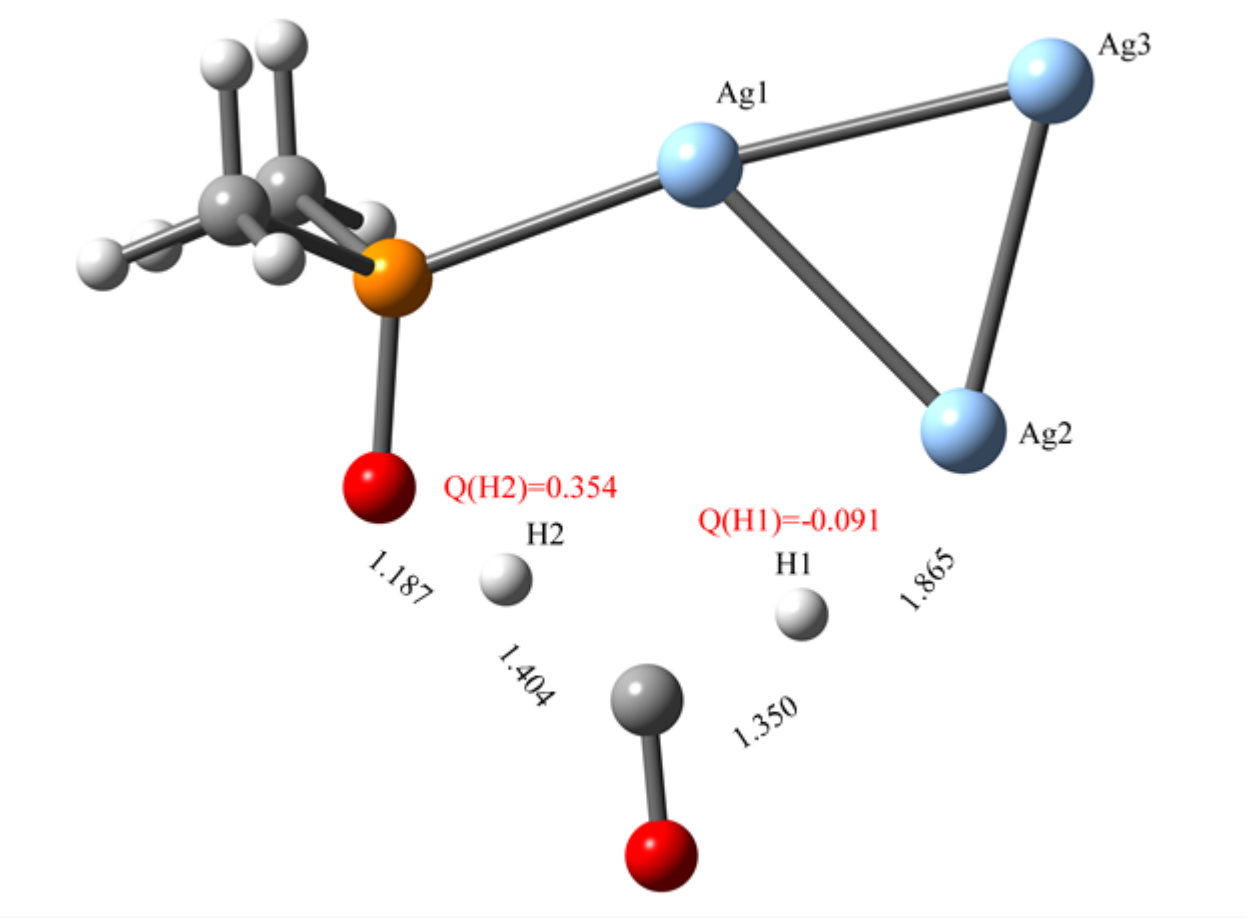


Figure 19. Optimized structure of **TSCO$_{AgMe}$**. Distances (Å) are given in black and net charges (a.u.) are given in red.

By comparing **CAgMe-2H** and **TSCO$_{AgMe}$** it can be figured out that the P-Ag1-Ag2 bond angle become wider in order to form a seven-membered cyclic TS. The net charge of H2 shows no significant change after the formation of TS while the net charge of H1 has increased from -0.153 to -0.091, which indicates that the CO hydrogenation reaction may be initiated by the electron transfer from H1 to CO. The activation energy for CO hydrogenation (EaCO) was also calculated as 20.07 kcal/mol for **CAgMe**. After combining all energy data, we are able to draw an energy profile for the whole **CAgMe** catalyzed reaction:

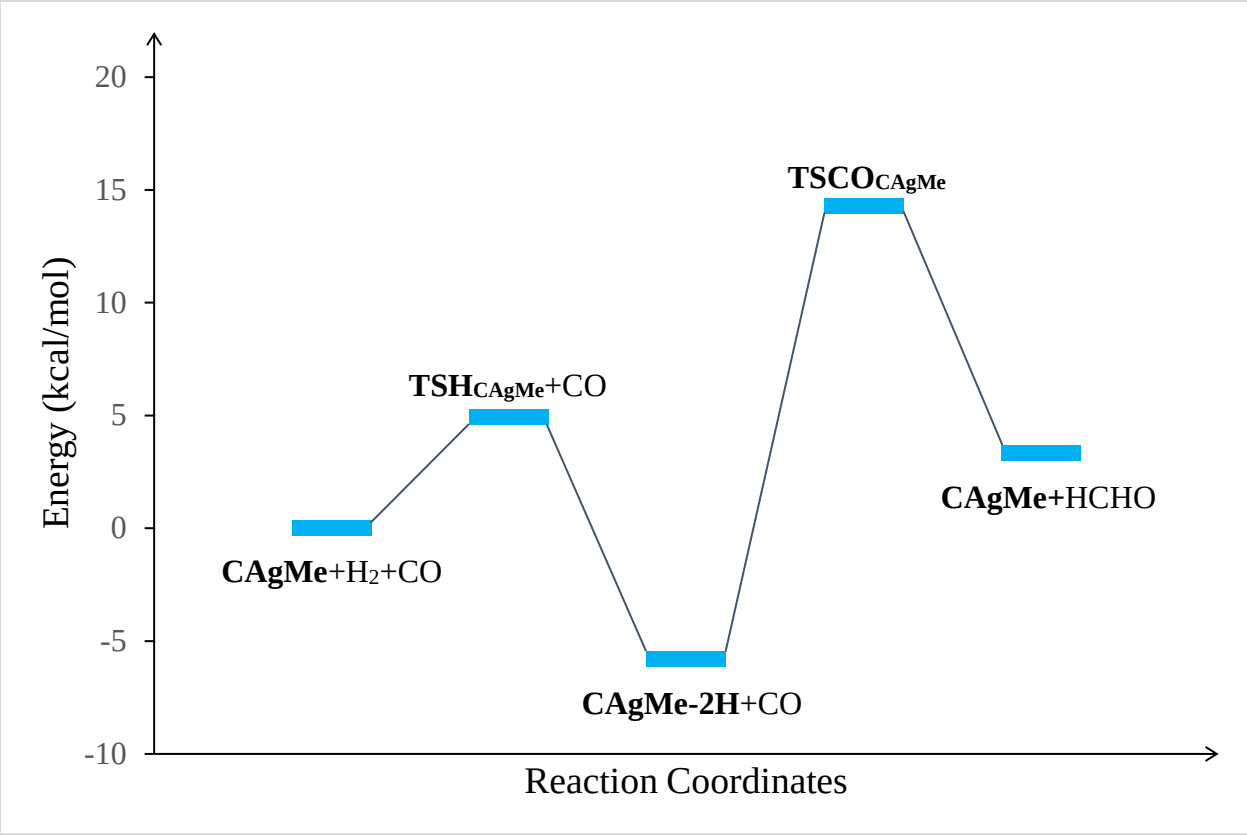


Figure 20. Reaction pathway of **CAgMe** catalyzed hydrogen activation and CO hydrogenation

Similar to the analysis part in hydrogen activation, we calculated all EaCOs for all catalysts. The results are listed in Table 3:

Table 3. List of catalysts and their E_aCO

Entry	Catalyst Name	Transition State (CO hydrogenation)	E_aCO (kcal/mol)
1	**CAgMe**	**$TSCO_{CAgMe}$**	20.07
2	**CAgiPr**	**$TSCO_{CAgiPr}$**	18.46
3	**CAgPh**	**$TSCO_{CAgPh}$**	18.34
4	**CAgCl**	**$TSCO_{CAgCl}$**	15.41
5	**CAgBr**	**$TSCO_{CAgBr}$**	15.93
6	**CAuMe**	**$TSCO_{CAuMe}$**	30.58
7	**CAuiPr**	**$TSCO_{CAuiPr}$**	30.91
8	**CAuPh**	**$TSCO_{CAuPh}$**	30.52
9	**CAuCl**	**$TSCO_{CAuCl}$**	22.08
10	**CAuBr**	**$TSCO_{CAuBr}$**	22.53
11	**CCuMe**	**$TSCO_{CCuMe}$**	21.54
12	**CCuiPr**	**$TSCO_{CCuiPr}$**	21.28
13	**CCuPh**	**$TSCO_{CCuPh}$**	19.97
14	**CCuCl**	**$TSCO_{CCuCl}$**	15.29

Like the hydrogenation activation stage, the energy barrier of CO hydrogenation is affected by different factors as well. Among all metals, Au based catalysts have the highest overall E_aCO. On contrary, Au based catalysts have the overall best catalytic performance in

hydrogen activation. We believe that the catalyst-2H complexes of Au based catalysts are more stable than the other two metals, due to the stronger interaction between Au and H. More stable catalyst-2H complex has a lower energy level and lower activity. Therefore, more energy is necessary to achieve the TSCO for Au based catalysts.

Substituent effect in CO hydrogenation stage is also opposite to hydrogen activation stage for all catalysts. EWGs pull the electrons toward them and alter the distribution of electron cloud, further make the catalyst-2H complex more active. As the result, catalysts with EWGs as their –R group usually has lower E_aCO than EDGs substituted catalysts.

In addition to the analysis of E_aCO, the HOMO-LUMO gap of catalyst-2H complexes (ΔE_{2HMO}) are obtained and analyzed as well. Similar to the last stage, ΔE_{2HMO} is plotted against E_aCO to visualize the relationship. Following figure shows the relationship between ΔE_{2HMO} and E_aCO:

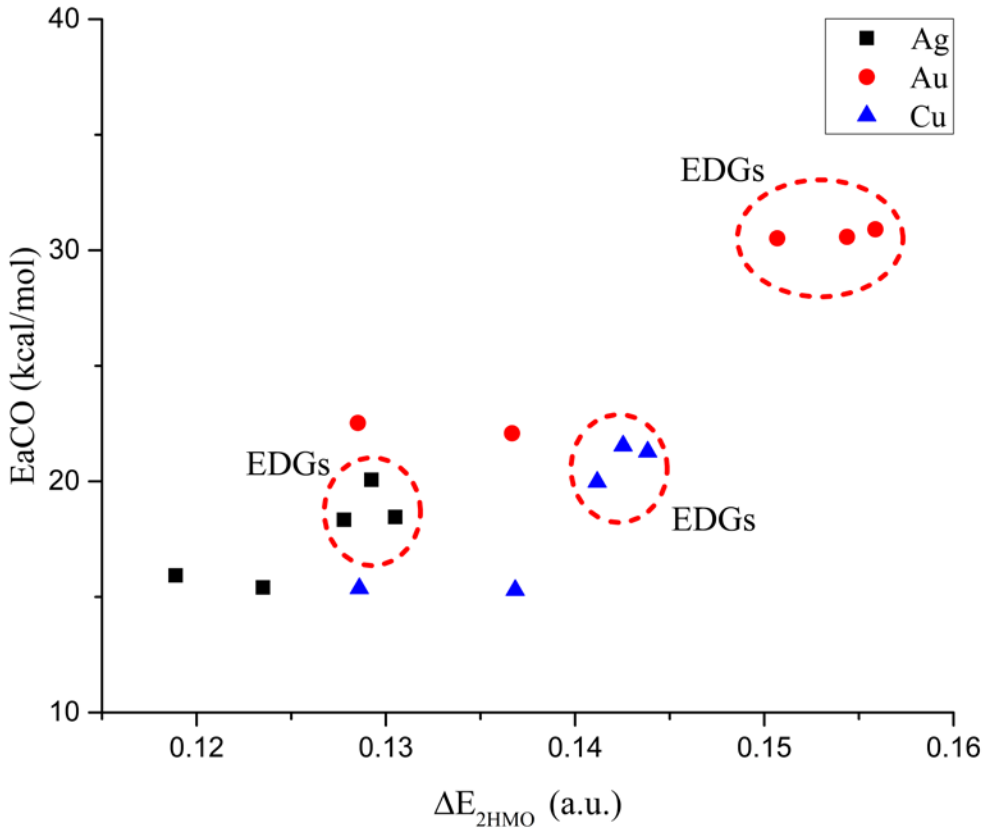


Figure 21. ΔE_{2HMO} (in a.u.) vs. E_aCO (kcal/mol). Red dashed circles are catalysts with EDGs as their –R groups.

The activation energy for CO hydrogenation also shows a positive correlation with $\Delta E_{2HM,}$ which indicates that electron transfer is critical during the reaction. The reversed substituent effects can be clearly found out in the figure as well. Compare with the hydrogen activation stage, the substituent effect is much stronger for Cu based catalysts, which may be attributed to the geometry. Once the catalyst-2H complex is formed, the Cu-O interaction is

eliminated and no longer is the bottleneck for the reaction. In addition, the geometries of all catalyst-2H complexes are quite similar as well.

3.4 Conclusion and Future Work

In this project, we applied DFT computational method in catalyst designing. A series of phosphine oxide modified Ag_3, Au_3 and Cu_3 catalysts that are able to catalyze hydrogen activation and CO hydrogenation reaction were successfully designed and evaluated. With the introduction of modification, the metal cluster catalysts were converted to a frustrated Lews pair and were capable to cleave the H-H bond asymmetrically with much lower energy barrier to overcome than unmodified nanoclusters by promoting electron transfer process. The activation energy is affected by both the metal and substituent group on P atom. Metals with higher H affinity are able to establish stronger interaction with hydrogen, so as to reduce the energy barrier. EDGs can reduce the energy barrier as well, through promoting the electron donation from the Lewis base side. Au based catalysts with EDGs substituted phosphine oxide ligand showed the best catalytic performance in hydrogen activation reaction.

In the CO hydrogenation stage, high H affinity and EDGs showed opposite effect, since they are able to stabilize the catalyt-2H complexes, which increase the energy barrier to form TSCO. In CO hydrogenation reaction, Ag based catalysts with EWGs are the most efficient candidates.

In the future, experimental research can be carryout based on this study. In addition, supporting material, such as oxides, zeolites or metal-organic framework (MOFs), will be

added to the catalytic system, further increase the reactivity and stability. Other computation chemistry tools, such as Vienna Ab initio Simulation Package (VASP) and Quantum Espresso, can be utilized to study the effect of supporting material.

CHAPTER 4: MODELLING OF REACTIVITY OF CATALYST WITH DFT CALCULATIONS

4.1 General Introduction

4.1.1 Background

The importance of catalysis in modern chemical industries cannot be overstated. Although numerous commercial catalysts have been developed since last century, efforts on catalyst develop never stopped.

Even though catalysis mechanism studies that have been accomplished recently significantly expanded researchers' understanding on the process, to develop new catalysts still require huge amount of time and cost to conduct experiments and the whole development cycle is filled with numerous failed attempts. In addition, modern catalysts are barely have only one or two component, most of them are complicated catalytic systems[51, 67-68]. To accelerate the development of new catalyst, researchers have invented High Throughput Screening devices to screen large amount of possible catalyst candidates[69]. However, the cost of the device and chemicals are extremely high.

To solve the problem, computation chemistry is becoming more and more attractive to researchers, due to its low cost and high efficiency. In the year of 2016, Latimer and et al. reported their remarkable work on modelling heterogeneous catalysts for methane activation reaction[70]. In the beginning of their work, researchers were able to identify a radical-like reaction pathway for methane activation on surface of material. Based on the data, they described a generalized relationship between H affinity (E_H) and TS energy (E_{TS})[70]:

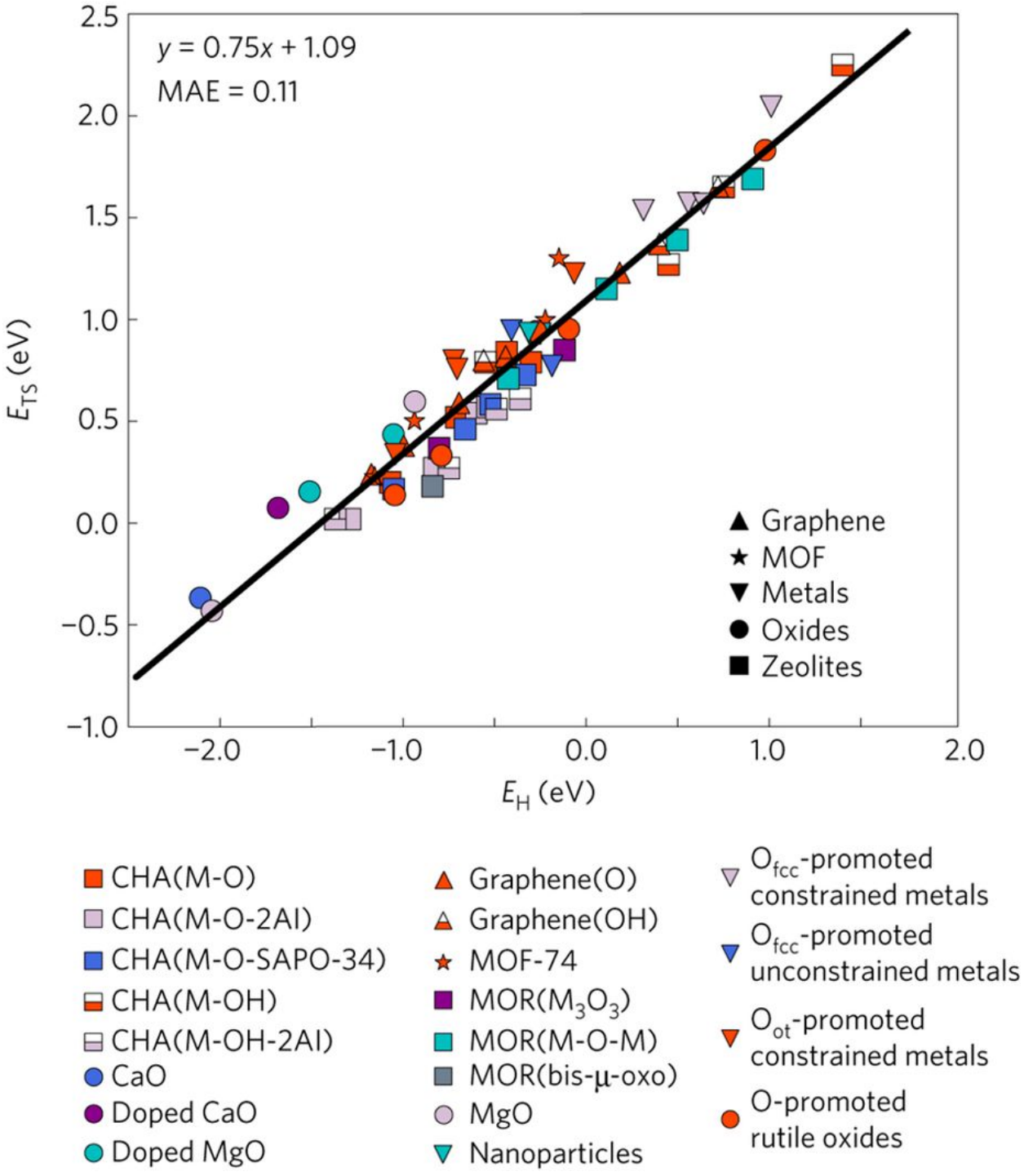


Figure 22. Relationship between E_H and E_{TS} for different heterogeneous catalyst for methane C-H bond activation via a radical-like mechanism

Latimer's group has successfully revealed a linear relationship between H affinity and energy barrier for C-H bond activation, yet the only heterogeneous catalysts, such as zeolites, oxides and MOFs, were considered. In addition, the behavior of electrons during the reaction was not well explained. In order to further study the catalysis mechanism and derive a better explanation for the electron behavior during reaction, we chose frustrated Lewis pairs (FLPs) as the sample catalysts to study the C-H activation.

C-H activation is one of the hottest topics in recent chemistry research[71-76]. Since C-H bond is relatively inert due to its high bonding energy and low polarity, to cleave the C-H bond selectively could greatly benefits the synthesis of new chemicals or even development of new drugs. In addition, C-H bond activation could improve atom economy in synthesis as well. As the simplest hydrocarbon, methane usually shows low reactivity. To utilize naturally abundant methane through C-H activation is of great significance.

Traditionally, most C-H activation reactions are catalyzed by transition metal based catalysts[77-80]. One typical example is the work reported by Chen and co-workers on 2009[81]. Following figure shows the catalytic cycle and reaction equation[81]:

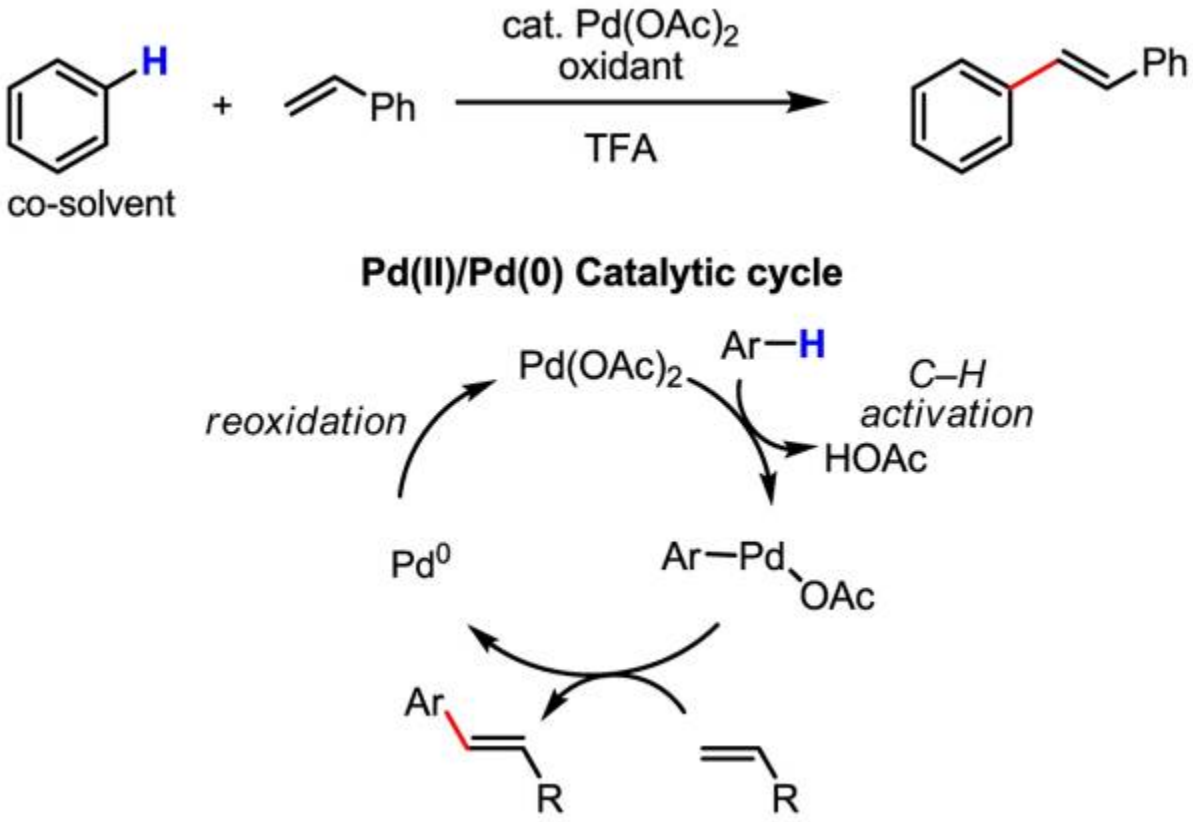


Figure 23. Pd catalyzed sp^2 C-H activation

Transition metal could weaken the C-H bond via coordination. Therefore, transition metals with variable oxidation states and good ability to form complexes are ideal candidates for researchers. By altering metal centers, ligands and substrates, plentiful of new chemicals were synthesized via C-H activation[73, 82].

One major problem with transition metal catalysts is that most catalysts are based on precious metals, whose high cost hinders commercial use in industry. Hence, metal-free FLP catalysts are attracting more attention.

FLP was first discovered and named by Dr. Stephan Douglas about a decade ago[61]. In his pioneering research, FLP was used to activate dihydrogen gas. From then on, FLPs' substrate scope was widely expanded by continuous efforts made by scientists, from simple hydrogen to sulfur oxide, nitrous oxides, and even carbon dioxide[63]. At the same time, scientists have expanded the component of FLP from small organic molecules to many other novel chemicals, such as transition metals, metal cluster, and etc[83-85].

In 2007, Bertrand has reported a breakthrough on small molecule activation[86]. They found that N-heterocyclic carbenes (NHCs) can work as both acid and base so as to activate hydrogen and ammonia under mild condition. On example reaction is shown below:

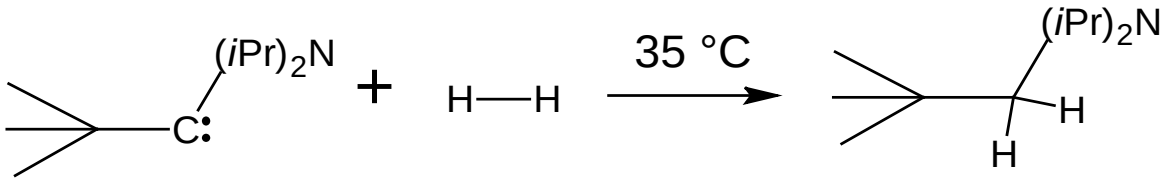


Figure 24. Hydrogen activation by NHC under mild condition.

Due to its capability to donate electrons, NHCs can be paired with another Lewis acid to form a FLP as well. With this idea, Wang and co-workers published their computational work on hydrogen and methane activation by FLPs on 2010[87]. Along with other "traditional" FLPs, such as $(Mes)_3P/B(C_6F_5)_3$, they simulated the catalytic performance of $NHC/B(C_6F_5)_3$ FLPs. According their results, NHC FLPs are able to catalyze the activation of both hydrogen and methane. Moreover, NHC FLPs even showed much better catalytic reactivity than well-know "traditional" FLP catalysts.

After invention of FLP, its catalytic mechanism has initiate discussion and controversy[88-89]. Generally, there're two major models to explain FLPs' high catalytic performance. One is electric field (EF) model and the other is electron transfer (ET) model. EF model believes that the main driving force of catalysis between Lewis acid and Lewis base is the electric field generated by both positive charge center and negative charge center. Strong EWGs around Lewis acid and strong EDGs around Lewis base generate both positive and negative centers with high net charge and electric field is generated consequently

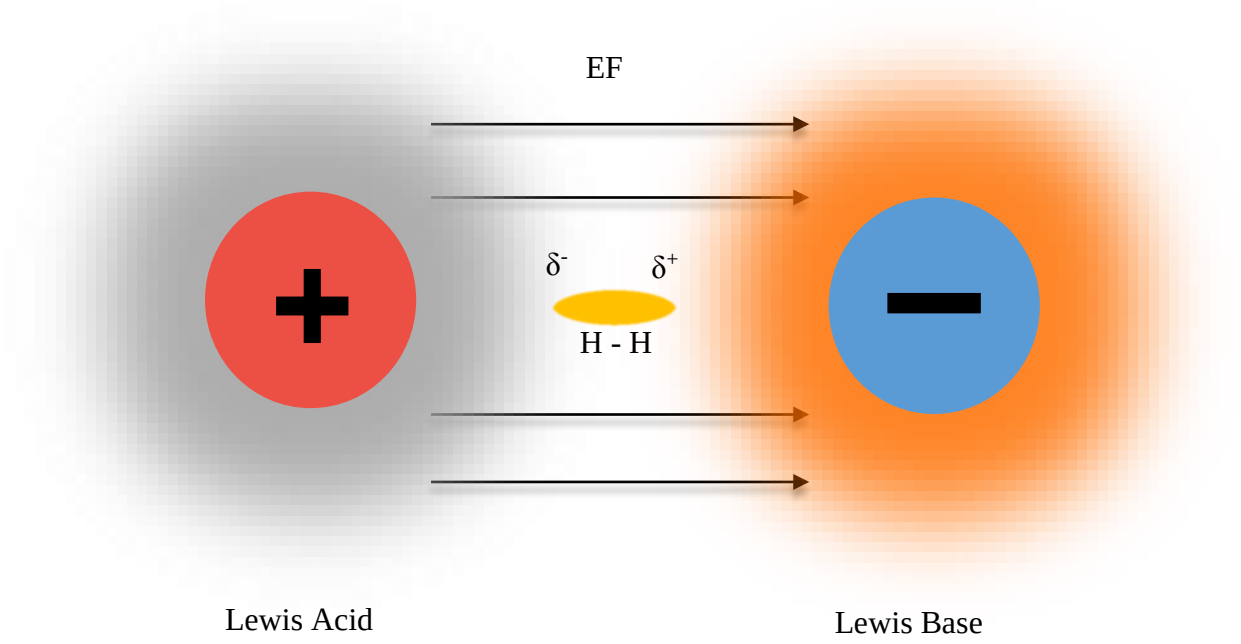


Figure 25. Illustration of EF model. Substrate molecule H-H (yellow) can be considered as a small dipole in the EF generated by FLP.

As shown in the illustration, the substrate molecule will be induced to a small dipole, with δ^+ and δ^- charges. Assume the EF generated by FLP is uniform, the torque on the substrate molecule (τ) can be calculated:

$$\tau = pE \tag{4.1}$$

Where p is the dipole moment and E is the electric field intensity.

According to the equation above, by increasing the EF intensity, the torque on the molecule can be increased, thus promoting the charge separation on the substrate molecule and further weakening the bond. Therefore, stronger Lewis acid/base pair with higher net charge difference may have higher catalytic performance.

Another model is ET model. ET model attributes the motivation of catalysis to electron transfer process, rather than static electric interaction. Following figure demonstrates the mechanism of ET.

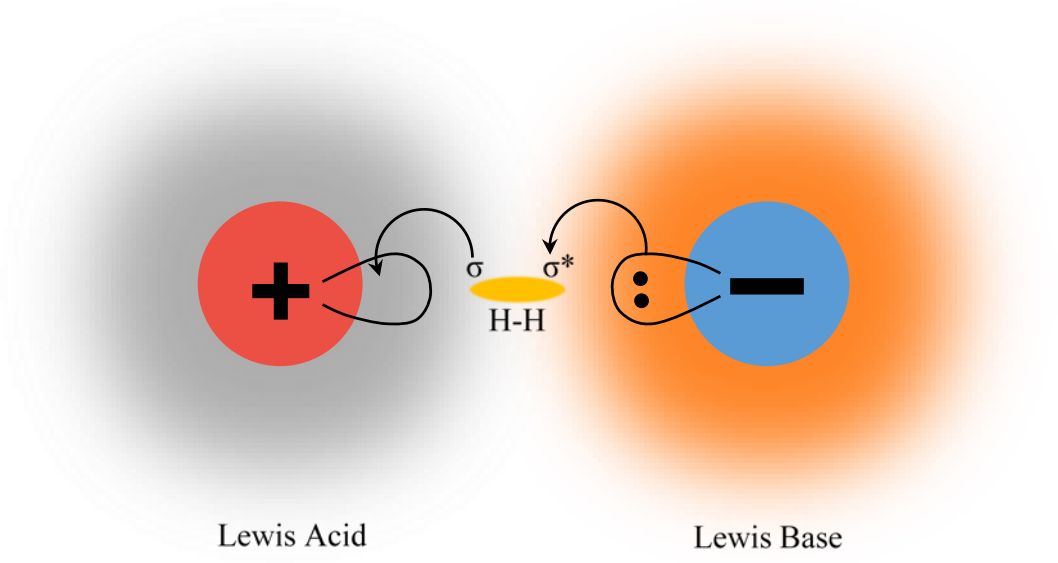


Figure 26. Illustration of ET model. Electrons flow from electron-rich Lewis base to the σ* orbit of H_2, then to the empty orbital of Lewis acid.

In a FLP catalyst, direct electron transfer between acid and base is hindered by bulky groups around acid/base centers. Substrate molecule works as the medium of electron transfer and the bond is eventually weakened during the ET.

In order to understand the mechanisms better, Papai and co-workers performed computational research on FLPs catalyzed H_2 activation reaction[90]. In their work, both EF and ET models were studied. After simulation, they believe the contribution of EF model is very small in the activation, while ET process is the major driving force for H_2 to be activated by FLP. In addition, they found that the activation is affected by many criteria, including H-H distance and charges. Although Papai's work provided plenty of evidence in mechanism study, they did not derive any mathematical model to predict the reactivity of catalyst.

Inspired by all these research mentioned above, we proposed a series of borane/NHC FLP catalysts and studied their catalytic performances in methane activation. Generally, to study the energy barrier of one reaction, TS must be found and optimized. However, the process to find and optimize TS is difficult and time-consuming, since there will be lots of attempts committed especially for novel reactions. In this work, we will use borane/NHC FLP catalyzed methane activation to derive a mathematical model to predict catalysts' reactivity, without complicated and difficult TS optimization.

4.1.2 List of NHCs/Boranes Studied in This Work

In this work, seven NHCs and five boranes were designed and simulated, and all 35 combinations were evaluated as FLP catalysts in methane activation. Following tables list all NHCs and boranes mentioned in this work.

Table 4. List of NHCs studied in this project

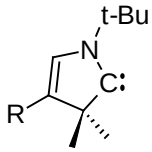
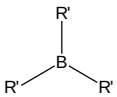
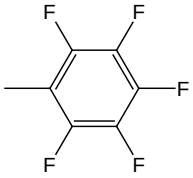
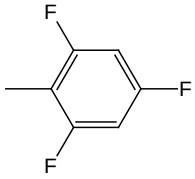
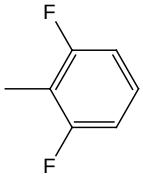
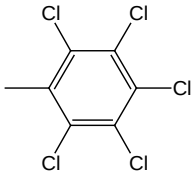
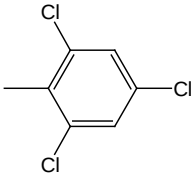
 -R = -H, -Br, -F, -N(*i*Pr)$_2$, -N(Me)$_2$, -OH, -Ph	**-R**	**Compound**
	-H	**NHC1**
	-Br	**NHC2**
	-F	**NHC3**
	-N(*i*Pr)$_2$	**NHC4**
	-N(Me)$_2$	**NHC5**
	-OH	**NHC6**
	-Ph	**NHC7**

Table 5. List of boranes studied in this project

Compound	**B5F**	**B3F**	**B2F**	**B5Cl**	**B3Cl**
-R' 					

As listed in Table 4 and 5, FLPs with different catalytic performance can be achieved by combining NHCs and boranes with different alkanity/acidity.

4.2 Research Methods

In this work, all calculation and simulation were performed with Gaussian 09 software package. DFT method with B3LYP functional were applied for all geometry optimizations (including TS), frequency calculations and energy calculations. In order to balance accuracy and cost, we chose 6-311G(d,p) basis set. In addition, intrinsic reaction coordinate (IRC) calculations were performed for all TS as verification. Free energies were discussed in this chapter unless specified.

4.3 Results and Discussion

4.3.1 Transition State and Reaction pathway

As the first stage of our research, one example **NHC1/B5F** FLP was chosen to study the TS and reaction pathway. Before finding TS, both **NHC1** and **B5F** were first optimized. Their optimized structures are shown below:

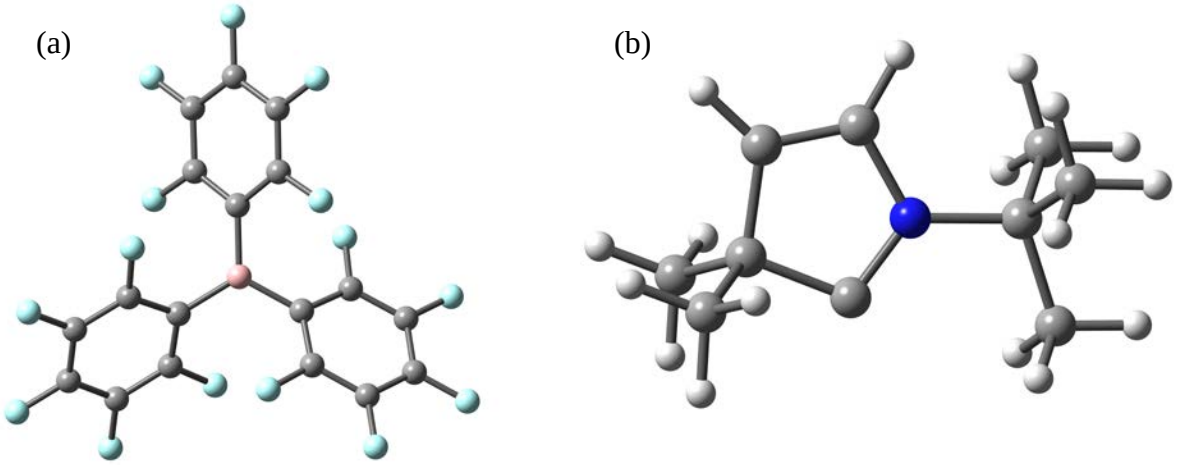


Figure 27. Optimized structure of (a) **B5F** and (b) **NHC1**. Color scheme: gray, C; white, H; blue, N; light blue, F; pink, B.

It can be clearly observed from optimized structures of **B5F** that B atom is surrounded with symmetrical $–C_6F_5$ groups. The dihedral angle between each planar $–C_6F_5$ group is about 39°. The net charge on B atom is 0.723 a.u.. For **NHC1** carbene, the multiplicity is singlet, and the net charge on the carbene C atom is -0.018.

Unlike symmetric H-H bond, the C-H bond is polarized. In optimized methane molecule, C atom has a -0.437 a.u. net charge while H atom has a 0.109 a.u.. To keep the simulation consistent, methane molecule is “placed” between borane and NHC with C atom towards borane and H atom towards NHC in this work. The reaction equation is shown in the following figure:

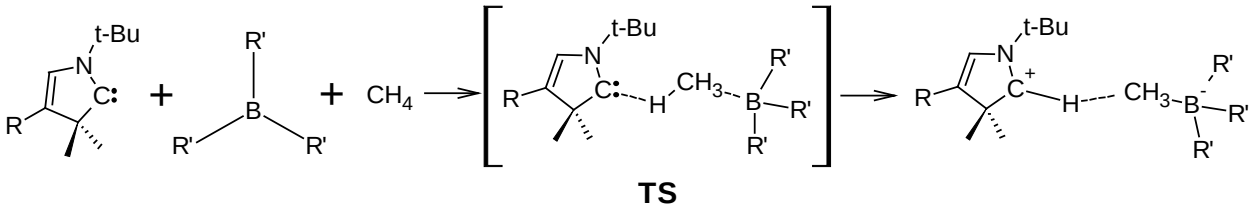


Figure 28. Methane activation by borane/NHC FLP.

After TS search, similar TSs were found for all combinations of boranes/NHCs, which indicates that all combinations can work as catalyst for methane activation though the energy barrier for each catalysts is much different. Following figure shows an example of TS with **B5F/NHC1** catalyst.

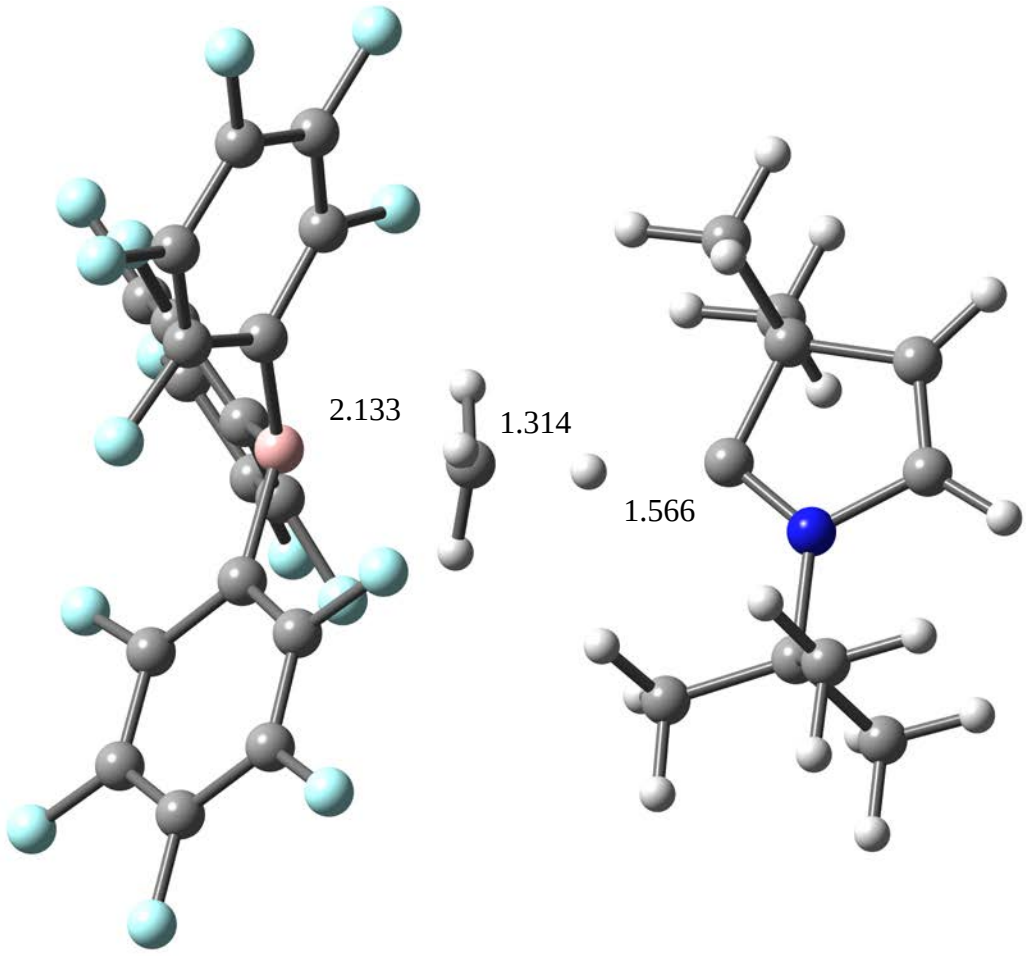


Figure 29. Optimized TS for methane activation by **B5F/NHC1**. Distances (Å) are given in black numbers.

From the figure above it can be clearly seen that the C-H bond is stretched out under the interaction with FLP catalyst. The C-H bond length has stretched to 1.314Å, from 1.09Å. The bond angles also showed significant change. The geometry of the CH_3 group near the borane is altering near planar. After the reaction, the C-H bond is cleaved. The activation energy (E_a) is calculated to be 47.93 kcal/mol for this specific borane/NHC combination. Following table listed activation energies for all combinations.

Table 6. List of activation energy of all borane/NHC combination for methane activation

Borane	NHC	Ea (kcal/mol)
B5F	NHC1	47.93
	NHC2	49.63
	NHC3	49.19
	NHC4	45.56
	NHC5	46.09
	NHC6	47.09
	NHC7	48.12
B3F	NHC1	56.63
	NHC2	57.28
	NHC3	57.48
	NHC4	53.19
	NHC5	53.70
	NHC6	55.82
	NHC7	54.72
B2F	NHC1	57.69
	NHC2	58.42
	NHC3	58.37
	NHC4	54.73
	NHC5	55.35
	NHC6	56.86
	NHC7	57.59
B5Cl	NHC1	68.01
	NHC2	69.88
	NHC3	69.42
	NHC4	64.86
	NHC5	65.83
	NHC6	67.26
	NHC7	68.32
B3Cl	NHC1	69.33
	NHC2	71.03
	NHC3	70.56
	NHC4	66.40
	NHC5	67.31
	NHC6	68.58
	NHC7	69.54

The bonding energy of C-H bond is about 105 kcal/mol[66]. All FLP catalysts showed their capability to lower the energy barrier by a large amount. Generally speaking, FLP catalysts with **B5F** as Lewis acid have the overall highest reactivity while FLPs with **B3Cl** have the lowest. The results meet our expectation that stronger and more EWGs around B could enhance the acidity, thus help to lower the energy barrier. Similar effects can be found in NHCs as well. NHCs with strong EDGs attached, such as **NHC4** and **NHC5**, showed better catalytic performance than other NHCs. As the electron donor in FLP, NHCs' electron density can be increased by attached EDGs via conjugation system.

4.3.2 Borane/NHC Complexes

Although E_a can be calculated after TS optimization, the process can be extremely difficult since TS search is more expensive than ground state optimization and time-consuming. In order to explore the relationship between E_a and FLP catalyst itself, we obtained optimized structures of borane/NHC complexes without methane involved at ground state for all 35 combinations. Following figure gives an example of **B5F/NHC1** complex.

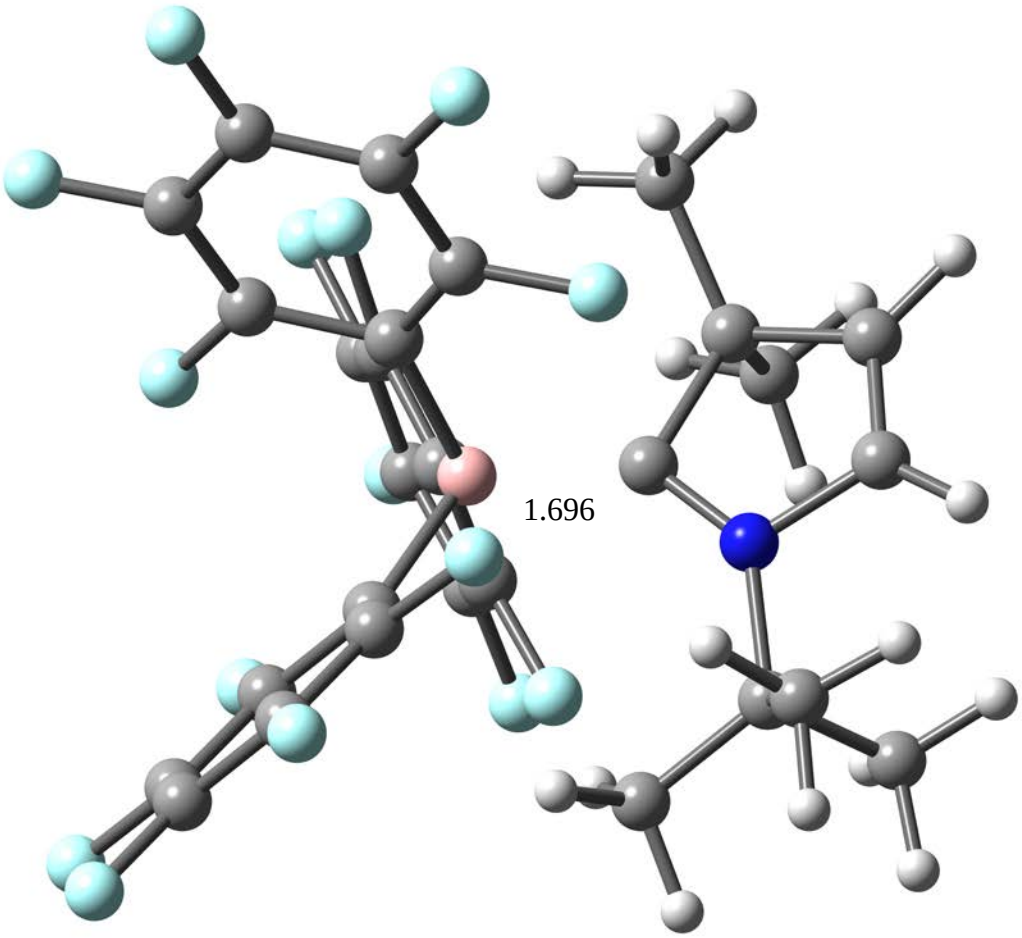


Figure 30. Optimized structure of **B5F/NHC1** complex. Distances (Å) are given in black numbers.

As expected, the geometry of **B5F** was greatly distorted, compared to Figure 29(a). The $-C_6F_5$ groups were pushed far away from approaching NHC in order to expose B center atom. The change on NHC's geometry was not that obvious, due to its stable cyclic structure. As expected, extra energy is needed to form such complex. For **B5F/NHC1**, the energy need to form complex is calculated to be 6.97 kcal/mol. After optimization, some physical properties

were obtained from calculation and used in exploration. List for the physical properties can be found in Appendix D.

4.3.3 Electron Transfer (ET)

According to Papai's research[90], FLP catalysis is mainly motivated by ET process. During the reaction, electrons flow from Lewis base, or NHCs, to Lewis acid side, or boranes. As the result, both Lewis acid and base suffered change of net charge. Interestingly, the net charge on methane during the reaction has not changed significantly according to the TS calculation. In order to evaluate the ET process, we first evaluated the dipole moment for each of the borane/NHC complexes.

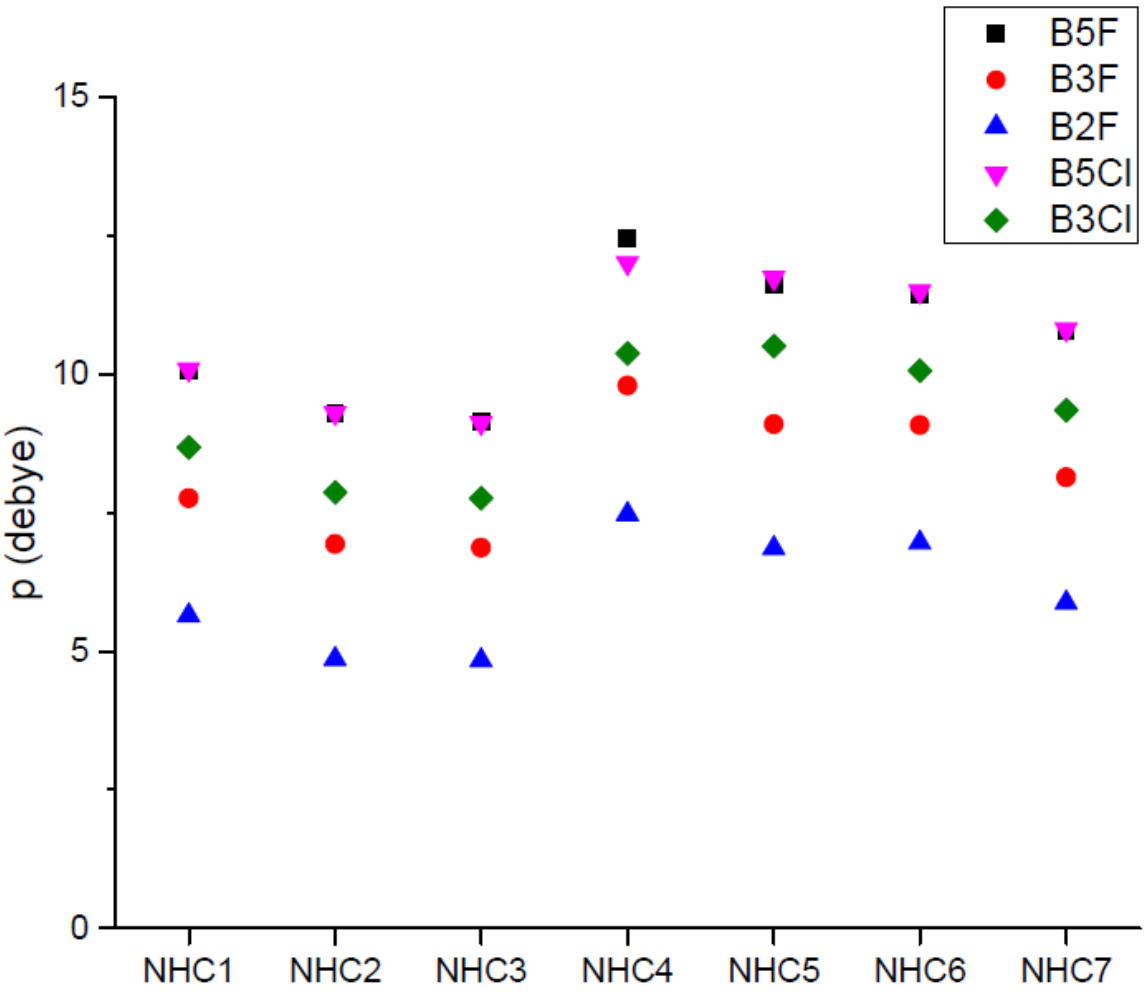


Figure 31. Dipole moment (**p**) for all borane/NHC combination

The dipole moment (**p**) can be calculated as following:

$$\boldsymbol{p} = \Delta Q \times \boldsymbol{d} \tag{4.1}$$

Where ΔQ is the charge difference and **d** is the distance between positive and negative charge center. According to Figure 31, **B5F** and **B5Cl** have almost the same dipole moment, even though $-C_6F_5$ and $-C_6Cl_5$ are totally different groups.

Another thing to notice in Figure 31 is that there the tendency of **p** in every group of boranes. Stronger EDGs on NHCs (for example, **NHC4**, **NHC5**) can significantly increase the dipole moment, which can be attributed to greater electron density separation.

Moreover, we plotted the dipole moment against Ea, which allows us to further explore the influencing factor of reactivity. Following figure shows the relationship between **p** and **E_a**.

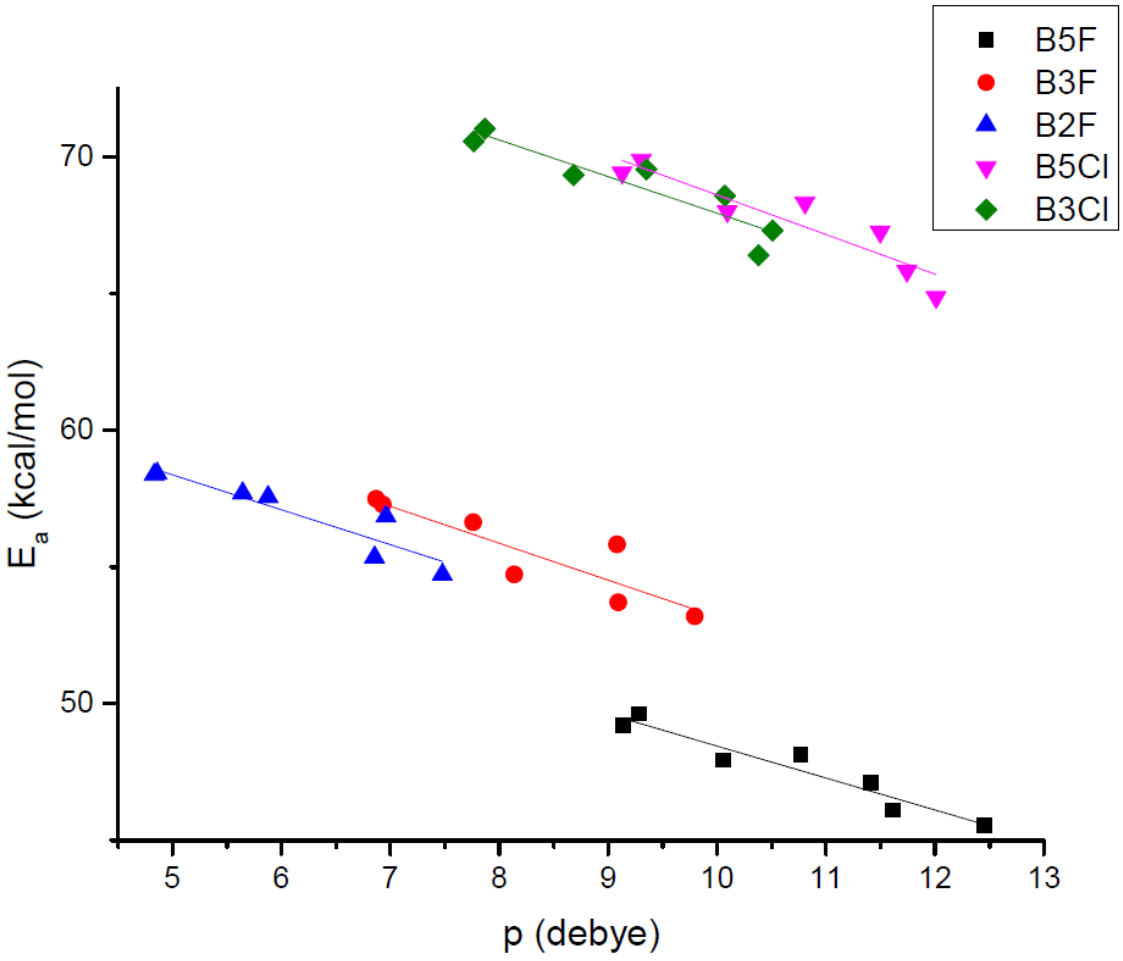


Figure 32. Relationship between **p** and E_a. Data organized according to borane.

Figure 32 clearly shows good linear relationships between **p** and E_a. However, linear relationship only true for FLP catalysts with same borane. The result indicates that there're more factors need to be considered.

Furthermore, we chose the net charge transferred (ΔQ, in a.u.) as the measurement of ET in order to eliminate the influence of distance in dipole moment,. ΔQ was measured by adding all net charges on each atom of borane. After gathering all ΔQ data, we plotted lnΔQ against E_a as shown in following figure:

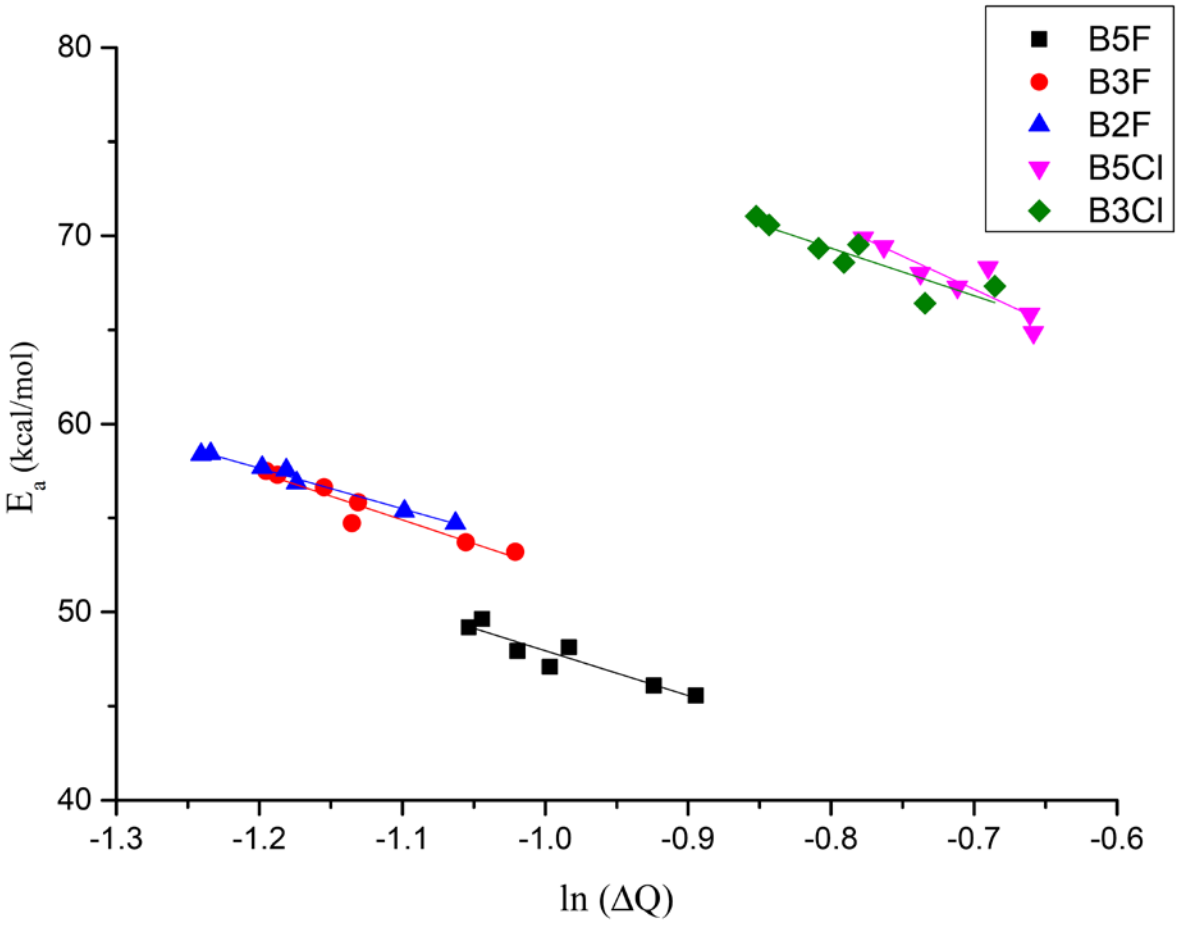


Figure 33. Relationship between lnΔQ and E_a. Data was organized according to borane used in FLP catalysts.

After plotting it can be found that situation is quite similar to **p** vs E_a. Linear relationships exist in each group of catalyst, but **B3F**/**B2F** and **B5Cl**/**B3Cl** are quite close to each other. Another thing to notice is that even though FLPs with Cl have more electron transferred, their E_as are still much higher than FLPs with F. This indicates that ET is only part of the energy barrier in methane activation.

Although we can use p or ΔQ to describe the relationship to Ea for a certain borane contained FLP, we still need to optimize borane/NHC complex first. Therefore, another physical property that is easier to calculate could further simplify the calculation. To describe ET process, a well-accepted theory is Marcus Theory. According to Marcus Theory, the ET process can be written as:

$$k = Aexp(\frac{-\Delta E_{MO}}{RT}) \tag{4.2}$$

Where k is the rate constant, A is a constant, R is the ideal gas constant, T is the temperature and ΔE_{MO} is the energy gap. In our study, ΔE_{MO} can be calculated according to following equation:

$$\Delta E_{MO} = E_{LUMO,Borane} - E_{HOMO,NHC} \tag{4.3}$$

Both HOMO and LUMO energy levels can be easily calculated through optimization while no borane/NHC complex optimization is needed. Equation (4.2) could establish a relationship between amount of electrons transferred and the energy gap, or ΔE_{MO}. Hence, we plotted ΔE_{MO} against lnΔQ, in order to figure out their relationship.

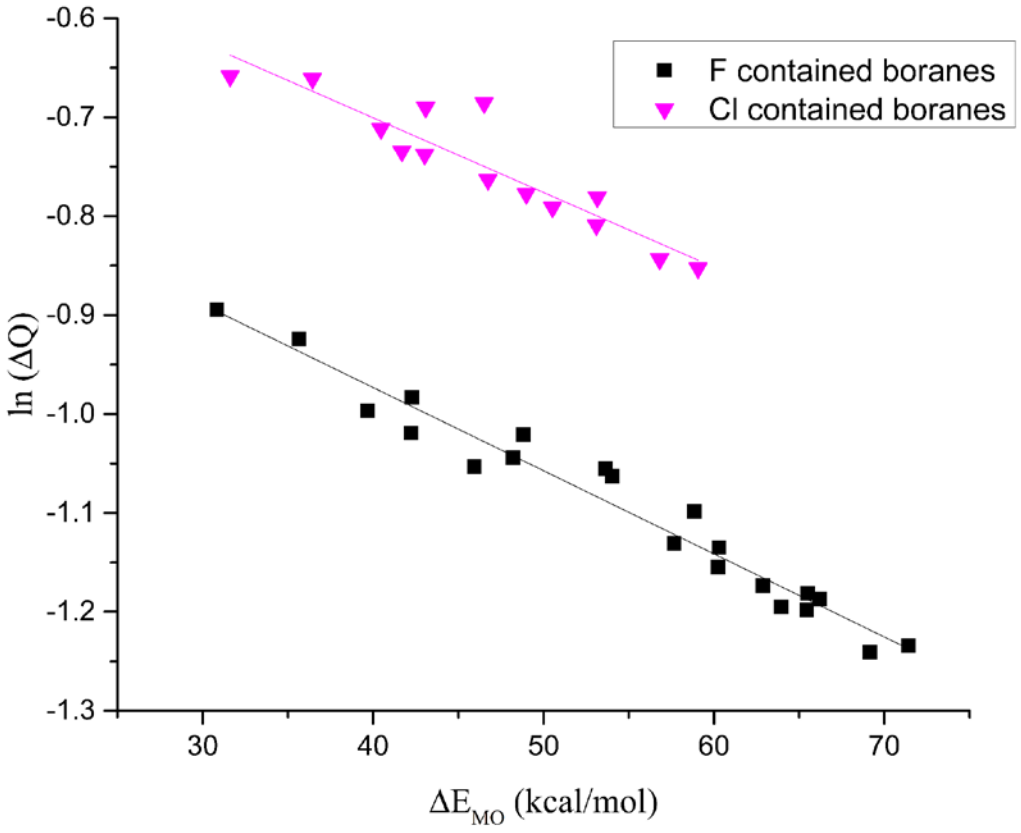


Figure 34. Relationship between ΔE_{MO} and $\ln\Delta Q$. Only two groups of linear relationships were found.

Only two data groups can be found in Figure 34, one is F contained FLPs and the other one is Cl contained FLPs. Figure 34 shows that in each data group ΔE_{MO} is linearly correlated to $\ln\Delta Q$, which meets our expectation from equation (4.2): higher ΔE_{MO} can lower the amount of electron transferred, and then degrade the catalytic performance in methane activation. Based on the observation, we plotted ΔE_{MO} against E_a to further prove:

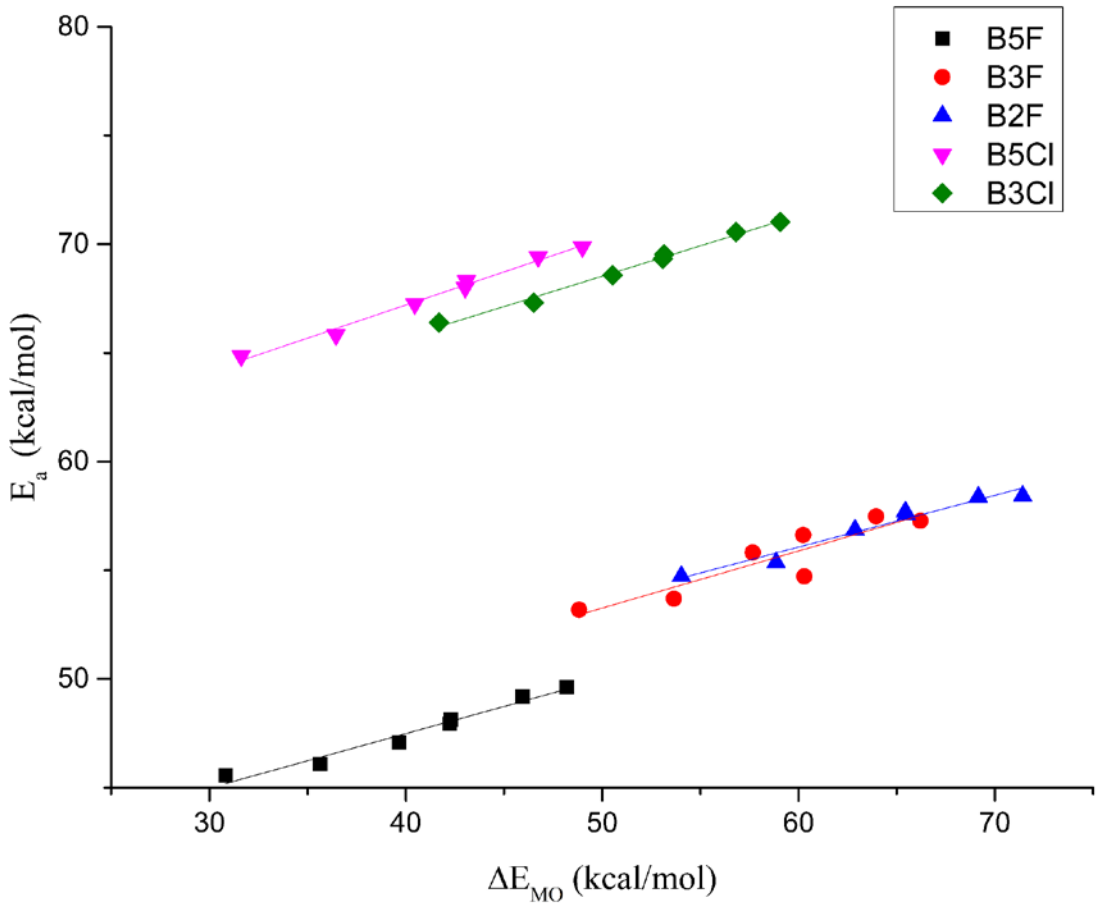


Figure 35. Relationship between ΔE_{MO} and E_a.

Although there are still five groups with similar slope in Figure 35, linear relationship between ΔE_{MO} and E_a can be well established for the most widely used borane, **B5F**. To use ΔE_{MO} as the description for Ea is much easier than ΔQ or p, since no borane/NHC complex optimization is needed anymore. For **B5F**, Ea can be calculated as:

$$E_a = 0.25\Delta E_{MO} + 37.49 \quad (4.4)$$

Equation (4.4) can be used to predict the reactivity of FLP catalyst with **B5F** borane, which can be used in most situations. The slope of the equation reflects how the energy gap in ET process affect the energy barrier and the interception of the equation reflects the energy barrier even when there's no gap between NHC's HOMO and borane's LUMO. Above all, in order to find the best FLP catalyst, the matching for HOMO/LUMO orbitals must be considered first.

4.3.4 Geometry Correction

To further expand our conclusions in last section to all of the data from calculation, further correction to equation (4.4) is necessary. In order to find a parameter that can describe and unify the difference between F contained FLPs and Cl contained FLPs, we first explored the geometry differences. Following figures give a comparison between **B5F** and **B5Cl** and their corresponding TSs.

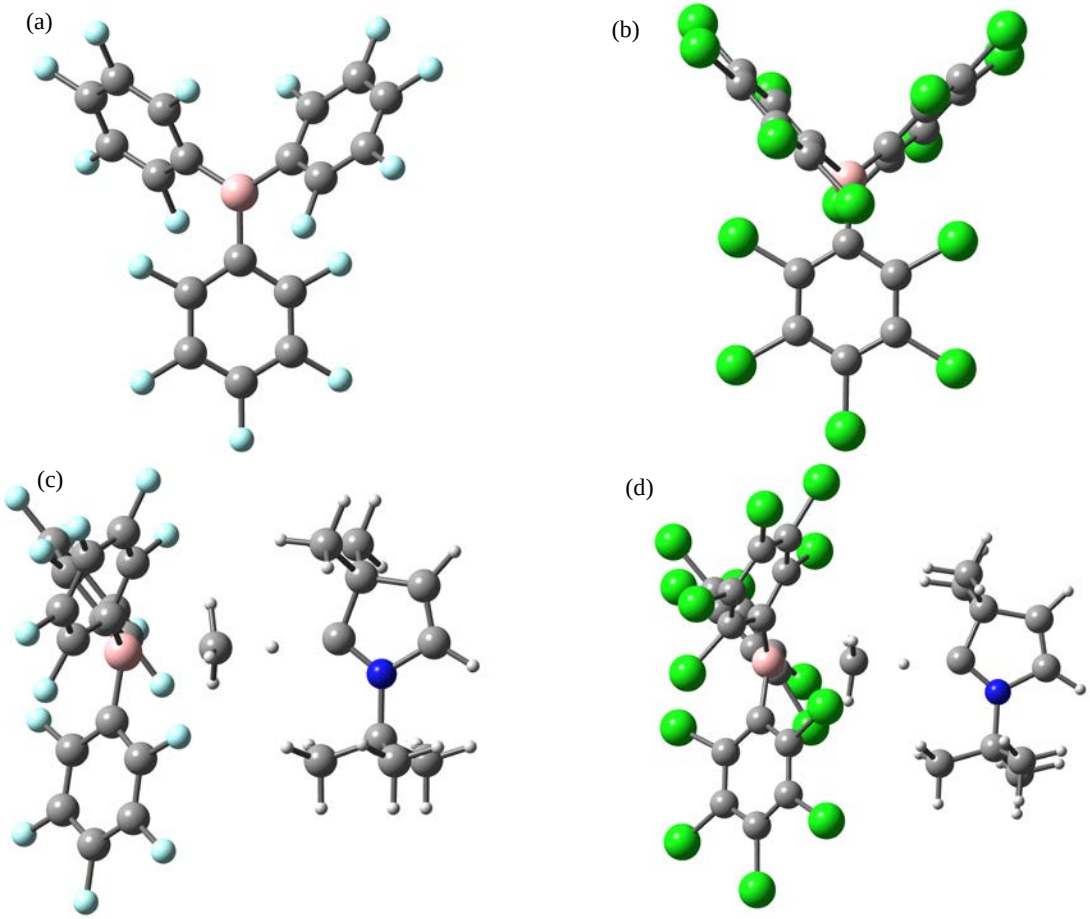


Figure 36. Optimized geometries of (a)**B5F**, (b)**B5Cl**, (c)TS of **B5F/NHC1** and (d)TS of **B5Cl/NHC1**. Color scheme: gray, C; white, H; pink, B; green, Cl; blue, N.

Although both **B5F** and **B5Cl** have similar centrosymmetric geometries, there're significant difference on dihedral angles between each aromatic groups. In **B5F**, the dihedral angle between each $–C_6F_5$ groups is about 39° but in **B5Cl**, the angle between each $–C_6Cl_5$ is about 54°. The reason for the difference may be attributed to the difference between F's and Cl's van der Waals radii. Cl's van der Waals radius is 175pm, which is about 18% larger than F atom (149pm). Large van der Waals radius and more electrons create greater repulsive

between Cl atoms on adjacent $–C_6Cl_5$ groups, which push the planar groups far from each other. The difference on dihedral angle can be clearly seen on side view of boranes:

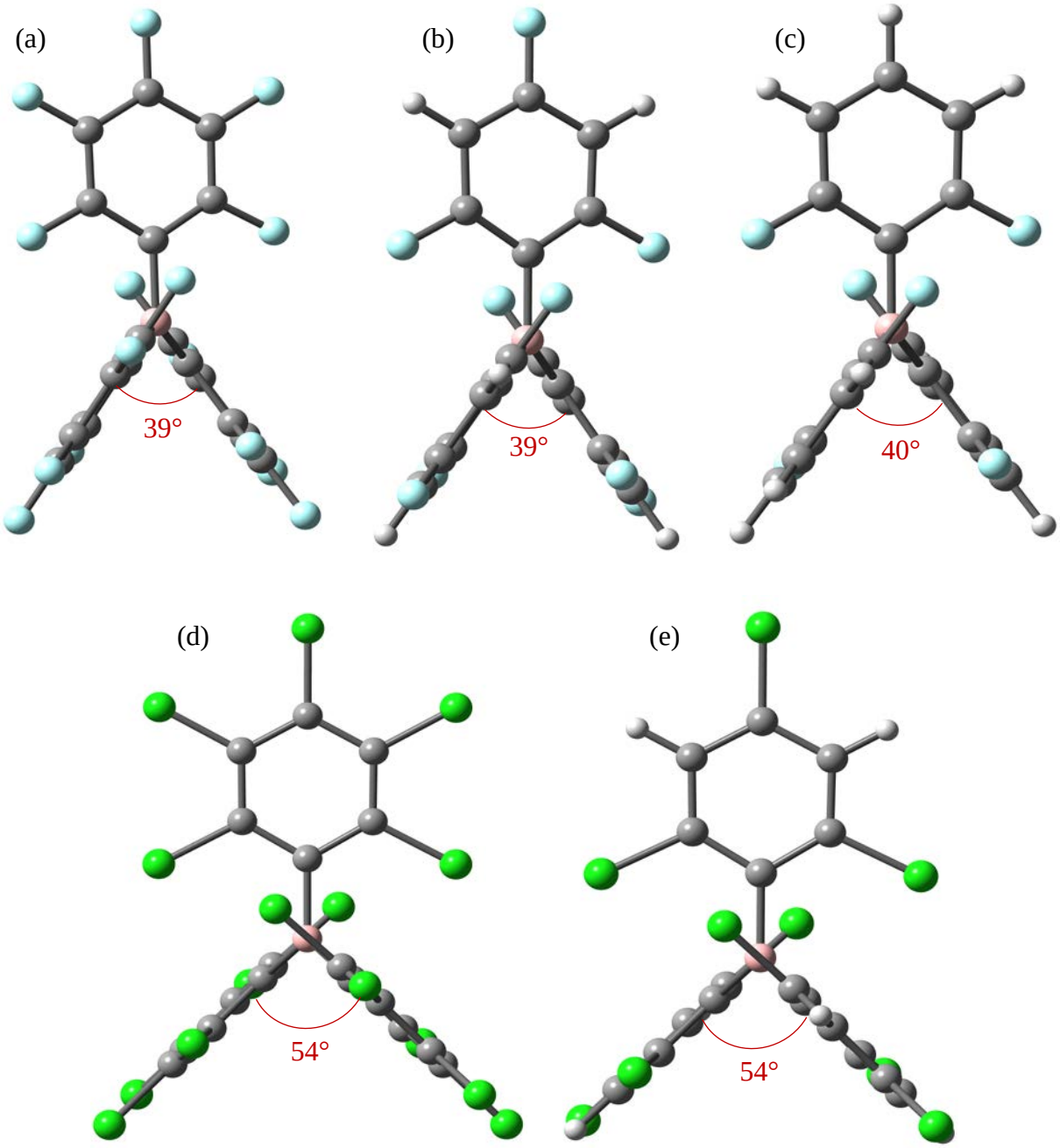


Figure 37. Side view of (a)**B5F**, (b)**B3F**, (c)**B2F**, (d)**B5Cl** and (e)**B3Cl**. Dihedral angles are given in red.

According to Figure 37, dihedral angles of aromatic rings in all F containing FLPs are almost the same, and so do Cl containing FLPs. Larger dihedral angle in Cl containing FLPs prompt stronger shielding to the B atom, which may require more energy to distort the geometry in order to expose B atom to a certain amount to form corresponding TS as shown in Figure 35(d). On contrary, shielding of B atom in F containing FLPs is less, due to smaller size of F atom. Therefore, less energy is needed to overcome the geometry change in order to form TS as shown in Figure 35(c).

Unlike boranes, NHCs didn't shown any significant geometry change before and after forming TSs because their stable five-membered ring structures. In addition, the –R group is far away from reaction center, whose geometry cannot be affected by TS formation as well. As a result, NHCs has no significant effect on geometry of TS but only on electron distributions through the induct effect of conjugation.

In order to evaluate the impact to the geometry without optimizing TS, we calculated the formation energies of each borane/NHC complex, to reflect the energy barrier for boranes' geometry change. The formation energies were calculated as following:

$$\Delta E_F = E_{complex} - (E_{borane} + E_{NHC}) \tag{4.5}$$

Where $E_{complex}$ is the energy of borane/NHC complex, E_{borane} and E_{NHC} are energies of borane and NHC molecule, respectively. After calculation, we plotted all ΔE_F for boranes with each NHCs:

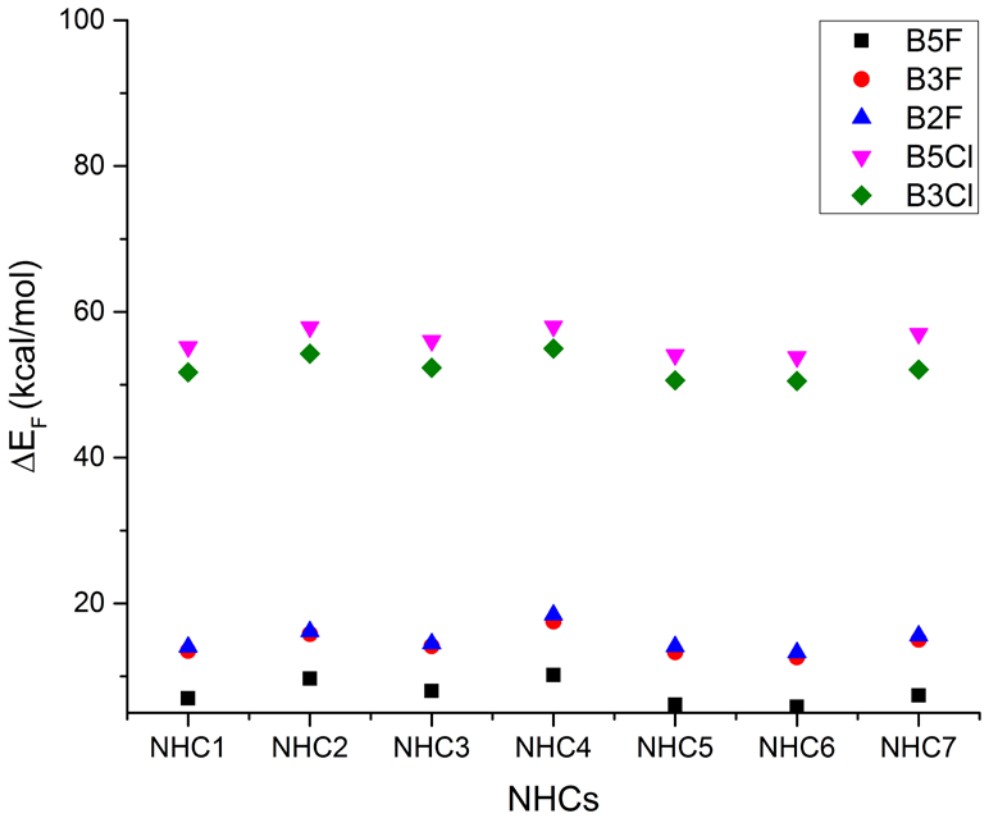


Figure 38. ΔE_F of borane/NHC complex

As expected, there's no significant difference on ΔE_F for each borane with different NHCs. Moreover, **B5F** has the lowest ΔE_F, **B5Cl** have the highest. According to Figure 36, F containing and Cl containing boranes have similar dihedral angles respectively. This is also reflected by analysis of ΔE_F. All F containing boranes have similar low ΔE_F while Cl containing boranes have similar high ΔE_F.

As a correction to ΔE_{MO}, the geometrical mean values of ΔE_F and ΔE_{MO} were calculated and plotted with E_a:

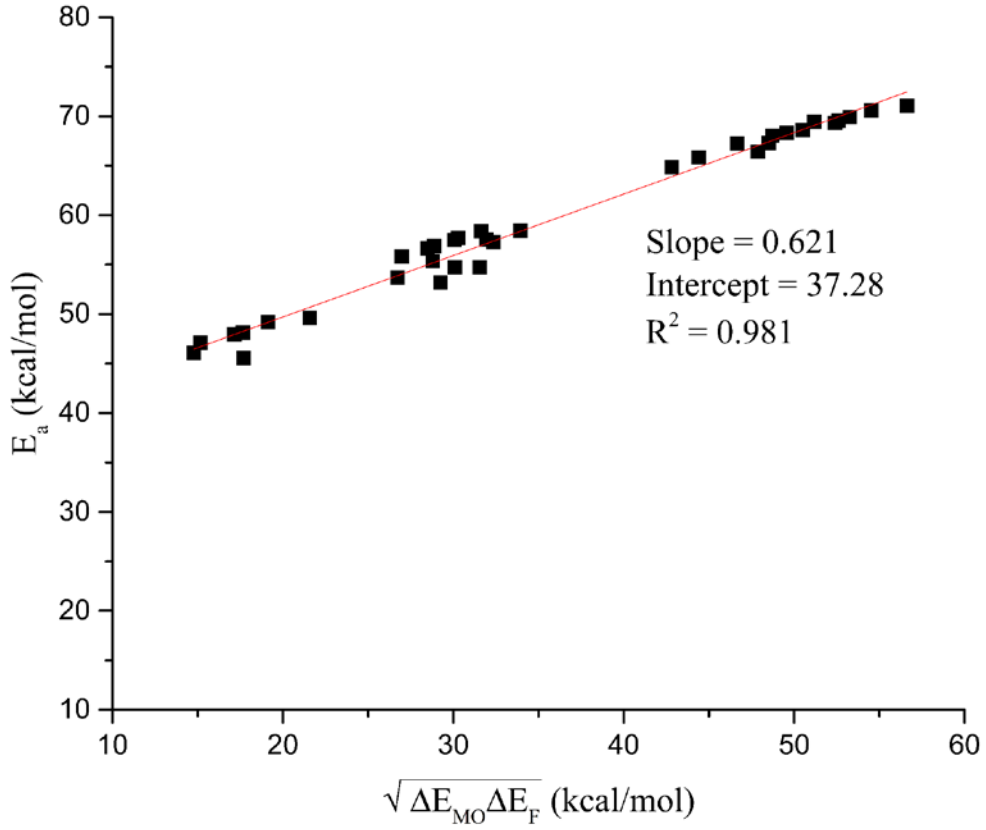


Figure 39. Relationship between E_a and geometrical mean values of ΔE_F and ΔE_{MO}.

As shown in Figure 38, E_a shows significant linear correlation to the geometrical mean value of ΔE_F and ΔE_{MO} with R^2=0.981. Equation to describe the relationship is:

$$E_a = 0.621\sqrt{\Delta E_{MO}\Delta E_F} + 37.28 \quad (4.6)$$

Equation (4.6) gives a simple way to predict the reactivity of FLP catalysts for methane activation without performing expensive and time-consuming TS optimization. Prediction might be even simpler to use equation (4.4) if most reactive **B5F** is used as Lewis acid in FLP.

4.4 Conclusion

In this project, we chose borane/NHC FLPs catalyzed methane activation reaction as the example to establish a mathematical model for catalysts' reactivity using DFT method and Gaussian software. After evaluating physical properties of FLP we were able to establish a linear relationship between E_a and ΔE_{MO} for each borane. Further corrections using formation energy ΔE_F helped us to generalize the model to all FLP catalysts tested. Our work agrees to Papai's result on H_2 activation that ET process is the major driving force of catalysis. The mathematical model established in this work would be useful to predict reactivity of catalysts before performing TS optimization.

APPENDIX A. LIST OF MOLECULAR COORDINATES OF ALL COMPOUND STUDIED IN CHAPTER 3

1. Ag based catalysts

CAgMe

Ag	-0.66154700	0.15567100	-0.00005500
Ag	1.97646700	1.26211600	0.00070300
Ag	1.76741400	-1.37193300	-0.00068700
P	-3.11842400	-0.20469800	-0.00026600
C	-3.82418400	0.73566600	-1.42791400
H	-4.91818000	0.66544800	-1.41564000
H	-3.52286500	1.78741400	-1.37781400
H	-3.45768900	0.30456300	-2.36267800
C	-3.82389700	0.73365800	1.42885300
H	-3.45736200	0.30108000	2.36292100
H	-3.52237200	1.78541900	1.38029200
H	-4.91791000	0.66368100	1.41662600
O	-3.53556300	-1.66405900	-0.00127000

CAgiPr

P	-2.72368700	-0.26627900	0.07401500
C	-3.84432900	-0.50577700	1.54353600
H	-4.70446900	0.14892500	1.34519300
C	-3.75202700	-0.72341300	-1.42529500
H	-4.80329100	-0.56016100	-1.15005200
O	-2.65699300	1.37218700	0.04221400
H	-1.75051000	1.72842900	-0.14326700
H	-0.25083700	2.51673500	-0.46827000
Ag	-0.35637500	-1.17132400	0.13560500
Ag	2.34698700	-1.11649200	0.02241200
Ag	0.92556500	1.29342300	-0.31667800
C	-3.54747400	-2.20132200	-1.79787800
H	-3.78372300	-2.88594100	-0.97844000
H	-4.18815800	-2.46584100	-2.64620400
H	-2.50911200	-2.38505700	-2.09718500
C	-4.33489300	-1.95232900	1.69737900
H	-4.94241100	-2.04108700	2.60441300
H	-4.95430200	-2.27680700	0.85675100
H	-3.49686500	-2.65251400	1.79653500
C	-3.13399600	-0.00961600	2.81239200
H	-2.79471600	1.02307300	2.70227700
H	-3.81795200	-0.05574200	3.66695800
H	-2.26439700	-0.63461200	3.04787000
C	-3.40314800	0.19646200	-2.60585200

H	-4.01958800	-0.06565900	-3.47275600
H	-3.57272700	1.24696600	-2.36279400
H	-2.35305100	0.08329300	-2.89952800

CAgPh

Ag	-0.49054400	0.28631300	0.21264700
Ag	2.09320900	1.08000100	1.16034000
Ag	1.98474600	-0.56043800	-0.91302700
P	-2.94730600	-0.03455900	0.04476600
O	-3.46404100	-1.46284300	-0.00677000
C	-3.72192900	0.86052300	1.46567900
C	-4.66787800	0.16129400	2.22599300
C	-3.38617800	2.17288500	1.82408600
C	-5.27777500	0.77265400	3.32376000
H	-4.90934700	-0.85834500	1.94015600
C	-3.99991100	2.78478500	2.91686200
H	-2.64361800	2.72174600	1.24870600
C	-4.94672300	2.08388100	3.66998100
H	-6.01149600	0.22479500	3.90916800
H	-3.73947000	3.80565800	3.18396500
H	-5.42035500	2.55867900	4.52489900
C	-3.53484800	0.90785600	-1.43361800
C	-4.54739700	0.32531300	-2.20775100
C	-3.00246000	2.14453400	-1.81898200
C	-5.03390900	0.98351500	-3.33866400
H	-4.93316900	-0.64574100	-1.91107400
C	-3.49367100	2.80567800	-2.94546800
H	-2.19375500	2.59105200	-1.24338500
C	-4.51156200	2.22522400	-3.70699700
H	-5.81933400	0.52620400	-3.93459500
H	-3.07776800	3.76721400	-3.23478000
H	-4.88895800	2.73578900	-4.58877600

CAgCl

Ag	-0.62911600	-0.21337500	-0.00072300
Ag	1.66394800	1.40815400	0.01215800
Ag	1.98299600	-1.23739800	-0.01471900
P	-3.11553400	-0.35230500	0.00083900
O	-3.91796400	-1.60709400	0.00393500
Cl	-3.67750700	0.91709300	-1.63640300
Cl	-3.67470700	0.92343400	1.63431100

CAgBr

Ag	-0.45950100	-2.51242300	-0.14820600
Ag	0.73514700	-0.03171600	0.50660200
Ag	2.22472900	-2.04667200	-0.58523000
P	-2.25662900	-0.91501300	0.85651000
O	-1.44335400	0.35474100	1.14338400
Br	-4.04901900	-0.31298700	-0.45075000
Br	-3.30189900	-1.52822800	2.81000200

CAgMe-2H

P	-2.73624100	-0.12118800	0.00013400
C	-3.80819700	-0.54655900	1.43013500
H	-4.75630600	-0.00277100	1.37323000
H	-4.00521000	-1.62325000	1.43974100
H	-3.29803800	-0.27557900	2.35760300
C	-3.80199500	-0.53952800	-1.43667000
H	-3.28799000	-0.26355600	-2.36054400
H	-3.99839200	-1.61627100	-1.45273700
H	-4.75064100	0.00346800	-1.38108600
O	-2.75450400	1.51278300	0.00515800
H	-1.85054400	1.92061500	0.00349300
H	-0.37137700	2.80038500	0.00032100
Ag	-0.33496100	-0.94056300	0.00046300
Ag	2.36115100	-0.77099100	-0.00021900
Ag	0.84741300	1.61132100	0.00009400

CAgiPr-2H

P	-2.72368700	-0.26627900	0.07401500
C	-3.84432900	-0.50577700	1.54353600
H	-4.70446900	0.14892500	1.34519300
C	-3.75202700	-0.72341300	-1.42529500
H	-4.80329100	-0.56016100	-1.15005200
O	-2.65699300	1.37218700	0.04221400
H	-1.75051000	1.72842900	-0.14326700
H	-0.25083700	2.51673500	-0.46827000
Ag	-0.35637500	-1.17132400	0.13560500
Ag	2.34698700	-1.11649200	0.02241200
Ag	0.92556500	1.29342300	-0.31667800
C	-3.54747400	-2.20132200	-1.79787800

H	-3.78372300	-2.88594100	-0.97844000
H	-4.18815800	-2.46584100	-2.64620400
H	-2.50911200	-2.38505700	-2.09718500
C	-4.33489300	-1.95232900	1.69737900
H	-4.94241100	-2.04108700	2.60441300
H	-4.95430200	-2.27680700	0.85675100
H	-3.49686500	-2.65251400	1.79653500
C	-3.13399600	-0.00961600	2.81239200
H	-2.79471600	1.02307300	2.70227700
H	-3.81795200	-0.05574200	3.66695800
H	-2.26439700	-0.63461200	3.04787000
C	-3.40314800	0.19646200	-2.60585200
H	-4.01958800	-0.06565900	-3.47275600
H	-3.57272700	1.24696600	-2.36279400
H	-2.35305100	0.08329300	-2.89952800

CAgPh-2H

P	-2.77513900	-0.15542700	-0.06918900
O	-2.96139400	1.46222400	0.06258000
H	-2.11833600	1.93740200	0.28951900
H	-0.77498400	2.91294400	0.64853800
Ag	-0.29189000	-0.69735100	-0.24780900
Ag	2.36419300	-0.21149600	-0.14042500
Ag	0.57295600	1.90022300	0.39685300
C	-3.89434900	-0.52464700	-1.47064400
C	-4.41153600	-1.81760700	-1.64483700
C	-4.17399700	0.46524300	-2.42309800
C	-5.20118100	-2.11339000	-2.75499000
H	-4.21391100	-2.59017400	-0.90632000
C	-4.96844900	0.16377900	-3.53086700
H	-3.78516900	1.46808500	-2.28235200
C	-5.48039000	-1.12336700	-3.70062900
H	-5.60354300	-3.11471900	-2.87852200
H	-5.18844100	0.93832000	-4.25997700
H	-6.09652300	-1.35510500	-4.56454800
C	-3.63314400	-0.86112500	1.38612500
C	-3.14939600	-2.03692500	1.97450800
C	-4.76751200	-0.23286200	1.92418700
C	-3.80428600	-2.59527000	3.07471100
H	-2.25533400	-2.51366600	1.57857200
C	-5.41090700	-0.78547500	3.02979300
H	-5.13042100	0.69035800	1.48304400

C	-4.93389100	-1.96888700	3.60205100
H	-3.42479100	-3.50782300	3.52496600
H	-6.28477900	-0.29372600	3.44727400
H	-5.43870500	-2.39629900	4.46361300

CAgCl-2H

P	-2.70570200	-0.06122000	0.00293900
O	-2.72796200	1.52906900	0.00798800
H	-1.80199100	1.96114500	0.00172900
H	-0.51621500	2.69724200	-0.00565200
Ag	-0.25663700	-1.04417200	0.00199200
Ag	2.41363100	-0.72856100	-0.00213500
Ag	0.77696300	1.56628100	-0.00530900
Cl	-3.92778800	-0.54006000	-1.61396700
Cl	-3.93541300	-0.54625800	1.61180800

CAgBr-2H

P	1.80836400	0.22451500	-0.01662000
O	1.71932600	1.81424400	-0.10804000
H	0.76517500	2.17835200	-0.11922000
H	-0.57451300	2.82029300	-0.14332400
Ag	-0.55808100	-0.94226500	0.03976200
Ag	-3.24418200	-0.81245100	0.04001600
Ag	-1.76899400	1.58844900	-0.07960200
Br	3.13898900	-0.11911800	1.77563700
Br	3.16896400	-0.31133300	-1.73655500

TSH_{CAgMe}

P	2.71167700	0.03086000	-0.00002600
C	3.73807800	-0.52506000	-1.43084200
H	4.71655700	-0.03264900	-1.40419100
H	3.87395600	-1.61138200	-1.40573500
H	3.23499600	-0.25322600	-2.36209100
C	3.73824200	-0.52495200	1.43071300
H	3.23527900	-0.25302800	2.36200000
H	3.87409600	-1.61127900	1.40568300
H	4.71672700	-0.03256200	1.40389900

O	2.61404900	1.57771200	-0.00009100
H	1.25391500	2.38771100	0.00003500
H	0.57324700	2.86965900	0.00010100
Ag	0.42428000	-0.98279500	0.00007300
Ag	-0.84874700	1.51337500	0.00001100
Ag	-2.38243200	-0.70606400	-0.00003700

TSH_{CAgiPr}

P	2.40670700	0.29371100	0.01264700
C	3.46467100	-0.05431300	-1.49587400
H	4.38180800	0.52624100	-1.31940900
C	3.46585300	-0.27046800	1.46908700
H	4.50912400	-0.17464900	1.13484200
O	2.21215500	1.83327700	0.08684800
H	0.79840900	2.54921800	0.26758500
H	0.09198900	2.97618200	0.35992800
Ag	0.18005600	-0.85752500	-0.08004200
Ag	-1.24742400	1.53950900	0.16287500
Ag	-2.64591100	-0.75219900	-0.07962700
C	3.24550800	0.67564100	2.65733300
H	3.41706100	1.71591200	2.37395700
H	2.21807200	0.59907300	3.03362900
H	3.92016800	0.41352700	3.48074400
C	3.19898100	-1.72971700	1.86314800
H	3.86727000	-2.03558800	2.67678600
H	2.16842800	-1.85056700	2.21900600
H	3.34382200	-2.42657200	1.03265300
C	3.82981700	-1.53271200	-1.67477200
H	4.38864100	-1.67491700	-2.60701700
H	4.45298900	-1.91100300	-0.85934400
H	2.93084300	-2.15935400	-1.73378600
C	2.76559400	0.51354600	-2.73824400
H	1.83872700	-0.03467700	-2.95126000
H	2.51267100	1.56747100	-2.59843300
H	3.41276400	0.42440900	-3.61848200

TSH_{CAgPh}

P	1.47178600	0.00804400	0.47210600
O	1.18720300	0.00788700	2.00082900
H	-0.24613400	0.01571500	2.54613400

H	-1.01299200	0.01982300	2.90790900
C	2.55855800	1.45144300	0.10413100
C	3.13550600	2.14581200	1.17549700
C	2.80529100	1.88027100	-1.20671000
C	3.96052800	3.24605600	0.93500300
H	2.92186800	1.81513700	2.18741000
C	3.63513500	2.97578700	-1.44587800
H	2.34430800	1.36244700	-2.04554700
C	4.21414000	3.66049000	-0.37402900
H	4.40433800	3.78124700	1.77015900
H	3.82357300	3.30057500	-2.46553700
H	4.85422300	4.51846300	-0.55976800
C	2.53833100	-1.44935200	0.10004900
C	3.10337800	-2.15630900	1.16950900
C	2.78094400	-1.87647900	-1.21212700
C	3.91265000	-3.26752600	0.92589000
H	2.89302600	-1.82652400	2.18240100
C	3.59508700	-2.98302800	-1.45438600
H	2.32902800	-1.34858700	-2.04961700
C	4.16228500	-3.68040900	-0.38438600
H	4.34727600	-3.81244100	1.75958600
H	3.78046200	-3.30642600	-2.47504800
H	4.79007300	-4.54689000	-0.57257500
Ag	-0.64189000	0.02427800	-0.87186300
Ag	-3.44374600	0.04291200	-1.01961800
Ag	-2.25223400	0.03066000	1.41041800

TSH_{CAgCl}

P	2.64294500	0.07250700	-0.00354200
O	2.58698300	1.61899300	0.00500400
H	1.46728400	2.16773400	0.00894100
H	0.60429200	2.67880000	0.01259900
Ag	0.28893500	-0.99443100	-0.00932400
Ag	-0.84191500	1.57496000	0.00627100
Ag	-2.42097200	-0.68199500	-0.00697500
Cl	3.86606700	-0.47710700	1.61707900
Cl	3.86616500	-0.45894300	-1.63010200

TSH_{CAgBr}

P	2.63366800	0.08528800	-0.00325300

O	2.57757300	1.63467000	0.00592400
H	1.45798200	2.18251200	0.00898600
H	0.59359900	2.68978100	0.01181600
Ag	0.28352500	-0.99817800	-0.00913400
Ag	-0.84253000	1.57228200	0.00580800
Ag	-2.42633400	-0.68231700	-0.00663700
Br	3.94164100	-0.52448200	1.76379400
Br	3.94133200	-0.50352600	-1.77761800

$TSCO_{CAgMe}$

P	2.75239000	-0.69953600	-0.00005600
C	3.57695200	-1.50867500	-1.43246000
H	4.65910400	-1.34714300	-1.38933600
H	3.36613600	-2.58321700	-1.42804600
H	3.19265700	-1.07949200	-2.36102500
C	3.57727500	-1.50869900	1.43214600
H	3.19325700	-1.07946500	2.36080200
H	3.36637800	-2.58322400	1.42781200
H	4.65942900	-1.34724900	1.38873300
O	3.24130800	0.80918300	-0.00012300
H	2.47590400	1.71665300	0.00004000
H	0.35037900	2.51072600	-0.00023300
C	1.65578800	2.85665800	0.00014900
O	1.83790800	4.02152400	0.00050000
Ag	0.26719100	-0.96702200	0.00011400
Ag	-2.48383100	-0.94599500	0.00008200
Ag	-1.18852800	1.45778500	-0.00019400

$TSCO_{CAgiPr}$

P	0.46865000	1.36739900	0.13311400
O	1.17406700	2.77675400	0.35458000
H	0.58227900	3.79733800	0.25043500
H	-1.32219700	4.95192300	-0.20169600
C	-0.02670700	5.06234000	0.15314300
O	0.32952100	6.17612300	0.30874800
Ag	-1.95164300	1.54318900	-0.48648100
Ag	-4.57906600	2.04454400	-1.15269900
Ag	-2.96060200	4.18399500	-0.66094500
C	0.75690300	0.40952100	1.71063400
H	0.36135500	-0.59764900	1.51883300

C	1.47346500	0.50219800	-1.17883200
H	2.50789100	0.49927600	-0.81191400
C	1.00366900	-0.94295300	-1.39662100
H	-0.05684000	-0.97731700	-1.67589700
H	1.57093700	-1.40578900	-2.21160600
H	1.13811800	-1.56540200	-0.50665600
C	1.42487000	1.32143100	-2.47694800
H	1.75955500	2.34863500	-2.31003900
H	2.07185500	0.86903700	-3.23673500
H	0.40684000	1.35499200	-2.88468600
C	2.24593900	0.31916200	2.08120300
H	2.36446900	-0.18919800	3.04483500
H	2.82495300	-0.24069900	1.34058200
H	2.68114200	1.31906700	2.16855700
C	-0.06146500	1.04864500	2.84412000
H	-1.13145000	1.07260000	2.60948100
H	0.06616300	0.48221100	3.77300000
H	0.26851000	2.07632600	3.02766500

$TSCO_{CAgPh}$

P	1.87335400	-0.24410500	-0.12220000
O	2.41506000	1.24565600	-0.22883100
H	1.69873100	2.16873000	-0.21580300
H	-0.42101300	3.02413200	-0.12316600
C	0.90345200	3.35213900	-0.20966900
O	1.09641500	4.51268800	-0.25932700
Ag	-0.61578400	-0.47963500	0.02532700
Ag	-3.35583000	-0.34597000	0.17074300
Ag	-1.96200900	2.00312400	0.00353000
C	2.74838100	-0.97057600	1.32124400
C	3.87419100	-0.32521500	1.85050100
C	2.29659600	-2.16128000	1.90523300
C	4.54542400	-0.87554600	2.94316800
H	4.20543500	0.60823000	1.40651600
C	2.97486700	-2.71425900	2.99183500
H	1.40793200	-2.65553100	1.51760900
C	4.10052200	-2.07109800	3.51180400
H	5.41555900	-0.36963000	3.35210400
H	2.61923900	-3.63827400	3.43888300
H	4.62373800	-2.49630300	4.36353200
C	2.58903300	-1.11243800	-1.57528100
C	3.58917600	-0.49151800	-2.33502800

C	2.13563600	-2.38733400	-1.93975300
C	4.13568300	-1.14711000	-3.43954300
H	3.92183300	0.50346300	-2.05691900
C	2.68959200	-3.04371500	-3.03876700
H	1.34340400	-2.86847300	-1.36964700
C	3.69064900	-2.42325300	-3.79037500
H	4.90871000	-0.66000100	-4.02733100
H	2.33411300	-4.03253600	-3.31445900
H	4.11616800	-2.93048000	-4.65156200

$TSCO_{CAgCl}$

P	2.67362300	-0.67321200	-0.07029700
O	3.18025500	0.78811500	-0.30712000
H	2.56339900	1.68798500	-0.12331300
H	0.31135600	2.48390700	0.09449900
C	1.80487900	2.97491300	0.07352700
O	1.87588300	4.12537000	0.20537800
Ag	0.13216100	-1.15465300	-0.09825400
Ag	-2.56457300	-0.97805600	-0.09378600
Ag	-1.06116900	1.36247900	0.04720200
Cl	3.55357000	-1.28092200	1.73468500
Cl	3.77452900	-1.77073400	-1.46246600

$TSCO_{CAgBr}$

P	2.73455400	-0.55661700	-0.34966500
O	3.10934900	0.96469300	-0.39922100
H	2.48338900	1.76334500	0.05192900
H	0.22047200	2.29559700	0.46102300
C	1.65852500	2.89154400	0.59357000
O	1.64227800	3.96242400	1.04042500
Ag	0.24923700	-1.23370700	-0.65383800
Ag	-2.45062500	-1.15980200	-0.70640300
Ag	-1.05491500	1.12141400	0.08105300
Br	4.19863200	-1.46861700	-1.81384500
Br	3.49079600	-1.33503900	1.65549700

2. Au based catalysts

CAuMe

P	-3.43744000	-0.24742400	0.00049200
C	-4.00609300	0.73148700	-1.44737800
H	-5.10119700	0.76133600	-1.45548300
H	-3.60582400	1.74866200	-1.40010800
H	-3.65822100	0.25091000	-2.36420900
C	-4.00618100	0.73983900	1.44265200
H	-3.65823600	0.26462300	2.36224900
H	-3.60592200	1.75672400	1.38942900
H	-5.10128300	0.76970900	1.45063900
O	-3.94402800	-1.66840200	0.00451600
Au	-1.07544700	-0.03825000	0.00009900
Au	1.42864400	1.33205300	-0.00014100
Au	1.62045000	-1.25989600	0.00007200

CAuiPr

P	-3.20697700	-0.09938400	0.03456900
C	-3.90335400	0.65283000	-1.52870400
H	-4.98597700	0.50000200	-1.40706300
C	-3.91128300	0.88961600	1.46905100
H	-4.90916900	1.18836300	1.11395100
O	-3.57646400	-1.56393500	0.12717800
Au	-0.85523200	0.27057800	-0.02401500
Au	1.57938800	1.76553100	-0.12362500
Au	1.90002200	-0.81378300	-0.06227200
C	-4.07978400	-0.03777000	2.68139500
H	-3.10413300	-0.35523400	3.06628500
H	-4.60190600	0.49142600	3.48685200
H	-4.64138200	-0.93711000	2.42210900
C	-3.11420500	2.14907800	1.83399200
H	-3.65369000	2.72538300	2.59465300
H	-2.13722900	1.87960100	2.24963900
H	-2.93587700	2.80458300	0.97780000
C	-3.62435600	2.14952700	-1.71064400
H	-4.01395300	2.48570700	-2.67829300
H	-4.09863900	2.76006400	-0.93701000
H	-2.54794900	2.35730400	-1.69839700
C	-3.43165700	-0.17322500	-2.73386300
H	-3.94190200	0.16097300	-3.64437900

H	-2.35287000	-0.05292900	-2.89013500
H	-3.63773600	-1.23615100	-2.58728400

CAuPh

P	-3.30524000	-0.14088500	-0.01918100
O	-3.61613900	-1.61629700	-0.09519700
Au	-1.02439100	0.45612600	0.21451700
Au	1.23820100	1.51380000	1.65819900
Au	1.72961700	0.48626000	-0.68028100
C	-3.92116100	0.74841400	-1.50467100
C	-4.87013700	0.08216000	-2.29300400
C	-3.49387800	2.03124300	-1.87173800
C	-5.40029900	0.70529400	-3.42371700
H	-5.17256100	-0.92233600	-2.01352500
C	-4.03009400	2.65332300	-2.99938700
H	-2.72956400	2.53751000	-1.28748700
C	-4.98505700	1.99122100	-3.77540200
H	-6.13445100	0.18481600	-4.03232500
H	-3.69589700	3.64868200	-3.27845300
H	-5.39685300	2.47381100	-4.65734100
C	-4.14280700	0.62901000	1.42513200
C	-4.94164700	-0.20482600	2.21839200
C	-4.00761700	1.98398900	1.75877500
C	-5.60605300	0.31691700	3.33038500
H	-5.03038300	-1.25304300	1.95029000
C	-4.67617500	2.50207100	2.86702000
H	-3.37879700	2.63405900	1.15648800
C	-5.47543800	1.66815400	3.65492800
H	-6.22532400	-0.33261500	3.94271900
H	-4.57262400	3.55389800	3.11870300
H	-5.99227900	2.07242100	4.52080500

CAuCl

P	-3.37702900	-0.29642800	-0.00309100
O	-3.98638700	-1.65189300	-0.01068200
Au	-1.03845300	-0.07861000	0.00026600
Au	1.39818100	1.35242700	-0.01985000
Au	1.53572000	-1.25387600	0.02927000
Cl	-4.03669900	0.87480200	-1.61440100
Cl	-4.04104600	0.85847000	1.61801600

CAuBr

P	-2.64001300	-0.76777900	-0.00769700
O	-3.07073400	-2.19234100	-0.02261500
Au	-0.34505300	-0.24013000	-0.00269700
Au	1.94269400	1.42267400	0.00901300
Au	2.31857200	-1.16245700	-0.00663900
Br	-3.50328100	0.41094900	-1.75629700
Br	-3.50285500	0.37386700	1.76549300

CAuMe-2H

P	-3.00325500	0.03095400	-0.00000500
C	-4.04813600	-0.34135000	1.45085700
H	-4.97849800	0.23298700	1.40722800
H	-4.27635500	-1.41100600	1.47299800
H	-3.50213400	-0.07857100	2.35952300
C	-4.05136700	-0.34717800	-1.44694400
H	-3.50770900	-0.08666200	-2.35768000
H	-4.27863000	-1.41710200	-1.46521700
H	-4.98212600	0.22649100	-1.40290300
O	-2.91612300	1.66722800	-0.00417000
Au	-0.82424000	-0.78469800	-0.00000500
Au	1.80682200	-1.01034300	0.00002600
Au	0.84147700	1.63965000	-0.00001500
H	-1.99140900	1.97995300	-0.00333800
H	0.39098800	3.15884000	-0.00115900

CAuiPr-2H

P	-3.02662400	-0.09213800	-0.06511400
C	-3.99692500	-0.59517500	1.44361800
H	-5.05625400	-0.45567100	1.18665300
C	-4.05649100	-0.44003500	-1.56781300
H	-4.97843400	0.13574000	-1.40403900
O	-3.05751300	1.55260500	-0.04906500
Au	-0.78006000	-0.71245400	-0.07174900
Au	1.86584200	-0.70972700	0.02324200
Au	0.67048400	1.82398200	0.30695100

H	-2.16805200	1.92778400	0.09358200
H	0.08768000	3.28845900	0.47447400
C	-4.40525800	-1.92782500	-1.72310500
H	-4.95418800	-2.07619700	-2.65873000
H	-3.50283700	-2.54752200	-1.76902900
H	-5.03736100	-2.29754000	-0.91140400
C	-3.74434300	-2.07000300	1.80191300
H	-2.69504900	-2.22732700	2.07280900
H	-4.35937700	-2.34674600	2.66462700
H	-3.98512700	-2.75799800	0.98775300
C	-3.34360300	0.11204000	-2.81315400
H	-3.10777300	1.17323400	-2.70556400
H	-2.41126000	-0.42996100	-3.00540300
H	-3.98987300	-0.00726300	-3.68912300
C	-3.64249200	0.32744000	2.62207800
H	-2.57814700	0.25525900	2.87261400
H	-3.87132400	1.37216800	2.40380600
H	-4.21393900	0.02416500	3.50555600

CAuPh-2H

P	2.05151600	0.01446900	0.37544800
O	1.78902500	-0.03334800	1.99542600
Au	-0.04425800	-0.04040600	-0.64973300
Au	-2.63808600	-0.08725100	-1.14825200
Au	-1.95516400	0.02743400	1.58595400
H	0.83498700	-0.00081600	2.19989800
H	-1.67753800	0.09006800	3.14466800
C	3.15879700	-1.40273400	0.09874000
C	3.58702100	-2.20219700	1.16714000
C	3.56794700	-1.70541300	-1.20991600
C	4.42829400	-3.29040400	0.92482700
H	3.25826100	-1.97208500	2.17469500
C	4.40862400	-2.79150400	-1.44293600
H	3.22697000	-1.09807700	-2.04467900
C	4.83984800	-3.58464000	-0.37541400
H	4.75797900	-3.90886700	1.75434000
H	4.72176100	-3.02342800	-2.45642900
H	5.49042300	-4.43441700	-0.56004000
C	3.05306200	1.50765600	0.09137000
C	4.42328900	1.53606700	0.39835500
C	2.42755200	2.66331600	-0.40090900
C	5.15253400	2.70997000	0.21880900

H	4.91641800	0.64444100	0.77284900
C	3.16263400	3.83535300	-0.57911500
H	1.36833600	2.64249600	-0.64252400
C	4.52359800	3.85840600	-0.26961800
H	6.21172000	2.72856800	0.45749000
H	2.67337000	4.72604600	-0.96122800
H	5.09637400	4.77021800	-0.41167900

CAuCl-2H

P	-2.95125900	0.04429100	-0.00004800
O	-2.83233200	1.64650600	-0.00061700
Au	-0.79376200	-0.86761100	0.00044300
Au	1.82149300	-0.98945800	0.00079100
Au	0.72317500	1.63274700	0.00023000
H	-1.89189100	1.94282400	-0.00049800
H	0.24456700	3.14255600	0.00019500
Cl	-4.17716100	-0.32221300	1.60501000
Cl	-4.17732800	-0.32314400	-1.60474400

CAuBr-2H

P	-2.95539300	0.04417800	0.00064000
O	-2.82822700	1.65085600	0.00034600
Au	-0.79045800	-0.86903800	-0.00056600
Au	1.82664800	-0.98611400	-0.00178100
Au	0.72029200	1.63476600	-0.00053500
H	-1.88554300	1.94042300	-0.00007200
H	0.25231700	3.14779100	-0.00050000
Br	-4.27175300	-0.35879300	1.75312200
Br	-4.27439600	-0.35909500	-1.74976900

TSH_{CAuMe}

P	-2.91632400	0.18952800	0.00000800
C	-3.92474600	-0.31264100	1.44787900
H	-4.86841900	0.24349700	1.44786800
H	-4.12638600	-1.38738200	1.41554600
H	-3.37480800	-0.07939300	2.36209400
C	-3.92481700	-0.31268800	-1.44779800

H	-3.37492500	-0.07946800	-2.36204800
H	-4.12645500	-1.38742700	-1.41542000
H	-4.86849000	0.24345000	-1.44775800
O	-2.63807900	1.69740700	-0.00002400
Au	-0.86787800	-0.96338000	-0.00001200
Au	1.99359100	-0.73817700	0.00000800
Au	0.62363100	1.50199700	-0.00000400
H	-1.08575000	2.51315800	-0.00001200
H	-0.42608300	3.02861100	-0.00001300

TSH_{CAuiPr}

P	-2.87716900	0.01017500	-0.00964100
C	-3.94237400	-0.46740600	1.45742800
H	-4.96781900	-0.22275400	1.14270800
C	-3.88716700	-0.29386900	-1.54818600
H	-4.76191300	0.35849200	-1.40892900
O	-2.49559900	1.49557700	0.05816200
Au	-0.88983300	-1.25942600	-0.06012700
Au	1.99327500	-1.19178800	-0.03241900
Au	0.74749900	1.11279300	0.07110100
H	-0.85716900	2.26281100	0.11520600
H	-0.17686500	2.73391600	0.14484100
C	-3.10088600	0.20341900	-2.77002800
H	-2.20811100	-0.41091000	-2.93645600
H	-3.72375900	0.14143000	-3.66928000
H	-2.78132400	1.24011900	-2.63990600
C	-3.57205800	0.41489600	2.65897200
H	-4.24823000	0.20696500	3.49580800
H	-2.55022400	0.20494800	2.99512800
H	-3.63103700	1.47631100	2.41096100
C	-3.86805300	-1.95805000	1.81772200
H	-2.86148000	-2.22139700	2.16036500
H	-4.56827000	-2.17961000	2.63118100
H	-4.11062500	-2.61368700	0.97802000
C	-4.35827100	-1.74329400	-1.72062900
H	-5.05691700	-2.05132100	-0.93787600
H	-4.87335300	-1.85470400	-2.68125700
H	-3.51069100	-2.43853400	-1.71674600

TSH_{CAuPh}

P	-2.92787300	0.12464700	0.06381900
O	-2.47334600	1.56154600	0.35655200
Au	-1.05379200	-1.26590100	-0.21308900
Au	1.79885200	-1.42667700	-0.23152000
Au	0.74158400	0.93120400	0.25122300
H	-0.82521700	2.13245100	0.49021900
H	-0.10151800	2.54537200	0.58207100
C	-3.98410200	-0.48382500	1.43258800
C	-4.48231900	0.45443500	2.34657300
C	-4.30442100	-1.83956400	1.58315300
C	-5.30599000	0.03773800	3.39373400
H	-4.21135100	1.49909900	2.23048800
C	-5.13150800	-2.25088300	2.62758400
H	-3.89643300	-2.57445900	0.89358800
C	-5.63342300	-1.31211700	3.53340400
H	-5.68868600	0.76698300	4.10219000
H	-5.37695100	-3.30293100	2.74113800
H	-6.27177600	-1.63499700	4.35091100
C	-3.97751300	0.09979600	-1.43843000
C	-4.46614500	1.32159800	-1.92038800
C	-4.30244700	-1.09022600	-2.10299600
C	-5.28494400	1.34746000	-3.05068200
H	-4.19181500	2.23827100	-1.40788500
C	-5.12458500	-1.06040300	-3.22869500
H	-3.90210400	-2.03722200	-1.74953300
C	-5.61698400	0.15876300	-3.70299700
H	-5.66028700	2.29632000	-3.42344000
H	-5.37370400	-1.98511500	-3.74132600
H	-6.25155200	0.18115000	-4.58440800

TSH_{CAuCl}

P	-2.82569300	0.20843300	0.00007200
O	-2.60041700	1.71566200	-0.00015600
Au	-0.76601600	-0.92691300	0.00015700
Au	1.97704600	-0.75879800	0.00000900
Au	0.64358500	1.55278200	-0.00016300
H	-1.24961700	2.35519000	-0.00019600
H	-0.52283300	2.89509400	-0.00023900
Cl	-4.03873400	-0.28896500	1.61593300
Cl	-4.03883700	-0.28941200	-1.61557400

TSH_{CAuBr}

P	-2.82711600	0.20903400	0.00000500
O	-2.59728700	1.71829300	-0.00029200
Au	-0.76031400	-0.92982900	0.00005400
Au	1.98396100	-0.75565600	0.00008000
Au	0.64206100	1.55083600	-0.00011000
H	-1.24413700	2.36066100	-0.00018000
H	-0.51886100	2.89987000	-0.00016800
Br	-4.13224800	-0.33563800	1.76268800
Br	-4.13264400	-0.33625000	-1.76218600

$TSCO_{CAuMe}$

P	3.01055500	-0.57556800	-0.00001200
C	3.81888900	-1.35278100	-1.44879200
H	4.89357100	-1.14472100	-1.43264600
H	3.64903000	-2.43358300	-1.43652900
H	3.38752700	-0.93726300	-2.36218100
C	3.81886900	-1.35258200	1.44888600
H	3.38747800	-0.93695500	2.36221200
H	3.64903300	-2.43338900	1.43675800
H	4.89354800	-1.14450200	1.43273800
O	3.35882900	0.94765200	-0.00011500
Au	0.70521400	-0.97361400	-0.00000200
Au	-2.05030800	-0.89086900	0.00002300
Au	-0.82216200	1.48782400	-0.00003300
H	2.49733700	1.96962200	-0.00004700
H	0.44910100	2.65050400	-0.00003600
C	1.79235300	3.01588800	0.00003200
O	1.97462000	4.16944000	0.00012200

$TSCO_{CAuiPr}$

P	2.92461200	-0.73399300	0.03114400
C	3.78814800	-1.49110100	-1.44651500
H	4.84079200	-1.58505800	-1.14277300
C	3.77199900	-1.36129700	1.56700400
H	4.81718600	-1.04614500	1.43741700
O	3.19250300	0.80957900	-0.00212500
Au	0.62835800	-1.22046700	0.04040200

Au	-2.13728800	-1.24376400	0.02599300
Au	-1.00666000	1.17611800	-0.08359400
H	2.28715800	1.79079900	-0.08070400
H	0.21880600	2.39318900	-0.13403800
C	1.54043700	2.80403600	-0.14706700
O	1.68312800	3.96232600	-0.21381200
C	3.70423800	-0.52535300	-2.63875000
H	2.66449500	-0.38970600	-2.95863000
H	4.11390200	0.45572900	-2.39154500
H	4.26174300	-0.93631500	-3.48750000
C	3.24032300	-2.87706700	-1.81879100
H	2.19656800	-2.80527900	-2.14304200
H	3.82169600	-3.29355700	-2.64891700
H	3.28019300	-3.59027800	-0.99213900
C	3.71637300	-2.88622000	1.73030700
H	4.27460700	-3.41072600	0.95020800
H	4.15495600	-3.17015800	2.69319100
H	2.68275900	-3.25070700	1.71771300
C	3.19225200	-0.63567200	2.79101100
H	3.25086000	0.44918800	2.67513300
H	2.14215800	-0.90854400	2.94753500
H	3.75007400	-0.91661000	3.69095100

$TSCO_{CAuPh}$

P	-2.12620300	0.41562200	-0.00133700
O	-1.88418500	1.96140600	-0.01647000
Au	-0.12575400	-0.80866600	-0.00967900
Au	2.46134000	-1.74797600	-0.04635100
Au	2.19506600	0.91785600	-0.01343700
H	-0.70868600	2.58957400	0.00727300
H	1.44763200	2.46794000	0.00921000
C	0.33246900	3.30453400	0.02282500
O	0.58920200	4.44343700	0.04228500
C	-3.17007900	-0.00557800	1.44227200
C	-4.52969900	0.34662400	1.45368200
C	-2.61040800	-0.62394700	2.56840600
C	-5.31257500	0.08041700	2.57555300
H	-4.97460900	0.82302300	0.58517200
C	-3.39711500	-0.88982700	3.69050400
H	-1.55890000	-0.89884600	2.56377900
C	-4.74753500	-0.53823300	3.69422500
H	-6.36400800	0.35284100	2.57681400

H	-2.95532700	-1.37132700	4.55793700
H	-5.36086700	-0.74710600	4.56609500
C	-3.14519800	0.02082700	-1.46715300
C	-3.60121400	1.05758600	-2.29113800
C	-3.46580400	-1.30908000	-1.77795000
C	-4.37978100	0.76434200	-3.41334500
H	-3.33972300	2.08191800	-2.04574100
C	-4.24548300	-1.59612900	-2.89662100
H	-3.10154000	-2.11761400	-1.14854900
C	-4.70293300	-0.55901800	-3.71565600
H	-4.73121900	1.57035300	-4.05115100
H	-4.49191400	-2.62697900	-3.13382500
H	-5.30573700	-0.78511700	-4.59054500

$TSCO_{CAuCl}$

P	2.93669700	-0.56687800	-0.00029800
O	3.30260000	0.92887500	0.00006700
Au	0.64307200	-1.02438900	-0.00039500
Au	-2.04888600	-0.93727700	-0.00028900
Au	-0.76685800	1.45838900	0.00052100
H	2.52990400	1.94553400	0.00041600
H	0.38563400	2.66367300	0.00089600
C	1.87948400	3.06656000	0.00073800
O	2.01411400	4.21396100	0.00092700
Cl	3.92667600	-1.41363100	-1.61504600
Cl	3.92665600	-1.41443200	1.61404500

$TSCO_{CAuBr}$

P	2.45173900	-0.29257600	-0.00020100
O	2.81465200	1.20751400	0.00017400
Au	0.15039900	-0.74890300	-0.00023500
Au	-2.54256200	-0.65936900	-0.00008500
Au	-1.25579200	1.73359300	0.00055300
H	2.04059100	2.22011100	0.00052100
H	-0.10253000	2.93949000	0.00084900
C	1.38689500	3.34123600	0.00088200
O	1.52378200	4.48871800	0.00120300
Br	3.51378800	-1.21322800	1.76021700
Br	3.51368500	-1.21232300	-1.76115200

3. Cu based catalysts

CCuMe

P	-3.03787100	0.20021900	0.04363900
C	-1.88268800	-0.16375800	-1.34576100
H	-1.07216600	0.57291200	-1.36401500
H	-1.46104500	-1.16863600	-1.23915000
H	-2.42852300	-0.10920900	-2.29092000
C	-1.91915700	0.12430400	1.50654600
H	-2.48861800	0.36575700	2.40746800
H	-1.49776800	-0.88058200	1.61405700
H	-1.10727600	0.85158900	1.39754700
O	-3.50631800	1.70946400	-0.11464600
Cu	-5.12877800	-0.77266900	0.11599200
Cu	-5.46567300	1.68033100	-0.13395100
Cu	-7.35729400	0.21601100	-0.00917500

CCuiPr

P	-3.03640900	0.00274200	0.07265600
C	-1.83393100	-0.35596500	-1.32989800
H	-0.86742700	0.07166700	-1.02692900
C	-1.95845500	0.17544600	1.59193800
H	-1.25880500	0.98572300	1.34060100
O	-3.64868900	1.45147500	-0.17373600
Cu	-5.02874700	-1.16439900	0.17567100
Cu	-5.59649600	1.22109200	-0.24929000
Cu	-7.34080400	-0.40650200	-0.08349800
C	-1.66887900	-1.86638200	-1.55786100
H	-2.62129200	-2.31673200	-1.86095800
H	-0.94221100	-2.05375100	-2.35689600
H	-1.32460000	-2.39510200	-0.66438000
C	-2.30086400	0.35095500	-2.61068400
H	-3.26065000	-0.05257400	-2.95444900
H	-2.42968300	1.42323700	-2.45050800
H	-1.56978700	0.19668600	-3.41273500
C	-1.16375400	-1.09399600	1.92667800
H	-0.44447800	-1.35448700	1.14494800
H	-0.59954900	-0.95006400	2.85519200
H	-1.82874100	-1.95296500	2.07703400
C	-2.82510600	0.63057300	2.77483300
H	-3.36733000	1.54869600	2.53580100

H	-3.55869100	-0.13996700	3.04327100
H	-2.20160100	0.81674900	3.65681900

CCuPh

Cu	-0.07523100	-1.21816500	0.53297900
Cu	-1.73641900	-2.97144400	-0.06155800
Cu	0.51720700	-3.58120400	0.46574100
P	-2.08759800	-0.16070400	0.11903300
O	-2.95043400	-1.43677400	-0.26136800
C	-2.26591100	1.01503400	-1.28398300
C	-2.87941500	0.57643100	-2.46454100
C	-1.75723500	2.32048100	-1.21503100
C	-2.98758200	1.43658500	-3.55981400
H	-3.27478700	-0.43350800	-2.50694800
C	-1.86816500	3.17665000	-2.30952700
H	-1.28441200	2.67555600	-0.30237900
C	-2.48226300	2.73516700	-3.48538000
H	-3.46855300	1.09109600	-4.47091300
H	-1.47760300	4.18853900	-2.24587900
H	-2.56547600	3.40255700	-4.33852500
C	-2.93281400	0.68525400	1.51428900
C	-2.20648500	1.46231900	2.42550400
C	-4.31786500	0.54063300	1.68047000
C	-2.85899000	2.11269000	3.47514100
H	-1.12709500	1.55075000	2.32107900
C	-4.96612000	1.18257300	2.73524200
H	-4.87316300	-0.08326200	0.98653600
C	-4.23928200	1.97313900	3.62999700
H	-2.28948300	2.71603000	4.17658400
H	-6.03901100	1.06594600	2.86137500
H	-4.74687600	2.47138100	4.45117200

CCuCl

Cu	-0.02961200	-0.79429200	-0.43569200
Cu	0.46408500	1.19523000	0.92803900
Cu	2.19360600	0.13279300	-0.35233500
P	-2.02325700	-0.11979100	0.63108300
O	-1.47422300	1.10669600	1.39540000
Cl	-2.96036500	-1.35924600	2.05542000
Cl	-3.68584500	0.54593400	-0.47995300

CCuBr

Cu	-0.52856000	1.27054100	0.14602800
Cu	1.86530500	1.01028200	0.08128600
Cu	0.49743600	-0.95004800	-0.12110600
P	-2.25673500	-0.33628700	-0.01016100
O	-1.38225800	-1.60515300	-0.16752400
Br	-3.71388700	-0.30757800	-1.77117400
Br	-3.65799300	-0.70654200	1.75761300

CCuMe-2H

P	-2.13592000	-0.09307000	-0.00051000
C	-3.18364700	-0.51488100	1.44713100
H	-4.14154800	0.01183900	1.39331200
H	-3.36225900	-1.59444100	1.47554700
H	-2.66738500	-0.22099000	2.36422600
C	-3.20421600	-0.55213200	-1.42118600
H	-2.70012100	-0.28527100	-2.35315200
H	-3.38607600	-1.63147000	-1.41684800
H	-4.15988000	-0.02126400	-1.36856500
O	-2.16676400	1.54087300	-0.02526500
H	-1.24987100	1.92511200	-0.01876500
H	0.28290900	2.58311900	-0.00380600
Cu	0.06573100	-0.76194000	-0.00079800
Cu	2.43404500	-0.79647400	0.00093700
Cu	1.26175300	1.37581100	-0.00075400

CCuiPr-2H

P	-2.12073700	-0.23855100	-0.06066600
C	-3.18056400	-0.69291100	1.41417000
H	-4.22744800	-0.53731700	1.11872500
C	-3.19621600	-0.48861200	-1.55963300
H	-4.06361600	0.16595500	-1.39526400
O	-2.04046100	1.39981700	-0.03033700
H	-1.11566900	1.71677300	0.14869000
H	0.43754600	2.25541000	0.45999300
Cu	0.04102900	-1.03530300	-0.05463100

Cu	2.40507600	-1.20788500	0.05130900
Cu	1.34865800	1.00182200	0.32752600
C	-2.97185800	-2.16896400	1.79409100
H	-1.93466800	-2.34558300	2.10143600
H	-3.61825000	-2.43466800	2.63774500
H	-3.19717600	-2.85693700	0.97440700
C	-3.67914800	-1.93738700	-1.71849200
H	-4.32342500	-2.25701900	-0.89480400
H	-4.25814600	-2.03441900	-2.64318900
H	-2.83645200	-2.63569500	-1.78583700
C	-2.44275700	-0.00217300	-2.80758500
H	-2.11119700	1.03281000	-2.69534400
H	-1.56237900	-0.62578300	-3.00330200
H	-3.09432400	-0.05987100	-3.68643200
C	-2.85903900	0.23186800	2.59891300
H	-1.81363100	0.12515000	2.91101400
H	-3.02898800	1.28088700	2.34991600
H	-3.48982600	-0.03154300	3.45507400

CCuPh-2H

P	-2.18255800	-0.13314000	-0.03461200
O	-1.88368400	1.46294500	0.15748600
H	-0.90725600	1.64197700	0.23670400
H	0.70970900	1.98217000	0.31745800
Cu	-0.15428000	-1.19923600	-0.31370200
Cu	2.16200900	-1.66223400	-0.49966300
Cu	1.42974700	0.63881600	0.01007700
C	-3.18194500	-0.62924200	1.41379300
C	-4.41004500	-0.01211400	1.70417300
C	-2.68998900	-1.62089200	2.27346900
C	-5.12904800	-0.38519900	2.83742400
H	-4.79838900	0.75712800	1.04333500
C	-3.41567800	-1.99853100	3.40528800
H	-1.73615400	-2.09620300	2.05718900
C	-4.63372600	-1.37968700	3.68698200
H	-6.07661200	0.09702300	3.05944000
H	-3.02806500	-2.76902000	4.06522000
H	-5.19859700	-1.66971000	4.56830900
C	-3.37561200	-0.13432300	-1.42136100
C	-3.48687000	0.98305600	-2.25980600
C	-4.13093800	-1.28500200	-1.69899700
C	-4.35058200	0.95027500	-3.35690100

H	-2.90816800	1.87374100	-2.03954500
C	-4.98948300	-1.31290400	-2.79650100
H	-4.05953200	-2.15576800	-1.05183600
C	-5.10003400	-0.19491800	-3.62818800
H	-4.43705700	1.82272400	-3.99822000
H	-5.57424000	-2.20504700	-3.00134800
H	-5.76898800	-0.21828100	-4.48358400

CCuCl-2H

P	-2.09875000	-0.04845000	-0.00005700
O	-2.12413900	1.54088900	-0.00071500
H	-1.17913700	1.94054000	-0.00078100
H	0.15088900	2.52970600	-0.00096900
Cu	0.10173500	-0.84389700	0.00026800
Cu	2.45245800	-0.76333200	0.00059700
Cu	1.18280700	1.35287500	-0.00041200
Cl	-3.30788400	-0.54882000	1.61189200
Cl	-3.30811400	-0.55010900	-1.61142500

CCuBr-2H

P	-2.09766100	-0.04235200	-0.00006200
O	-2.12328000	1.55137300	-0.00077900
H	-1.17822000	1.94914000	-0.00086800
H	0.15693800	2.53712800	-0.00091200
Cu	0.09739100	-0.84806300	0.00027300
Cu	2.44740600	-0.76683400	0.00060400
Cu	1.17622800	1.34999100	-0.00037200
Br	-3.39105200	-0.59726300	-1.75790500
Br	-3.39080500	-0.59575300	1.75844800

TSH_{CCuMe}

P	2.06279400	-0.01570300	-0.02008500
C	3.16164100	-0.65621000	-1.35651500
H	4.09308300	-0.08011800	-1.38358000
H	3.39068200	-1.71453300	-1.19265400
H	2.65613100	-0.54838300	-2.31942500
C	3.10792300	-0.28306200	1.47804200

H	2.57098400	0.07388600	2.36070100
H	3.32847200	-1.34821000	1.60654900
H	4.04588300	0.27623300	1.38884700
O	1.85150000	1.51549000	-0.24478600
H	0.54670500	2.28094700	-0.00587000
H	-0.16263700	2.74934800	0.10968800
Cu	-0.04060100	-0.93226400	0.06055600
Cu	-1.08316000	1.29412400	-0.01502000
Cu	-2.45694900	-0.63571900	-0.01222100

TSH_{CCuiPr}

P	1.65751300	0.27877600	0.03308200
C	2.75058600	-0.32875500	-1.37740100
H	3.78917700	-0.14110700	-1.06916600
C	2.74699000	0.16054300	1.55115700
H	3.61255300	0.79769700	1.31853400
O	1.34296700	1.79855500	-0.16770100
H	-0.01661000	2.37040900	-0.64085900
H	-0.74802700	2.72761800	-0.89321000
Cu	-0.37956300	-0.78071800	0.20150800
Cu	-1.56752000	1.29481900	-0.36221400
Cu	-2.81875200	-0.64228200	0.16799500
C	2.56642900	-1.83121700	-1.63658900
H	1.53709600	-2.04463900	-1.94988700
H	3.23329500	-2.16826800	-2.43892700
H	2.77363700	-2.44124300	-0.75256100
C	2.46122200	0.49351400	-2.64094500
H	1.43773600	0.32059600	-2.99583200
H	2.56983700	1.56358900	-2.45269500
H	3.14418100	0.20318600	-3.44781100
C	3.23252200	-1.26285000	1.85308400
H	3.88041700	-1.65885500	1.06576800
H	3.80555500	-1.27819100	2.78736000
H	2.38763600	-1.95206900	1.97590500
C	2.00191200	0.77212200	2.74575100
H	1.66359300	1.78615600	2.51916000
H	1.12262900	0.16958000	3.00796900
H	2.65219400	0.81047700	3.62739600

TSH_{CCuPh}

P	2.12848600	0.03697200	0.06795800
O	1.83628800	1.54839400	-0.18565500
H	0.41251800	2.07769200	-0.41738500
H	-0.35603700	2.42914300	-0.55350700
Cu	0.14221500	-1.07840500	0.34354500
Cu	-1.13819100	0.95473700	-0.12367300
Cu	-2.29389000	-1.04605400	0.40384100
C	3.15033900	-0.59568800	-1.32824000
C	3.82772800	0.32001100	-2.14468800
C	3.24717800	-1.96571000	-1.60344500
C	4.60606600	-0.13342600	-3.21041000
H	3.72604300	1.38137100	-1.93836100
C	4.03126800	-2.41886100	-2.66544200
H	2.70093300	-2.68157800	-0.99200800
C	4.71237000	-1.50208600	-3.46971100
H	5.12839100	0.58095700	-3.84104000
H	4.10266600	-3.48334000	-2.87159000
H	5.31664200	-1.85324200	-4.30150000
C	3.25758500	-0.06927500	1.52032400
C	3.78155900	1.11390300	2.05607500
C	3.58015000	-1.29701500	2.11456200
C	4.62810100	1.06637900	3.16558500
H	3.51247600	2.05935100	1.59486300
C	4.42979400	-1.34317800	3.21964700
H	3.16642700	-2.22107000	1.71574100
C	4.95484200	-0.16005500	3.74714800
H	5.03176500	1.98765500	3.57698900
H	4.67794800	-2.29902300	3.67298200
H	5.61149700	-0.19549300	4.61195600

TSH_{CCuCl}

P	2.01160100	0.06732500	0.02028700
O	1.92420200	1.61135800	-0.04671300
H	0.76789900	2.10204100	-0.06790800
H	-0.11984200	2.56786100	-0.08817800
Cu	-0.12669900	-0.85592000	0.06127600
Cu	-1.20948000	1.34677000	-0.03409800
Cu	-2.50329600	-0.68459200	0.05514500
Cl	3.23144200	-0.39105100	1.66314100
Cl	3.23061600	-0.53179500	-1.57724600

TSH_{CCuBr}

P	2.01020400	0.07725700	0.02362400
O	1.92277800	1.62413400	-0.04846300
H	0.76557600	2.11290000	-0.07114200
H	-0.12372800	2.57369800	-0.09259500
Cu	-0.12173200	-0.86120000	0.06573300
Cu	-1.20155900	1.34063800	-0.03714800
Cu	-2.49722400	-0.69059700	0.05499800
Br	3.31273000	-0.42710800	1.81896500
Br	3.31350200	-0.59221200	-1.71634700

$TSCO_{CCuMe}$

P	2.16729000	-0.57605900	-0.00003000
C	3.02366100	-1.35346300	-1.43154100
H	4.09872200	-1.14937100	-1.38900200
H	2.85639000	-2.43575600	-1.42710800
H	2.62356100	-0.94027400	-2.36084200
C	3.02384500	-1.35323000	1.43149700
H	2.62383400	-0.93991400	2.36077900
H	2.85660900	-2.43553000	1.42724500
H	4.09889500	-1.14911100	1.38881000
O	2.57455000	0.95368700	-0.00019200
H	1.72062900	1.83157500	-0.00008300
H	-0.45319000	2.31338300	-0.00036000
C	0.81008800	2.84035700	0.00002100
O	0.82098100	4.01695200	0.00036800
Cu	-0.10123500	-0.89687100	0.00009500
Cu	-2.50487200	-1.11003500	0.00012800
Cu	-1.57474100	1.07514000	-0.00023200

$TSCO_{CCuiPr}$

P	2.11719700	-0.70184800	0.04191000
C	2.98795900	-1.48884000	-1.42468000
H	4.02256600	-1.68106600	-1.10706600
C	3.03040900	-1.32573400	1.54633700
H	4.07488700	-1.02178100	1.38897300
O	2.44722800	0.85098100	-0.00159700
H	1.55578900	1.67970600	-0.10932200

H	-0.63989100	2.06825400	-0.13597500
C	0.59814700	2.64121500	-0.21791000
O	0.55846900	3.80915800	-0.36022600
Cu	-0.14108500	-1.12952800	0.09813300
Cu	-2.53991200	-1.43031100	0.16910400
Cu	-1.69828500	0.77942900	-0.01624500
C	2.32613700	-2.81697800	-1.82468800
H	1.29541300	-2.64966500	-2.15961800
H	2.87243500	-3.27949300	-2.65468000
H	2.29327800	-3.53971200	-1.00457100
C	3.01328800	-0.50662800	-2.60498000
H	3.56646800	-0.94298300	-3.44433600
H	1.99757800	-0.28809500	-2.95657800
H	3.48162500	0.43977500	-2.32835900
C	2.96420000	-2.85070300	1.70624500
H	3.47544900	-3.37814000	0.89601200
H	3.44188000	-3.15129500	2.64546200
H	1.92566700	-3.20270200	1.74026200
C	2.49375400	-0.60211800	2.79026900
H	1.44789300	-0.87385100	2.98109600
H	3.07606300	-0.88129600	3.67555000
H	2.54820500	0.48274100	2.67056700

$TSCO_{CCuPh}$

P	2.14720200	-0.63466800	0.00671700
O	2.67952100	0.85423700	-0.10468100
H	1.91522600	1.78577200	-0.11476000
H	-0.23639200	2.41235500	-0.02921100
C	1.06749900	2.87233500	-0.12837700
O	1.13502800	4.04346500	-0.19796800
Cu	-0.12957800	-0.84541200	0.14872600
Cu	-2.53595200	-0.84380800	0.28669800
Cu	-1.41555400	1.24963100	0.10413200
C	3.01557300	-1.36033200	1.45375700
C	4.13768600	-0.71675400	1.99236200
C	2.55546200	-2.54902000	2.03584300
C	4.79767700	-1.26675400	3.09204400
H	4.47438500	0.21550300	1.54971800
C	3.22180200	-3.10152700	3.13010600
H	1.66935800	-3.04093600	1.63936700
C	4.34427300	-2.46004100	3.65903800
H	5.66564700	-0.76275100	3.50802200

H	2.85998000	-4.02389100	3.57571300
H	4.85875900	-2.88498500	4.51623300
C	2.85043600	-1.51754500	-1.44269400
C	3.89590400	-0.93945100	-2.17491400
C	2.33882800	-2.76202100	-1.83394100
C	4.43023000	-1.60828400	-3.27701100
H	4.27157000	0.03498200	-1.87869300
C	2.88005800	-3.43270400	-2.93115800
H	1.50987700	-3.20566300	-1.28588400
C	3.92699200	-2.85557600	-3.65374800
H	5.23894800	-1.15486800	-3.84342300
H	2.47903100	-4.39767100	-3.22822800
H	4.34340700	-3.37317000	-4.51325500

$TSCO_{CCuCl}$

P	2.04102700	-0.65724700	0.03259100
O	2.42861100	0.84970700	-0.07610300
H	1.64944500	1.67017600	-0.12043000
H	-0.68666400	2.01449500	-0.11330900
C	0.69447700	2.77274800	-0.18179500
O	0.54095600	3.91934100	-0.25658500
Cu	-0.20433200	-1.22035000	0.08902600
Cu	-2.55632900	-1.51283800	0.13097900
Cu	-1.64810400	0.72945300	-0.02057700
Cl	3.09033100	-1.35624100	1.69710000
Cl	3.06985200	-1.58178200	-1.53136000

$TSCO_{CCuBr}$

P	2.03917300	-0.64917100	0.02497600
O	2.43276300	0.85973500	-0.08664800
H	1.65362800	1.67799200	-0.12407200
H	-0.68486200	2.01893900	-0.10552600
C	0.69214000	2.77921600	-0.17729100
O	0.53639800	3.92599900	-0.24728400
Cu	-0.20085600	-1.22527700	0.08670600
Cu	-2.55064600	-1.51578300	0.13413600
Cu	-1.63789200	0.72722700	-0.01315500
Br	3.15343200	-1.41736900	1.84104600
Br	3.12890400	-1.66699700	-1.67913300

Ag_3 (No modification)

Ag	0.00000000	0.00000000	0.53965700
Ag	0.00000000	2.56938600	-0.26982900
Ag	0.00000000	-2.56938600	-0.26982900

Au_3 (No modification)

Au	-2.48687500	-0.29466900	0.00012400
Au	0.00001900	0.58934500	0.00001200
Au	2.48685500	-0.29467600	-0.00013600

Cu_3 (No modification)

Cu	0.00000000	0.00000000	1.23664200
Cu	0.00000000	1.40288700	-0.61832100
Cu	0.00000000	-1.40288700	-0.61832100

TSH_{Ag3}

H	2.70021300	3.67907000	-0.28848300
H	1.98197200	4.97805600	-0.97858900
Ag	0.84558400	3.75537800	-0.60496300
Ag	-0.14321900	1.33898500	0.32403200
Ag	2.59660400	1.89605400	0.49257300

TSH_{Au3}

H	1.84261400	4.45512400	-0.55007900
H	0.88539100	3.50003600	-0.39578900
Au	2.78608500	3.24098100	-0.10564700
Au	-0.65581800	2.93893500	-0.41709900
Au	5.19339700	2.37508500	0.41164100

TSH_{Cu3}

Cu	-0.83759300	-1.04447700	0.00000000

Cu	-0.44456400	1.32216600	0.00000000
Cu	1.43188500	-0.25037800	0.00000000
H	-2.42767100	-1.08311300	-0.00001100
H	-1.91447300	0.29108300	0.00000900

APPENDIX B. LIST OF HOMO/LUMO FOR ALL CATALYSTS/CATALYT-2H COMPLEXES IN CHAPTER 3

Entry	Catalyst Name	Catalyst HOMO (a.u.)	Catalyst LUMO (a.u.)	ΔE_{MO} (a.u.)	Catalyst-2H Complex	Catalyst-2H HOMO (a.u.)	Catalyst-2H LUMO (a.u.)	ΔE_{MO} (a.u.)
1	**CAgMe**	-0.18163	-0.12391	0.05772	**CAgMe-2H**	-0.20028	-0.07104	0.12924
2	**CAgiPr**	-0.17848	-0.12216	0.05632	**CAgiPr-2H**	-0.1976	-0.0671	0.1305
3	**CAgPh**	-0.1857	-0.12729	0.05841	**CAgPh-2H**	-0.19923	-0.07144	0.12779
4	**CAgCl**	-0.23363	-0.14942	0.08421	**CAgCl-2H**	-0.22777	-0.10426	0.12351
5	**CAgBr**	-0.2337	-0.11948	0.11422	**CAgBr-2H**	-0.22666	-0.10777	0.11889
6	**CAuMe**	-0.21842	-0.1594	0.05902	**CAuMe-2H**	-0.23314	-0.07877	0.15437
7	**CAuiPr**	-0.21368	-0.1568	0.05688	**CAuiPr-2H**	-0.22966	-0.07379	0.15587
8	**CAuPh**	-0.21599	-0.15983	0.05616	**CAuPh-2H**	-0.22924	-0.07856	0.15068
9	**CAuCl**	-0.26007	-0.18423	0.07584	**CAuCl-2H**	-0.25703	-0.12036	0.13667
10	**CAuBr**	-0.25251	-0.18272	0.06979	**CAuBr-2H**	-0.25518	-0.12666	0.12852
11	**CCuMe**	-0.19897	-0.07436	0.12461	**CCuMe-2H**	-0.20105	-0.05851	0.14254
12	**CCuiPr**	-0.19555	-0.07271	0.12284	**CCuiPr-2H**	-0.19868	-0.05484	0.14384
13	**CCuPh**	-0.19886	-0.07669	0.12217	**CCuPh-2H**	-0.19975	-0.05858	0.14117
14	**CCuCl**	-0.24189	-0.10842	0.13347	**CCuCl-2H**	-0.2293	-0.09246	0.13684
15	**CCuBr**	-0.23768	-0.11007	0.12761	**CCuBr-2H**	-0.22805	-0.09945	0.1286

APPENDIX C. LIST OF MOLECULAR COORDINATES OF ALL COMPOUND STUDIED IN CHAPTER 4

B5F

B	0.00232700	-0.00126000	-0.00037000
C	-0.48879100	1.48745700	-0.00174700
C	-1.58307300	1.90847900	-0.76560800
C	0.13768500	2.47825900	0.76233700
C	-2.02596900	3.22227100	-0.78595500
C	-0.29191200	3.79650700	0.78364700
C	-1.37762600	4.16950600	-0.00103900
C	-1.04317500	-1.16893100	0.00332900
C	-0.85713000	-2.33826700	-0.74336700
C	-2.22334100	-1.10792100	0.75358600
C	-1.77709900	-3.37549400	-0.76010200
C	-3.15441800	-2.13518100	0.77764700
C	-2.93005100	-3.27301100	0.01058200
C	1.53669500	-0.31989900	-0.00252100
C	2.45169500	0.43245500	-0.74853900
C	2.07980500	-1.37458300	0.74080400
C	3.81061100	0.15752100	-0.77233500
C	3.43562400	-1.66409800	0.75779100
C	4.30396600	-0.89472500	-0.00887800
F	2.02466600	1.45142400	-1.51108700
F	4.64559600	0.88755600	-1.51519800
F	5.60581600	-1.16544600	-0.01205900
F	3.91400500	-2.66771400	1.49669700
F	1.28528600	-2.13955600	1.50600300
F	-1.56953200	-4.46523500	-1.50274500
F	-3.81789100	-4.26292800	0.01407800
F	-4.25738200	-2.04414900	1.52411800
F	-2.48089600	-0.03615300	1.51984200
F	0.32206200	4.70626000	1.54371400
F	-1.79601500	5.43186500	-0.00077500
F	-3.06211100	3.58560200	-1.54531100
F	-2.23524700	1.03351400	-1.54789800
F	0.23431500	-2.48111100	-1.51187800
F	1.18292200	2.16553300	1.54487100

B3F

B	-0.00433900	0.00018300	-0.00068800
C	-0.76685400	-1.36835400	-0.00531600

C	-1.93727300	-1.59504900	0.73263900
C	-0.33884200	-2.47980900	-0.74509700
C	-2.62800900	-2.79426400	0.76678600
C	-0.98792500	-3.70216600	-0.77851400
C	-2.13089700	-3.83253300	-0.00536100
C	-0.80461200	1.34696000	0.00450800
C	-0.40645500	2.47034800	0.74297900
C	-1.98245000	1.54043800	-0.73117300
C	-1.08943600	3.67407300	0.77720800
C	-2.70647400	2.71987000	-0.76444700
C	-2.23711300	3.77202300	0.00626500
C	1.56268200	0.02161600	-0.00065600
C	2.33906500	-0.86843300	0.75392200
C	2.31476400	0.93259000	-0.75478300
C	3.72301600	-0.87258100	0.78890900
C	3.69808200	0.97517800	-0.78850000
C	4.37805600	0.06061800	0.00057200
F	1.71071900	-1.77231300	1.53352800
F	5.72109900	0.07933200	0.00125100
F	1.66226700	1.81839100	-1.53527700
F	-2.91975300	4.92859800	0.00660200
F	-2.44247800	0.52765000	-1.49354500
F	-2.78090500	-5.00777900	-0.00494800
F	-2.42365600	-0.59581100	1.49655400
F	0.70067700	2.38209800	1.50787300
F	0.76383500	-2.36024400	-1.51219000
H	-3.59899100	2.81280900	-1.36696000
H	-0.74034400	4.49941300	1.38152400
H	4.22206100	1.69148400	-1.40543700
H	4.26613600	-1.57420000	1.40617000
H	-3.51631500	-2.91237600	1.37110000
H	-0.61711700	-4.51717400	-1.38391400

B2F

B	-0.00325400	0.00096400	-0.00075400
C	-0.76624500	-1.36861200	-0.00483500
C	-1.91507000	-1.60321900	0.76137100
C	-0.35700500	-2.46594500	-0.77311700
C	-2.60155900	-2.80554000	0.78997300
C	-1.01284700	-3.68531200	-0.80310900
C	-2.14239100	-3.85036000	-0.00682700

C	-0.80457200	1.34833300	0.00317300
C	-0.42272400	2.45939900	0.76607000
C	-1.96416900	1.54779200	-0.75705200
C	-1.11301700	3.65957200	0.79635300
C	-2.68485100	2.72994900	-0.78503700
C	-2.25128300	3.78986100	0.00609400
C	1.56470500	0.02198900	0.00004400
C	2.33654700	-0.84774300	0.78017400
C	2.31472200	0.91148900	-0.77896700
C	3.72103000	-0.84668600	0.81104500
C	3.69877700	0.94677000	-0.80759600
C	4.40140700	0.05912300	0.00231300
F	1.69866700	-1.72836100	1.58421600
F	1.65518200	1.77503000	-1.58404900
F	-2.40011800	0.53887700	-1.54434700
F	-2.37457700	-0.60907000	1.55418300
F	0.67091700	2.35473400	1.55400900
F	0.72889600	-2.32750700	-1.56667600
H	-3.56180900	2.80294900	-1.41468700
H	-0.75559200	4.46229700	1.42778000
H	4.19923400	1.65717800	-1.45236000
H	4.23890400	-1.54376700	1.45660000
H	-3.47237400	-2.90541800	1.42443100
H	-0.63624700	-4.47574000	-1.43889300
H	-2.80346400	4.72196200	0.00710700
H	5.48468100	0.07335100	0.00317300
H	-2.66765200	-4.79788900	-0.00750800

B5Cl

B	-1.27573900	-0.12470100	0.00053800
C	0.31592300	-0.12340600	0.00498200
C	1.04981900	0.71461200	0.85928200
C	1.05588000	-0.96019600	-0.84530600
C	2.44839000	0.72558200	0.87793900
C	2.45454600	-0.96867800	-0.85646900
C	3.15363800	-0.12090900	0.01259800
C	-2.06754800	-1.49119300	0.19143900
C	-1.81597000	-2.34152700	1.27967400
C	-3.04583300	-1.91033800	-0.72381500
C	-2.49543900	-3.55100800	1.45771300
C	-3.73914600	-3.11651500	-0.57822100

C	-3.46081900	-3.94066000	0.52011600
C	-2.06878400	1.24042100	-0.19499200
C	-3.05327900	1.65777200	0.71439900
C	-1.81259900	2.09102100	-1.28196000
C	-3.74830600	2.86241700	0.56440500
C	-2.49355000	3.29902900	-1.46427700
C	-3.46528300	3.68685600	-0.53251000
Cl	-0.67148000	-1.84498700	2.50186300
Cl	-2.15586100	-4.56459500	2.82456800
Cl	-4.30876600	-5.43825500	0.71928100
Cl	-4.93099600	-3.60018100	-1.74307800
Cl	-3.36257300	-0.93703900	-2.13902500
Cl	-0.66006000	1.59659100	-2.49741800
Cl	-3.37622700	0.68416400	2.12798400
Cl	-4.94807800	3.34381200	1.72205000
Cl	-4.31526900	5.18255800	-0.73714500
Cl	-2.14806500	4.31299100	-2.82937300
Cl	0.21203900	-1.97578900	-1.98889100
Cl	3.32572400	-2.01181800	-1.93551400
Cl	4.88610500	-0.11933600	0.01719800
Cl	3.31193000	1.77024600	1.96163500
Cl	0.19803800	1.72862300	1.99839300

B3Cl

B	-1.27078100	-0.12470500	0.00060600
C	0.31171400	-0.12341600	0.00512700
C	1.06851300	0.71499200	0.84367900
C	1.07459900	-0.96053000	-0.82922600
C	2.45695900	0.72826000	0.87088900
C	2.46319000	-0.97132200	-0.84880400
C	3.14181100	-0.12091400	0.01290000
C	-2.05963500	-1.48313300	0.18935700
C	-1.82188200	-2.35649000	1.26623600
C	-3.05089900	-1.91672500	-0.70946200
C	-2.50182000	-3.55294300	1.45291000
C	-3.74568200	-3.11154500	-0.57325300
C	-3.46066100	-3.91943800	0.51865700
C	-2.06082600	1.23235100	-0.19295300
C	-3.05838400	1.66415300	0.69973400
C	-1.81832100	2.10593500	-1.26859800
C	-3.75482800	2.85747900	0.55899900

C	-2.49959000	3.30093100	-1.45968800
C	-3.46487200	3.66566100	-0.53139700
Cl	-0.66324200	-1.92412400	2.51661900
Cl	-4.32611700	-5.42699400	0.72161100
Cl	-3.41992600	-0.96917000	-2.14435300
Cl	-0.65134900	1.67563600	-2.51191300
Cl	-3.43410500	0.71615100	2.13258900
Cl	-4.33225500	5.17132800	-0.74008000
Cl	0.27906500	-2.02039500	-1.98562600
Cl	4.89183600	-0.11931900	0.01764700
Cl	0.26470100	1.77339600	1.99570600
H	-4.49962600	3.14887100	1.28540700
H	-2.28490300	3.92660100	-2.31393200
H	2.98761200	1.38129500	1.54852300
H	2.99871900	-1.62340000	-1.52351200
H	-4.48543800	-3.40430800	-1.30424600
H	-2.29099400	-4.17839700	2.30827300

S 1.1.2 NHCs

NHC1

C	-0.58143900	-0.85488200	0.00026600
C	-1.52003300	1.37031000	0.00034300
C	-0.19294900	1.43763900	0.00007200
N	0.34080300	0.09061800	0.00008900
H	-2.19986300	2.21168700	0.00040500
H	0.45852100	2.29862800	-0.00011900
C	-1.90922800	-0.09493400	0.00055400
C	1.81957900	-0.14586100	-0.00019400
C	2.41684800	0.49308300	-1.26718600
H	2.25627400	1.57348500	-1.29943900
H	3.49463900	0.31644300	-1.30041700
H	1.96960000	0.05411800	-2.16213400
C	2.41728800	0.49273000	1.26677000
H	1.97030700	0.05355300	2.16174700
H	3.49508200	0.31603400	1.29961000
H	2.25677300	1.57313100	1.29935500
C	2.09700500	-1.65151500	-0.00045200
H	1.66372400	-2.13205000	-0.87756300
H	3.17930400	-1.80943000	-0.00068800

H	1.66406800	-2.13229200	0.87669500
C	-2.70555200	-0.47888700	-1.26540600
H	-2.90292100	-1.55270900	-1.27040100
H	-3.66029000	0.05523700	-1.29238800
H	-2.14878400	-0.23045600	-2.17232500
C	-2.70469200	-0.47864100	1.26716400
H	-3.65938500	0.05553300	1.29471100
H	-2.90210100	-1.55245400	1.27248000
H	-2.14726800	-0.23006800	2.17363900

NHC2

C	-0.95409400	1.38029300	-0.00001500
C	0.88565300	-0.15061900	-0.00004400
C	-0.25588500	-0.83594000	-0.00007800
H	-0.41821200	-1.90197300	-0.00011400
N	-1.33883600	0.11458600	-0.00003600
C	0.57633300	1.33252300	0.00004400
C	-2.76447600	-0.35130700	-0.00002400
C	-3.00269700	-1.19118200	-1.26745000
H	-2.36668700	-2.07913100	-1.30132100
H	-4.04174300	-1.52750900	-1.30018100
H	-2.80701500	-0.59584600	-2.16242300
C	-3.69415300	0.86442700	0.00008600
H	-3.52758400	1.48873700	-0.87758500
H	-4.72943300	0.51234800	0.00008600
H	-3.52754200	1.48861200	0.87783700
C	-3.00262100	-1.19135200	1.26730500
H	-2.80688800	-0.59613300	2.16234600
H	-4.04166300	-1.52768700	1.30005400
H	-2.36660500	-2.07930300	1.30102200
C	1.10041000	2.03680000	-1.26843000
H	0.78206100	3.08049300	-1.26557400
H	2.19248600	1.99712800	-1.30021600
H	0.71273000	1.56251600	-2.17308300
C	1.10030000	2.03661700	1.26867300
H	2.19237300	1.99694800	1.30054800
H	0.78194300	3.08030700	1.26594500
H	0.71254500	1.56219400	2.17322000
Br	2.61885000	-0.92397500	-0.00006300

NHC3

C	-0.19656400	-1.11002400	0.01239300
C	-1.45838500	0.90877000	-0.04861700
C	-0.16745400	1.22412600	-0.04912200
H	0.31074500	2.18951900	-0.07152400
N	0.56009600	-0.02605400	-0.01196400
C	-1.63546400	-0.58175400	-0.01016900
C	2.05889900	-0.02730900	-0.00203300
C	2.55623900	0.66952900	-1.28092400
H	2.22958100	1.71064200	-1.33765600
H	3.64850800	0.66315500	-1.30642100
H	2.18935800	0.14689900	-2.16738900
C	2.56499900	-1.47160600	0.03198400
H	2.21762400	-2.03225300	-0.83570800
H	3.65852400	-1.45860600	0.03851200
H	2.20655400	-1.99496800	0.91818000
C	2.53879500	0.72420800	1.25236600
H	2.16052600	0.23951700	2.15541400
H	3.63063000	0.72096900	1.29274900
H	2.21016600	1.76630200	1.25993700
C	-2.35598500	-1.10559400	-1.27016200
H	-2.40321300	-2.19533100	-1.24000300
H	-3.37258200	-0.70572900	-1.31974400
H	-1.82603200	-0.81188900	-2.17937700
C	-2.37013400	-1.03800800	1.26784800
H	-3.38715800	-0.63651600	1.28453700
H	-2.41720000	-2.12782400	1.29526100
H	-1.85028200	-0.69588700	2.16587100
F	-2.48863900	1.76840400	-0.07760600

NHC4

C	1.63792100	1.53892800	-0.00021400
C	-0.38483500	0.15289300	-0.00000200
C	0.73720700	-0.60591000	0.00011900
H	0.85973200	-1.67266600	0.00026700
N	1.89629500	0.25394500	-0.00003300
C	0.10426400	1.62432200	-0.00018600
C	3.27291100	-0.33351200	0.00003400
C	3.44412600	-1.19113600	1.26709400

H	2.74145300	-2.02697600	1.29899400
H	4.45547100	-1.60395500	1.30279200
H	3.29053300	-0.58191200	2.16101600
C	4.31064000	0.79285600	-0.00007500
H	4.19943400	1.43048900	0.87672000
H	5.31058500	0.34914200	-0.00003100
H	4.19943300	1.43031500	-0.87699700
C	3.44413800	-1.19139500	-1.26684900
H	3.29057900	-0.58234800	-2.16089600
H	4.45547600	-1.60424300	-1.30244100
H	2.74144800	-2.02722500	-1.29859500
C	-0.27232500	2.40398600	1.28017700
H	0.27172000	3.35009400	1.28981200
H	-1.34063900	2.62175900	1.34961100
H	0.01767700	1.84237900	2.17188900
C	-0.27243600	2.40367900	-1.28069800
H	-1.34076200	2.62140900	-1.35009700
H	0.27158600	3.34979700	-1.29059500
H	0.01750600	1.84186800	-2.17230100
N	-1.69727400	-0.28195600	-0.00001700
C	-2.83730300	0.65322900	0.00003700
H	-2.40991300	1.64904500	-0.00012900
C	-2.03854100	-1.72013800	0.00011300
H	-3.12959900	-1.74786400	0.00014900
C	-1.60507100	-2.44949600	1.28383400
H	-1.97733400	-3.47782200	1.26762900
H	-0.52264100	-2.48597800	1.40350300
H	-2.01892500	-1.95091900	2.16294800
C	-3.69446300	0.53922800	1.27232300
H	-4.46908400	1.31155100	1.27252400
H	-4.19961200	-0.42782500	1.34516800
H	-3.08063800	0.67104700	2.16594200
C	-1.60515700	-2.44966700	-1.28353700
H	-2.01909000	-1.95121200	-2.16268300
H	-0.52273500	-2.48614000	-1.40328400
H	-1.97739600	-3.47799900	-1.26716600
C	-3.69478000	0.53895700	-1.27201000
H	-4.19996300	-0.42810400	-1.34452600
H	-4.46939200	1.31129000	-1.27218300
H	-3.08117600	0.67057600	-2.16581000

NHC5

C	0.63224000	-1.37016600	0.07649500
C	-1.15662300	0.28056800	0.03591100
C	0.04969000	0.88089000	-0.02524600
H	0.30119100	1.92675600	-0.07285700
N	1.07604700	-0.13438600	0.00972700
C	-0.89707300	-1.23351600	0.08613200
C	2.52223200	0.24949300	-0.03898200
C	2.78708600	0.99368500	-1.36047600
H	2.19034000	1.90477600	-1.44457500
H	3.84090300	1.27590900	-1.42503800
H	2.55069400	0.35085400	-2.21172200
C	3.38961300	-1.01046500	0.02716700
H	3.17281500	-1.68127900	-0.80374700
H	4.44205700	-0.71460100	-0.01086200
H	3.20570400	-1.56711500	0.94615300
C	2.83240000	1.15421600	1.16763000
H	2.60706700	0.63330700	2.10127300
H	3.89242500	1.42000800	1.17009200
H	2.25621500	2.08190800	1.14670400
C	-1.39227400	-2.01286500	-1.15439000
H	-0.96573600	-3.01712800	-1.13089000
H	-2.48019700	-2.10037400	-1.18393200
H	-1.06207300	-1.52959900	-2.07764100
C	-1.43269400	-1.85955200	1.38922600
H	-2.52220500	-1.78783800	1.44973100
H	-1.14683700	-2.91202500	1.43646700
H	-1.01450400	-1.35469600	2.26341500
N	-2.38021100	0.91223800	0.19317500
C	-3.58332800	0.33979900	-0.39753700
H	-4.45571500	0.83596500	0.03319200
H	-3.62440100	0.46049700	-1.49149100
H	-3.65834500	-0.72014000	-0.16643700
C	-2.35818800	2.36537000	0.20786600
H	-2.08348300	2.79850700	-0.76801500
H	-3.34546900	2.73951500	0.48447000
H	-1.63840300	2.71501100	0.95178000

NHC6

C	-0.19457600	-1.10913200	-0.00016000
C	-1.46439500	0.93333700	0.00007400
C	-0.16036400	1.22768600	0.00012300

H	0.34120000	2.18310500	0.00019300
N	0.56370900	-0.03026100	0.00005900
C	-1.62768100	-0.56897500	-0.00005500
C	2.06060500	-0.03800000	0.00002600
C	2.55531900	0.68345900	-1.26667200
H	2.23458700	1.72748500	-1.29853100
H	3.64748300	0.67030000	-1.30049200
H	2.17793300	0.18280200	-2.16140000
C	2.56267700	-1.48442100	-0.00040700
H	2.20654900	-2.02478200	-0.87730000
H	3.65650400	-1.47577800	-0.00042800
H	2.20658300	-2.02529500	0.87618300
C	2.55540400	0.68272300	1.26711200
H	2.17805100	0.18156400	2.16157400
H	3.64757000	0.66951300	1.30086800
H	2.23470700	1.72673800	1.29958900
C	-2.35792500	-1.05358100	-1.26908500
H	-2.41684100	-2.14337100	-1.26745300
H	-3.36913800	-0.63933300	-1.30632400
H	-1.82579100	-0.74356300	-2.17203800
C	-2.35785400	-1.05381800	1.26892600
H	-3.36906200	-0.63957300	1.30630800
H	-2.41677400	-2.14360700	1.26708900
H	-1.82566300	-0.74397700	2.17190700
O	-2.55559400	1.73756700	0.00011300
H	-2.28188100	2.66173500	0.00019400

NHC7

C	1.65482200	1.32141400	0.25420800
C	-0.46641000	0.16928600	-0.05618900
C	0.56396000	-0.67388100	-0.18878200
H	0.54974400	-1.73132700	-0.40713100
N	1.80261200	0.03574700	-0.00707000
C	0.14304900	1.54810800	0.24232300
C	3.11741500	-0.67544300	-0.11661800
C	3.15806400	-1.79717000	0.93678800
H	2.37999600	-2.54677300	0.77346300
H	4.12303400	-2.30827100	0.89792900
H	3.02988800	-1.38314900	1.93972700
C	4.25579400	0.31534600	0.14058500
H	4.17896800	0.75452800	1.13522900

H	5.20861000	-0.21459900	0.05367200
H	4.23357400	1.13579800	-0.57634000
C	3.24195800	-1.25500300	-1.53706100
H	3.19378800	-0.45558900	-2.28017800
H	4.20037400	-1.76829100	-1.64680700
H	2.45161100	-1.97621900	-1.75883800
C	-0.28930100	2.05359600	1.63606900
H	0.21153900	2.99708300	1.86117800
H	-1.37141300	2.20919100	1.66540000
H	-0.02665600	1.33445300	2.41599300
C	-0.15360500	2.62532500	-0.82550700
H	-1.19789600	2.94340800	-0.78820800
H	0.47722700	3.49589900	-0.63686500
H	0.06510300	2.26026900	-1.83221600
C	-1.88784000	-0.22238000	-0.08633200
C	-2.85869800	0.52325800	-0.77472400
C	-2.30924900	-1.38358500	0.58546300
C	-4.18987300	0.11739900	-0.79952700
H	-2.56747700	1.41228400	-1.31764000
C	-3.63944600	-1.78949700	0.55857100
H	-1.58349500	-1.95713500	1.15075100
C	-4.58781800	-1.04001300	-0.13437900
H	-4.91817400	0.70705400	-1.34540000
H	-3.93742900	-2.68757400	1.08854300
H	-5.62592500	-1.35185800	-0.15179400

S 1.1.3 CH_4

CH_4

C	0.00000000	0.00000000	0.00000000
H	0.62958700	0.62958700	0.62958700
H	-0.62958700	-0.62958700	0.62958700
H	-0.62958700	0.62958700	-0.62958700
H	0.62958700	-0.62958700	-0.62958700

S 1.2 Optimized complexes

S 1.2.1 **B5F**-NHC Complexes

NHC1

C	-0.28401100	-0.44328800	-2.16066000
C	-0.40605400	0.18887800	-4.46150400
H	-0.55711400	0.74203200	-5.37628800
C	0.16947500	-0.99188000	-4.33516400
H	0.62054900	-1.62108800	-5.07914600
N	0.15435800	-1.41763800	-2.95461300
C	-0.92663400	0.61349500	-3.12470000
C	0.50320300	-2.91502200	-2.80770200
C	-0.50794500	-3.66264100	-3.71117900
H	-0.49252100	-3.34707000	-4.75349600
H	-0.26786600	-4.72701000	-3.68659100
H	-1.52303000	-3.53714100	-3.32733200
C	0.34648700	-3.50874500	-1.40908100
H	-0.56306500	-3.18437700	-0.91523600
H	0.29415300	-4.59309000	-1.52843700
H	1.19777800	-3.30129500	-0.77422500
C	1.95212400	-3.11872800	-3.28380500
H	2.63563200	-2.51757300	-2.68457800
H	2.21552000	-4.17081700	-3.15334600
H	2.10143300	-2.87402400	-4.33657900
C	-2.47039000	0.30708700	-3.18026100
H	-2.97927800	0.72255100	-2.31518800
H	-2.87762800	0.77911700	-4.07640800
H	-2.67326200	-0.76336000	-3.23604800
C	-0.75107900	2.12378300	-2.89158500
H	-1.38895800	2.64707600	-3.60962800
H	-1.05201700	2.43418900	-1.89568900
H	0.27311600	2.44142300	-3.06845000
B	-0.22851800	-0.11163600	-0.49927100
C	-1.81587500	0.19937700	-0.09720300
C	-2.73792800	-0.84767500	-0.12712700
C	-2.38457900	1.42433200	0.25374700
C	-4.08012700	-0.73731900	0.19593900
C	-3.72748700	1.59091300	0.58571500
C	-4.58379700	0.50202800	0.56608500
C	0.80452900	1.19093300	-0.27945600
C	1.80768300	1.58955200	-1.15657100
C	0.86178300	1.82098100	0.96783900
C	2.74326300	2.57902500	-0.87759300
C	1.77515500	2.81291300	1.29462200
C	2.72491500	3.20293100	0.35938300
C	0.49778300	-1.16982000	0.57063200

C	1.85428000	-1.47501300	0.42045400
C	-0.03533500	-1.61476400	1.78205800
C	2.62457600	-2.16147800	1.34435500
C	0.69746200	-2.31269700	2.74176700
C	2.03675400	-2.58941200	2.52747400
F	-1.31672900	-1.38231100	2.12316000
F	0.11271900	-2.70778700	3.87911800
F	2.75039300	-3.25965100	3.43610200
F	3.91231900	-2.43744100	1.09493700
F	2.49042300	-1.12968500	-0.72782100
F	-1.66601100	2.56795100	0.25023900
F	-4.19789500	2.79975400	0.91553000
F	-5.87317000	0.64373400	0.88281000
F	-4.88986400	-1.80301100	0.14525200
F	-2.33138400	-2.08429700	-0.51006500
F	1.92693700	1.00963900	-2.37897500
F	3.66013600	2.92666300	-1.79204800
F	3.61296400	4.15745500	0.65277800
F	1.75818200	3.38693300	2.50396500
F	0.01267300	1.45325500	1.94774900

NHC2

C	-0.28490900	-0.43721200	-2.16345200
C	-0.37946300	0.18776200	-4.45772500
C	0.19231800	-0.99758800	-4.32979700
H	0.64240800	-1.62112500	-5.07790200
N	0.16027200	-1.41333600	-2.95344800
C	-0.92841100	0.62252400	-3.12712700
C	0.50296800	-2.91657200	-2.80440400
C	-0.50801000	-3.65702900	-3.71341400
H	-0.48418100	-3.34315200	-4.75620300
H	-0.27463000	-4.72278300	-3.68683300
H	-1.52457200	-3.52535900	-3.33574300
C	0.33517500	-3.50731500	-1.40603900
H	-0.57529400	-3.17795500	-0.91743500
H	0.27696700	-4.59127600	-1.52592500
H	1.18421900	-3.30477800	-0.76663600
C	1.95288100	-3.12605000	-3.27341400
H	2.63659400	-2.52707800	-2.67239500
H	2.21056400	-4.17909000	-3.13962800
H	2.10846800	-2.88522200	-4.32618600

C	-2.46576300	0.29202700	-3.19241300
H	-2.98081600	0.70057200	-2.32834700
H	-2.87128300	0.76060100	-4.09096300
H	-2.65284000	-0.78117700	-3.24840600
C	-0.77096100	2.12884200	-2.87341600
H	-1.42198300	2.65816900	-3.57255900
H	-1.06556500	2.40899100	-1.86754600
H	0.24716000	2.46269300	-3.05400700
B	-0.23301900	-0.10349200	-0.50108900
C	-1.81973500	0.20709900	-0.09714400
C	-2.74267400	-0.83910400	-0.13200800
C	-2.38665800	1.42958400	0.26561200
C	-4.08352300	-0.73095000	0.19689200
C	-3.72840900	1.59414500	0.60348600
C	-4.58524200	0.50576500	0.57870000
C	0.80218700	1.19733200	-0.28259100
C	1.80137300	1.59790500	-1.16316300
C	0.86579700	1.82271000	0.96669200
C	2.74020500	2.58446600	-0.88535400
C	1.78232000	2.81207200	1.29249100
C	2.72840300	3.20378200	0.35416800
C	0.49460700	-1.16503200	0.56352800
C	1.85116300	-1.46864400	0.41079200
C	-0.03734700	-1.61434600	1.77384100
C	2.62307600	-2.15699400	1.33187800
C	0.69715500	-2.31439100	2.73072100
C	2.03663600	-2.58897400	2.51431700
F	-1.31874500	-1.38455800	2.11605900
F	0.11393100	-2.71355200	3.86714300
F	2.75165500	-3.26104900	3.42009800
F	3.91060600	-2.43097000	1.08028100
F	2.48512900	-1.12016000	-0.73781200
F	-1.66745200	2.57260800	0.26889700
F	-4.19676100	2.80033900	0.94432900
F	-5.87304700	0.64541300	0.90124400
F	-4.89357200	-1.79585600	0.14075700
F	-2.33795700	-2.07267200	-0.52712300
F	1.91232100	1.02206800	-2.38881700
F	3.65332200	2.93343800	-1.80232700
F	3.61931100	4.15538400	0.64700600
F	1.77201700	3.38154300	2.50381100
F	0.02088300	1.45216800	1.94905600
Br	-0.60948100	1.11519900	-6.07723100

NHC3

C	-0.28692800	-0.44838700	-2.15687000
C	-0.41374500	0.18149800	-4.42840500
C	0.16226300	-1.00273300	-4.34296300
H	0.59354500	-1.61555800	-5.10982900
N	0.14994000	-1.41622300	-2.96105400
C	-0.93498400	0.61905800	-3.10532400
C	0.50948400	-2.91388000	-2.81584700
C	-0.49736500	-3.66941600	-3.71706300
H	-0.47968000	-3.36283100	-4.76185200
H	-0.25369700	-4.73262700	-3.68353200
H	-1.51402700	-3.54504200	-3.33710200
C	0.35700400	-3.50326300	-1.41545900
H	-0.55405500	-3.18179600	-0.92218300
H	0.30997800	-4.58814100	-1.53114500
H	1.20784600	-3.28927400	-0.78258600
C	1.95874800	-3.10432100	-3.29417600
H	2.63855900	-2.50064200	-2.69332800
H	2.22974800	-4.15499100	-3.16859100
H	2.10434100	-2.85393900	-4.34616500
C	-2.47837300	0.31391900	-3.17511900
H	-2.99375900	0.75763600	-2.32861200
H	-2.86591000	0.76342600	-4.09162700
H	-2.68384300	-0.75696700	-3.20000300
C	-0.75218000	2.13028600	-2.88809500
H	-1.37807800	2.64822700	-3.61850800
H	-1.06294900	2.44442400	-1.89690300
H	0.27525700	2.44143800	-3.05603600
B	-0.22863000	-0.11638200	-0.49569200
C	-1.81630300	0.19737100	-0.09768900
C	-2.73881200	-0.84927100	-0.12954100
C	-2.38440400	1.42263300	0.25292200
C	-4.08140500	-0.73806900	0.19149700
C	-3.72766200	1.59002300	0.58328200
C	-4.58462600	0.50155000	0.56181800
C	0.80612500	1.18539900	-0.28196300
C	1.80814200	1.57978100	-1.16207500
C	0.86683400	1.81860500	0.96353500
C	2.74743600	2.56686600	-0.88765200
C	1.78381200	2.80859700	1.28609300
C	2.73309200	3.19351800	0.34812500
C	0.49477300	-1.17275800	0.57667000
C	1.85175700	-1.47800900	0.43076000

C	-0.04162700	-1.61507300	1.78766100
C	2.61970900	-2.16225000	1.35820100
C	0.68886900	-2.31046600	2.75097400
C	2.02879000	-2.58739600	2.54084800
F	-1.32377900	-1.38171900	2.12481900
F	0.10119100	-2.70287800	3.88749800
F	2.73998300	-3.25535500	3.45270400
F	3.90781700	-2.43890600	1.11258500
F	2.49058000	-1.13576800	-0.71714600
F	-1.66463500	2.56557700	0.25000100
F	-4.19756900	2.79878900	0.91289800
F	-5.87405100	0.64388900	0.87672100
F	-4.89168900	-1.80298300	0.13910400
F	-2.33173900	-2.08611200	-0.51148900
F	1.92187700	0.99736200	-2.38501700
F	3.66292500	2.90980300	-1.80464200
F	3.62423500	4.14586800	0.63765600
F	1.77078600	3.38545600	2.49383300
F	0.01833000	1.45535000	1.94544400
F	-0.63033400	0.89034800	-5.53196700

NHC4

C	-0.45841700	-0.41611400	-2.09716600
C	-0.66339300	0.25904000	-4.42446100
C	-0.14345500	-0.98083300	-4.28907500
H	0.22555000	-1.65089900	-5.03611700
N	-0.10348400	-1.39088800	-2.92055400
C	-1.13573200	0.66688400	-3.02626100
C	0.18079200	-2.90656900	-2.79035800
C	-0.91309200	-3.61123200	-3.63139600
H	-0.93305600	-3.30939400	-4.67660200
H	-0.72831700	-4.68650400	-3.59890400
H	-1.89981500	-3.42726700	-3.19974200
C	0.07050000	-3.49689800	-1.38473800
H	-0.79218300	-3.12711400	-0.84184900
H	-0.04596800	-4.57648300	-1.50224600
H	0.96423200	-3.33939100	-0.79567400
C	1.58807100	-3.19039000	-3.34387900
H	2.33665100	-2.62931500	-2.78527600
H	1.79811900	-4.25597300	-3.22466600
H	1.69263900	-2.95220900	-4.40304200

C	-2.66711400	0.31951200	-2.95518000
H	-3.10043200	0.69670200	-2.03338600
H	-3.19077200	0.78566600	-3.79043100
H	-2.83814800	-0.75624400	-3.01221200
C	-0.92783300	2.14845500	-2.66909400
H	-1.74265300	2.75845900	-3.05898800
H	-0.91786700	2.30445100	-1.59767500
H	0.00684000	2.52713900	-3.07663700
B	-0.25891500	-0.09144700	-0.44495300
C	-1.78743100	0.28301900	0.11839100
C	-2.75855600	-0.71880100	0.16575900
C	-2.26255800	1.52514700	0.54288200
C	-4.05684300	-0.55134300	0.61845100
C	-3.55857900	1.74929200	1.00305800
C	-4.46448000	0.70303200	1.05046900
C	0.84735300	1.16715600	-0.28613500
C	1.77396400	1.56635700	-1.24448200
C	1.04710200	1.75348000	0.96780500
C	2.76758500	2.51318900	-1.02503300
C	2.02349700	2.70201200	1.23700200
C	2.89295100	3.09223200	0.22731400
C	0.52390200	-1.19084300	0.54404100
C	1.85274000	-1.53128500	0.27046600
C	0.08389700	-1.65036500	1.78669600
C	2.67712300	-2.26475200	1.10769400
C	0.87358800	-2.39526500	2.66230500
C	2.17976100	-2.70691800	2.32626800
F	-1.15553400	-1.38938700	2.24354400
F	0.37668200	-2.80201000	3.83735800
F	2.94743500	-3.42146500	3.15443500
F	3.93051900	-2.57009400	0.74188900
F	2.40060400	-1.17386200	-0.91792500
F	-1.49241300	2.63507000	0.49602900
F	-3.93578100	2.97363500	1.39351100
F	-5.71071400	0.89867100	1.49062100
F	-4.91751300	-1.57831600	0.63448300
F	-2.45375200	-1.96710100	-0.26612500
F	1.74981200	1.03734000	-2.49442600
F	3.60418000	2.86491900	-2.01356400
F	3.84035400	4.00608200	0.46258200
F	2.14219800	3.23488400	2.46012300
F	0.27670300	1.38801000	2.01247000
N	-0.74070500	0.97767700	-5.59667600
C	-0.04933400	0.36353700	-6.76013900

H	0.81331500	-0.13876500	-6.31546900
C	-1.67714600	2.12002500	-5.75251900
H	-2.20136300	2.17975400	-4.80669000
C	-2.76807100	1.88856600	-6.81079200
H	-3.49760900	2.70087000	-6.75090700
H	-2.37290400	1.88369200	-7.82760100
H	-3.29613400	0.94795100	-6.64106700
C	0.54407500	1.36787200	-7.75416500
H	1.16292500	0.81540200	-8.46604700
H	-0.21391700	1.89848400	-8.33224400
H	1.18268600	2.09708200	-7.25409400
C	-0.98689400	3.48261600	-5.94410500
H	-1.71110400	4.28019500	-5.75408200
H	-0.15974500	3.60478300	-5.24396100
H	-0.60508100	3.62372900	-6.95461700
C	-0.88679200	-0.70826600	-7.48689500
H	-1.39738600	-1.36544900	-6.78049000
H	-1.64093200	-0.26264400	-8.13703800
H	-0.23503400	-1.32565800	-8.11223000

NHC5

C	-0.37808700	-0.41989700	-2.12467800
C	-0.50612000	0.23741500	-4.44417800
C	0.03845800	-0.97901100	-4.30003300
H	0.43232500	-1.63336800	-5.05143900
N	0.04454100	-1.39043600	-2.93115500
C	-1.04277900	0.63047100	-3.06856700
C	0.40948000	-2.88677500	-2.78494000
C	-0.63054600	-3.65341100	-3.63832200
H	-0.65796300	-3.34911600	-4.68324600
H	-0.38211800	-4.71583600	-3.60976700
H	-1.63037500	-3.53057500	-3.21552100
C	0.31977900	-3.47657800	-1.37794500
H	-0.56698600	-3.15674100	-0.84298500
H	0.26835100	-4.56153100	-1.49266600
H	1.19916500	-3.26417000	-0.78406400
C	1.84101000	-3.08644400	-3.31324800
H	2.54095500	-2.47089200	-2.74798600
H	2.11772000	-4.13430900	-3.17629100
H	1.95018000	-2.85530000	-4.37359600
C	-2.56108000	0.21916400	-3.15840800

H	-3.10662400	0.58246900	-2.29109100
H	-2.97249900	0.68224800	-4.05770200
H	-2.69053400	-0.86107900	-3.23369200
C	-0.99756700	2.12065700	-2.70629100
H	-1.74110300	2.65084000	-3.30483900
H	-1.25144600	2.29291300	-1.66685200
H	-0.02216400	2.56014700	-2.89583800
B	-0.28071100	-0.09197800	-0.46785300
C	-1.86477100	0.17265000	-0.00482900
C	-2.76867200	-0.89040900	-0.05179700
C	-2.44763700	1.36585200	0.42525400
C	-4.10088600	-0.82393400	0.32130700
C	-3.78156700	1.48882800	0.80848600
C	-4.61681500	0.38502900	0.76640300
C	0.73079000	1.23235400	-0.25587700
C	1.68253600	1.68210000	-1.16558800
C	0.83017300	1.83020400	1.00463800
C	2.60567300	2.68681600	-0.90008600
C	1.73299100	2.83603800	1.31877600
C	2.62941700	3.27570400	0.35372000
C	0.50747700	-1.14429600	0.56346200
C	1.86664000	-1.40722300	0.36576000
C	0.02313100	-1.62721700	1.78026600
C	2.68320600	-2.08800700	1.25354600
C	0.80360900	-2.32149400	2.70415500
C	2.14332100	-2.55479900	2.44481100
F	-1.25535800	-1.44052300	2.16002800
F	0.26501500	-2.75518400	3.85063800
F	2.90313200	-3.22084300	3.31912800
F	3.97055700	-2.32254200	0.96148100
F	2.45680500	-1.02492800	-0.79503500
F	-1.75416900	2.52525300	0.45554000
F	-4.26365300	2.67181200	1.20946200
F	-5.89777800	0.48447700	1.13163000
F	-4.89000500	-1.90432800	0.24870200
F	-2.35418100	-2.10216100	-0.50028600
F	1.75802600	1.14586800	-2.41156600
F	3.47026200	3.08489200	-1.84568800
F	3.50668400	4.24482500	0.63364900
F	1.75735500	3.37604200	2.54392600
F	0.03647900	1.41475800	2.01172200
N	-0.81585800	0.85721700	-5.64124000
C	-0.67143800	0.04024600	-6.84276500
H	-1.19839900	-0.90645200	-6.71407700

H	-1.11761200	0.57115300	-7.68523300
H	0.38050700	-0.16860900	-7.09232100
C	-0.40784400	2.24810000	-5.87441700
H	0.65925600	2.31609600	-6.13007400
H	-0.98966200	2.64950400	-6.70649800
H	-0.59049500	2.86684400	-5.00395200

NHC6

C	-0.29405600	-0.45463200	-2.16168000
C	-0.41757300	0.18907000	-4.45241400
C	0.15329000	-1.00677500	-4.34687400
H	0.59093100	-1.63305600	-5.10079200
N	0.13994700	-1.42068600	-2.96550000
C	-0.93919900	0.60899500	-3.11365900
C	0.49552100	-2.91603200	-2.81564300
C	-0.51403400	-3.67648400	-3.71009300
H	-0.49742300	-3.37460700	-4.75607000
H	-0.27315300	-4.74018400	-3.66993600
H	-1.52970200	-3.54658500	-3.32929500
C	0.34625700	-3.50151900	-1.41279400
H	-0.56202600	-3.17577500	-0.91753600
H	0.29630100	-4.58675700	-1.52433900
H	1.19968200	-3.28759800	-0.78334500
C	1.94382700	-3.11558000	-3.29488700
H	2.62580800	-2.50637900	-2.70203100
H	2.21338000	-4.16531100	-3.15813200
H	2.08803000	-2.87648800	-4.34966100
C	-2.47807400	0.28894300	-3.18534300
H	-2.99877100	0.71958000	-2.33515000
H	-2.86856100	0.74204500	-4.09864500
H	-2.67242100	-0.78408200	-3.21749500
C	-0.77223200	2.11936600	-2.88492900
H	-1.40083100	2.63680400	-3.61273100
H	-1.08479700	2.42378000	-1.89144500
H	0.25229600	2.44100000	-3.05132000
B	-0.23184700	-0.11871500	-0.50223500
C	-1.81835300	0.19520800	-0.09535100
C	-2.74168500	-0.85100800	-0.12303800
C	-2.38576300	1.42054300	0.25621500
C	-4.08381400	-0.73856000	0.19948200
C	-3.72868400	1.58922600	0.58752000

C	-4.58638600	0.50163400	0.56822700
C	0.80336600	1.18449300	-0.29035100
C	1.80182100	1.58136400	-1.17377800
C	0.86741900	1.81801800	0.95481200
C	2.73911900	2.57116600	-0.90185200
C	1.78255900	2.81061300	1.27461000
C	2.72751300	3.19813800	0.33359700
C	0.49727300	-1.17183100	0.57168200
C	1.85431000	-1.47541600	0.42222500
C	-0.03441400	-1.61354500	1.78490700
C	2.62597000	-2.15742800	1.34832000
C	0.69989700	-2.30673600	2.74694200
C	2.03948400	-2.58203300	2.53323200
F	-1.31604300	-1.38227500	2.12600200
F	0.11617200	-2.69873500	3.88606600
F	2.75473300	-3.24793900	3.44407500
F	3.91420100	-2.43245800	1.09936300
F	2.49007200	-1.13403900	-0.72753000
F	-1.66592400	2.56352700	0.25435000
F	-4.19752700	2.79898600	0.91681700
F	-5.87592800	0.64499600	0.88453800
F	-4.89485100	-1.80369900	0.15049900
F	-2.33692200	-2.08960000	-0.50141300
F	1.91541500	1.00004400	-2.39659900
F	3.65144500	2.91668200	-1.82203600
F	3.61751000	4.15326200	0.62000700
F	1.77212700	3.38757000	2.48281800
F	0.02356400	1.45286000	1.94038200
O	-0.65364500	0.96868000	-5.52077000
H	-0.33843800	0.54200500	-6.32601800

NHC7

C	-0.30805000	-0.39165300	-2.14900400
C	-0.42084800	0.29044600	-4.45701300
C	0.14168200	-0.90424500	-4.32722900
H	0.58891500	-1.51874600	-5.08615100
N	0.13340800	-1.34997800	-2.96018500
C	-0.95798000	0.67421400	-3.09110100
C	0.49940200	-2.84708400	-2.84055200
C	-0.51365000	-3.59070100	-3.74503000
H	-0.50922600	-3.25912700	-4.78239100

H	-0.26447600	-4.65325700	-3.73842100
H	-1.52606000	-3.47976800	-3.34964200
C	0.36728900	-3.46842400	-1.45100000
H	-0.53732600	-3.16194800	-0.93776500
H	0.32270100	-4.55071800	-1.59085900
H	1.22627600	-3.26652600	-0.82449600
C	1.94527900	-3.02829600	-3.33484900
H	2.62858400	-2.42990700	-2.73246600
H	2.22009500	-4.07962700	-3.22319500
H	2.08224400	-2.76525200	-4.38468700
C	-2.48968400	0.30922100	-3.17368400
H	-3.01721300	0.66930900	-2.29496500
H	-2.90629400	0.80321900	-4.05337300
H	-2.65038700	-0.76530200	-3.27226100
C	-0.86448900	2.17275900	-2.77316000
H	-1.50132300	2.71085600	-3.47866800
H	-1.21582300	2.40106200	-1.77225200
H	0.14683300	2.55311000	-2.88079400
B	-0.24957500	-0.09271400	-0.48282400
C	-1.84061200	0.17578600	-0.05933400
C	-2.74436600	-0.88607700	-0.12214300
C	-2.42939900	1.37425500	0.34633300
C	-4.08522600	-0.81408300	0.21688800
C	-3.77212300	1.50234400	0.69580900
C	-4.60855800	0.39962300	0.64044800
C	0.76278100	1.22254600	-0.23713600
C	1.74811900	1.66526900	-1.11360800
C	0.82525700	1.81635600	1.02759500
C	2.66955400	2.66251200	-0.81618600
C	1.72526100	2.81423800	1.37327600
C	2.65627600	3.24885400	0.43901700
C	0.50538000	-1.16333100	0.55418900
C	1.86584800	-1.43861400	0.38433700
C	-0.00949200	-1.65070400	1.75698900
C	2.65642300	-2.13533100	1.28313600
C	0.74403100	-2.36089600	2.69121300
C	2.08640500	-2.60649200	2.45854500
F	-1.29259400	-1.45196500	2.11333100
F	0.17644400	-2.79798500	3.82201200
F	2.82006500	-3.28791300	3.34280200
F	3.94704100	-2.38033200	1.01636300
F	2.48519000	-1.05023600	-0.75923600
F	-1.73302800	2.53092900	0.38369400
F	-4.26135600	2.68840300	1.07723800

F	-5.89751900	0.50450900	0.97327300
F	-4.87521600	-1.89249600	0.13102000
F	-2.32004300	-2.09987200	-0.55607100
F	1.86207600	1.12729300	-2.35622900
F	3.56738700	3.05512800	-1.73198200
F	3.53123600	4.21013000	0.74990000
F	1.71380100	3.35113400	2.59966400
F	-0.00364000	1.40396500	2.00692400
C	-0.62900300	1.00663100	-5.73229000
C	-0.06435200	2.27035600	-5.96058800
C	-1.37392700	0.40890600	-6.75976900
C	-0.24123200	2.91346500	-7.18157000
H	0.53878300	2.73594300	-5.19190200
C	-1.55421200	1.05733700	-7.97882500
H	-1.82187100	-0.56421000	-6.59326000
C	-0.98893300	2.31178800	-8.19225300
H	0.21137100	3.88467000	-7.34553300
H	-2.13708100	0.58222700	-8.75962700
H	-1.12741400	2.81747500	-9.14092800

S 1.2.2 **B3F**-NHC Complexes

NHC1

C	-0.28986100	-0.44520800	-2.16253600
C	-0.41049200	0.19136300	-4.46437200
H	-0.56066600	0.74674100	-5.37802800
C	0.16752400	-0.98833600	-4.33950400
H	0.62395200	-1.61339700	-5.08408100
N	0.14900500	-1.41800200	-2.96066900
C	-0.93596600	0.60980100	-3.12674900
C	0.50436200	-2.90970200	-2.81112000
C	-0.48391000	-3.66647400	-3.73294700
H	-0.45063300	-3.35362600	-4.77579200
H	-0.23822400	-4.72947400	-3.70072500
H	-1.50692100	-3.54535300	-3.36914700
C	0.32350300	-3.50544400	-1.41585300
H	-0.59872800	-3.18457000	-0.94335300
H	0.28121500	-4.59050000	-1.53627400
H	1.15595100	-3.29084600	-0.75910500
C	1.96185200	-3.10275000	-3.26487600

H	2.62862400	-2.49029900	-2.65862900
H	2.23451900	-4.15173000	-3.12728500
H	2.12166600	-2.85884600	-4.31668100
C	-2.47749800	0.29658000	-3.18535000
H	-2.98910200	0.69977000	-2.31611400
H	-2.88658500	0.77296000	-4.07881600
H	-2.67310300	-0.77479800	-3.24968600
C	-0.76671600	2.11933400	-2.88779000
H	-1.40932000	2.64333500	-3.60171500
H	-1.06319600	2.42215000	-1.88854900
H	0.25611900	2.44115800	-3.06430700
B	-0.23199500	-0.11410300	-0.49877500
C	-1.81802300	0.20114700	-0.09969000
C	-2.76124600	-0.83029800	-0.12116400
C	-2.40154100	1.41986400	0.25804800
C	-4.10319700	-0.73806100	0.20400800
C	-3.73654700	1.61148100	0.60081600
C	-4.56997200	0.51067600	0.57712800
C	0.80376600	1.18620700	-0.29175000
C	1.81560100	1.59380500	-1.15689000
C	0.88383400	1.82860700	0.95108300
C	2.76725900	2.57278000	-0.90069700
C	1.79181600	2.81846100	1.29380700
C	2.72696400	3.18092600	0.33978500
C	0.49451200	-1.17525700	0.56578000
C	1.85514900	-1.48231700	0.44193200
C	-0.02508600	-1.63751200	1.78037500
C	2.64337800	-2.16081400	1.35623800
C	0.68762200	-2.33347000	2.75348200
C	2.02504800	-2.58129300	2.52204700
F	-1.32052200	-1.41354900	2.09743200
F	2.48786700	-1.12227800	-0.71219300
F	-1.66340700	2.55907000	0.24538500
F	-2.34693400	-2.06684000	-0.52223200
F	1.91629400	1.00017100	-2.38392200
F	0.02906400	1.45081000	1.93007400
H	3.68980300	-2.35062200	1.16218300
H	0.20109700	-2.64950900	3.66574600
H	-4.74924200	-1.60394900	0.16955700
H	-4.09776100	2.59270500	0.87538700
H	1.77251800	3.27270500	2.27458600
H	3.51409600	2.83163400	-1.63809900
F	-5.86901000	0.65626300	0.90846800
F	2.74717800	-3.24735000	3.44663200

F	3.63026700	4.14015000	0.63340200

NHC2

C	-0.29050000	-0.43916700	-2.16451200
C	-0.38175700	0.19113900	-4.45832800
C	0.19206100	-0.99312900	-4.33319800
H	0.64786300	-1.61176000	-5.08218700
N	0.15550600	-1.41364600	-2.95869200
C	-0.93722300	0.61955600	-3.12817400
C	0.50442800	-2.91114100	-2.80756300
C	-0.48396500	-3.66019800	-3.73497200
H	-0.44225400	-3.34862200	-4.77803000
H	-0.24529600	-4.72467800	-3.70127300
H	-1.50827500	-3.53269000	-3.37723200
C	0.31298400	-3.50446300	-1.41290300
H	-0.60990000	-3.17893600	-0.94510300
H	0.26490700	-4.58910800	-1.53450400
H	1.14355500	-3.29492400	-0.75212600
C	1.96276500	-3.11011600	-3.25452000
H	2.62982500	-2.49901500	-2.64736100
H	2.22991300	-4.15985500	-3.11258500
H	2.12855300	-2.87123500	-4.30656000
C	-2.47207100	0.28163100	-3.19818600
H	-2.99007600	0.67620500	-2.32941700
H	-2.87933700	0.75604300	-4.09319900
H	-2.65136200	-0.79234500	-3.26463400
C	-0.78718400	2.12493000	-2.86770600
H	-1.44392900	2.65464600	-3.56167200
H	-1.07675500	2.39622100	-1.85826400
H	0.22904600	2.46412000	-3.04813100
B	-0.23653500	-0.10623600	-0.49977900
C	-1.82190000	0.20889700	-0.09918900
C	-2.76621100	-0.82145700	-0.12752500
C	-2.40327400	1.42475600	0.27212500
C	-4.10679200	-0.73157700	0.20301600
C	-3.73693000	1.61392000	0.62113600
C	-4.57123900	0.51397400	0.59002000
C	0.80163400	1.19207400	-0.29485900
C	1.80838100	1.60194300	-1.16460600
C	0.88909400	1.82991400	0.94979200
C	2.76223200	2.57911300	-0.91134900

C	1.79999000	2.81780200	1.29013800
C	2.72965900	3.18289400	0.33164700
C	0.49071600	-1.17110700	0.55921300
C	1.85149800	-1.47659800	0.43308300
C	-0.02830500	-1.63835000	1.77214200
C	2.64084400	-2.15735300	1.34456500
C	0.68568100	-2.33691400	2.74231600
C	2.02336700	-2.58233000	2.50934700
F	-1.32400000	-1.41740600	2.08949700
F	2.48230700	-1.11312100	-0.72112000
F	-1.66410300	2.56311900	0.26769200
F	-2.35371400	-2.05415400	-0.54285700
F	1.89978800	1.01185900	-2.39469700
F	0.03966700	1.44901600	1.93207400
H	3.68737200	-2.34554300	1.14948800
H	0.20007700	-2.65680400	3.65372700
H	-4.75373300	-1.59651200	0.16222500
H	-4.09651600	2.59280500	0.90597500
H	1.78705500	3.26887300	2.27248400
H	3.50412400	2.84059500	-1.65277600
F	-5.86856300	0.65714300	0.92731900
F	2.74646100	-3.25067700	3.43100800
F	3.63504700	4.14022400	0.62314500
Br	-0.60810600	1.12297700	-6.07835200

NHC3

C	-0.29289200	-0.45058900	-2.15810600
C	-0.41697500	0.18489400	-4.42976300
C	0.16184500	-0.99779700	-4.34687700
H	0.59946600	-1.60539000	-5.11452900
N	0.14512000	-1.41646700	-2.96626000
C	-0.94430800	0.61561500	-3.10666400
C	0.51165800	-2.90807500	-2.81871900
C	-0.46945500	-3.67266300	-3.74130200
H	-0.42985600	-3.36920900	-4.78652800
H	-0.22089400	-4.73452400	-3.69887700
H	-1.49522500	-3.55221800	-3.38518600
C	0.33159300	-3.50081900	-1.42259100
H	-0.59358000	-3.18375400	-0.95294200
H	0.29548200	-4.58628700	-1.54026300
H	1.16152700	-3.27984000	-0.76518500

C	1.97053800	-3.08707600	-3.27149200
H	2.63213700	-2.47327000	-2.66106500
H	2.25055300	-4.13483000	-3.13997200
H	2.12897900	-2.83556200	-4.32172900
C	-2.48530200	0.30266000	-3.17983200
H	-3.00374900	0.73292200	-2.32826800
H	-2.87507100	0.75714300	-4.09329400
H	-2.68266200	-0.76953800	-3.21397300
C	-0.76891400	2.12610700	-2.88237600
H	-1.40123400	2.64515100	-3.60694000
H	-1.07376100	2.43124100	-1.88688800
H	0.25661800	2.44256500	-3.05127400
B	-0.23252600	-0.11923500	-0.49455400
C	-1.81883700	0.19900400	-0.09950900
C	-2.76287000	-0.83173800	-0.12343800
C	-2.40158000	1.41815300	0.25788100
C	-4.10537100	-0.73815700	0.19865800
C	-3.73713300	1.61101800	0.59765800
C	-4.57163600	0.51097300	0.57153500
C	0.80497400	1.18030500	-0.29419700
C	1.81488000	1.58430500	-1.16297900
C	0.88906900	1.82565100	0.94686800
C	2.76931900	2.56160300	-0.91218900
C	1.80018700	2.81418900	1.28462900
C	2.73365900	3.17242600	0.32725800
C	0.49132200	-1.17877900	0.57187500
C	1.85245600	-1.48537400	0.45202700
C	-0.03168200	-1.63964700	1.78557200
C	2.63832500	-2.16239600	1.36927500
C	0.67873200	-2.33389000	2.76147100
C	2.01691400	-2.58148700	2.53401600
F	-1.32797600	-1.41554100	2.09843700
F	2.48776600	-1.12726200	-0.70144200
F	-1.66175600	2.55637500	0.24721900
F	-2.34818200	-2.06864600	-0.52313500
F	1.90956800	0.98823300	-2.39066000
F	0.03563500	1.45182900	1.92831000
H	3.68530100	-2.35232600	1.17830800
H	0.18989100	-2.64896800	3.67283500
H	-4.75229200	-1.60336300	0.16305900
H	-4.09803400	2.59239100	0.87215200
H	1.78461100	3.27095400	2.26431700
H	3.51423800	2.81778200	-1.65245500
F	-5.87086400	0.65761600	0.90012700

F	2.73658600	-3.24606200	3.46117000
F	3.63953700	4.13004400	0.61630400
F	-0.63011200	0.89776000	-5.53384400

NHC4

C	-0.45699400	-0.41830700	-2.10044900
C	-0.66509000	0.25949700	-4.42770300
C	-0.14622100	-0.97916900	-4.29655100
H	0.22846700	-1.64551100	-5.04452100
N	-0.10630100	-1.39284500	-2.92652000
C	-1.13616100	0.66477700	-3.02837000
C	0.18238900	-2.90335400	-2.79526000
C	-0.89902900	-3.61548000	-3.64655800
H	-0.91246000	-3.31348100	-4.69200600
H	-0.70809500	-4.68975500	-3.61250200
H	-1.89031900	-3.43674100	-3.22319300
C	0.06078900	-3.49417200	-1.39053900
H	-0.80926900	-3.12546000	-0.85834100
H	-0.04955100	-4.57470400	-1.50914100
H	0.94510600	-3.33096200	-0.78927600
C	1.59575100	-3.17894800	-3.33804900
H	2.33248400	-2.60017600	-2.78184200
H	1.81853600	-4.24054800	-3.20597600
H	1.70200200	-2.95053200	-4.39959200
C	-2.66706400	0.31660400	-2.95587200
H	-3.09848300	0.68760400	-2.03084600
H	-3.19254700	0.78563700	-3.78873800
H	-2.83622900	-0.75924400	-3.01749800
C	-0.92755900	2.14561600	-2.66946100
H	-1.75093700	2.75451100	-3.04425400
H	-0.89821700	2.29623100	-1.59775300
H	0.00027700	2.52749400	-3.08957500
B	-0.25721800	-0.09450100	-0.44353900
C	-1.78492700	0.28540500	0.11195300
C	-2.77563600	-0.69985000	0.16749900
C	-2.27406500	1.52192800	0.54414800
C	-4.07542200	-0.55030600	0.61949000
C	-3.56042900	1.77030700	1.01425800
C	-4.44519500	0.71140600	1.05230100
C	0.85222500	1.15905700	-0.29596400
C	1.79221400	1.56356300	-1.24102500

C	1.07307800	1.75735100	0.95179100
C	2.80271200	2.49636600	-1.04388200
C	2.04850000	2.70006000	1.23948300
C	2.90494500	3.05986300	0.21385700
C	0.51983200	-1.19787900	0.54281800
C	1.85467500	-1.54467300	0.29920000
C	0.08889400	-1.67054200	1.78739700
C	2.69328400	-2.26863800	1.13050700
C	0.85643900	-2.41092500	2.68310400
C	2.16067900	-2.69615200	2.33517100
F	-1.16802000	-1.41470800	2.21685500
F	2.93478000	-3.40603300	3.18287500
F	2.40163500	-1.17904100	-0.89553700
F	-1.48490800	2.62633200	0.48711600
F	-5.69994800	0.91146600	1.50663200
F	-2.46360600	-1.94794400	-0.28337500
F	1.74954700	1.02139000	-2.49406700
F	3.87113100	3.97371000	0.45070900
F	0.29275200	1.38552700	1.99412200
N	-0.73878000	0.98671100	-5.59856800
C	-0.04898300	0.37637200	-6.76268300
H	0.81706700	-0.12243100	-6.32015900
C	-1.68770800	2.11757900	-5.75181100
H	-2.20422900	2.17617900	-4.80179200
C	-2.78468000	1.87372300	-6.80149200
H	-3.52272500	2.67817700	-6.73768200
H	-2.39679700	1.87121700	-7.82132900
H	-3.30105500	0.92760600	-6.62645600
C	0.53592400	1.38344700	-7.75928900
H	1.15719300	0.83522300	-8.47251800
H	-0.22738600	1.90836400	-8.33585000
H	1.16957200	2.11823100	-7.26087000
C	-1.01339600	3.48709100	-5.95203000
H	-1.74597000	4.27768300	-5.76426900
H	-0.18721100	3.62068900	-5.25285000
H	-0.63453900	3.62784400	-6.96386900
C	-0.88103900	-0.70034500	-7.48968900
H	-1.38912200	-1.35855600	-6.78260800
H	-1.63662500	-0.25858500	-8.14100300
H	-0.22616100	-1.31593200	-8.11381100
H	-4.76174000	-1.38523000	0.63553800
H	-3.84461000	2.76178700	1.33815300
H	2.13751500	3.12049800	2.23142000
H	3.48647000	2.75414800	-1.84054800

H	3.71283700	-2.48693300	0.84492200
H	0.43719700	-2.73202100	3.62650400

NHC5

C	-0.38330900	-0.42136700	-2.12756600
C	-0.51629400	0.23914700	-4.44631400
C	0.03238100	-0.97436700	-4.30686600
H	0.42932000	-1.62465300	-5.06061500
N	0.03909000	-1.39022000	-2.93781400
C	-1.05366400	0.62680600	-3.07006800
C	0.41233600	-2.88056300	-2.79065500
C	-0.60942700	-3.65640000	-3.65840500
H	-0.62597800	-3.35301200	-4.70397400
H	-0.35331800	-4.71700500	-3.62586600
H	-1.61553400	-3.54022700	-3.24874200
C	0.30679100	-3.47334900	-1.38564100
H	-0.59021800	-3.15747800	-0.86525600
H	0.26447300	-4.55886400	-1.50270700
H	1.17266900	-3.25462300	-0.77480700
C	1.85130900	-3.06732400	-3.30346400
H	2.53612000	-2.43977700	-2.73309900
H	2.13943800	-4.11151300	-3.16099100
H	1.96708000	-2.83664700	-4.36361500
C	-2.57024500	0.21042700	-3.15901800
H	-3.11449100	0.56164500	-2.28606400
H	-2.98562900	0.67904800	-4.05382500
H	-2.69376300	-0.86992900	-3.24324800
C	-1.01331600	2.11605700	-2.70543700
H	-1.75355400	2.64578300	-3.30930700
H	-1.27213600	2.28440400	-1.66675900
H	-0.03671400	2.55660300	-2.88528000
B	-0.28385400	-0.09423100	-0.46765000
C	-1.86693900	0.17163000	-0.00750700
C	-2.78958900	-0.87861400	-0.04469100
C	-2.46562700	1.35606600	0.43265300
C	-4.12025400	-0.83423600	0.33341100
C	-3.79055500	1.49946400	0.83339300
C	-4.60041200	0.38258400	0.78568500
C	0.72835000	1.22873400	-0.26853100
C	1.68986300	1.68724500	-1.16557200
C	0.84930300	1.83955000	0.98695700

C	2.62872200	2.68222400	-0.92316000
C	1.74729000	2.84287800	1.31782600
C	2.62995800	3.25479600	0.33470700
C	0.50560500	-1.14912400	0.55768800
C	1.86996900	-1.41299400	0.38625100
C	0.03587800	-1.64954900	1.77690000
C	2.70483000	-2.08373100	1.26453200
C	0.79741800	-2.34134300	2.71528900
C	2.13426200	-2.54360100	2.43976900
F	-1.25759100	-1.47414400	2.13243200
F	2.90346300	-3.20444500	3.33028100
F	2.45557300	-1.01649100	-0.78058200
F	-1.75530800	2.51350400	0.45191500
F	-5.88924700	0.48081000	1.17180900
F	-2.36560500	-2.08757200	-0.51466900
F	1.74861700	1.13627400	-2.41548000
F	3.52300900	4.22818300	0.61531900
F	0.04999400	1.41368600	1.99286800
N	-0.83017100	0.86551600	-5.64264000
C	-0.69524300	0.05008100	-6.84531000
H	-1.22898500	-0.89284500	-6.71654900
H	-1.13910000	0.58576800	-7.68637800
H	0.35451500	-0.16770400	-7.09897400
C	-0.39349000	2.24763700	-5.87149800
H	0.67457800	2.29517300	-6.13043500
H	-0.96885800	2.66586600	-6.70018900
H	-0.56043600	2.86503900	-4.99667000
H	-4.16140100	2.45771100	1.16949700
H	-4.74697000	-1.71330800	0.28030700
H	1.76121900	3.26850000	2.31145800
H	3.33598500	2.97927100	-1.68484800
H	0.34817700	-2.68960400	3.63494100
H	3.74999700	-2.23932100	1.03611500

NHC6

C	-0.29814500	-0.45629800	-2.16396000
C	-0.41878000	0.19164400	-4.45518400
C	0.15449300	-1.00256600	-4.35166800
H	0.59880600	-1.62412500	-5.10597400
N	0.13675000	-1.42090600	-2.97084600
C	-0.94589000	0.60591100	-3.11665500

C	0.49974500	-2.91022000	-2.81840200
C	-0.48363000	-3.68023500	-3.73453300
H	-0.44516700	-3.38161200	-4.78101500
H	-0.23732500	-4.74243100	-3.68542800
H	-1.50857800	-3.55484400	-3.37772500
C	0.32282200	-3.49889500	-1.41963600
H	-0.60007600	-3.17826300	-0.94832800
H	0.28468800	-4.58482500	-1.53282000
H	1.15513800	-3.27688500	-0.76548000
C	1.95795300	-3.09732700	-3.27189600
H	2.62142300	-2.47806000	-2.66894800
H	2.23665200	-4.14411000	-3.12963300
H	2.11525900	-2.85664200	-4.32483100
C	-2.48263300	0.27906800	-3.19202500
H	-3.00625700	0.69739900	-2.33754500
H	-2.87469700	0.73664000	-4.10277600
H	-2.66957000	-0.79502600	-3.23270500
C	-0.78546100	2.11548400	-2.88163200
H	-1.41975700	2.63396300	-3.60422300
H	-1.09263700	2.41141800	-1.88423100
H	0.23744100	2.44161500	-3.04842300
B	-0.23560800	-0.12093000	-0.50147200
C	-1.82125100	0.19665400	-0.09908700
C	-2.76557200	-0.83405400	-0.11925900
C	-2.40401300	1.41558900	0.25895400
C	-4.10797700	-0.73992200	0.20387700
C	-3.73947400	1.60923300	0.59950100
C	-4.57422400	0.50964000	0.57487400
C	0.80151200	1.18010100	-0.30109200
C	1.80908500	1.58721900	-1.17157300
C	0.88715100	1.82521500	0.93993900
C	2.76139400	2.56720200	-0.92135100
C	1.79612200	2.81620900	1.27706700
C	2.72667700	3.17747700	0.31820900
C	0.49286200	-1.17738900	0.56715700
C	1.85417200	-1.48256700	0.44491200
C	-0.02630000	-1.63737900	1.78276100
C	2.64298200	-2.15762300	1.36139600
C	0.68701700	-2.32970900	2.75815400
C	2.02486600	-2.57606000	2.52802100
F	-1.32226300	-1.41489500	2.09891900
F	2.48749700	-1.12525000	-0.70983100
F	-1.66445400	2.55415200	0.24982200
F	-2.35240400	-2.07276900	-0.51481400

F	1.90561700	0.99267400	-2.39914900
F	0.03699200	1.44900000	1.92375300
H	3.68976100	-2.34634300	1.16822600
H	0.20043700	-2.64406000	3.67096600
H	-4.75453900	-1.60546300	0.17039300
H	-4.09956900	2.59105700	0.87336700
H	1.78088800	3.27216300	2.25711700
H	3.50419800	2.82574900	-1.66291500
F	-5.87389700	0.65679400	0.90418600
F	2.74775500	-3.23888500	3.45469200
F	3.63108900	4.13779600	0.60595600
O	-0.65207700	0.97332800	-5.52538900
H	-0.33746300	0.54216700	-6.32825100

NHC7

C	-0.38952800	-0.41371600	-2.15070300
C	-0.54583800	0.26048000	-4.46270400
C	0.03133600	-0.93185500	-4.33026300
H	0.46815000	-1.55289800	-5.08987200
N	0.03623200	-1.37649900	-2.96722900
C	-1.08207900	0.63323900	-3.09215900
C	0.38728800	-2.87405700	-2.84375400
C	-0.63658000	-3.61258100	-3.74054300
H	-0.64035600	-3.28035400	-4.77793400
H	-0.39348700	-4.67673400	-3.73519900
H	-1.64520600	-3.49545400	-3.33747900
C	0.25033200	-3.48394400	-1.44944800
H	-0.65072200	-3.15968000	-0.94050600
H	0.19247200	-4.56700300	-1.58139700
H	1.10810700	-3.28566000	-0.82021400
C	1.82744900	-3.07609300	-3.34668600
H	2.51914400	-2.46921800	-2.76311100
H	2.09658000	-4.12708400	-3.21813000
H	1.95427600	-2.83431400	-4.40340800
C	-2.60301700	0.21924400	-3.08367600
H	-3.09026600	0.57938300	-2.18250500
H	-3.10004900	0.66434500	-3.94434900
H	-2.72915600	-0.86245600	-3.14646000
C	-0.97540400	2.13418900	-2.79081400
H	-1.69160300	2.66939900	-3.41688000
H	-1.20394000	2.36605300	-1.75641600

H	0.01456100	2.51621600	-3.02570300
B	-0.27369900	-0.09632700	-0.48714100
C	-1.84149100	0.19566000	-0.00189500
C	-2.77571000	-0.84445700	0.01191000
C	-2.41543600	1.40097000	0.41382300
C	-4.09737800	-0.77222900	0.41566400
C	-3.73006100	1.57227700	0.83681300
C	-4.55350600	0.46410400	0.83964300
C	0.75745600	1.21378000	-0.30878400
C	1.71551700	1.65568400	-1.21732400
C	0.89466600	1.83165600	0.94150100
C	2.66552400	2.64337200	-0.99068400
C	1.80559500	2.82772100	1.25726900
C	2.68323300	3.22441200	0.26314400
C	0.51718100	-1.16473800	0.52310000
C	1.87301500	-1.45321200	0.32587900
C	0.06358300	-1.65508500	1.75307400
C	2.71284000	-2.14040300	1.18637900
C	0.83106400	-2.36139700	2.67557800
C	2.15768700	-2.59009300	2.37283900
F	-1.21687400	-1.45212400	2.13804200
F	2.44370800	-1.06291600	-0.85045800
F	-1.69008600	2.54784100	0.38497700
F	-2.37516900	-2.06999700	-0.43416800
F	1.75889500	1.09089000	-2.46132500
F	0.09719500	1.42196100	1.95577100
H	3.75038800	-2.31404300	0.93728800
H	0.39418700	-2.70003700	3.60472100
H	-4.73579400	-1.64433600	0.40207300
H	-4.08289000	2.54437400	1.15183500
H	1.83190200	3.26100800	2.24731700
H	3.36705500	2.92983100	-1.76159300
F	-5.83253500	0.58985700	1.24824900
F	2.93171400	-3.26559800	3.24733700
F	3.58734900	4.19099300	0.52929600
C	-0.62229000	1.01699900	-5.72435700
C	-1.70977800	1.83251300	-6.07707400
C	0.44602700	0.92243200	-6.63547700
C	-1.73762700	2.50151700	-7.29733600
H	-2.55232000	1.94325700	-5.40886800
C	0.41581500	1.58974500	-7.85394900
H	1.32253900	0.34500200	-6.36595600
C	-0.67926800	2.38166700	-8.19357500
H	-2.59289300	3.11950600	-7.54609300

H	1.25645300	1.50277500	-8.53305500
H	-0.70192500	2.90779800	-9.14084900

S 1.2.3 **B2F**-NHC Complexes

NHC1

C	-0.28806100	-0.44320500	-2.15978400
C	-0.40719200	0.19425700	-4.46152800
H	-0.55569400	0.75054100	-5.37493000
C	0.16855800	-0.98654500	-4.33679200
H	0.62458900	-1.61196800	-5.08139800
N	0.14862700	-1.41696200	-2.95856100
C	-0.93320700	0.61252100	-3.12398100
C	0.50015100	-2.90870500	-2.80916500
C	-0.49352900	-3.66285700	-3.72740700
H	-0.46456300	-3.34831000	-4.76999900
H	-0.25008600	-4.72651900	-3.69753200
H	-1.51430800	-3.53941100	-3.35817900
C	0.32290000	-3.50393800	-1.41319200
H	-0.59623000	-3.17956600	-0.93717900
H	0.27642100	-4.58900300	-1.53369300
H	1.15813900	-3.29097300	-0.75949600
C	1.95573500	-3.10650200	-3.26742000
H	2.62475600	-2.49440900	-2.66338400
H	2.22596700	-4.15607700	-3.12885700
H	2.11313800	-2.86460000	-4.32017700
C	-2.47495200	0.30042000	-3.18386400
H	-2.98667700	0.70068300	-2.31333800
H	-2.88282900	0.77950800	-4.07666900
H	-2.67066900	-0.77076300	-3.25106500
C	-0.76303300	2.12152300	-2.88330900
H	-1.40528200	2.64651600	-3.59713400
H	-1.05967900	2.42297200	-1.88366300
H	0.26048300	2.44177100	-3.05814700
B	-0.23140800	-0.11420200	-0.49653300
C	-1.81957200	0.19640800	-0.10071000
C	-2.76115300	-0.83681200	-0.12483900
C	-2.40680800	1.41530600	0.25128500
C	-4.10302000	-0.73906600	0.19506900
C	-3.74407800	1.59734900	0.58724000

C	-4.60032800	0.50544200	0.56847800
C	0.80474500	1.18541200	-0.28616100
C	1.81665300	1.59431100	-1.15150000
C	0.88190900	1.82842300	0.95646700
C	2.76420600	2.57365400	-0.88816100
C	1.79199400	2.81779800	1.29215500
C	2.74330000	3.19984900	0.35172600
C	0.50003600	-1.17291100	0.56660600
C	1.85940300	-1.48554700	0.43667400
C	-0.01647600	-1.63095100	1.78411800
C	2.64330600	-2.16353900	1.35325700
C	0.70471000	-2.32639400	2.75038500
C	2.04883900	-2.59206400	2.53675600
F	-1.31283100	-1.39997000	2.10358800
F	2.48523400	-1.12938000	-0.72676300
F	-1.66621900	2.55676200	0.23759300
F	-2.33858100	-2.07564300	-0.52402400
F	1.91296900	0.99889500	-2.38254400
F	0.02127900	1.44902700	1.93360500
H	3.68738800	-2.34204000	1.12998800
H	2.62859700	-3.12444200	3.28107400
H	0.19521000	-2.62946400	3.65618300
H	-4.72573900	-1.62311900	0.15011500
H	-5.64454300	0.62264400	0.83189400
H	-4.08160700	2.59023100	0.85553100
H	1.74761700	3.25755300	2.28024900
H	3.46852900	3.96898600	0.58855900
H	3.49995700	2.81442500	-1.64481200

NHC2

C	-0.28872400	-0.43733000	-2.16136700
C	-0.37921600	0.19336400	-4.45471800
C	0.19221400	-0.99194000	-4.33026200
H	0.64688200	-1.61090000	-5.07969400
N	0.15494600	-1.41294900	-2.95620600
C	-0.93500900	0.62215700	-3.12495300
C	0.50051300	-2.91038400	-2.80522900
C	-0.49318800	-3.65701500	-3.72898200
H	-0.45627900	-3.34344600	-4.77176600
H	-0.25609400	-4.72200900	-3.69807900
H	-1.51524900	-3.52796000	-3.36542600

C	0.31310400	-3.50320400	-1.40980500
H	-0.60659400	-3.17437300	-0.93820400
H	0.26095700	-4.58782700	-1.53159800
H	1.14663100	-3.29524900	-0.75230800
C	1.95701200	-3.11356900	-3.25674000
H	2.62612700	-2.50258000	-2.65180400
H	2.22208100	-4.16377800	-3.11375100
H	2.12038800	-2.87673400	-4.30974400
C	-2.47012200	0.28552200	-3.19608300
H	-2.98798700	0.67757800	-2.32607500
H	-2.87629700	0.76230300	-4.09049500
H	-2.64960300	-0.78828600	-3.26486100
C	-0.78369300	2.12703300	-2.86315800
H	-1.44025500	2.65775600	-3.55679100
H	-1.07301200	2.39727500	-1.85332500
H	0.23326200	2.46442900	-3.04232400
B	-0.23590200	-0.10660700	-0.49720500
C	-1.82345000	0.20388400	-0.09995700
C	-2.76606800	-0.82826700	-0.13109800
C	-2.40866400	1.42011400	0.26492600
C	-4.10673600	-0.73275000	0.19364100
C	-3.74487200	1.59978900	0.60628600
C	-4.60182200	0.50869600	0.58019300
C	0.80283700	1.19099200	-0.28928400
C	1.80950100	1.60158000	-1.15961400
C	0.88734100	1.83017800	0.95479700
C	2.75924400	2.57936600	-0.89991200
C	1.80031600	2.81792800	1.28731200
C	2.74596600	3.20193700	0.34198800
C	0.49637700	-1.16903500	0.56046400
C	1.85595900	-1.47983500	0.42837700
C	-0.01956600	-1.63174500	1.77644300
C	2.64112100	-2.15955100	1.34245000
C	0.70314900	-2.32915900	2.74008600
C	2.04753000	-2.59231300	2.52489600
F	-1.31615100	-1.40373300	2.09630400
F	2.47982600	-1.12037700	-0.73525200
F	-1.66728700	2.56085500	0.25897400
F	-2.34518700	-2.06327900	-0.54449600
F	1.89594400	1.00922700	-2.39356400
F	0.03218400	1.44820600	1.93556000
H	3.68533700	-2.33613600	1.11835000
H	0.19467000	-2.63576800	3.64524800
H	-4.73043200	-1.61572600	0.14199100

H	-4.08105600	2.59043400	0.88425000
H	1.76239500	3.25521700	2.27675500
H	3.48981700	2.82250200	-1.66073300
Br	-0.60353400	1.12553000	-6.07594100
H	-5.64517600	0.62425400	0.84756400
H	3.47281200	3.97023500	0.57639100
H	2.62833900	-3.12605000	3.26738100

NHC3

C	-0.29123700	-0.44902200	-2.15492600
C	-0.41419600	0.18657700	-4.42649800
C	0.16190600	-0.99730400	-4.34375600
H	0.59872400	-1.60552100	-5.11141200
N	0.14425000	-1.41627200	-2.96336600
C	-0.94190700	0.61770000	-3.10380400
C	0.50660600	-2.90789500	-2.81557900
C	-0.48051200	-3.66988300	-3.73400400
H	-0.44654300	-3.36422200	-4.77892000
H	-0.23357600	-4.73232100	-3.69467200
H	-1.50377300	-3.54776100	-3.37132000
C	0.33069000	-3.49966500	-1.41847100
H	-0.59105100	-3.17877300	-0.94486100
H	0.29000300	-4.58516300	-1.53603300
H	1.16387500	-3.28047200	-0.76461400
C	1.96349400	-3.09213000	-3.27322100
H	2.62763700	-2.47834300	-2.66560800
H	2.24092900	-4.14043600	-3.13998700
H	2.11936400	-2.84350500	-4.32465400
C	-2.48310400	0.30560900	-3.17797400
H	-3.00162100	0.73347300	-2.32522500
H	-2.87173600	0.76212400	-4.09108600
H	-2.68036900	-0.76653200	-3.21413100
C	-0.76575300	2.12776300	-2.87820900
H	-1.39790600	2.64759400	-3.60258200
H	-1.07053700	2.43174200	-1.88230400
H	0.26038300	2.44268900	-3.04568600
B	-0.23164200	-0.11939900	-0.49203300
C	-1.82000100	0.19443500	-0.09993500
C	-2.76251700	-0.83795500	-0.12623900
C	-2.40635300	1.41409000	0.25068500
C	-4.10511700	-0.73837900	0.18979100

C	-3.74437200	1.59788000	0.58268600
C	-4.60181000	0.50691300	0.56154200
C	0.80640100	1.17955300	-0.28921900
C	1.81581700	1.58458100	-1.15898100
C	0.88794200	1.82625000	0.95121600
C	2.76603200	2.56272000	-0.90209400
C	1.80106600	2.81479600	1.28087800
C	2.75004800	3.19225800	0.33623900
C	0.49755900	-1.17628600	0.57305800
C	1.85741600	-1.48843500	0.44673800
C	-0.02188300	-1.63230400	1.79010000
C	2.63938700	-2.16440100	1.36632400
C	0.69751300	-2.32547900	2.75928400
C	2.04221200	-2.59092900	2.54919100
F	-1.31892700	-1.40089300	2.10589200
F	2.48542700	-1.13443900	-0.71639300
F	-1.66388800	2.55443900	0.23849000
F	-2.33972100	-2.07742800	-0.52324800
F	1.90538200	0.98622100	-2.39052100
F	0.02924200	1.45115100	1.93146400
H	3.68405500	-2.34297400	1.14591300
H	0.18615500	-2.62710200	3.66450800
H	-4.72892900	-1.62161000	0.14378400
H	-4.08160000	2.59111500	0.85000100
H	1.76075300	3.25778700	2.26769500
H	3.49933300	2.80060300	-1.66198300
F	-0.62547400	0.89986600	-5.53173600
H	3.47731600	3.96080500	0.56850100
H	2.62047800	-3.12156700	3.29587400
H	-5.64661200	0.62545400	0.82188200

NHC4

C	-0.45688400	-0.41740300	-2.09830400
C	-0.66675400	0.25876500	-4.42529700
C	-0.15218100	-0.98094300	-4.29466100
H	0.22187800	-1.64794800	-5.04252400
N	-0.11124600	-1.39424600	-2.92391100
C	-1.13522700	0.66637300	-3.02591900
C	0.17296100	-2.90461700	-2.79178800
C	-0.91490700	-3.61365500	-3.63757600
H	-0.93456600	-3.30932400	-4.68240600

H	-0.72578600	-4.68841800	-3.60664800
H	-1.90287700	-3.43350200	-3.20709000
C	0.05656400	-3.49403000	-1.38596800
H	-0.80917200	-3.12135200	-0.84963100
H	-0.05873100	-4.57435000	-1.50357000
H	0.94420600	-3.33281900	-0.78904600
C	1.58303000	-3.18575300	-3.34065600
H	2.32289300	-2.60739200	-2.78828400
H	1.80305600	-4.24779200	-3.20677700
H	1.68537800	-2.96039400	-4.40337800
C	-2.66700000	0.32193000	-2.95051000
H	-3.09545500	0.69228000	-2.02386400
H	-3.19275900	0.79313200	-3.78219400
H	-2.83860100	-0.75351200	-3.01277000
C	-0.92281400	2.14680100	-2.66838600
H	-1.74459800	2.75724300	-3.04471300
H	-0.89468400	2.29860100	-1.59671000
H	0.00707800	2.52480100	-3.08726100
B	-0.25597700	-0.09438800	-0.44187100
C	-1.78525400	0.28234500	0.11251300
C	-2.77515300	-0.70409100	0.16880000
C	-2.27736900	1.52035100	0.53827800
C	-4.07391600	-0.54769000	0.61831600
C	-3.56589300	1.76063500	1.00408200
C	-4.47295900	0.71201900	1.05349100
C	0.85491500	1.15788800	-0.29468100
C	1.79456800	1.56145800	-1.24134400
C	1.07455600	1.75876800	0.95213900
C	2.80228000	2.49429500	-1.03914600
C	2.05205900	2.70105500	1.23004800
C	2.92603900	3.07756300	0.21560300
C	0.52747300	-1.19527700	0.54163900
C	1.85960900	-1.54837000	0.28883100
C	0.10314400	-1.66229500	1.79074000
C	2.69561700	-2.27203500	1.12086800
C	0.88049600	-2.40207300	2.67736200
C	2.19111600	-2.70764100	2.34278200
F	-1.15261600	-1.39756300	2.22634400
F	2.39609200	-1.18645200	-0.91591200
F	-1.48565700	2.62664500	0.47615300
F	-2.45656600	-1.95556700	-0.28026700
F	1.74568800	1.01555600	-2.49707300
F	0.28938200	1.38714600	1.99457900
N	-0.73663500	0.98793100	-5.59672300

C	-0.04540400	0.37782400	-6.75903900
H	0.81973100	-0.12124600	-6.31492000
C	-1.68761100	2.11598200	-5.75139100
H	-2.20396000	2.17493900	-4.80130500
C	-2.78437600	1.86950400	-6.80091600
H	-3.52409600	2.67259100	-6.73792400
H	-2.39633600	1.86674500	-7.82081000
H	-3.29878300	0.92246400	-6.62499500
C	0.54107000	1.38499700	-7.75477800
H	1.16392200	0.83725600	-8.46710500
H	-0.22161900	1.90973400	-8.33252600
H	1.17322500	2.12008300	-7.25486000
C	-1.01623800	3.48686400	-5.95298700
H	-1.75080200	4.27624700	-5.76745400
H	-0.19166300	3.62273300	-5.25241000
H	-0.63601900	3.62686400	-6.96452700
C	-0.87534100	-0.69919200	-7.48859400
H	-1.38555200	-1.35681500	-6.78256600
H	-1.62892300	-0.25754600	-8.14243200
H	-0.21864100	-1.31532100	-8.11040000
H	-4.73931500	-1.40132200	0.62393600
H	-3.82551800	2.76345700	1.31834800
H	2.11755600	3.10908700	2.23052500
H	3.47179500	2.73327000	-1.85565000
H	3.70972900	-2.47937300	0.80393000
H	0.44063200	-2.70796800	3.61808100
H	-5.48025800	0.87373500	1.41794300
H	2.81399100	-3.27522400	3.02360700
H	3.70214200	3.80937400	0.40512400

NHC5

C	-0.38185900	-0.41977000	-2.12558700
C	-0.50930400	0.24272000	-4.44328600
C	0.03480400	-0.97224300	-4.30497800
H	0.43096000	-1.62283400	-5.05903000
N	0.03870200	-1.38964400	-2.93605900
C	-1.04878400	0.63022500	-3.06834600
C	0.40759300	-2.88015500	-2.78924700
C	-0.61891400	-3.65245100	-3.65462900
H	-0.63922400	-3.34628300	-4.69950000
H	-0.36499500	-4.71376100	-3.62545200

H	-1.62279600	-3.53452300	-3.24005700
C	0.30465200	-3.47302500	-1.38408700
H	-0.58931100	-3.15371300	-0.86073000
H	0.25779600	-4.55848800	-1.50169900
H	1.17287900	-3.25661800	-0.77581700
C	1.84501400	-3.07156200	-3.30520000
H	2.53154500	-2.44460800	-2.73630500
H	2.13058800	-4.11638600	-3.16152400
H	1.95948600	-2.84291400	-4.36605900
C	-2.56619700	0.21691600	-3.16104800
H	-3.11105900	0.56640500	-2.28782600
H	-2.97835200	0.68858400	-4.05587900
H	-2.69117800	-0.86309100	-3.24776600
C	-1.00720700	2.11918500	-2.70345200
H	-1.73984300	2.65054800	-3.31552300
H	-1.27603000	2.28859100	-1.66736800
H	-0.02704400	2.55564400	-2.87270200
B	-0.28696200	-0.09569600	-0.46558000
C	-1.87319800	0.16482700	-0.01218500
C	-2.79391700	-0.88731800	-0.05409100
C	-2.47731200	1.34951900	0.42072200
C	-4.12554400	-0.83770200	0.31625700
C	-3.80543000	1.48307100	0.81144000
C	-4.63771400	0.37395000	0.76863400
C	0.72536100	1.22642900	-0.26117900
C	1.68976100	1.68535600	-1.15590100
C	0.83999600	1.83865100	0.99420400
C	2.62448400	2.68013400	-0.90411500
C	1.73906900	2.84173800	1.31972500
C	2.64115600	3.27240100	0.35242700
C	0.50552300	-1.14838500	0.55918700
C	1.86873200	-1.41840600	0.38331800
C	0.03724100	-1.64359200	1.78117600
C	2.69794800	-2.08884400	1.26519000
C	0.80570900	-2.33429100	2.71368900
C	2.15052400	-2.55558700	2.45696800
F	-1.25752700	-1.45999700	2.13785500
F	2.44876700	-1.02627800	-0.79210500
F	-1.76539600	2.50976600	0.43972700
F	-2.36031800	-2.09817800	-0.52231900
F	1.74725700	1.13197100	-2.40937100
F	0.03229300	1.41153700	1.99662700
N	-0.81848200	0.87486900	-5.63950600
C	-0.69330000	0.05914000	-6.84256500

H	-1.23788000	-0.87765900	-6.71435400
H	-1.13083900	0.60068600	-7.68344400
H	0.35388100	-0.17109500	-7.09705300
C	-0.35370400	2.24813900	-5.86549800
H	0.71443600	2.27415800	-6.12806600
H	-0.92307100	2.68189700	-6.69061600
H	-0.50394400	2.86492800	-4.98712500
H	-4.15414100	2.45369600	1.14022400
H	-4.72856200	-1.73400000	0.24952700
H	1.72581200	3.25277400	2.32101800
H	3.32254000	2.95851900	-1.68335000
H	0.33174500	-2.66924900	3.62755200
H	3.73979500	-2.23325000	1.00906400
H	3.35782300	4.05213700	0.58069400
H	2.76688400	-3.08364200	3.17452700
H	-5.67413400	0.45284100	1.07383600

NHC6

C	-0.29729700	-0.45484700	-2.16110800
C	-0.41823800	0.19226200	-4.45238900
C	0.15232400	-1.00297500	-4.34892400
H	0.59551900	-1.62527100	-5.10339000
N	0.13457900	-1.42113000	-2.96801700
C	-0.94478700	0.60761900	-3.11411700
C	0.49326300	-2.91045700	-2.81517700
C	-0.49733600	-3.67780900	-3.72583800
H	-0.46564900	-3.37722800	-4.77212300
H	-0.25287000	-4.74064000	-3.67984900
H	-1.51930900	-3.55038700	-3.36131100
C	0.32200600	-3.49785700	-1.41517400
H	-0.59657300	-3.17276100	-0.93862100
H	0.27836600	-4.58378700	-1.52822600
H	1.15863500	-3.27833900	-0.76578600
C	1.94896400	-3.10318400	-3.27494600
H	2.61565500	-2.48389500	-2.67562700
H	2.22513300	-4.15049500	-3.13096300
H	2.10274800	-2.86570700	-4.32925200
C	-2.48188200	0.28216600	-3.18914900
H	-3.00470200	0.69874000	-2.33330600
H	-2.87347700	0.74137800	-4.09945000
H	-2.66921900	-0.79181400	-3.23113800

C	-0.78287500	2.11682800	-2.87844200
H	-1.41757500	2.63615800	-3.60031700
H	-1.08894300	2.41200100	-1.88043600
H	0.24058800	2.44106700	-3.04487600
B	-0.23452000	-0.12076300	-0.49922400
C	-1.82194500	0.19248600	-0.09892200
C	-2.76483500	-0.83985500	-0.12045300
C	-2.40809900	1.41198200	0.25276700
C	-4.10685700	-0.73985000	0.19832300
C	-3.74557500	1.59640900	0.58714100
C	-4.60334600	0.50581900	0.56900600
C	0.80349400	1.17951800	-0.29727300
C	1.81035200	1.58736700	-1.16915000
C	0.88727100	1.82622800	0.94303500
C	2.75863100	2.56805700	-0.91339700
C	1.79850700	2.81703200	1.27150200
C	2.74438700	3.19741100	0.32497600
C	0.49990900	-1.17447900	0.56772800
C	1.85992400	-1.48515700	0.43840400
C	-0.01492400	-1.62933100	1.78713600
C	2.64543100	-2.15857600	1.35706600
C	0.70802600	-2.31990700	2.75567500
C	2.05249000	-2.58397000	2.54245400
F	-1.31152100	-1.39974900	2.10680500
F	2.48514500	-1.13285200	-0.72666100
F	-1.66622600	2.55282200	0.24052000
F	-2.34397200	-2.08108300	-0.51391900
F	1.90109000	0.99044700	-2.40058000
F	0.03213000	1.44916800	1.92608300
H	3.68970600	-2.33602600	1.13380600
H	0.19941700	-2.62051300	3.66280700
H	-4.73028700	-1.62352600	0.15520600
H	-4.08176900	2.59013200	0.85401300
H	1.75905800	3.25928100	2.25870200
H	3.48948900	2.80800400	-1.67505900
O	-0.64959100	0.97354900	-5.52445500
H	-0.33371000	0.53962300	-6.32515400
H	3.47028500	3.96779000	0.55572800
H	2.63362100	-3.11256400	3.28842500
H	-5.64770200	0.62469500	0.83118900

NHC7

C	-0.38887600	-0.41188800	-2.14783900
C	-0.54564000	0.26216600	-4.45959600
C	0.02976100	-0.93093700	-4.32740400
H	0.46567100	-1.55225100	-5.08741500
N	0.03426600	-1.37602900	-2.96496500
C	-1.08167100	0.63525800	-3.08897500
C	0.38226700	-2.87357300	-2.84158600
C	-0.64687100	-3.60973200	-3.73434900
H	-0.65558100	-3.27544900	-4.77120700
H	-0.40535500	-4.67432400	-3.73191400
H	-1.65297900	-3.49135300	-3.32540900
C	0.24998300	-3.48306700	-1.44662900
H	-0.64793400	-3.15640400	-0.93381000
H	0.18890100	-4.56612700	-1.57868200
H	1.11047500	-3.28574300	-0.82087500
C	1.82026800	-3.07950600	-3.34952900
H	2.51408100	-2.47266300	-2.76852400
H	2.08753500	-4.13092400	-3.21985900
H	1.94422200	-2.83992000	-4.40722400
C	-2.60283700	0.22211700	-3.08064600
H	-3.08917600	0.57911200	-2.17774600
H	-3.09983600	0.67016200	-3.94003300
H	-2.72909900	-0.85940400	-3.14637000
C	-0.97416800	2.13583200	-2.78661800
H	-1.69072800	2.67173900	-3.41201800
H	-1.20220700	2.36671200	-1.75184700
H	0.01639900	2.51655800	-3.02066500
B	-0.27278500	-0.09641000	-0.48485500
C	-1.84242500	0.19085800	-0.00140700
C	-2.77514800	-0.85098700	0.01023800
C	-2.42010800	1.39636200	0.40938200
C	-4.09665200	-0.77333900	0.41025500
C	-3.73695000	1.55798500	0.82681100
C	-4.58289400	0.45832500	0.83688800
C	0.75896000	1.21320000	-0.30479400
C	1.71613700	1.65594300	-1.21467600
C	0.89425000	1.83246700	0.94498700
C	2.66236800	2.64420200	-0.98226600
C	1.80686300	2.82878700	1.25196200
C	2.70002200	3.24462400	0.26983200
C	0.52418100	-1.16216700	0.52298600
C	1.87832200	-1.45607600	0.31814500
C	0.07525700	-1.64803100	1.75651000
C	2.71487200	-2.14292400	1.18012900

C	0.85205600	-2.35337300	2.67097100
C	2.18600800	-2.60059500	2.38359800
F	-1.20555500	-1.43799700	2.14562500
F	2.44044500	-1.06924700	-0.86772700
F	-1.69272100	2.54566400	0.37835500
F	-2.36675000	-2.07845600	-0.43580800
F	1.75359000	1.08873000	-2.46232900
F	0.09210400	1.42136600	1.95872900
H	3.74808600	-2.30501600	0.90082100
H	0.39291200	-2.67889000	3.59572100
H	-4.71225300	-1.66314000	0.38474800
H	-4.06645000	2.54202700	1.13475800
H	1.80952000	3.24777300	2.25002100
H	3.35129700	2.91242500	-1.77296400
C	-0.62121100	1.01793700	-5.72163000
C	-1.70772400	1.83453900	-6.07499000
C	0.44678800	0.92211300	-6.63306100
C	-1.73520600	2.50266300	-7.29578600
H	-2.54944000	1.94679200	-5.40603900
C	0.41682900	1.58816200	-7.85227600
H	1.32287300	0.34442700	-6.36274700
C	-0.67747500	2.38092700	-8.19253800
H	-2.58988500	3.12157100	-7.54459200
H	1.25732300	1.49967600	-8.53147400
H	-0.69991300	2.90622200	-9.14034500
H	3.42562100	4.02027000	0.48313900
H	2.80838200	-3.14051500	3.08694100
H	-5.61086100	0.55957000	1.16330200

S 1.2.4 **B5Cl**-NHC Complexes

NHC1

C	-0.28022300	-0.48776200	-2.29974000
C	-0.45822600	0.08021300	-4.61997900
H	-0.65737400	0.59395600	-5.54834100
C	0.17883200	-1.06745700	-4.47078900
H	0.64704600	-1.68524200	-5.21241100
N	0.20882700	-1.46344600	-3.08895200
C	-1.05941100	0.45926000	-3.30472400
C	0.61939000	-2.96459600	-2.97334500

C	-0.48324200	-3.73447300	-3.74036200
H	-0.61325600	-3.39444000	-4.76750800
H	-0.20480100	-4.78952800	-3.77390500
H	-1.44394100	-3.65480800	-3.22976900
C	0.70426900	-3.56909700	-1.57251100
H	-0.10002900	-3.26164900	-0.91656400
H	0.63819000	-4.65258200	-1.69362600
H	1.65492800	-3.36236200	-1.09788900
C	1.98942500	-3.16358400	-3.65412600
H	2.73307800	-2.48262800	-3.24243200
H	2.32024400	-4.18375000	-3.44919000
H	1.96510400	-3.04906100	-4.73788400
C	-2.53913000	-0.08020100	-3.47297700
H	-3.15069800	0.19585500	-2.61998100
H	-2.96323300	0.39737900	-4.35837700
H	-2.57418300	-1.15831100	-3.61526900
C	-1.20400900	1.97560900	-3.09634500
H	-1.50282600	2.41240100	-4.05326400
H	-1.99020000	2.20468500	-2.38535800
H	-0.29618100	2.47437700	-2.78118900
B	-0.16745400	-0.05186000	-0.60000700
C	-1.79625100	0.37705100	-0.27992600
C	-2.79431400	-0.61951400	-0.39063100
C	-2.32478100	1.64497900	0.07120700
C	-4.14832100	-0.44324000	-0.08772000
C	-3.67485400	1.85245900	0.42111200
C	-4.59041800	0.80269800	0.35707600
C	0.94866000	1.25798500	-0.38472800
C	1.79397800	1.85673300	-1.34458500
C	1.15299700	1.77580100	0.92131700
C	2.67859600	2.91467000	-1.07611400
C	2.06174000	2.79620800	1.23449300
C	2.81679200	3.39253700	0.22440300
C	0.49177900	-1.21848500	0.51416600
C	1.86425500	-1.56099500	0.41883300
C	-0.13217100	-1.82062800	1.64421100
C	2.54954000	-2.41521200	1.29627700
C	0.50622500	-2.74715800	2.49192100
C	1.85707400	-3.04513500	2.32605800
Cl	1.90092900	1.25023100	-2.99405800
Cl	0.19016100	1.21927100	2.26884300
Cl	3.91449500	4.68908300	0.58319600
Cl	2.84957900	-0.98078300	-0.91178400
Cl	-1.73880400	-1.39319100	2.20573800

Cl	2.66450600	-4.15936300	3.38502600
Cl	-2.36660400	-2.24124200	-0.91394800
Cl	-6.25395100	1.04277200	0.79065100
Cl	-1.37615600	3.12219000	0.03701200
Cl	-5.29101100	-1.74753800	-0.23407200
Cl	-4.24634100	3.41697200	0.92773200
Cl	3.64179600	3.63514600	-2.33878300
Cl	2.25007800	3.36709000	2.86761800
Cl	4.25051800	-2.74295800	1.10533500
Cl	-0.34936000	-3.52664000	3.79518100

NHC2

C	-0.28264400	-0.48251200	-2.30521400
C	-0.43180600	0.08286100	-4.62056600
C	0.19579800	-1.07289300	-4.46813900
H	0.65967600	-1.68728700	-5.21420500
N	0.21002300	-1.46055200	-3.09100700
C	-1.06436800	0.46866200	-3.30981900
C	0.61609300	-2.96787900	-2.97404000
C	-0.49007800	-3.73090100	-3.74171800
H	-0.61588800	-3.39219400	-4.77000900
H	-0.21763300	-4.78754200	-3.77355100
H	-1.45115400	-3.64519500	-3.23298100
C	0.69704900	-3.56849300	-1.57179800
H	-0.10679500	-3.25651700	-0.91759500
H	0.62655000	-4.65186200	-1.69131900
H	1.64814700	-3.36444300	-1.09685900
C	1.98561600	-3.17161200	-3.65347600
H	2.73083000	-2.49075000	-3.24452900
H	2.31378900	-4.19154600	-3.44350600
H	1.96237700	-3.06333100	-4.73798100
C	-2.53452400	-0.08847800	-3.48515000
H	-3.14478700	0.16270600	-2.62458500
H	-2.96329900	0.40281900	-4.36037100
H	-2.55493800	-1.16422600	-3.64749600
C	-1.21759300	1.97625800	-3.07195600
H	-1.47846200	2.44123700	-4.02486500
H	-2.03360900	2.17734800	-2.38679400
H	-0.32533900	2.46437600	-2.70198300
B	-0.17200100	-0.04456200	-0.60181000
C	-1.80026700	0.38200900	-0.27921700

C	-2.79803700	-0.61479700	-0.39029200
C	-2.32831100	1.64849400	0.07869700
C	-4.15152500	-0.44020600	-0.08385600
C	-3.67727300	1.85343400	0.43437600
C	-4.59272000	0.80361400	0.36789800
C	0.94456300	1.26392000	-0.38696000
C	1.78823000	1.86338600	-1.34753300
C	1.15201800	1.77919800	0.91961300
C	2.67596000	2.91883000	-1.07941800
C	2.06324500	2.79749200	1.23246400
C	2.81769200	3.39386000	0.22182200
C	0.48980300	-1.21348900	0.50761300
C	1.86239600	-1.55482600	0.40931000
C	-0.13172000	-1.81691400	1.63843600
C	2.55041300	-2.40810300	1.28554400
C	0.50946200	-2.74292400	2.48469500
C	1.86053300	-3.03889700	2.31659000
Cl	1.88963900	1.26085700	-2.99884300
Cl	0.19154500	1.22110200	2.26802400
Cl	3.91894800	4.68701800	0.58061100
Cl	2.84423300	-0.97513100	-0.92417000
Cl	-1.73794900	-1.39244000	2.20267800
Cl	2.67130200	-4.15181400	3.37401900
Cl	-2.37060900	-2.23552300	-0.91747500
Cl	-6.25484600	1.04102700	0.80710700
Cl	-1.38177100	3.12651000	0.04474000
Cl	-5.29407200	-1.74404800	-0.23309200
Cl	-4.24769100	3.41504700	0.95008100
Cl	3.63759100	3.63880000	-2.34278600
Cl	2.25592400	3.36518100	2.86599500
Cl	4.25125700	-2.73380300	1.09141100
Cl	-0.34285400	-3.52389200	3.78892800
Br	-0.71923700	0.93320900	-6.27320400

NHC3

C	-0.28298200	-0.49480800	-2.29078500
C	-0.46929400	0.07652300	-4.57989700
C	0.16508100	-1.07753700	-4.47427700
H	0.60482800	-1.68205600	-5.24195900
N	0.20159000	-1.46338600	-3.09214200
C	-1.06982300	0.46567300	-3.27501100

C	0.62190200	-2.96500900	-2.98098200
C	-0.48222600	-3.74115300	-3.73907100
H	-0.61917100	-3.40764000	-4.76728500
H	-0.19953200	-4.79510500	-3.76875900
H	-1.44032400	-3.66322900	-3.22338200
C	0.71874200	-3.56448700	-1.57923300
H	-0.08272700	-3.25804300	-0.91925100
H	0.65570000	-4.64849500	-1.69656800
H	1.67189900	-3.35248200	-1.11236600
C	1.98763300	-3.15232600	-3.67147500
H	2.73151200	-2.47284500	-3.25764400
H	2.32248400	-4.17343900	-3.47843600
H	1.95616300	-3.02709900	-4.75386300
C	-2.54930200	-0.06915100	-3.46138300
H	-3.16941200	0.22041000	-2.62014000
H	-2.94974800	0.40500700	-4.35985400
H	-2.58804600	-1.14889500	-3.59064500
C	-1.19310700	1.98553900	-3.07402400
H	-1.32247700	2.44313000	-4.05740700
H	-2.07323700	2.22833600	-2.48675900
H	-0.33324100	2.44532600	-2.60596300
B	-0.16551500	-0.05742900	-0.59422600
C	-1.79635100	0.37092000	-0.28120200
C	-2.79196500	-0.62882400	-0.39015500
C	-2.32883100	1.64008800	0.05879100
C	-4.14783500	-0.45317600	-0.09561600
C	-3.68218000	1.84784000	0.39712500
C	-4.59527600	0.79584200	0.33560700
C	0.95009800	1.25424300	-0.38694500
C	1.79345800	1.84963500	-1.35049800
C	1.15629700	1.77690000	0.91669500
C	2.68080300	2.90671000	-1.08760100
C	2.06734600	2.79677300	1.22482800
C	2.82227300	3.38796000	0.21148500
C	0.49367100	-1.21967100	0.52078300
C	1.86573800	-1.56361300	0.42540500
C	-0.13088800	-1.81810800	1.65238100
C	2.54973500	-2.41838900	1.30324900
C	0.50651000	-2.74395000	2.50150800
C	1.85656800	-3.04526600	2.33457900
Cl	1.89580100	1.24006400	-3.00060700
Cl	0.19399500	1.22592700	2.26649700
Cl	3.92336900	4.68285000	0.56424700
Cl	2.85207500	-0.98427300	-0.90529300

Cl	-1.73624900	-1.38587100	2.21333500
Cl	2.66240300	-4.15959000	3.39436300
Cl	-2.35964800	-2.25342700	-0.90164900
Cl	-6.26183600	1.03612800	0.75617300
Cl	-1.38072100	3.11713500	0.03211400
Cl	-5.28710900	-1.76086800	-0.23695900
Cl	-4.26015900	3.41500700	0.88738000
Cl	3.64188500	3.62179200	-2.35416300
Cl	2.25906800	3.37264700	2.85550300
Cl	4.24971400	-2.74989900	1.11147800
Cl	-0.34948800	-3.51834200	3.80722400
F	-0.74201800	0.73232500	-5.70275900

NHC4

C	-0.36907900	-0.50470600	-2.17392200
C	-0.64424200	0.05351200	-4.52560500
C	-0.15838700	-1.18263100	-4.35372600
H	0.13678300	-1.88509100	-5.10766100
N	-0.06527700	-1.54317200	-2.98039300
C	-1.10593900	0.50163900	-3.13007400
C	0.19249100	-3.07931300	-2.85504200
C	-1.05411700	-3.74653800	-3.48511900
H	-1.24274700	-3.42277000	-4.50806000
H	-0.89441300	-4.82642100	-3.50317000
H	-1.94793500	-3.54713100	-2.89235700
C	0.35648100	-3.66248400	-1.45214000
H	-0.34119400	-3.26187400	-0.72888900
H	0.16973100	-4.73540500	-1.53516700
H	1.36659300	-3.54692200	-1.08104100
C	1.46121000	-3.44392700	-3.65536600
H	2.30688300	-2.83041500	-3.34722100
H	1.70709800	-4.48558500	-3.43877500
H	1.34167000	-3.36379500	-4.73584800
C	-2.62548100	0.06578300	-3.19707000
H	-3.15854200	0.39725300	-2.31086700
H	-3.05878900	0.56510700	-4.06519300
H	-2.75025400	-1.00888100	-3.31147300
C	-1.15174600	2.00715200	-2.86401900
H	-1.67237000	2.47691700	-3.70046000
H	-1.73957600	2.22514400	-1.98240700
H	-0.17991000	2.47677200	-2.75568300

B	-0.07317300	-0.07412000	-0.49312400
C	-1.62480900	0.50346500	-0.02426300
C	-2.72103800	-0.39137500	-0.05172200
C	-1.99783900	1.80988200	0.38503700
C	-4.02318200	-0.08658800	0.35962200
C	-3.28576200	2.14034700	0.85327200
C	-4.30346700	1.18755900	0.85189500
C	1.17280100	1.12731800	-0.37611300
C	1.97924300	1.64466600	-1.41255600
C	1.54033000	1.62785100	0.90085900
C	2.96887600	2.62614300	-1.23766600
C	2.55602900	2.56910000	1.11957900
C	3.26204900	3.09796600	0.03883300
C	0.56913400	-1.29281700	0.57784600
C	1.89108700	-1.76134700	0.36961700
C	-0.00702000	-1.82969000	1.76455600
C	2.56965800	-2.66871400	1.19739100
C	0.61553600	-2.80602100	2.56701400
C	1.91493100	-3.22618900	2.29155900
Cl	1.89848700	1.00771800	-3.05200800
Cl	0.66709200	1.15381000	2.33834600
Cl	4.48982300	4.30199900	0.28199200
Cl	2.80257900	-1.28751700	-1.05209700
Cl	-1.51524200	-1.25589900	2.45536000
Cl	2.70730900	-4.40263000	3.29376400
Cl	-2.49724500	-2.04901000	-0.58560600
Cl	-5.89520400	1.58180400	1.42252800
Cl	-0.92389900	3.19627500	0.26956100
Cl	-5.29930300	-1.26909600	0.29371600
Cl	-3.65578400	3.74218400	1.42813400
Cl	3.87302600	3.25604600	-2.59081600
Cl	2.94074300	3.12685200	2.72287500
Cl	4.21071700	-3.15331700	0.86479900
Cl	-0.19180800	-3.49781100	3.94883700
N	-0.98767800	0.67438400	-5.72023500
C	-0.24622400	1.93691400	-6.01735800
H	-0.08641900	2.38844300	-5.04081300
C	-1.56009600	-0.19534400	-6.78949500
H	-1.82566600	-1.11095400	-6.25872000
C	1.16143500	1.72243000	-6.60988600
H	1.73606100	2.64733100	-6.50986100
H	1.70345000	0.94093400	-6.07343200
H	1.13755700	1.46155800	-7.66843300
C	-1.04402400	2.94831100	-6.84523900

H	-1.14727900	2.64123700	-7.88792400
H	-2.04065000	3.11034700	-6.43036900
H	-0.51466000	3.90462400	-6.84238200
C	-0.60793800	-0.60008000	-7.92723200
H	-0.39419900	0.23287000	-8.59972300
H	0.34186500	-0.98469300	-7.55037500
H	-1.07810600	-1.38615300	-8.52503900
C	-2.88255600	0.35276800	-7.35452400
H	-3.55651400	0.65057900	-6.54928600
H	-2.73868000	1.20718700	-8.01566700
H	-3.37602600	-0.43166500	-7.93584000

NHC5

C	-0.33996600	-0.55606200	-2.31303100
C	-0.50044500	-0.04762600	-4.67550000
C	0.05114600	-1.25112800	-4.46293400
H	0.43780800	-1.94192000	-5.18424300
N	0.08373300	-1.58139800	-3.07846300
C	-1.09097000	0.37996200	-3.33382700
C	0.44039700	-3.09291900	-2.90471900
C	-0.71844900	-3.85966200	-3.58618000
H	-0.88034300	-3.56082500	-4.62118800
H	-0.47541100	-4.92405900	-3.58101500
H	-1.65343800	-3.72482900	-3.04059700
C	0.56637000	-3.63510300	-1.48160200
H	-0.19851200	-3.27244100	-0.80773200
H	0.46268800	-4.72031400	-1.54990800
H	1.54295000	-3.43825700	-1.05813700
C	1.77487900	-3.37973400	-3.62605600
H	2.55365900	-2.69508300	-3.29230200
H	2.08628900	-4.39355100	-3.36605200
H	1.70889000	-3.33645500	-4.71325400
C	-2.56615200	-0.17370200	-3.48648100
H	-3.18290800	0.14778500	-2.65208800
H	-2.97207500	0.25378500	-4.40519000
H	-2.59954100	-1.25837700	-3.56186200
C	-1.26263500	1.88156200	-3.09746600
H	-1.80725200	2.29568000	-3.94770700
H	-1.87958600	2.06529200	-2.22883300
H	-0.33275200	2.42878600	-2.98341600
B	-0.16886100	-0.07007500	-0.63244500

C	-1.77979300	0.40778200	-0.25855400
C	-2.80942500	-0.56064300	-0.33004600
C	-2.26285800	1.69082100	0.10758300
C	-4.15032500	-0.34019300	0.00379900
C	-3.59350000	1.93784100	0.50137900
C	-4.54291100	0.91774800	0.45962800
C	0.98393200	1.22029200	-0.48464500
C	1.80232000	1.77716500	-1.49126200
C	1.24996200	1.76860200	0.79799900
C	2.70546500	2.83397400	-1.28934300
C	2.18281700	2.78529800	1.04617900
C	2.89972700	3.34773800	-0.01010500
C	0.49887500	-1.21793700	0.49745000
C	1.86030000	-1.59293200	0.37185800
C	-0.10326300	-1.77289200	1.66256700
C	2.55410400	-2.43366300	1.25556100
C	0.54068000	-2.68758600	2.51875000
C	1.88007000	-3.01779500	2.32379800
Cl	1.85826500	1.10415300	-3.11888800
Cl	0.34162900	1.25843300	2.20116000
Cl	4.02161000	4.64418000	0.26701100
Cl	2.81378300	-1.08114300	-1.00870300
Cl	-1.68272300	-1.29300000	2.25848500
Cl	2.69630500	-4.11612500	3.39319600
Cl	-2.44240900	-2.20799900	-0.81367000
Cl	-6.18691600	1.20904900	0.93591800
Cl	-1.28197500	3.14721200	0.02139900
Cl	-5.33784500	-1.60778400	-0.11272100
Cl	-4.10194000	3.51708800	1.03064900
Cl	3.62381700	3.50971500	-2.61049400
Cl	2.44745500	3.39572600	2.65452900
Cl	4.24180300	-2.80339500	1.02487700
Cl	-0.29213400	-3.41071700	3.86889800
N	-0.79708700	0.52861600	-5.89556800
C	-0.28072700	1.87319500	-6.19019600
H	-0.92512800	2.35616300	-6.92838500
H	-0.25011800	2.48789000	-5.29781800
H	0.73862000	1.81915600	-6.59803000
C	-0.73105000	-0.34400100	-7.06435400
H	-1.29906800	-1.25689000	-6.88056700
H	-1.17722000	0.17425900	-7.91526300
H	0.30148400	-0.61277300	-7.33713900

NHC6

C	-0.28983200	-0.50116000	-2.29534600
C	-0.47129400	0.08382100	-4.60506600
C	0.16667900	-1.07735200	-4.47675000
H	0.62076500	-1.69186100	-5.22967300
N	0.19620100	-1.46614800	-3.09580700
C	-1.07353400	0.45404300	-3.28468800
C	0.61024300	-2.96589700	-2.98026400
C	-0.49685200	-3.74386100	-3.73249100
H	-0.63357800	-3.41245000	-4.76124800
H	-0.21816500	-4.79910300	-3.75700800
H	-1.45393200	-3.65916200	-3.21599400
C	0.70795500	-3.56194600	-1.57666600
H	-0.09018900	-3.24892100	-0.91599100
H	0.63978500	-4.64615600	-1.68962400
H	1.66324900	-3.35261200	-1.11283700
C	1.97502200	-3.16556300	-3.67080100
H	2.71950000	-2.47827700	-3.27106900
H	2.31125600	-4.18295000	-3.46103000
H	1.94079000	-3.05937800	-4.75528000
C	-2.54464300	-0.09727100	-3.47118900
H	-3.16593100	0.17120800	-2.62376300
H	-2.95355300	0.38409900	-4.36173400
H	-2.57008400	-1.17604400	-3.61387900
C	-1.21329000	1.96981400	-3.06935600
H	-1.34297300	2.43692100	-4.04740400
H	-2.09710800	2.19745300	-2.48116600
H	-0.35948800	2.43234800	-2.59241400
B	-0.17060000	-0.06031700	-0.60208400
C	-1.80071600	0.36852200	-0.28024400
C	-2.79734700	-0.63100100	-0.38466200
C	-2.33207400	1.63819200	0.05997400
C	-4.15276900	-0.45319700	-0.08886700
C	-3.68467900	1.84754500	0.40008000
C	-4.59888400	0.79672700	0.34049700
C	0.94634200	1.25383200	-0.39749900
C	1.78601900	1.84894800	-1.36470300
C	1.15727800	1.77834000	0.90464100
C	2.67254300	2.90763400	-1.10589300
C	2.06840500	2.79941700	1.20857200
C	2.81856700	3.39061900	0.19189800
C	0.49405400	-1.21841300	0.51686500
C	1.86620300	-1.56143200	0.41841600

C	-0.12629300	-1.81495000	1.65177300
C	2.55323700	-2.41429700	1.29575700
C	0.51403100	-2.73917200	2.50043600
C	1.86361600	-3.04013700	2.32996800
Cl	1.88373600	1.23623600	-3.01355500
Cl	0.20089000	1.22829300	2.25936700
Cl	3.91967300	4.68763700	0.53928700
Cl	2.84848600	-0.98396600	-0.91616000
Cl	-1.72985900	-1.38186300	2.21773700
Cl	2.67330500	-4.15293900	3.38909500
Cl	-2.36813100	-2.25850100	-0.88910600
Cl	-6.26544300	1.03941000	0.76198700
Cl	-1.38366400	3.11513900	0.03091100
Cl	-5.29424200	-1.76004600	-0.22674900
Cl	-4.26102800	3.41605300	0.88971300
Cl	3.62815500	3.62358300	-2.37707600
Cl	2.26624100	3.37707200	2.83836500
Cl	4.25322200	-2.74536600	1.09969500
Cl	-0.33774700	-3.51219200	3.81018700
O	-0.75869600	0.81311800	-5.69413300
H	-0.43019700	0.37734500	-6.48928200

NHC7

C	-0.34048100	-0.45356100	-2.29444100
C	-0.59028800	0.14015700	-4.63069100
C	0.02541600	-1.03314700	-4.47294900
H	0.43541800	-1.67208600	-5.23015500
N	0.10595400	-1.42999000	-3.10475100
C	-1.14090300	0.50973300	-3.26813600
C	0.52641400	-2.93309300	-3.01268900
C	-0.60787400	-3.70873400	-3.72439000
H	-0.79961000	-3.35925300	-4.73852700
H	-0.31793500	-4.75960500	-3.78483000
H	-1.53989300	-3.64765100	-3.16113900
C	0.69245000	-3.53956900	-1.61988900
H	-0.07254500	-3.23622700	-0.91748500
H	0.62274400	-4.62308400	-1.73906700
H	1.66897100	-3.33007600	-1.20205400
C	1.86286900	-3.12217700	-3.76143500
H	2.61613100	-2.42396200	-3.39829100
H	2.21971300	-4.13405200	-3.55959600

H	1.78114000	-3.02447700	-4.84398600
C	-2.62378600	-0.03678700	-3.34236400
H	-3.19295100	0.27534500	-2.47381900
H	-3.09963600	0.38579000	-4.22627400
H	-2.65852500	-1.12111800	-3.42895000
C	-1.19275600	2.02234000	-2.97388700
H	-0.66305500	2.58818600	-3.73743900
H	-2.22430200	2.37690100	-2.94472300
H	-0.74672800	2.27512700	-2.02336000
B	-0.18983600	-0.03752600	-0.58342400
C	-1.82195500	0.35702800	-0.21357800
C	-2.79934700	-0.66415600	-0.30664000
C	-2.37635900	1.60948100	0.15419400
C	-4.15349200	-0.51941000	0.00905500
C	-3.73309100	1.78932400	0.49848700
C	-4.62506200	0.72041600	0.44074200
C	0.91768900	1.28361700	-0.37575000
C	1.72767900	1.90374300	-1.35331200
C	1.15521600	1.78684200	0.92995600
C	2.61283800	2.96383700	-1.09663000
C	2.06361700	2.81188800	1.22948500
C	2.78563000	3.42538800	0.20582300
C	0.51878600	-1.20916000	0.49281800
C	1.88991900	-1.53747800	0.34396000
C	-0.05799800	-1.82712400	1.63953600
C	2.61487800	-2.39283400	1.18747100
C	0.62097300	-2.75240200	2.45650100
C	1.96746300	-3.03608400	2.23810600
Cl	1.77954800	1.32799500	-3.01501700
Cl	0.24107000	1.20034300	2.29781500
Cl	3.88488100	4.72483500	0.54959600
Cl	2.81895100	-0.93557400	-1.01705900
Cl	-1.65029800	-1.42564900	2.25908200
Cl	2.82451400	-4.15000100	3.25792200
Cl	-2.34538700	-2.27712600	-0.83239700
Cl	-6.29407100	0.92580600	0.87216100
Cl	-1.45211200	3.10256100	0.18748500
Cl	-5.26534500	-1.85301100	-0.11267800
Cl	-4.34163100	3.34245700	0.99946200
Cl	3.53299900	3.70837200	-2.37716100
Cl	2.29368600	3.36467400	2.86385400
Cl	4.30983300	-2.70539700	0.92839800
Cl	-0.17738400	-3.54825800	3.78598500
C	-0.77686600	0.83397200	-5.91384300

C	-1.78970700	1.78211200	-6.13580200
C	0.09926100	0.55446400	-6.98051800
C	-1.93672200	2.39761000	-7.37601700
H	-2.47509700	2.04864800	-5.34419300
C	-0.04826800	1.17001300	-8.21564500
H	0.92535300	-0.13057700	-6.83043800
C	-1.07248400	2.09345800	-8.42270000
H	-2.73069300	3.12149200	-7.51915200
H	0.64603200	0.93877700	-9.01535000
H	-1.18585200	2.57829600	-9.38523200

S 1.2.5 **B3Cl-**NHC Complexes

NHC1

C	-0.28054900	-0.48879700	-2.31428000
C	-0.46291500	0.10587400	-4.62932500
H	-0.66067400	0.63247900	-5.55078000
C	0.15844600	-1.05169000	-4.49579300
H	0.61299100	-1.67014800	-5.24551600
N	0.19398100	-1.45829100	-3.11635000
C	-1.03869400	0.48726400	-3.30382200
C	0.59858500	-2.95658400	-3.00687900
C	-0.50208800	-3.72386300	-3.77910300
H	-0.62170000	-3.38883500	-4.80927100
H	-0.23082200	-4.78108900	-3.80415300
H	-1.46539600	-3.63268700	-3.27548300
C	0.67510900	-3.55852100	-1.60560700
H	-0.14131200	-3.25653500	-0.96224900
H	0.62281000	-4.64322400	-1.72510100
H	1.61594700	-3.33721700	-1.11885100
C	1.97106800	-3.15333200	-3.68286400
H	2.71233800	-2.47634500	-3.26030200
H	2.29881500	-4.17634200	-3.48675700
H	1.95167900	-3.02668400	-4.76557700
C	-2.53445700	-0.01059800	-3.44773200
H	-3.12636600	0.29684600	-2.59167000
H	-2.95521100	0.46237700	-4.33731300
H	-2.60057300	-1.09021700	-3.56933500
C	-1.13400200	2.00446300	-3.08186400
H	-1.52027700	2.44564200	-4.00542100

H	-1.83759200	2.24919600	-2.29533700
H	-0.18734100	2.48255300	-2.86267800
B	-0.17596100	-0.08487300	-0.61297400
C	-1.79392400	0.32515400	-0.27736000
C	-2.80827600	-0.65782900	-0.37962900
C	-2.35325600	1.57796400	0.08578700
C	-4.15681000	-0.49870600	-0.08789400
C	-3.69550900	1.79132500	0.41022300
C	-4.59099000	0.74360700	0.33488900
C	0.92166800	1.21695800	-0.39773100
C	1.80583200	1.81244500	-1.32492400
C	1.12254900	1.76063400	0.90028000
C	2.69891700	2.84915600	-1.05849100
C	2.01536300	2.77582700	1.22733800
C	2.79230400	3.33343300	0.23018600
C	0.48931500	-1.23231500	0.48847300
C	1.86636100	-1.57297300	0.42759800
C	-0.10349100	-1.82463100	1.63996900
C	2.56645900	-2.38780100	1.31281600
C	0.54264900	-2.68424400	2.53109400
C	1.88194000	-2.96467600	2.36274900
H	3.61997300	-2.57322700	1.16351700
H	-0.00301100	-3.09154400	3.36916500
H	-4.83992100	-1.33002100	-0.18058300
H	-4.02542300	2.77731200	0.70219200
H	2.08038400	3.12945700	2.24580000
H	3.32646500	3.24087600	-1.84525200
Cl	1.98917900	1.24648900	-3.00208500
Cl	0.18876000	1.23282500	2.30064100
Cl	3.91079600	4.63187000	0.60442300
Cl	2.92072400	-1.03225500	-0.89087100
Cl	-1.74231300	-1.49554200	2.23115000
Cl	2.71391800	-4.02317700	3.48632700
Cl	-2.44482900	-2.30883400	-0.91606700
Cl	-6.27777000	0.99488800	0.74024900
Cl	-1.46390800	3.11300500	0.11698800

NHC2

C	-0.30951400	-0.38750900	-2.46921200
C	-0.46011600	0.20448800	-4.77857900
C	0.15249000	-0.96045900	-4.64233400

H	0.60447700	-1.57423400	-5.39629000
N	0.17021100	-1.35912700	-3.26754700
C	-1.06971600	0.59244200	-3.45888100
C	0.56877600	-2.86393000	-3.15679100
C	-0.53508600	-3.62272900	-3.93185600
H	-0.64843500	-3.28857300	-4.96319400
H	-0.27112100	-4.68179100	-3.95520500
H	-1.49939100	-3.52456200	-3.43160300
C	0.63794600	-3.46292600	-1.75435000
H	-0.17878200	-3.15548800	-1.11408900
H	0.57957200	-4.54737900	-1.87314500
H	1.57870100	-3.24638300	-1.26523900
C	1.94154600	-3.06683500	-3.82927900
H	2.68463700	-2.39127200	-3.40777700
H	2.26482500	-4.09024800	-3.62822100
H	1.92531200	-2.94578300	-4.91276000
C	-2.55527000	0.07308400	-3.61311600
H	-3.14828400	0.35264100	-2.74922200
H	-2.98026700	0.56079100	-4.49229300
H	-2.60405400	-1.00472700	-3.75698300
C	-1.17944700	2.10092300	-3.20817300
H	-1.52391200	2.56704500	-4.13396800
H	-1.92164700	2.31396500	-2.44865100
H	-0.24775400	2.57550600	-2.92774000
B	-0.20838700	0.01797300	-0.76471100
C	-1.82537700	0.42688200	-0.42704600
C	-2.84048500	-0.55523700	-0.52924400
C	-2.38236400	1.67904900	-0.05724500
C	-4.18791600	-0.39628300	-0.23240100
C	-3.72305900	1.89134600	0.27394900
C	-4.61959300	0.84448800	0.19775400
C	0.89017800	1.31799400	-0.54874900
C	1.77215700	1.91528600	-1.47655500
C	1.09432400	1.85783000	0.75034100
C	2.66745600	2.94986300	-1.20978700
C	1.98969600	2.87060900	1.07769200
C	2.76523900	3.42986500	0.08024600
C	0.45900400	-1.13236500	0.33132300
C	1.83627700	-1.47152600	0.26717400
C	-0.13136500	-1.72652700	1.48317800
C	2.53917200	-2.28550600	1.15086200
C	0.51785400	-2.58572600	2.37246000
C	1.85740500	-2.86380500	2.20191000
Cl	1.94782600	1.35538500	-3.15626200

Cl	0.16229300	1.32812600	2.15089600
Cl	3.88650000	4.72504200	0.45551800
Cl	2.88661200	-0.93074800	-1.05443900
Cl	-1.76966600	-1.40101500	2.07663400
Cl	2.69286300	-3.92114600	3.32345300
Cl	-2.47951500	-2.20495300	-1.07149100
Cl	-6.30409800	1.09483800	0.61115800
Cl	-1.49266300	3.21315100	-0.02789300
Br	-0.74649600	1.07728300	-6.42087600
H	2.05777800	3.22138900	2.09694900
H	3.29260000	3.34368200	-1.99742600
H	-0.02573500	-2.99449500	3.21116900
H	3.59268700	-2.46936900	0.99957700
H	-4.87198100	-1.22673200	-0.32591800
H	-4.05140600	2.87640900	0.57079600

NHC3

C	-0.31277000	-0.40189200	-2.45436700
C	-0.49444800	0.20057700	-4.73629800
C	0.12576100	-0.96207600	-4.64736100
H	0.55759600	-1.56330600	-5.42222200
N	0.16291000	-1.36178100	-3.26847000
C	-1.08040600	0.58404600	-3.42342800
C	0.57381800	-2.86094600	-3.16367100
C	-0.52925000	-3.63085300	-3.92937500
H	-0.65269500	-3.30056100	-4.96050500
H	-0.25684400	-4.68776900	-3.95115600
H	-1.49062900	-3.53910900	-3.42213000
C	0.65757300	-3.45837500	-1.76140200
H	-0.15763300	-3.15644100	-1.11620400
H	0.60704900	-4.54344400	-1.87775100
H	1.59977000	-3.23343200	-1.27929900
C	1.94246300	-3.05012600	-3.84743200
H	2.68518100	-2.37586700	-3.42303700
H	2.27169600	-4.07451100	-3.66156800
H	1.91722200	-2.91433800	-4.92893900
C	-2.56982100	0.07492500	-3.59900600
H	-3.17649100	0.37398800	-2.75130500
H	-2.96969000	0.55481100	-4.49489700
H	-2.62573600	-1.00463600	-3.72664000
C	-1.17541300	2.10253700	-3.20076100

H	-1.32514500	2.57315900	-4.17529700
H	-2.03465800	2.34977300	-2.58592000
H	-0.29618200	2.54315100	-2.75022100
B	-0.20311400	0.00559600	-0.75706500
C	-1.82112400	0.41835000	-0.42968600
C	-2.83545000	-0.56521500	-0.52794300
C	-2.38033200	1.67549200	-0.08248700
C	-4.18502100	-0.40234900	-0.24334200
C	-3.72437900	1.89288700	0.23256200
C	-4.62025100	0.84495400	0.16415900
C	0.89471900	1.30894400	-0.54796700
C	1.77539300	1.90320400	-1.47869600
C	1.09910800	1.85410200	0.74868600
C	2.67497200	2.93496900	-1.21575900
C	1.99835300	2.86453100	1.07257800
C	2.77655800	3.41698800	0.07329800
C	0.46370400	-1.13699000	0.34378700
C	1.84070700	-1.47714300	0.28046900
C	-0.12751600	-1.72606500	1.49746900
C	2.54219900	-2.29012100	1.16607300
C	0.52049600	-2.58303900	2.38964800
C	1.85949300	-2.86401200	2.21907800
Cl	1.93903900	1.34565600	-3.16153500
Cl	0.16048000	1.33549000	2.14859600
Cl	3.90383100	4.70808000	0.44436500
Cl	2.89246100	-0.93769600	-1.04132200
Cl	-1.76577300	-1.39503800	2.08789800
Cl	2.69361000	-3.91940100	3.34359700
Cl	-2.47118200	-2.22056200	-1.05151600
Cl	-6.30832900	1.10141500	0.55920600
Cl	-1.48777200	3.20736900	-0.05481200
F	-0.76280600	0.87456500	-5.85066500
H	3.29950100	3.32575100	-2.00539800
H	2.06735600	3.21905800	2.09049800
H	-0.02341600	-2.98820700	3.22991400
H	3.59544000	-2.47611900	1.01547700
H	-4.86849100	-1.23397400	-0.33070900
H	-4.05501900	2.88191400	0.51331700

NHC4

C	-0.36773500	-0.51735900	-2.19021700

C	-0.64584700	0.05952000	-4.53671100
C	-0.17630000	-1.18340100	-4.37665400
H	0.10420400	-1.88625600	-5.13603000
N	-0.07685600	-1.55072700	-3.00442700
C	-1.08290000	0.51053200	-3.13591600
C	0.18061900	-3.08195100	-2.87967500
C	-1.05998100	-3.75572100	-3.51455000
H	-1.24379500	-3.43846900	-4.54053300
H	-0.89744100	-4.83537300	-3.52542400
H	-1.95679500	-3.55426700	-2.92697900
C	0.33760600	-3.65681200	-1.47373500
H	-0.37835000	-3.26492500	-0.76346700
H	0.17311100	-4.73386600	-1.55456700
H	1.33890500	-3.51676800	-1.08869400
C	1.45550200	-3.44011200	-3.67264500
H	2.29586000	-2.82538200	-3.35233200
H	1.70170300	-4.48309900	-3.46227300
H	1.34396200	-3.35040200	-4.75344000
C	-2.61271200	0.10943800	-3.18338000
H	-3.12652900	0.45582900	-2.29162300
H	-3.04465700	0.61339700	-4.04975200
H	-2.76031500	-0.96350400	-3.28944600
C	-1.08626300	2.01390700	-2.85589300
H	-1.62869500	2.50327700	-3.66735600
H	-1.63107500	2.23672100	-1.94858800
H	-0.09984200	2.45866100	-2.78128000
B	-0.08366200	-0.10820200	-0.50804800
C	-1.62431000	0.45217600	-0.02923100
C	-2.73455700	-0.42723700	-0.04113900
C	-2.02741500	1.74806300	0.38939800
C	-4.03121500	-0.14108600	0.36761000
C	-3.30782800	2.08591500	0.83459100
C	-4.30430700	1.13113200	0.83255700
C	1.14176200	1.08797700	-0.38961100
C	1.99047900	1.59781400	-1.39595000
C	1.50529900	1.61557700	0.87943400
C	2.99022600	2.55392400	-1.22320300
C	2.50863200	2.54993200	1.11468400
C	3.23836900	3.03430800	0.04619600
C	0.56549700	-1.30462800	0.55293900
C	1.89656300	-1.76855000	0.38195900
C	0.02241300	-1.83357500	1.75822500
C	2.59551000	-2.63362700	1.21921200
C	0.66337000	-2.73990200	2.60590000

C	1.95442700	-3.13795100	2.33203400
Cl	1.97981400	0.99810700	-3.07112600
Cl	0.66245200	1.17361000	2.36531600
Cl	4.49367000	4.23293700	0.30485800
Cl	2.87572500	-1.34255300	-1.03338100
Cl	-1.52746000	-1.35881900	2.47784600
Cl	2.78291900	-4.25595800	3.40010700
Cl	-2.58086200	-2.10684100	-0.58747900
Cl	-5.91735200	1.53869400	1.38696300
Cl	-0.99994500	3.19584700	0.33630100
N	-0.99325400	0.69217900	-5.72632800
C	-0.23521900	1.94327200	-6.02409800
H	-0.06485300	2.39050600	-5.04733400
C	-1.58377700	-0.16527400	-6.79441800
H	-1.85774600	-1.07924000	-6.26517900
C	1.16679200	1.71097800	-6.62388300
H	1.75473700	2.62797600	-6.52583300
H	1.69944400	0.92102200	-6.09054800
H	1.13474600	1.45226500	-7.68286200
C	-1.02248900	2.96780900	-6.84609300
H	-1.13681500	2.66364700	-7.88856300
H	-2.01398700	3.14347000	-6.42453100
H	-0.47935400	3.91649900	-6.84541300
C	-0.64485500	-0.57865500	-7.94037600
H	-0.42519500	0.25370100	-8.61191200
H	0.30258200	-0.97605300	-7.57095900
H	-1.12863500	-1.35711000	-8.53745100
C	-2.90292700	0.40165600	-7.34897200
H	-3.56728900	0.70443600	-6.53765400
H	-2.75291700	1.25717200	-8.00750200
H	-3.41027400	-0.37398600	-7.93033600
H	-4.79662200	-0.90236000	0.33583700
H	-3.51330800	3.09534700	1.15893000
H	2.69518900	2.89961300	2.11940900
H	3.57858600	2.88397400	-2.06655700
H	0.15638500	-3.09086000	3.49232600
H	3.61186600	-2.91395500	0.98469600

NHC5

C	-0.33003200	-0.34544500	-2.49224000
C	-0.54722800	0.27826200	-4.83440100

C	0.07888000	-0.90169400	-4.67890800
H	0.49747100	-1.53769800	-5.43050700
N	0.12933000	-1.30030100	-3.31244800
C	-1.08574200	0.65846800	-3.45983400
C	0.56693500	-2.79276400	-3.21434100
C	-0.52638900	-3.59028100	-3.96609700
H	-0.66465900	-3.26701500	-4.99682700
H	-0.23362400	-4.64201600	-3.98233500
H	-1.48549600	-3.51333800	-3.45257100
C	0.68589900	-3.39730200	-1.81697000
H	-0.12082100	-3.11445900	-1.15389800
H	0.65285700	-4.48256500	-1.93826300
H	1.63363200	-3.15883300	-1.35302700
C	1.93390800	-2.95743300	-3.91081600
H	2.66346500	-2.25999800	-3.50081100
H	2.29006900	-3.97135500	-3.71656100
H	1.89565300	-2.83237100	-4.99289700
C	-2.58404700	0.18808200	-3.57155400
H	-3.16469900	0.53502400	-2.72316300
H	-2.99683500	0.63147700	-4.48030700
H	-2.67132500	-0.89470400	-3.65052700
C	-1.09141000	2.15475400	-3.10267400
H	-2.03863800	2.60973700	-3.39816700
H	-0.99295600	2.30675400	-2.03904500
H	-0.28204200	2.70004300	-3.57817100
B	-0.22773400	0.02762200	-0.77504400
C	-1.86242000	0.39402200	-0.42350400
C	-2.85174200	-0.61253400	-0.56197300
C	-2.46317300	1.61805800	-0.02860700
C	-4.20977700	-0.49223100	-0.29850400
C	-3.81906300	1.79404200	0.26167800
C	-4.68751200	0.73007300	0.13441200
C	0.85192000	1.34178400	-0.53169000
C	1.72550100	1.96079400	-1.45496100
C	1.04856500	1.87351500	0.77106600
C	2.59858200	3.01151400	-1.18060100
C	1.92050400	2.90498200	1.10615700
C	2.68226300	3.48772600	0.11222200
C	0.45439200	-1.12640500	0.31191000
C	1.83665400	-1.44619400	0.25220800
C	-0.13317400	-1.74369000	1.45334400
C	2.54434600	-2.26658800	1.12634300
C	0.52081700	-2.61052900	2.33169200
C	1.86384700	-2.87134600	2.16282500

Cl	1.92820800	1.40182500	-3.13423800
Cl	0.14515300	1.29788600	2.17289800
Cl	3.77448400	4.80685900	0.49544900
Cl	2.88935800	-0.87021000	-1.05222700
Cl	-1.77535000	-1.44053700	2.05145600
Cl	2.70562700	-3.94004600	3.27030800
Cl	-2.44378300	-2.24987600	-1.10583000
Cl	-6.39166100	0.93316000	0.49483100
Cl	-1.61289400	3.17267300	0.11199800
N	-0.89492200	0.84132400	-6.03948800
C	-0.49469800	0.11005400	-7.23586900
H	-0.83753400	-0.92485600	-7.17224000
H	-0.96143100	0.56965300	-8.10715000
H	0.59504900	0.10936200	-7.38826100
C	-0.97994700	2.29038600	-6.22764100
H	-1.57849100	2.75330500	-5.45038600
H	0.00829200	2.77019000	-6.24421400
H	-1.47043200	2.48174900	-7.18297400
H	-0.02216500	-3.03832400	3.16121900
H	3.60071400	-2.43540500	0.97765400
H	1.98300700	3.24821900	2.12830700
H	3.22019500	3.42022800	-1.96341600
H	-4.86827000	-1.33925800	-0.42176000
H	-4.17835800	2.76381500	0.57232200

NHC6

C	-0.31923300	-0.40716900	-2.46305100
C	-0.49680400	0.20858100	-4.76528900
C	0.12625700	-0.96171300	-4.65390600
H	0.57220800	-1.57309300	-5.41443700
N	0.15750000	-1.36383500	-3.27608300
C	-1.08423200	0.57346400	-3.43716100
C	0.56201600	-2.86138900	-3.16704000
C	-0.54413500	-3.63291100	-3.92706100
H	-0.66731800	-3.30508000	-4.95884200
H	-0.27603800	-4.69112700	-3.94343000
H	-1.50443200	-3.53403400	-3.41911700
C	0.64625400	-3.45554200	-1.76298300
H	-0.16605400	-3.14723200	-1.11738200
H	0.59068800	-4.54085700	-1.87517300
H	1.59048300	-3.23319400	-1.28351800

C	1.92971500	-3.06278400	-3.85064600
H	2.67321900	-2.38122700	-3.43939900
H	2.25979200	-4.08390500	-3.64870700
H	1.90211500	-2.94501400	-4.93434100
C	-2.56566100	0.04788200	-3.61324800
H	-3.17398900	0.32678800	-2.75981900
H	-2.97336300	0.53467000	-4.50164200
H	-2.60855800	-1.03100300	-3.75361400
C	-1.19529000	2.08818700	-3.19994500
H	-1.33445900	2.56975000	-4.16985600
H	-2.06409300	2.32112400	-2.59246200
H	-0.32604800	2.52977200	-2.73087500
B	-0.20851400	0.00369300	-0.76822700
C	-1.82579800	0.41664700	-0.43279600
C	-2.84105400	-0.56665300	-0.52601700
C	-2.38406000	1.67418400	-0.08540200
C	-4.19002100	-0.40234600	-0.23867100
C	-3.72725400	1.89314200	0.23244500
C	-4.62370400	0.84581400	0.16722100
C	0.89003800	1.30906200	-0.56014700
C	1.76769300	1.90371600	-1.49368800
C	1.09822800	1.85559900	0.73527900
C	2.66726500	2.93636600	-1.23384800
C	1.99778500	2.86675400	1.05647900
C	2.77249500	3.41896400	0.05455500
C	0.46341300	-1.13529500	0.33604300
C	1.84065500	-1.47407500	0.26962200
C	-0.12312400	-1.72258100	1.49296700
C	2.54597500	-2.28422100	1.15489100
C	0.52844200	-2.57693100	2.38522600
C	1.86713900	-2.85658800	2.21111200
Cl	1.92610200	1.34546100	-3.17654900
Cl	0.16411700	1.33815100	2.13918300
Cl	3.90065400	4.71144300	0.42162000
Cl	2.88817200	-0.93661000	-1.05660600
Cl	-1.76004100	-1.39221200	2.08836100
Cl	2.70623400	-3.90898600	3.33565700
Cl	-2.48051900	-2.22491900	-1.04335100
Cl	-6.31165200	1.10397900	0.56514700
Cl	-1.49151400	3.20647500	-0.06087500
O	-0.77959500	0.95429500	-5.84599900
H	-0.45886600	0.52122500	-6.64558600
H	2.06946800	3.22182400	2.07400600
H	3.28890700	3.32733800	-2.02564500

H	-0.01249400	-2.98084100	3.22800200
H	3.59896100	-2.46928200	1.00146700
H	-4.87398600	-1.23387800	-0.32270800
H	-4.05654300	2.88282300	0.51237400

NHC7

C	-0.31273100	-0.33104200	-2.48467500
C	-0.47587800	0.31668000	-4.81125900
C	0.14259900	-0.84997800	-4.66803600
H	0.61099600	-1.44645600	-5.42755800
N	0.17416800	-1.27985000	-3.30290400
C	-1.07038600	0.65616500	-3.45836000
C	0.60205100	-2.77498300	-3.22148300
C	-0.48339700	-3.54481300	-4.01226200
H	-0.59855300	-3.19544500	-5.03806200
H	-0.19836100	-4.59799000	-4.05146200
H	-1.45144600	-3.47379700	-3.51454000
C	0.68493400	-3.40364200	-1.83239600
H	-0.13563500	-3.12569200	-1.18382600
H	0.64711100	-4.48641000	-1.97324100
H	1.62248100	-3.17982000	-1.34046500
C	1.97961500	-2.93837300	-3.89642400
H	2.70945800	-2.25873300	-3.45855400
H	2.32143800	-3.96001900	-3.71792800
H	1.96198600	-2.79145100	-4.97638700
C	-2.55006400	0.11868200	-3.62682900
H	-3.15385700	0.38112700	-2.76409600
H	-2.97798700	0.60666500	-4.50447800
H	-2.58435800	-0.95877300	-3.77861400
C	-1.22139700	2.15071700	-3.15713500
H	-1.70289500	2.61791100	-4.01860300
H	-1.87296200	2.31293600	-2.30882300
H	-0.28520800	2.66580300	-2.97598500
B	-0.22547400	0.03091500	-0.77055700
C	-1.85353100	0.39701300	-0.42189700
C	-2.84858800	-0.60165000	-0.55869700
C	-2.43870200	1.62349500	-0.01063100
C	-4.20042200	-0.47934900	-0.26381800
C	-3.78446300	1.79789900	0.32174400
C	-4.65945800	0.73696700	0.20498300
C	0.84598000	1.34750700	-0.51454400

C	1.71995700	1.98465000	-1.42343400
C	1.03536400	1.85995300	0.79792500
C	2.59095700	3.03237500	-1.12876100
C	1.90606300	2.88500200	1.15299400
C	2.67166900	3.48532600	0.17211800
C	0.46044300	-1.13237700	0.30314400
C	1.84426400	-1.44350300	0.23793300
C	-0.12311800	-1.76720500	1.43661700
C	2.55872800	-2.26639100	1.10405400
C	0.53793800	-2.63706300	2.30664000
C	1.88326400	-2.88506900	2.13582100
Cl	1.92465400	1.45988800	-3.11244600
Cl	0.11693200	1.27167100	2.18455900
Cl	3.76208900	4.79699500	0.58225100
Cl	2.88966900	-0.85072100	-1.06486300
Cl	-1.76989100	-1.48774400	2.03157200
Cl	2.73359600	-3.95616500	3.23366800
Cl	-2.45317400	-2.22905100	-1.14176700
Cl	-6.35116300	0.93978700	0.61748400
Cl	-1.58351100	3.17674800	0.07331100
C	-0.71157500	1.00278600	-6.09698400
C	-0.28083200	2.32137800	-6.31004200
C	-1.34003300	0.32491700	-7.15271400
C	-0.47107700	2.93722900	-7.54308300
H	0.22821300	2.85384000	-5.51693000
C	-1.53441800	0.94569600	-8.38373000
H	-1.68946600	-0.68955100	-6.99796400
C	-1.10049800	2.25383300	-8.58205100
H	-0.12226800	3.95247100	-7.69376300
H	-2.02701800	0.40751200	-9.18558600
H	-1.25076700	2.73839700	-9.53996300
H	-4.86660600	-1.32038400	-0.38698000
H	-4.13350600	2.76560200	0.65025900
H	1.96336200	3.21206400	2.18073900
H	3.21318500	3.45585700	-1.90320900
H	-0.00179000	-3.07781600	3.13151600
H	3.61616900	-2.42635000	0.95306800

S 1.3 Optimized TSs for CH_4 Activaiton

S 1.3.1 **B5F**-NHC TSs

NHC1

C	-3.77231400	0.83755700	0.98888100
C	-5.54843800	2.30885300	1.54908500
H	-6.12290200	3.16128500	1.87988800
C	-6.03701400	1.16448700	1.08937200
H	-7.05516600	0.84243600	0.95015400
N	-4.93449400	0.28552100	0.75592300
C	-4.04142500	2.22646600	1.53259300
C	-5.19356800	-1.09358800	0.21677500
C	-6.02121000	-1.86446500	1.25673000
H	-6.99224000	-1.40286300	1.44022100
H	-6.20113300	-2.87783200	0.89597600
H	-5.48635800	-1.93110700	2.20553100
C	-3.86723300	-1.81041800	-0.02395100
H	-3.29122300	-1.90455300	0.89620800
H	-4.07676100	-2.81282200	-0.39917700
H	-3.25627200	-1.29444900	-0.76300300
C	-5.96175700	-0.95409500	-1.10608300
H	-5.38308100	-0.38075100	-1.83186300
H	-6.14458700	-1.94440700	-1.52482600
H	-6.92918100	-0.46734200	-0.97425100
C	-3.44321900	2.35182500	2.95285200
H	-2.35979900	2.23702400	2.92154100
H	-3.67274000	3.33687200	3.36303000
H	-3.85231500	1.59706300	3.62596600
C	-3.42042500	3.28805700	0.59499500
H	-3.65525500	4.28746100	0.96557800
H	-2.33649500	3.18249900	0.55908800
H	-3.81195400	3.20127200	-0.41968300
C	-1.01608800	0.26078700	0.39654500
H	-2.29232700	0.43875300	0.67642100
H	-1.12581400	0.44455900	-0.66011400
H	-0.64177800	1.05076400	1.02686700
H	-0.97369100	-0.75487500	0.75507100
B	1.05216400	-0.07294500	-0.12188300
C	1.77356600	0.11539700	1.31571700
C	1.37561700	-0.60139900	2.44739000
C	2.85974200	0.96437700	1.53546500
C	1.94811900	-0.45816100	3.70028100
C	3.46920400	1.13217200	2.77360000
C	3.01078600	0.41764500	3.86709800
C	1.30527000	1.09669700	-1.21374900
C	1.00894400	2.43751000	-0.95613200

C	1.86149400	0.87250800	-2.47456700
C	1.18115400	3.46302100	-1.87039000
C	2.06095700	1.87332600	-3.41894600
C	1.71768700	3.18012900	-3.11787100
C	1.01255700	-1.58734700	-0.69909600
C	1.89383900	-2.59066600	-0.29150800
C	0.11058000	-1.99297800	-1.68520300
C	1.85512300	-3.89424000	-0.77302100
C	0.02986400	-3.28234200	-2.18428800
C	0.91539000	-4.24650700	-1.72665400
F	-0.75426700	-1.10275600	-2.22349200
F	-0.88046300	-3.60054700	-3.11547400
F	0.86078100	-5.49412400	-2.19940100
F	2.72528200	-4.80889000	-0.32947000
F	2.86561500	-2.33669800	0.60511700
F	3.39989900	1.67418600	0.52661700
F	4.50196200	1.97165900	2.91449800
F	3.58299300	0.56622600	5.06430600
F	1.50130400	-1.17007400	4.74348300
F	0.38084000	-1.51215800	2.35762900
F	0.52638100	2.80568800	0.25255300
F	0.85392200	4.72367100	-1.55536800
F	1.89992100	4.15433000	-4.01244000
F	2.59075900	1.58448000	-4.61337000
F	2.25897500	-0.35862100	-2.84809100

NHC2

C	-3.23210100	0.32590200	-0.46457600
C	-5.40446000	-0.57710700	-0.24762100
C	-5.46800800	0.75162100	-0.18244600
H	-6.31689800	1.40187200	-0.05576900
N	-4.12907800	1.27141800	-0.31699600
C	-3.96295100	-1.00436800	-0.42832000
C	-3.88317800	2.75792300	-0.29139600
C	-4.67247200	3.38871400	-1.45155500
H	-5.74905600	3.23057900	-1.35860000
H	-4.49712600	4.46630100	-1.46403700
H	-4.34493000	2.97852700	-2.40957200
C	-2.38988500	3.03674700	-0.46668100
H	-2.01521300	2.63260600	-1.40801900
H	-2.24069800	4.11853900	-0.47639100

H	-1.79793900	2.62382600	0.35031200
C	-4.36272700	3.29752100	1.06681800
H	-3.81950300	2.82118000	1.88585600
H	-4.17678000	4.37223800	1.11581400
H	-5.43225500	3.13980800	1.22285600
C	-3.73903500	-1.75642900	-1.76069300
H	-2.68122400	-1.99115800	-1.88559500
H	-4.30474300	-2.69062900	-1.75484800
H	-4.06733100	-1.16081800	-2.61507700
C	-3.45817600	-1.84736000	0.76796400
H	-4.03619900	-2.77178700	0.83113400
H	-2.40637700	-2.10433400	0.63862500
H	-3.57356200	-1.30794700	1.71059300
C	-0.36632200	0.12425600	-0.35970000
H	-1.66581800	0.29642300	-0.45455400
H	-0.37900600	0.32252300	0.70075600
H	-0.35340400	-0.89646700	-0.70716100
H	-0.09765000	0.91038600	-1.04831300
B	1.69533400	-0.07814500	0.02347100
C	2.18845700	-0.87326400	-1.29775800
C	1.93582600	-0.39413300	-2.58716300
C	2.90817100	-2.06974100	-1.26365800
C	2.31624000	-1.04802600	-3.74854600
C	3.31368300	-2.75634000	-2.40428300
C	3.01214500	-2.24641100	-3.65698600
C	1.71514500	-0.91242000	1.41558500
C	0.96965800	-2.07875000	1.60725100
C	2.48372800	-0.54040500	2.52102300
C	0.93368400	-2.79575300	2.79255600
C	2.48616000	-1.23580700	3.72669800
C	1.70081800	-2.36881700	3.86830400
C	2.17578200	1.46761800	0.13796700
C	3.29301600	1.97296000	-0.53109500
C	1.52218000	2.40546900	0.94079700
C	3.70281000	3.30021500	-0.45386100
C	1.88713700	3.73940800	1.03749500
C	2.99137500	4.19474400	0.33055200
F	0.46023800	2.03619900	1.70161100
F	1.19042400	4.58539300	1.81072200
F	3.36572900	5.47484000	0.41205700
F	4.78142500	3.71915000	-1.12675400
F	4.06569300	1.17205100	-1.28914600
F	3.27615200	-2.62731500	-0.09386400
F	3.99796000	-3.90253800	-2.29993000

F	3.39141700	-2.89323800	-4.76278400
F	2.02980800	-0.53266300	-4.95193400
F	1.29575600	0.78600300	-2.75948000
F	0.22597100	-2.58784000	0.59418400
F	0.17621600	-3.89592000	2.90495600
F	1.68591400	-3.04549300	5.02009500
F	3.24381900	-0.82032800	4.74915500
F	3.30025500	0.52995600	2.46981800
Br	-6.87380600	-1.75255100	-0.12850100

NHC3

C	3.70216100	-0.55037600	0.66368000
C	5.63107600	-1.88175200	0.55121100
C	5.99060100	-0.61010700	0.40421300
H	6.96100000	-0.16871500	0.25711800
N	4.77839500	0.17565400	0.47712000
C	4.14594200	-2.00227300	0.72553400
C	4.84336200	1.67551600	0.35320900
C	5.72239100	2.20753500	1.49821500
H	6.74324700	1.82215200	1.45289400
H	5.77725900	3.29625800	1.43696200
H	5.29616100	1.94131300	2.46815100
C	3.43555400	2.26242200	0.45977000
H	2.96604900	2.00655700	1.41032100
H	3.51013900	3.35004900	0.39699900
H	2.79060200	1.92254500	-0.35076500
C	5.45007600	2.01597800	-1.01854600
H	4.83785200	1.60564700	-1.82456800
H	5.48713800	3.10049700	-1.13894000
H	6.46808400	1.63634000	-1.12943200
C	3.77711500	-2.61705600	2.09631700
H	2.69320100	-2.65058500	2.21285000
H	4.16623400	-3.63587300	2.15804400
H	4.19806700	-2.03711100	2.92036500
C	3.50739000	-2.81371000	-0.42894500
H	3.91271400	-3.82808000	-0.42692000
H	2.42569600	-2.87177900	-0.30416500
H	3.72351000	-2.36158500	-1.39943000
C	0.86126300	-0.17462100	0.46008600
H	2.16560700	-0.26283800	0.59854700
H	0.94425600	-0.08511400	-0.61181700

H	0.61587400	-1.13170500	0.89189900
H	0.74060300	0.71138700	1.06408700
B	-1.18507600	0.03906700	-0.03365700
C	-1.89198700	-0.49595500	1.31963300
C	-1.59608300	0.04848500	2.57357400
C	-2.84804500	-1.51391900	1.35019100
C	-2.15215700	-0.39206000	3.76414200
C	-3.43515500	-1.98281400	2.52167800
C	-3.08249700	-1.42290600	3.73914300
C	-1.33001900	-0.90381400	-1.34609800
C	-0.84942200	-2.21537600	-1.39149100
C	-1.95338900	-0.48544800	-2.52401900
C	-0.92010200	-3.03372100	-2.50764400
C	-2.05627600	-1.27682700	-3.66432900
C	-1.53020000	-2.55895700	-3.66104400
C	-1.29606400	1.63329000	-0.31312300
C	-2.28758400	2.44250700	0.24669800
C	-0.41870400	2.31451400	-1.16052800
C	-2.37759700	3.81370900	0.02925200
C	-0.46280200	3.68007300	-1.39518500
C	-1.45444300	4.44147600	-0.79259100
F	0.55558500	1.64181900	-1.82510500
F	0.43588100	4.26545500	-2.20065500
F	-1.52051200	5.75858400	-1.00782400
F	-3.35124300	4.53080500	0.60316800
F	-3.24690500	1.91702400	1.03202500
F	-3.27920200	-2.09821600	0.21556400
F	-4.34303400	-2.96618500	2.48029200
F	-3.63485600	-1.86161700	4.87380500
F	-1.81185700	0.17193600	4.93109800
F	-0.72911000	1.08235600	2.67693300
F	-0.27731200	-2.77210200	-0.29553700
F	-0.41428500	-4.27488900	-2.47958000
F	-1.61496200	-3.33112700	-4.74794100
F	-2.66288700	-0.81012200	-4.76270500
F	-2.52129400	0.73282700	-2.61341700
F	6.43654900	-2.94327900	0.54719100

NHC4

C	-2.59515400	0.72442900	-0.73344100
C	-4.94204500	0.14387100	-0.70318200

C	-4.75460200	1.47062900	-0.93164500
H	-5.45916600	2.26048500	-1.10123000
N	-3.34812000	1.76602300	-0.94184100
C	-3.52658300	-0.46422400	-0.53927800
C	-2.87330700	3.17352800	-1.17585700
C	-3.39570600	3.63744600	-2.54717000
H	-4.48612000	3.66068800	-2.59051900
H	-3.03253600	4.64714100	-2.75016300
H	-3.03363900	2.97835100	-3.33956500
C	-1.34420200	3.21476800	-1.16953900
H	-0.92494800	2.57554300	-1.94756400
H	-1.02398900	4.24151400	-1.35998800
H	-0.93058600	2.90555800	-0.20958000
C	-3.42316600	4.06112200	-0.04581000
H	-3.07213700	3.70760200	0.92619700
H	-3.07085200	5.08566400	-0.18345200
H	-4.51460900	4.08146900	-0.03091800
C	-3.16560900	-1.49444600	-1.63667400
H	-2.10738700	-1.75018900	-1.56515200
H	-3.73852300	-2.41787200	-1.54373600
H	-3.34856900	-1.08068500	-2.63103900
C	-3.24403400	-1.00423900	0.88618500
H	-3.85262900	-1.87619500	1.12752500
H	-2.19693800	-1.29801600	0.97210300
H	-3.44657400	-0.23621200	1.63638700
C	0.18969300	0.17922800	-0.26975600
H	-1.05874600	0.49065000	-0.52444300
H	0.19847800	0.62922200	0.71139300
H	0.10859600	-0.89424900	-0.34257400
H	0.64729000	0.70968800	-1.09095600
B	2.27314000	-0.22243200	0.32277100
C	2.64829900	-1.39399600	-0.72131700
C	2.50804900	-1.23203700	-2.10414300
C	3.15409600	-2.63933400	-0.33993500
C	2.79242600	-2.21945700	-3.03420900
C	3.45724000	-3.65562500	-1.24075000
C	3.27077300	-3.44819400	-2.59804000
C	2.08708000	-0.65160200	1.86989200
C	1.16960200	-1.62265500	2.28210400
C	2.83817500	-0.09895500	2.91069900
C	0.96233500	-1.98629800	3.60313300
C	2.66972000	-0.44194500	4.24871200
C	1.72065300	-1.38828400	4.60079000
C	2.95209700	1.22096600	0.06346800

C	4.12548500	1.39342800	-0.67524800
C	2.42661600	2.40716700	0.58380700
C	4.70504900	2.63362400	-0.92244700
C	2.96420000	3.66369100	0.35214600
C	4.11763600	3.78032600	-0.41131500
F	1.32768800	2.38018500	1.37505400
F	2.38665700	4.76050400	0.86396400
F	4.65624300	4.98123800	-0.64331300
F	5.82859800	2.72811700	-1.64472500
F	4.78597400	0.33454200	-1.18185300
F	3.40172400	-2.92234800	0.95361700
F	3.93479600	-4.82924000	-0.80635700
F	3.55463900	-4.41312700	-3.47805200
F	2.62243000	-1.99755500	-4.34498400
F	2.08338600	-0.05285900	-2.61044300
F	0.41743700	-2.28288400	1.37020700
F	0.04760600	-2.91301600	3.92325300
F	1.54126300	-1.72733500	5.88090800
F	3.42133500	0.13079700	5.19747600
F	3.80525600	0.80562400	2.66362300
N	-6.13362500	-0.53398000	-0.64720500
C	-6.21822800	-1.97932700	-0.34046200
H	-5.19876400	-2.32337100	-0.21096000
C	-7.42772100	0.15293700	-0.87634800
H	-8.17459900	-0.63540900	-0.77867300
C	-6.95058700	-2.25257900	0.98296400
H	-8.00472900	-1.96691700	0.93867500
H	-6.91211500	-3.32020900	1.21545100
H	-6.48374700	-1.70743700	1.80613700
C	-6.81377900	-2.79079400	-1.50227200
H	-6.76084700	-3.85847400	-1.27288800
H	-7.86461800	-2.54989100	-1.68265000
H	-6.25975200	-2.61270700	-2.42638600
C	-7.77603600	1.19020200	0.20469700
H	-7.71634200	0.74478200	1.19965700
H	-7.12100800	2.06098100	0.19081900
H	-8.79961500	1.54298200	0.05203400
C	-7.57972600	0.69618200	-2.30688400
H	-7.41527500	-0.09832900	-3.03763200
H	-8.59373400	1.08072300	-2.44531100
H	-6.88352700	1.50407900	-2.53165000

NHC5

C	-3.45967900	0.12369000	-0.50306700
C	-5.60932000	-0.93352600	-0.35749000
C	-5.72179800	0.41041700	-0.24457300
H	-6.58901600	1.02864500	-0.09936000
N	-4.41079700	0.99981800	-0.32933500
C	-4.11789500	-1.24825800	-0.54651200
C	-4.24410100	2.49184800	-0.24090900
C	-5.03633800	3.13015400	-1.39544600
H	-6.10497700	2.91582400	-1.33373100
H	-4.91070800	4.21463600	-1.36605900
H	-4.66845300	2.76926000	-2.35875400
C	-2.76449500	2.85864200	-0.36620000
H	-2.34779000	2.51881100	-1.31505800
H	-2.67197800	3.94602700	-0.32125700
H	-2.16950000	2.43645300	0.44375000
C	-4.78158300	2.95724100	1.12361300
H	-4.23627900	2.47413000	1.93747000
H	-4.64623800	4.03682300	1.21754500
H	-5.84499300	2.74217900	1.24563400
C	-3.75390200	-1.86394700	-1.92020400
H	-2.67013600	-1.85965100	-2.04524100
H	-4.09542400	-2.89572600	-2.00591600
H	-4.19249800	-1.28825400	-2.73873300
C	-3.57286400	-2.10282200	0.62209600
H	-4.06770600	-3.07561300	0.65520600
H	-2.50044300	-2.26894600	0.51093100
H	-3.74828600	-1.60864000	1.58028700
C	-0.58979700	0.07188000	-0.38789100
H	-1.89588000	0.17529200	-0.48549200
H	-0.57957700	0.26436200	0.67386700
H	-0.48698400	-0.94557300	-0.73119700
H	-0.32302100	0.86686000	-1.06753200
B	1.55441600	-0.04108600	0.02476300
C	2.06679700	-0.83710100	-1.28283300
C	1.79591400	-0.38934400	-2.58041300
C	2.82662500	-2.00831400	-1.22888600
C	2.19483200	-1.05303000	-3.72997700
C	3.25174300	-2.70238200	-2.35752400
C	2.93009500	-2.22599800	-3.61830400
C	1.57443100	-0.85129100	1.42523200
C	0.88111300	-2.05008100	1.61577500
C	2.29426200	-0.42512600	2.54421200
C	0.84642000	-2.74749200	2.81272500
C	2.29608900	-1.09958200	3.76145800

C	1.56178400	-2.26647600	3.90127600
C	1.93795500	1.52741900	0.11160000
C	3.00692800	2.09349500	-0.58754900
C	1.24106800	2.43252600	0.91687600
C	3.33173500	3.44518700	-0.53646900
C	1.52149700	3.78822400	0.98707500
C	2.57977500	4.30304400	0.25081700
F	0.22281900	2.00623800	1.70312400
F	0.78878700	4.59977600	1.76370800
F	2.87247500	5.60575000	0.30771200
F	4.36799900	3.92286700	-1.23699200
F	3.81379400	1.33290600	-1.35173300
F	3.21657100	-2.53075600	-0.04997300
F	3.97475800	-3.82308500	-2.23414900
F	3.32783700	-2.88055600	-4.71337300
F	1.88904000	-0.57071200	-4.94244600
F	1.11701000	0.76360800	-2.77259300
F	0.19198400	-2.61001500	0.59316200
F	0.14020900	-3.88170100	2.92466200
F	1.54716600	-2.92469000	5.06410900
F	3.00543900	-0.63246200	4.79663400
F	3.06142800	0.68100300	2.49482200
N	-6.61823000	-1.85073100	-0.18379800
C	-6.59871000	-3.14278300	-0.86198400
H	-7.31938500	-3.80214500	-0.37549000
H	-6.86437100	-3.06671800	-1.92620600
H	-5.62038100	-3.60981600	-0.78169500
C	-7.94813500	-1.31915200	0.07684700
H	-8.37821900	-0.80792600	-0.79793600
H	-8.61256500	-2.13585800	0.36060800
H	-7.90628800	-0.60912900	0.90604100

NHC6

C	3.71129700	-0.53557500	0.67763500
C	5.65640700	-1.88548100	0.58647500
C	6.00097900	-0.60179500	0.42648200
H	6.96412900	-0.14296600	0.27688700
N	4.78662000	0.18555800	0.48636300
C	4.15984500	-1.98394100	0.75674600
C	4.84961200	1.68172200	0.34245600
C	5.72640300	2.23366900	1.48009500

H	6.74872900	1.85184800	1.43980400
H	5.77589700	3.32192700	1.40543800
H	5.30151100	1.97687000	2.45316700
C	3.44154000	2.27061600	0.44010600
H	2.97153600	2.02643600	1.39342000
H	3.51533000	3.35747200	0.36243600
H	2.79699300	1.91843100	-0.36542200
C	5.45565400	2.00717000	-1.03352700
H	4.84475300	1.58324600	-1.83350900
H	5.48903300	3.09016100	-1.16879900
H	6.47446600	1.62833700	-1.13932100
C	3.78709400	-2.58313900	2.13177300
H	2.70273100	-2.61850600	2.24564100
H	4.18184700	-3.59863000	2.20834600
H	4.20198000	-1.99003300	2.94994000
C	3.52548800	-2.80579300	-0.39082000
H	3.93497400	-3.81825900	-0.38080500
H	2.44327800	-2.86463200	-0.26920300
H	3.74201100	-2.35948400	-1.36427200
C	0.87053300	-0.16609800	0.47139800
H	2.17340400	-0.25195100	0.60921100
H	0.93580300	-0.07787000	-0.60190700
H	0.61303000	-1.12038200	0.90297000
H	0.73172900	0.72144200	1.06953600
B	-1.20922600	0.04005800	-0.03578000
C	-1.90782700	-0.50787700	1.31408800
C	-1.61744700	0.03264000	2.57125700
C	-2.85373400	-1.53574200	1.33884600
C	-2.16798100	-0.42190100	3.75912800
C	-3.43495000	-2.01833800	2.50755500
C	-3.08717400	-1.46252100	3.72825000
C	-1.33186000	-0.89896200	-1.35036900
C	-0.84794600	-2.20978100	-1.39032100
C	-1.93718300	-0.47891300	-2.53715900
C	-0.89914800	-3.02521000	-2.50966200
C	-2.01992100	-1.26767100	-3.68078100
C	-1.49140300	-2.54872000	-3.67166600
C	-1.31749000	1.63387600	-0.30486700
C	-2.30380100	2.44218500	0.26559800
C	-0.44235900	2.31785400	-1.15291300
C	-2.39063100	3.81510200	0.05812700
C	-0.48379000	3.68509900	-1.37754900
C	-1.46981200	4.44541100	-0.76424500
F	0.52517100	1.64666500	-1.82682800

F	0.41179500	4.27378000	-2.18415100
F	-1.53293500	5.76432100	-0.97028700
F	-3.35930900	4.53140200	0.64189800
F	-3.26084900	1.91422200	1.05216100
F	-3.28032600	-2.11652900	0.20065200
F	-4.33311400	-3.01061200	2.46050000
F	-3.63414300	-1.91425000	4.86061500
F	-1.83331900	0.13830800	4.92965600
F	-0.76229200	1.07459500	2.68085900
F	-0.29219100	-2.76653700	-0.28741000
F	-0.39194600	-4.26570600	-2.47695500
F	-1.55710000	-3.31869700	-4.76173900
F	-2.60997500	-0.79978400	-4.78796500
F	-2.50589900	0.73863300	-2.63261300
O	6.39917900	-3.00815700	0.61109600
H	7.33239000	-2.80056100	0.48517600

NHC7

C	-3.01579800	0.68745500	-0.53512100
C	-5.28691300	-0.01038900	-0.21843500
C	-5.17788500	1.32060300	-0.14361600
H	-5.94364600	2.06050600	0.02530500
N	-3.80512500	1.71400900	-0.34132400
C	-3.87832100	-0.55786200	-0.46918500
C	-3.41506900	3.16767000	-0.33405700
C	-4.16931300	3.86506200	-1.47962400
H	-5.25319900	3.80042600	-1.36277100
H	-3.90031000	4.92316300	-1.50102700
H	-3.89993200	3.42424100	-2.44214300
C	-1.90662000	3.30031400	-0.54738500
H	-1.59597500	2.85477200	-1.49317000
H	-1.65177000	4.36211600	-0.56852600
H	-1.34000300	2.83424000	0.25917300
C	-3.80289200	3.76498700	1.02961100
H	-3.29737800	3.23690000	1.84111800
H	-3.49839300	4.81302400	1.06563600
H	-4.87943000	3.72711100	1.20904300
C	-3.71357000	-1.33749300	-1.79586100
H	-2.65692300	-1.54609800	-1.97111800
H	-4.23914400	-2.29225200	-1.74616700
H	-4.09667300	-0.76890800	-2.64628800

C	-3.41894700	-1.43726600	0.72204000
H	-4.08883100	-2.29452200	0.82030300
H	-2.40480800	-1.80620000	0.56284600
H	-3.44327700	-0.87891900	1.66075100
C	-0.18483300	0.21158900	-0.44971200
H	-1.46231500	0.50541800	-0.54895300
H	-0.17185300	0.36747900	0.61774700
H	-0.24121100	-0.79573800	-0.83060700
H	0.17627900	0.98996400	-1.10410300
B	1.88585600	-0.18663000	-0.05289400
C	2.30756800	-0.97388200	-1.39980800
C	2.10860500	-0.42648300	-2.67163800
C	2.90956500	-2.23441600	-1.40752900
C	2.42783300	-1.07367800	-3.85489600
C	3.25082300	-2.91670700	-2.57135500
C	3.00444400	-2.33615400	-3.80527600
C	1.80639100	-1.06251700	1.30760700
C	0.95978400	-2.16589000	1.44901100
C	2.58048100	-0.79005700	2.43826100
C	0.83613300	-2.90869800	2.61229300
C	2.49649000	-1.51614200	3.62261700
C	1.61311000	-2.57989000	3.71513900
C	2.48189900	1.31048000	0.11391800
C	3.63624400	1.74999100	-0.53890700
C	1.89960100	2.26975600	0.94645900
C	4.14467300	3.03956200	-0.42151900
C	2.36462600	3.56851600	1.08363300
C	3.50131300	3.96065000	0.39038800
F	0.81008400	1.96036700	1.69336600
F	1.73209600	4.44101700	1.88218900
F	3.97117800	5.20582800	0.51092700
F	5.25334300	3.39631900	-1.08159300
F	4.34766400	0.91634200	-1.32145500
F	3.21853600	-2.86406800	-0.25740900
F	3.82170900	-4.12644100	-2.50768500
F	3.32350600	-2.97746000	-4.93330500
F	2.19747300	-0.49144100	-5.03970900
F	1.58631900	0.81452600	-2.80293600
F	0.19647600	-2.57951500	0.40887300
F	-0.01687800	-3.94072900	2.67807100
F	1.51404000	-3.28471600	4.84593500
F	3.26533200	-1.19738900	4.67137100
F	3.48796700	0.20578600	2.43420700
C	-6.52403500	-0.77608800	0.02666300

C	-7.30596300	-0.48454500	1.15664100
C	-6.96289800	-1.78950300	-0.83955600
C	-8.48639900	-1.17642300	1.40844300
H	-6.96891300	0.27603400	1.85163300
C	-8.14472800	-2.47936400	-0.58641400
H	-6.39697900	-2.02110300	-1.73206000
C	-8.91024700	-2.17749300	0.53771100
H	-9.07061900	-0.93852400	2.29013000
H	-8.47015500	-3.25236100	-1.27327100
H	-9.82773200	-2.71991600	0.73443800

S 1.3.2 **B3F**-NHC TSs

NHC1

C	-3.77650300	0.89264200	1.04423000
C	-5.60624300	2.28432700	1.66109300
H	-6.21095900	3.11259400	2.00248800
C	-6.05432200	1.10709600	1.23879200
H	-7.06086400	0.73232400	1.14607800
N	-4.92249300	0.27965600	0.87076300
C	-4.09744800	2.27813800	1.57538500
C	-5.13261500	-1.11563300	0.35132900
C	-5.88759700	-1.91856900	1.42531000
H	-6.87233200	-1.49963800	1.64387700
H	-6.03419100	-2.94280800	1.07633100
H	-5.31451300	-1.95429800	2.35469500
C	-3.78076900	-1.77209600	0.06837400
H	-3.16961300	-1.83498100	0.96945600
H	-3.95589700	-2.78736200	-0.29428600
H	-3.21674100	-1.23321400	-0.69297500
C	-5.95177900	-1.02243900	-0.94789200
H	-5.42033600	-0.43019900	-1.69606600
H	-6.10620900	-2.02462500	-1.35323300
H	-6.93506500	-0.57445000	-0.78737300
C	-3.43764600	2.47055200	2.96184900
H	-2.35129300	2.40975600	2.87902000
H	-3.69838700	3.45344200	3.36248900
H	-3.77333800	1.71156000	3.67202900
C	-3.57930800	3.34651100	0.58014000
H	-3.83590100	4.34380900	0.94695900

H	-2.49643300	3.28187400	0.47180800
H	-4.02910300	3.21940100	-0.40700300
C	-0.96939300	0.33888600	0.58188800
H	-2.24857500	0.51966100	0.76817800
H	-1.15286400	0.37585000	-0.48103300
H	-0.64621000	1.23454400	1.09095600
H	-0.92472400	-0.60512400	1.10514700
B	0.90191900	-0.00660100	-0.06578500
C	1.69989500	0.10354800	1.34257200
C	1.48854800	-0.79785900	2.39352400
C	2.61101800	1.10950500	1.68355100
C	2.09254800	-0.75833100	3.63880400
C	3.26522700	1.22162000	2.90623200
C	2.99087400	0.27031300	3.86911800
C	1.28855200	1.10633400	-1.19567600
C	0.60099600	2.25109200	-1.59298900
C	2.47874300	0.92541700	-1.91119000
C	0.99793000	3.12564800	-2.59761300
C	2.95184500	1.74406900	-2.92402000
C	2.18198500	2.84636500	-3.25302300
C	0.81463900	-1.47857100	-0.76813300
C	1.69316600	-2.54134600	-0.52136100
C	-0.10676100	-1.78132900	-1.77491600
C	1.65340900	-3.78075700	-1.14751400
C	-0.22014200	-2.98942900	-2.44793400
C	0.68036400	-3.98296400	-2.10828200
F	-1.00209800	-0.82220600	-2.16145000
F	0.61154300	-5.17520700	-2.73815600
F	2.68591200	-2.38401500	0.37971600
F	2.90678700	2.08023700	0.78755100
F	3.60717500	0.34662300	5.06779400
F	0.60010200	-1.81165900	2.20531000
F	-0.56874900	2.58817700	-0.97259200
F	2.60163700	3.67366600	-4.23434900
F	3.26543700	-0.12652900	-1.57852700
H	1.87455400	-1.50477700	4.38967600
H	3.96339300	2.02720500	3.08607200
H	3.88741800	1.53173300	-3.42224400
H	0.40149600	3.99183100	-2.84784900
H	-0.96701100	-3.13453100	-3.21586400
H	2.37185600	-4.54856200	-0.89638300

NHC2

C	-3.27814600	0.27148400	-0.45577200
C	-5.51319800	-0.50058500	-0.41393100
C	-5.50522700	0.82982000	-0.46491000
H	-6.32294700	1.53017200	-0.48723900
N	-4.13156800	1.26863700	-0.48856200
C	-4.08852700	-1.01176900	-0.38941000
C	-3.80650800	2.73846900	-0.53651700
C	-4.44397500	3.32777200	-1.80674000
H	-5.53239000	3.23672800	-1.80903100
H	-4.20200000	4.39033000	-1.87333400
H	-4.05467300	2.83327500	-2.69955900
C	-2.29039100	2.92821800	-0.57779900
H	-1.85188700	2.46047600	-1.45985600
H	-2.07473400	3.99797000	-0.61888500
H	-1.80489700	2.51945300	0.30846200
C	-4.38356800	3.39302800	0.73059400
H	-3.94368500	2.95048400	1.62704000
H	-4.14956800	4.45953500	0.72675000
H	-5.46949900	3.29276500	0.79299100
C	-3.76228200	-1.90455400	-1.60768100
H	-2.71313100	-2.20153400	-1.58362700
H	-4.38029000	-2.80475600	-1.58037200
H	-3.95545200	-1.38361500	-2.54790600
C	-3.77019400	-1.75095000	0.93310200
H	-4.39374000	-2.64472500	1.00818000
H	-2.72214000	-2.04677600	0.96149900
H	-3.97339400	-1.11739600	1.79917300
C	-0.39773400	-0.04079900	-0.36735500
H	-1.69337000	0.16458600	-0.41442200
H	-0.44425500	0.26502200	0.66682200
H	-0.43375100	-1.09218100	-0.60922800
H	-0.17385100	0.67060100	-1.14839000
B	1.55025100	-0.12534000	0.04420300
C	2.09376100	-0.83650000	-1.31071400
C	1.99016500	-0.22556800	-2.56669200
C	2.65223200	-2.11699500	-1.38990700
C	2.38511000	-0.77003600	-3.77677600
C	3.07954900	-2.73705300	-2.55971700
C	2.93707300	-2.03990700	-3.74345700
C	1.76366800	-0.96706000	1.42737900
C	0.85205600	-1.74087300	2.14260000
C	3.02773500	-0.94474800	2.02976600
C	1.10938700	-2.39994200	3.33844600
C	3.37447100	-1.57136900	3.21625400

C	2.38534700	-2.29510400	3.85911300
C	1.97435600	1.43501300	0.28737500
C	3.07380300	2.07086200	-0.30359500
C	1.31663600	2.26468400	1.19954800
C	3.46485900	3.38360600	-0.07299600
C	1.63516600	3.58392300	1.48868400
C	2.72378800	4.12465600	0.82840000
F	0.24616100	1.76740800	1.89313700
F	3.07431000	5.40429100	1.07806000
F	3.85491300	1.38059200	-1.16109000
F	2.80350000	-2.85489300	-0.26504200
F	3.33995400	-2.61033800	-4.89860100
F	1.44314600	1.01973600	-2.63528100
F	-0.41922600	-1.90053200	1.66471900
F	2.67594700	-2.92165200	5.01921600
F	4.02290900	-0.27768500	1.39739900
Br	-7.05617900	-1.58539800	-0.36344900
H	0.34050100	-2.97698200	3.83285900
H	4.37914600	-1.50376000	3.60957000
H	3.50848200	-3.72904400	-2.53291800
H	2.27394900	-0.21994400	-4.70065800
H	4.32891800	3.79740700	-0.57396200
H	1.06746700	4.15138500	2.21276000

NHC3

C	3.72643400	-0.60011800	0.71401800
C	5.67698300	-1.89275400	0.92286700
C	6.03269300	-0.62576500	0.73424700
H	7.00690000	-0.17293800	0.67139500
N	4.80876000	0.13519900	0.61231400
C	4.18366900	-2.03445800	0.92400100
C	4.86736000	1.62251100	0.38831000
C	5.63767800	2.25220400	1.56193900
H	6.66803800	1.89571300	1.62441800
H	5.67065700	3.33592900	1.43291500
H	5.14000700	2.03691700	2.51025800
C	3.44937100	2.19119000	0.33256800
H	2.90532500	2.00474600	1.25930300
H	3.51569800	3.27185100	0.18983900
H	2.87392300	1.77624200	-0.49471200
C	5.58857600	1.87309500	-0.94728900

H	5.04983100	1.39873100	-1.77046600
H	5.63113300	2.94681000	-1.14126000
H	6.61376500	1.49599000	-0.94211900
C	3.65910300	-2.57437200	2.27484600
H	2.57008100	-2.63074200	2.25991000
H	4.05842100	-3.57613900	2.44923700
H	3.96213200	-1.93378200	3.10587700
C	3.70492200	-2.92574700	-0.24832100
H	4.10549300	-3.93450200	-0.12343400
H	2.61695700	-2.97623300	-0.27092900
H	4.04813800	-2.53581900	-1.20894700
C	0.86359200	-0.24810800	0.47180000
H	2.16665800	-0.32777400	0.57960900
H	1.00994800	-0.02100800	-0.57299400
H	0.66836400	-1.26761400	0.76856200
H	0.74970800	0.54083200	1.20115700
B	-1.05359100	0.00352500	-0.04791400
C	-1.77564000	-0.52698400	1.30536900
C	-1.62796800	0.12561800	2.53582100
C	-2.54658900	-1.68986000	1.41266200
C	-2.16902000	-0.27693100	3.74514000
C	-3.12987500	-2.16352600	2.58348400
C	-2.92845600	-1.43511300	3.73949100
C	-1.35409400	-0.85621300	-1.40284300
C	-0.56012800	-1.79828600	-2.05310700
C	-2.57676300	-0.65156700	-2.05453000
C	-0.88755100	-2.46037200	-3.23009700
C	-2.98655500	-1.26597400	-3.22708800
C	-2.11226300	-2.17206500	-3.80186000
C	-1.16911300	1.59818300	-0.38331900
C	-2.15677000	2.45613200	0.11731700
C	-0.32896100	2.24129800	-1.29666800
C	-2.28492800	3.80417700	-0.19236400
C	-0.38187500	3.57921100	-1.66036200
C	-1.37800400	4.34640700	-1.08361700
F	0.65456300	1.51694500	-1.91381900
F	-1.47112900	5.65352600	-1.40817300
F	-3.09147900	1.96803700	0.96001800
F	-2.76432400	-2.45499900	0.31727200
F	-3.47918200	-1.86396300	4.89486100
F	-0.87503300	1.25862900	2.57915000
F	0.65505200	-2.13799200	-1.52624300
F	-2.46719000	-2.79514500	-4.94587000
F	-3.46372700	0.20195400	-1.48865200

F	6.49300500	-2.93502900	1.08425300
H	-0.20908500	-3.17586400	-3.67323400
H	-3.95277400	-1.05059900	-3.66144400
H	-3.72051600	-3.06899400	2.57809600
H	-2.00894200	0.29634200	4.64751800
H	-3.07817100	4.39659000	0.24191100
H	0.31248700	3.99225800	-2.37857100

NHC4

C	-2.58646200	0.73105600	-0.72793800
C	-4.92836000	0.13438300	-0.70919600
C	-4.74945500	1.46196300	-0.93895800
H	-5.45878100	2.24647100	-1.11392800
N	-3.34499100	1.76726300	-0.94247800
C	-3.50964500	-0.46338400	-0.53698900
C	-2.87682400	3.17583400	-1.18097900
C	-3.39832500	3.63132200	-2.55551900
H	-4.48879500	3.65044700	-2.60161100
H	-3.03812400	4.64129900	-2.76251500
H	-3.03173900	2.96982500	-3.34379700
C	-1.34803200	3.22343400	-1.17079000
H	-0.92301000	2.58387900	-1.94529100
H	-1.03122900	4.25073100	-1.36423300
H	-0.93462100	2.91681200	-0.21009000
C	-3.43486400	4.06515500	-0.05630000
H	-3.08319700	3.71849900	0.91794500
H	-3.08931900	5.09145600	-0.19851600
H	-4.52654700	4.07822700	-0.04350100
C	-3.13252300	-1.49139800	-1.63157900
H	-2.07185700	-1.73493800	-1.55478600
H	-3.69597000	-2.42087400	-1.53963300
H	-3.31590000	-1.08098800	-2.62730800
C	-3.23006800	-1.00062100	0.89008400
H	-3.83115500	-1.87938400	1.12628800
H	-2.18000800	-1.28119600	0.98120800
H	-3.44564400	-0.23520900	1.63936400
C	0.18546200	0.21496700	-0.20208200
H	-1.08638900	0.52200500	-0.49057200
H	0.16895300	0.69398400	0.76440300
H	0.07369900	-0.85604700	-0.25576500
H	0.61618800	0.73409400	-1.04380800

B	2.22263600	-0.19713800	0.32770100
C	2.57479900	-1.37361800	-0.72502900
C	2.41567500	-1.22870200	-2.10908100
C	3.08189500	-2.63074600	-0.37851900
C	2.66489400	-2.20108200	-3.06397900
C	3.36205900	-3.66012800	-1.27026300
C	3.13867300	-3.42119600	-2.61228500
C	2.08190800	-0.63138900	1.88205200
C	1.18070700	-1.59945300	2.33993500
C	2.85910200	-0.10152800	2.91892400
C	0.99895900	-1.98759700	3.65729200
C	2.74593700	-0.43551600	4.26372700
C	1.80050200	-1.38110000	4.60938400
C	2.93133800	1.23460900	0.06024700
C	4.10209100	1.40459200	-0.68769300
C	2.46005200	2.44286900	0.58531200
C	4.72564100	2.61970100	-0.94529300
C	3.01432600	3.69559800	0.37478500
C	4.15614500	3.75655000	-0.40525600
F	1.36076700	2.42536200	1.39078000
F	4.73144900	4.95688100	-0.63388500
F	4.72445700	0.31935500	-1.20382700
F	3.35556500	-2.90570700	0.91822000
F	3.39797700	-4.39707900	-3.50924000
F	1.98666400	-0.03286000	-2.59435500
F	0.39709100	-2.24763600	1.43244700
F	1.65919500	-1.73212100	5.90568700
F	3.82687700	0.80019500	2.63274300
N	-6.11581400	-0.55178300	-0.65610600
C	-6.19003100	-1.99819900	-0.35347500
H	-5.16828500	-2.33427600	-0.22135100
C	-7.41388700	0.12594300	-0.88768500
H	-8.15571200	-0.66744000	-0.79161900
C	-6.92474100	-2.28097300	0.96670800
H	-7.98091700	-2.00318400	0.91985100
H	-6.87898700	-3.34901300	1.19621000
H	-6.46465600	-1.73456100	1.79283100
C	-6.77521700	-2.81144100	-1.51938400
H	-6.71556600	-3.87930100	-1.29233300
H	-7.82706900	-2.57745100	-1.70340400
H	-6.21859900	-2.62720300	-2.44072300
C	-7.77095100	1.16053300	0.19306300
H	-7.71303100	0.71401300	1.18765700
H	-7.11895900	2.03360200	0.18275800

H	-8.79537200	1.50946600	0.03702400
C	-7.56724300	0.66866800	-2.31837600
H	-7.39572300	-0.12447300	-3.04900000
H	-8.58367800	1.04617000	-2.45866600
H	-6.87610600	1.48129100	-2.54157400
H	2.58258700	4.57969700	0.82265300
H	5.62966200	2.66225300	-1.53658800
H	3.75265000	-4.60468800	-0.91822800
H	2.51380500	-2.00203800	-4.11571700
H	0.27761300	-2.74814300	3.92153500
H	3.38763100	0.02387500	5.00255300

NHC5

C	-3.48810600	0.03674600	-0.51066100
C	-5.68564800	-0.93647500	-0.46736400
C	-5.75348600	0.41338100	-0.42240900
H	-6.60432900	1.06711800	-0.35791700
N	-4.41804100	0.95167100	-0.44515200
C	-4.19803900	-1.31121100	-0.54010800
C	-4.20437400	2.43892400	-0.41105300
C	-4.91041600	3.05382500	-1.63268000
H	-5.98865600	2.88284200	-1.61946700
H	-4.74357300	4.13309300	-1.64323000
H	-4.50787100	2.63702400	-2.55880400
C	-2.70858500	2.75126100	-0.46879800
H	-2.25384100	2.36492700	-1.38151600
H	-2.57922300	3.83574900	-0.45584300
H	-2.17317200	2.33568600	0.38476900
C	-4.79822800	2.98099700	0.90107100
H	-4.30841300	2.52156500	1.76254000
H	-4.63912100	4.06025800	0.95361400
H	-5.87192100	2.79770900	0.97683800
C	-3.76588700	-2.00113500	-1.85750700
H	-2.67686400	-2.04376700	-1.90602700
H	-4.14328500	-3.02193100	-1.92433200
H	-4.12279300	-1.44597700	-2.72838000
C	-3.76882500	-2.13109400	0.69833400
H	-4.29367700	-3.08854200	0.72909000
H	-2.69613600	-2.32262400	0.67999700
H	-4.00108800	-1.59344200	1.62021200
C	-0.59313400	-0.07115200	-0.38030700

H	-1.89172800	0.04552800	-0.45514500
H	-0.62730300	0.24896000	0.64959600
H	-0.53568000	-1.12754000	-0.59604700
H	-0.36349300	0.63290000	-1.16657900
B	1.41187800	-0.07192200	0.06011300
C	1.96695900	-0.80995200	-1.27026600
C	1.85077700	-0.24244100	-2.54613800
C	2.55243100	-2.08065600	-1.30718200
C	2.25890000	-0.81927800	-3.73685000
C	2.99426600	-2.72985500	-2.45546800
C	2.83814700	-2.07507000	-3.66148600
C	1.63801600	-0.85901800	1.46973400
C	0.74718900	-1.63113100	2.21265500
C	2.90060800	-0.77759500	2.06985700
C	1.02494300	-2.23829800	3.43152300
C	3.26569300	-1.35079600	3.27765700
C	2.29736800	-2.07887200	3.94671800
C	1.76023300	1.50843200	0.25064700
C	2.82537800	2.17593900	-0.36732000
C	1.06870400	2.33246000	1.14347000
C	3.15271600	3.51304100	-0.18270100
C	1.32415500	3.67465600	1.38563600
C	2.38026500	4.24602600	0.69883300
F	0.03347700	1.80413700	1.86240700
F	2.66835700	5.54931500	0.90304400
F	3.63701500	1.49445800	-1.20371600
F	2.71731100	-2.77816400	-0.15866400
F	3.25448500	-2.67468700	-4.79725600
F	1.27480800	0.98453900	-2.65734400
F	-0.51780300	-1.84194900	1.74478200
F	2.60554600	-2.65477600	5.12880100
F	3.87522500	-0.10372800	1.41233000
N	-6.73936000	-1.80838100	-0.31401100
C	-6.73477000	-3.12168200	-0.94932800
H	-7.50811100	-3.73627100	-0.48530700
H	-6.93606900	-3.07119300	-2.02931700
H	-5.78226400	-3.62315900	-0.79797900
C	-8.05900000	-1.21574400	-0.15457600
H	-8.41787100	-0.72608900	-1.07305800
H	-8.77157400	-1.99339900	0.12270900
H	-8.03560300	-0.47277700	0.64596900
H	3.99292700	3.95202000	-0.70243800
H	0.73290100	4.23766200	2.09412300
H	3.44449100	-3.71089400	-2.39552700

H	2.13582300	-0.30312600	-4.67864000
H	4.26774800	-1.23940700	3.66767200
H	0.27210900	-2.81705900	3.94812300

NHC6

C	3.73806700	-0.58942800	0.70950800
C	5.71034500	-1.89186800	0.91837000
C	6.04526400	-0.60994900	0.72959600
H	7.00980900	-0.13441000	0.66499600
N	4.81635500	0.14719400	0.60870700
C	4.20641500	-2.01977100	0.91651900
C	4.86782100	1.63288400	0.38580400
C	5.63554500	2.26873200	1.55823200
H	6.66841800	1.91943600	1.61884400
H	5.65966400	3.35297200	1.43055500
H	5.14123900	2.04778900	2.50702100
C	3.44778400	2.19756900	0.33154200
H	2.90545300	2.00754900	1.25847900
H	3.50961000	3.27868100	0.18903200
H	2.87312500	1.77956300	-0.49469900
C	5.58555100	1.89058000	-0.95066300
H	5.04858000	1.41253600	-1.77288600
H	5.62066300	2.96472900	-1.14436500
H	6.61278400	1.51921200	-0.94738000
C	3.68516000	-2.56461400	2.26512000
H	2.59635600	-2.62930300	2.25065900
H	4.09476100	-3.56198300	2.44009700
H	3.98176800	-1.92045000	3.09613100
C	3.73128800	-2.90853500	-0.25737200
H	4.14173400	-3.91405500	-0.13969700
H	2.64344200	-2.96703400	-0.27839400
H	4.06847200	-2.50973300	-1.21688600
C	0.87192300	-0.24780300	0.46879300
H	2.17114100	-0.32414100	0.57611700
H	0.99684500	-0.02448200	-0.57954200
H	0.66601300	-1.26422500	0.76875100
H	0.74302700	0.54538400	1.19090100
B	-1.07068600	0.00164400	-0.05519700
C	-1.78256100	-0.54024500	1.29657100
C	-1.63425100	0.10461000	2.53131800
C	-2.54819000	-1.70740400	1.39766400

C	-2.16900900	-0.31020600	3.73929200
C	-3.12479900	-2.19277700	2.56695600
C	-2.92247600	-1.47220000	3.72766900
C	-1.36448800	-0.85306600	-1.41330000
C	-0.57413700	-1.80601200	-2.05274900
C	-2.57813900	-0.63638400	-2.07755300
C	-0.89656800	-2.46517200	-3.23279900
C	-2.98208500	-1.24766100	-3.25397200
C	-2.11156300	-2.16369000	-3.81832000
C	-1.18287000	1.59712100	-0.37875800
C	-2.16720500	2.45293800	0.13179500
C	-0.34426100	2.24513200	-1.29031200
C	-2.29300100	3.80386800	-0.16573500
C	-0.39533200	3.58644900	-1.64194600
C	-1.38730200	4.35124900	-1.05511800
F	0.63387500	1.52375300	-1.91723000
F	-1.47805000	5.66159900	-1.36806500
F	-3.10186000	1.95901300	0.97142100
F	-2.76789800	-2.46425300	0.29702300
F	-3.46690900	-1.91251700	4.88190600
F	-0.88811400	1.24108600	2.58076800
F	0.62877300	-2.15989100	-1.51122000
F	-2.46099400	-2.78415800	-4.96574900
F	-3.46322500	0.22597700	-1.52160400
O	6.46902200	-2.99231900	1.08863000
H	7.40548600	-2.76471500	1.05888400
H	-3.94141300	-1.02258500	-3.69855100
H	-0.22165700	-3.18932200	-3.66722000
H	0.29792500	4.00393600	-2.35864900
H	-3.08366500	4.39444300	0.27567200
H	-2.00836200	0.25692500	4.64543400
H	-3.71117200	-3.10096100	2.55677100

NHC7

C	-3.00788900	0.63957300	-0.40261900
C	-5.29158200	-0.03415400	-0.13666800
C	-5.18472900	1.29807500	-0.16462900
H	-5.95591200	2.04784400	-0.08872700
N	-3.80169400	1.67725200	-0.31740200
C	-3.87600300	-0.59767900	-0.29547000
C	-3.40574100	3.12795300	-0.37460600

C	-4.12493800	3.77109900	-1.57346900
H	-5.21204200	3.73286900	-1.47607600
H	-3.83626000	4.82149600	-1.64843700
H	-3.84335100	3.27342300	-2.50430900
C	-1.89182800	3.24408800	-0.55419400
H	-1.55871500	2.75711000	-1.47153600
H	-1.62942300	4.30247400	-0.61551700
H	-1.34717800	2.80882300	0.28360600
C	-3.83005500	3.79174500	0.94667800
H	-3.33945100	3.30975600	1.79513300
H	-3.53543300	4.84325400	0.93513800
H	-4.91019200	3.75152300	1.10341700
C	-3.75438200	-1.40719100	-1.61117800
H	-2.72948100	-1.75526000	-1.74883300
H	-4.41678800	-2.27498300	-1.56988800
H	-4.03470500	-0.80385800	-2.47763700
C	-3.39141500	-1.45576400	0.89823800
H	-3.96309800	-2.38362800	0.95053800
H	-2.33995200	-1.71647400	0.77191100
H	-3.50238300	-0.92289200	1.84556000
C	-0.18097200	0.18944900	-0.23522500
H	-1.48676300	0.47121100	-0.36153700
H	-0.16587300	0.45046100	0.81115400
H	-0.26887200	-0.84635900	-0.51999400
H	0.12176200	0.91369200	-0.97471800
B	1.86863800	-0.15484800	0.03705300
C	2.21695300	-1.03467200	-1.27747600
C	1.93039400	-0.60172200	-2.57789800
C	2.83640800	-2.28904800	-1.26124700
C	2.16190800	-1.31280900	-3.74396300
C	3.10877500	-3.06721200	-2.38092800
C	2.75477300	-2.55753000	-3.61498300
C	1.90986500	-0.93861200	1.45818100
C	1.10823000	-2.04556700	1.75844400
C	2.76250300	-0.60239000	2.51600400
C	1.08111200	-2.73280500	2.96106300
C	2.80402600	-1.23779500	3.75191600
C	1.94568800	-2.30111500	3.95250600
C	2.47223500	1.35150200	0.06165100
C	3.57367400	1.77033900	-0.69359100
C	1.97156100	2.37293600	0.87527100
C	4.10579100	3.05431000	-0.70016600
C	2.43580900	3.67786000	0.92799100
C	3.51299100	3.99571600	0.11890400

F	0.93363900	2.09440200	1.71664000
F	4.00088900	5.25474400	0.14058600
F	4.21749600	0.87786200	-1.48080000
F	3.23642600	-2.82087800	-0.08270300
F	3.00059700	-3.28512900	-4.72559100
F	1.38093400	0.63218000	-2.74769300
F	0.26928300	-2.52787400	0.79706200
F	1.95519000	-2.94362100	5.14001300
F	3.65073800	0.40718600	2.36105900
C	-6.56088100	-0.78591100	-0.08367800
C	-6.79202600	-1.79590200	0.86312200
C	-7.58466100	-0.48334800	-0.99592100
C	-8.00694500	-2.47385800	0.89687600
H	-6.03271700	-2.03257000	1.59673700
C	-8.79800500	-1.16398300	-0.96144300
H	-7.41458700	0.27916500	-1.74747100
C	-9.01324900	-2.16299200	-0.01513500
H	-8.16903700	-3.24406000	1.64238600
H	-9.57266200	-0.91727700	-1.67865700
H	-9.95675600	-2.69579200	0.01124700
H	4.96093600	3.29446700	-1.31644400
H	1.98883900	4.40408700	1.59241400
H	3.49507500	-0.91273900	4.51708800
H	0.42927900	-3.58309500	3.10507300
H	3.59082000	-4.02961900	-2.28030300
H	1.90702500	-0.89994200	-4.70995200

S 1.3.3 **B2F**-NHC TSs

NHC1

C	-3.76624800	0.89155000	1.04460800
C	-5.60015300	2.28727900	1.63938900
H	-6.20724200	3.11752700	1.97172900
C	-6.04551500	1.10894800	1.21714000
H	-7.05161800	0.73497800	1.11631500
N	-4.91124600	0.27897700	0.86283100
C	-4.09063100	2.27949500	1.56681100
C	-5.11717000	-1.11814800	0.34684700
C	-5.88565200	-1.91541000	1.41553000
H	-6.87207800	-1.49399300	1.62166000

H	-6.02996200	-2.94079400	1.06889500
H	-5.32274200	-1.94850000	2.35121100
C	-3.76326300	-1.77769100	0.08171100
H	-3.16137800	-1.83640100	0.98928100
H	-3.93578200	-2.79490700	-0.27689100
H	-3.19013700	-1.24477700	-0.67684800
C	-5.92160300	-1.02906200	-0.96185800
H	-5.38026100	-0.44122900	-1.70634100
H	-6.07316200	-2.03273200	-1.36466000
H	-6.90588400	-0.57846200	-0.81453300
C	-3.44159900	2.47740200	2.95748200
H	-2.35481800	2.41435200	2.88310700
H	-3.70408900	3.46257800	3.35151100
H	-3.78394700	1.72202500	3.66840600
C	-3.56334500	3.34293000	0.57088600
H	-3.82282300	4.34193500	0.93123100
H	-2.47991200	3.27683600	0.47078500
H	-4.00499600	3.21122000	-0.41932100
C	-0.95725000	0.33938300	0.60278500
H	-2.24036300	0.51857100	0.77968700
H	-1.15324100	0.37395700	-0.45823000
H	-0.64461300	1.23944900	1.11086400
H	-0.92002100	-0.60101400	1.13344100
B	0.89018200	-0.00331800	-0.05370800
C	1.69654000	0.10105700	1.35270200
C	1.49258800	-0.80691500	2.39951000
C	2.60170100	1.11127900	1.69653800
C	2.10438300	-0.76568300	3.64002500
C	3.25591400	1.21345200	2.91929300
C	3.00681100	0.26209500	3.89895000
C	1.27727200	1.10936500	-1.18542400
C	0.58035100	2.24444300	-1.59519800
C	2.47225000	0.93405500	-1.89437800
C	0.97948100	3.11177500	-2.60372300
C	2.93581200	1.75411000	-2.90932800
C	2.17165900	2.85943000	-3.26999100
C	0.80242100	-1.47360700	-0.76420200
C	1.68997300	-2.53229500	-0.53318600
C	-0.13068700	-1.77783900	-1.76015500
C	1.64304800	-3.76595700	-1.16895100
C	-0.24036400	-2.98466800	-2.43376000
C	0.66379700	-3.99533000	-2.12754500
F	-1.03858400	-0.81642100	-2.12942000
F	2.69299000	-2.37066300	0.35982600

F	2.88398000	2.09147500	0.80147300
F	0.60354100	-1.82456400	2.20491600
F	-0.60032700	2.57182700	-0.97950500
F	3.26509400	-0.11284000	-1.54821900
H	1.87396400	-1.53120400	4.36982200
H	3.94542700	2.03343200	3.07479800
H	3.87908500	1.52232300	-3.38702600
H	0.35556100	3.96368700	-2.84238300
H	-1.00731100	-3.10321000	-3.18853200
H	2.38116800	-4.51424400	-0.90994000
H	2.50667700	3.52168400	-4.05925500
H	3.50823200	0.32023200	4.85762600
H	0.61184000	-4.94897900	-2.63911500

NHC2

C	-3.26988700	0.25747600	-0.45652000
C	-5.50527000	-0.51111400	-0.39374600
C	-5.49599700	0.81926100	-0.44508100
H	-6.31311700	1.52056900	-0.45989200
N	-4.12208700	1.25603600	-0.48178200
C	-4.08130200	-1.02447200	-0.38147200
C	-3.79460000	2.72517000	-0.53371400
C	-4.44445300	3.31492200	-1.79744900
H	-5.53309600	3.22607700	-1.78838500
H	-4.20085600	4.37692800	-1.86731700
H	-4.06532900	2.81907600	-2.69389300
C	-2.27870800	2.91242200	-0.59036100
H	-1.84925900	2.44287400	-1.47586500
H	-2.06178000	3.98180200	-0.63538400
H	-1.78451500	2.50506700	0.29154300
C	-4.35747300	3.38110600	0.73904100
H	-3.90827100	2.93829100	1.63068400
H	-4.12179500	4.44726900	0.73218900
H	-5.44290000	3.28238900	0.81303300
C	-3.76620500	-1.91914700	-1.60121400
H	-2.71665100	-2.21517400	-1.58619900
H	-4.38356200	-2.81959500	-1.56649300
H	-3.96819800	-1.39979900	-2.54050500
C	-3.75184300	-1.76234300	0.93917800
H	-4.37616600	-2.65508700	1.02064000
H	-2.70383000	-2.05857300	0.95925100

H	-3.94630900	-1.12721700	1.80608400
C	-0.39027000	-0.05624800	-0.38722200
H	-1.68784000	0.15040600	-0.42472800
H	-0.44890100	0.26175900	0.64291000
H	-0.43392500	-1.10989900	-0.61881800
H	-0.17989800	0.64752200	-1.17912500
B	1.53563900	-0.12260400	0.03337900
C	2.09123800	-0.82944000	-1.32140800
C	1.99262500	-0.21505900	-2.57615800
C	2.64819600	-2.11042300	-1.40154300
C	2.39646500	-0.76096200	-3.78167800
C	3.08053300	-2.71984200	-2.57432800
C	2.95534700	-2.03583800	-3.77579000
C	1.75634100	-0.95981000	1.41958300
C	0.84182700	-1.70767700	2.15876500
C	3.02861700	-0.94913400	2.00474400
C	1.11198600	-2.35461200	3.35727800
C	3.37458800	-1.56909100	3.19385600
C	2.39597500	-2.27941100	3.88170400
C	1.95391900	1.44039800	0.28328800
C	3.05887200	2.07897400	-0.29414300
C	1.28300100	2.26857500	1.18782100
C	3.43876000	3.39218900	-0.05086200
C	1.60093600	3.58618600	1.47938700
C	2.69897000	4.15513800	0.84410800
F	0.20016700	1.76352000	1.86683700
F	3.84946400	1.38867500	-1.14718400
F	2.78746100	-2.85243800	-0.27385000
F	1.44051700	1.03284600	-2.64022200
F	-0.44377200	-1.84673000	1.69873200
F	4.02335100	-0.30005600	1.34691900
Br	-7.05038000	-1.59314100	-0.32888100
H	0.32038500	-2.90526900	3.84931000
H	4.39365000	-1.49477100	3.55116000
H	3.50577500	-3.71387300	-2.51936200
H	2.27709900	-0.18540800	-4.69063500
H	4.31228700	3.78403500	-0.55608400
H	1.00489600	4.12874300	2.20208300
H	2.63497900	-2.77653900	4.81413500
H	2.98087500	5.18027400	1.05255600
H	3.28811900	-2.49080100	-4.70104700

NHC3

C	3.71724600	-0.59745800	0.71673000
C	5.67250800	-1.88494500	0.91083600
C	6.02357000	-0.61591000	0.72722200
H	6.99621100	-0.15991600	0.66254700
N	4.79681200	0.14187800	0.61426100
C	4.17972400	-2.03145700	0.91627000
C	4.84872900	1.63034500	0.39706500
C	5.62420900	2.25707000	1.56889200
H	6.65602700	1.90337100	1.62403700
H	5.65310600	3.34147300	1.44447500
H	5.13247000	2.03616100	2.51901900
C	3.42855100	2.19455500	0.35227800
H	2.88985900	2.00116400	1.28069300
H	3.49055200	3.27631800	0.21567200
H	2.84937800	1.78342700	-0.47417400
C	5.56095900	1.88948400	-0.94173300
H	5.01758100	1.41814500	-1.76355400
H	5.59964000	2.96429300	-1.13052100
H	6.58707500	1.51462400	-0.94511800
C	3.66017200	-2.58165000	2.26478800
H	2.57122300	-2.63925700	2.25247300
H	4.06158200	-3.58402800	2.43104400
H	3.96458100	-1.94621400	3.09932600
C	3.69964400	-2.91596000	-0.26083800
H	4.10175300	-3.92498900	-0.14267200
H	2.61176700	-2.96641900	-0.28295100
H	4.04068000	-2.51934100	-1.21947700
C	0.85351200	-0.25484400	0.48970900
H	2.15916100	-0.32944400	0.58952300
H	1.01321600	-0.02150300	-0.55198100
H	0.67021700	-1.27836700	0.78092400
H	0.74535900	0.52735200	1.22741000
B	-1.03940600	-0.00413300	-0.04072700
C	-1.76951200	-0.52940500	1.31289700
C	-1.63221500	0.13232100	2.53969100
C	-2.52925800	-1.69911700	1.42442800
C	-2.17952000	-0.27130100	3.74490300
C	-3.11218600	-2.16290400	2.59856500
C	-2.93771300	-1.43843900	3.76973800
C	-1.33925500	-0.86464000	-1.39680700
C	-0.53065500	-1.78008800	-2.06737300
C	-2.57307900	-0.67990900	-2.03320400
C	-0.86257000	-2.43438800	-3.24628600
C	-2.97523600	-1.29478300	-3.20705900

C	-2.10079600	-2.18410700	-3.82359700
C	-1.15839500	1.58987000	-0.38759700
C	-2.15596400	2.44587100	0.09614100
C	-0.30936600	2.23224200	-1.29386300
C	-2.28093600	3.78992700	-0.22958600
C	-0.37002000	3.56699900	-1.66346100
C	-1.37442200	4.35746600	-1.11646700
F	0.68886600	1.50346300	-1.89322200
F	-3.09679100	1.95560700	0.93511700
F	-2.72862900	-2.47549000	0.32931000
F	-0.88264000	1.27278300	2.57569600
F	0.70324500	-2.09375600	-1.55490700
F	-3.46995700	0.15299300	-1.44534500
F	6.49324100	-2.92545000	1.06346300
H	-0.15246600	-3.12466800	-3.68360100
H	-3.95660800	-1.07676600	-3.60837500
H	-3.68999000	-3.07787500	2.56788900
H	-2.01217400	0.32901000	4.62998000
H	-3.09164500	4.35896400	0.20720200
H	0.34598200	3.95298800	-2.37780200
H	-2.38557300	-2.68247100	-4.74241700
H	-3.38566900	-1.77933200	4.69546600
H	-1.45606900	5.40321100	-1.38769000

NHC4

C	-2.57878400	0.73053700	-0.72747400
C	-4.92189500	0.13781200	-0.70887200
C	-4.74111500	1.46482400	-0.93860400
H	-5.44931800	2.25046600	-1.11352600
N	-3.33576600	1.76792200	-0.94216500
C	-3.50415400	-0.46202900	-0.53572200
C	-2.86448900	3.17536000	-1.18013400
C	-3.38663300	3.63309400	-2.55374100
H	-4.47718300	3.65430600	-2.59891400
H	-3.02458300	4.64253200	-2.76030600
H	-3.02188600	2.97147400	-3.34277700
C	-1.33556100	3.21980500	-1.17152200
H	-0.91247500	2.57928100	-1.94624400
H	-1.01695100	4.24643000	-1.36592100
H	-0.92051800	2.91322900	-0.21159200
C	-3.41956900	4.06507900	-0.05425300

H	-3.06682700	3.71708300	0.91909400
H	-3.07233400	5.09087800	-0.19623200
H	-4.51130500	4.07992300	-0.03987200
C	-3.12777700	-1.49207900	-1.62862200
H	-2.06726400	-1.73590300	-1.55141500
H	-3.69166400	-2.42120200	-1.53492500
H	-3.31100700	-1.08318000	-2.62505200
C	-3.22534100	-0.99783100	0.89221600
H	-3.82796200	-1.87544700	1.12925800
H	-2.17579800	-1.27980800	0.98461600
H	-3.44032000	-0.23099500	1.64026000
C	0.19366800	0.20505600	-0.20577800
H	-1.07321400	0.51588800	-0.49075500
H	0.16722600	0.68706400	0.75901800
H	0.06940600	-0.86432200	-0.26193900
H	0.61557900	0.72581600	-1.05097600
B	2.20006200	-0.20002200	0.32232300
C	2.56215700	-1.37355400	-0.73412700
C	2.40422200	-1.22718900	-2.11824600
C	3.07126800	-2.62993100	-0.38810400
C	2.65906600	-2.20148600	-3.06843200
C	3.35225100	-3.65258500	-1.28623300
C	3.13768000	-3.43639000	-2.64083700
C	2.06565300	-0.64129500	1.87828000
C	1.15276300	-1.59472800	2.34379000
C	2.86193400	-0.12615200	2.90799200
C	0.98192800	-1.97638800	3.66363200
C	2.74982200	-0.46395500	4.25114400
C	1.79441700	-1.39596100	4.63278800
C	2.91480600	1.23371400	0.06526200
C	4.09656600	1.40011000	-0.66582700
C	2.43760600	2.44383000	0.58065200
C	4.71970200	2.61667700	-0.91274700
C	3.00186800	3.69161300	0.37257600
C	4.16146800	3.77633300	-0.39127900
F	1.32252000	2.42644000	1.37270600
F	4.72344900	0.30762500	-1.16919800
F	3.34319900	-2.90282700	0.91272500
F	1.97202000	-0.02629600	-2.60050900
F	0.35013600	-2.23124600	1.43741900
F	3.84464500	0.75978700	2.60857400
N	-6.11094500	-0.54702200	-0.65662100
C	-6.18678500	-1.99257900	-0.35207000
H	-5.16550400	-2.32921400	-0.21810300

C	-7.40752200	0.13178800	-0.89054500
H	-8.15068800	-0.66053300	-0.79530000
C	-6.92335300	-2.27309900	0.96764000
H	-7.97921900	-1.99418300	0.91925100
H	-6.87889300	-3.34089700	1.19870100
H	-6.46341400	-1.72598600	1.79336900
C	-6.77119700	-2.80724700	-1.51746400
H	-6.71291700	-3.87487300	-1.28877200
H	-7.82256900	-2.57239000	-1.70342400
H	-6.21292900	-2.62483100	-2.43815800
C	-7.76532700	1.16765600	0.18887000
H	-7.71015500	0.72146300	1.18378100
H	-7.11150400	2.03935100	0.17953400
H	-8.78881800	1.51844100	0.03053100
C	-7.55797300	0.67408900	-2.32179100
H	-7.38711200	-0.11998000	-3.05158600
H	-8.57335300	1.05390800	-2.46382500
H	-6.86438500	1.48476900	-2.54439800
H	2.54273200	4.56180000	0.82419600
H	5.63175100	2.62783300	-1.49576400
H	3.74252400	-4.58834600	-0.90681200
H	2.49835200	-1.97433500	-4.11460000
H	0.24090000	-2.72743600	3.90600400
H	3.41927200	0.00032700	4.96398000
H	1.68993000	-1.67764200	5.67376400
H	3.35238500	-4.21783700	-3.36003400
H	4.63108200	4.73673100	-0.56746500

NHC5

C	-3.47785200	0.02544300	-0.52931800
C	-5.68373500	-0.92679100	-0.45524800
C	-5.73908900	0.42389900	-0.42834200
H	-6.58357200	1.08611000	-0.36581600
N	-4.39897300	0.94972200	-0.46850300
C	-4.20020700	-1.31617300	-0.53402100
C	-4.17124100	2.43513700	-0.45311900
C	-4.88187300	3.04282300	-1.67569200
H	-5.96131100	2.88007900	-1.65308700
H	-4.70694600	4.12064700	-1.69849800
H	-4.48907900	2.61365400	-2.60036000
C	-2.67324700	2.73318800	-0.52594700

H	-2.22862500	2.33093500	-1.43673100
H	-2.53385400	3.81654800	-0.52851800
H	-2.13488400	2.32480100	0.32907800
C	-4.74951700	2.99694700	0.85775600
H	-4.25590000	2.54284000	1.71984000
H	-4.58061900	4.07529900	0.89693600
H	-5.82414300	2.82372800	0.94473600
C	-3.78338800	-2.02968900	-1.84378300
H	-2.69510000	-2.08078700	-1.89945200
H	-4.16854200	-3.04879700	-1.89188300
H	-4.14276200	-1.48541500	-2.72055100
C	-3.76865000	-2.12107500	0.71355000
H	-4.30221600	-3.07304700	0.76244400
H	-2.69783200	-2.32179500	0.69096200
H	-3.98900400	-1.56719400	1.62870200
C	-0.58286700	-0.10162300	-0.40812400
H	-1.88193800	0.02192900	-0.47913100
H	-0.63524700	0.21836100	0.62120200
H	-0.53321000	-1.15829100	-0.62571400
H	-0.36174900	0.60283700	-1.19659400
B	1.39156100	-0.08240200	0.05335400
C	1.97050100	-0.79927900	-1.28125500
C	1.86778400	-0.21357400	-2.54997500
C	2.55790200	-2.06859900	-1.32949700
C	2.29591500	-0.77622300	-3.73946400
C	3.01563000	-2.69223200	-2.48489500
C	2.88537000	-2.03670800	-3.70166500
C	1.62064900	-0.87853800	1.45919400
C	0.72350400	-1.62951600	2.21640700
C	2.89024300	-0.81509400	2.04669500
C	1.00995200	-2.23491700	3.43308600
C	3.25063700	-1.39225300	3.25283600
C	2.28994400	-2.11038400	3.95773700
C	1.72941400	1.49940100	0.27074500
C	2.80399800	2.17863300	-0.31737500
C	1.01677500	2.30981500	1.15998000
C	3.11743200	3.51385200	-0.10139400
C	1.26867800	3.64759000	1.42293800
C	2.33774300	4.25727600	0.77606500
F	-0.03644500	1.76382600	1.84900100
F	3.63189300	1.50882200	-1.15164100
F	2.70279100	-2.78383700	-0.18525400
F	1.28416600	1.01571900	-2.64681000
F	-0.55530000	-1.81412700	1.76078700

F	3.86708300	-0.15424200	1.37312100
N	-6.74453300	-1.78665000	-0.28022000
C	-6.75673100	-3.10861500	-0.89655700
H	-7.52937900	-3.71098700	-0.41545600
H	-6.96930400	-3.07241200	-1.97508500
H	-5.80602800	-3.61423800	-0.74815300
C	-8.05714200	-1.17955400	-0.11979500
H	-8.41798900	-0.69860500	-1.04223500
H	-8.77514400	-1.94665400	0.17272400
H	-8.02131100	-0.42614800	0.67051000
H	3.97167200	3.93825300	-0.61328700
H	0.64431200	4.17519700	2.13260600
H	3.46388400	-3.67438500	-2.40474000
H	2.17008500	-0.22360900	-4.66169100
H	4.26601200	-1.27879300	3.61038500
H	0.23184500	-2.79185600	3.93940100
H	2.56686500	5.29974100	0.96223800
H	2.53973300	-2.57437800	4.90435500
H	3.23741200	-2.50284900	-4.61418000

NHC6

C	3.72848200	-0.59400200	0.70955900
C	5.70398700	-1.89416000	0.90043200
C	6.03578600	-0.61031700	0.71970600
H	6.99935800	-0.13275000	0.65449200
N	4.80494500	0.14547600	0.60952500
C	4.20037000	-2.02498800	0.90293000
C	4.85170000	1.63271600	0.39682800
C	5.62476000	2.26197600	1.56931400
H	6.65845500	1.91368700	1.62261400
H	5.64666500	3.34708300	1.44854100
H	5.13537400	2.03426100	2.51905900
C	3.43022400	2.19479000	0.35408300
H	2.89261700	1.99652200	1.28201500
H	3.48912700	3.27720600	0.22005500
H	2.85170400	1.78307400	-0.47248200
C	5.56142900	1.90112700	-0.94181900
H	5.01992200	1.42828000	-1.76402500
H	5.59370000	2.97671400	-1.12805300
H	6.58926200	1.53117000	-0.94726700
C	3.68373100	-2.58231300	2.24810300

H	2.59495600	-2.64725700	2.23614900
H	4.09454200	-3.58096700	2.41300100
H	3.98233100	-1.94520700	3.08389300
C	3.72245000	-2.90373000	-0.27753000
H	4.13232400	-3.91053600	-0.16848700
H	2.63458400	-2.96003900	-0.29842200
H	4.05851400	-2.49709400	-1.23412500
C	0.86129300	-0.25715300	0.48475600
H	2.16241500	-0.33096700	0.58411000
H	0.99988400	-0.02425200	-0.55996100
H	0.66523600	-1.27833700	0.77559100
H	0.74056600	0.52721200	1.21805200
B	-1.05517800	-0.00182900	-0.04674800
C	-1.77562900	-0.53852300	1.30539700
C	-1.63454100	0.11306100	2.53744100
C	-2.53394100	-1.71006600	1.40951300
C	-2.17584000	-0.30281900	3.74119700
C	-3.11073000	-2.18545100	2.58199900
C	-2.93184800	-1.47148800	3.75892900
C	-1.35320200	-0.85421700	-1.40696100
C	-0.55137300	-1.78106500	-2.07054600
C	-2.57958400	-0.65324600	-2.05256200
C	-0.88285300	-2.42940300	-3.25295100
C	-2.98034800	-1.26178600	-3.23033000
C	-2.11269200	-2.16198200	-3.84047600
C	-1.16738400	1.59407100	-0.37906100
C	-2.15892600	2.44982200	0.11724200
C	-0.31953800	2.24057500	-1.28370100
C	-2.27860800	3.79770100	-0.19398300
C	-0.37542800	3.57956300	-1.63893300
C	-1.37293700	4.36960900	-1.07899200
F	0.67059500	1.51309500	-1.89556400
F	-3.09987800	1.95482400	0.95357700
F	-2.73882300	-2.47577200	0.30802400
F	-0.88804500	1.25457200	2.58069300
F	0.67153000	-2.11272000	-1.54736000
F	-3.47151700	0.18957700	-1.47068700
O	6.46655600	-2.99420300	1.05946900
H	7.40198200	-2.76301700	1.02664800
H	-3.95565900	-1.03074700	-3.63909600
H	-0.17870900	-3.12935700	-3.68450800
H	0.33935700	3.96922000	-2.35250100
H	-3.08473800	4.36620700	0.25189400
H	-2.00536500	0.28965700	4.63094600

H	-3.68735500	-3.10095200	2.54552400
H	-1.45019100	5.41857800	-1.33892900
H	-2.39651300	-2.65585700	-4.76204700
H	-3.37477200	-1.82166700	4.68363400

NHC7

C	-3.04728400	0.55238600	-0.37697100
C	-5.36370500	-0.04673000	-0.18683600
C	-5.21557100	1.27970000	-0.25844900
H	-5.96621800	2.05356000	-0.23883900
N	-3.81691300	1.61315600	-0.36593900
C	-3.95956600	-0.65418900	-0.26014400
C	-3.37915900	3.05034600	-0.44419900
C	-4.04368700	3.68755700	-1.67741200
H	-5.13379500	3.68937200	-1.60974000
H	-3.71646800	4.72521000	-1.76991800
H	-3.75486100	3.15744100	-2.58793300
C	-1.85832400	3.12250900	-0.57922100
H	-1.51085500	2.61368400	-1.47902100
H	-1.56438400	4.17218200	-0.64780400
H	-1.35220400	2.68599400	0.28136200
C	-3.82363100	3.75438000	0.84966700
H	-3.36697800	3.27982900	1.72097600
H	-3.50448700	4.79854100	0.82340600
H	-4.90834000	3.74148100	0.97768900
C	-3.80411500	-1.52685500	-1.52998200
H	-2.78566200	-1.91168600	-1.60283100
H	-4.49506100	-2.37180300	-1.48157700
H	-4.02401600	-0.95696900	-2.43577500
C	-3.55336900	-1.46751600	0.99265400
H	-4.14167000	-2.38475000	1.05245900
H	-2.50037600	-1.74211800	0.93943900
H	-3.70538400	-0.89273600	1.90921700
C	-0.19449200	0.02345400	-0.36100800
H	-1.47083600	0.32532100	-0.38266600
H	-0.17864300	0.39241100	0.65310800
H	-0.31146000	-1.03598500	-0.53375100
H	0.06317400	0.66324400	-1.19244200
B	1.75889500	-0.17894600	0.01315000
C	2.19366100	-1.02043300	-1.30546000
C	2.11047900	-0.48187500	-2.59591900

C	2.61844900	-2.35376100	-1.31411800
C	2.41674100	-1.14309200	-3.77223000
C	2.94633700	-3.07854800	-2.45451000
C	2.84745100	-2.46455500	-3.69552100
C	1.95936000	-0.93660600	1.44613900
C	1.01546500	-1.54593600	2.27068700
C	3.25217000	-1.00146700	1.98067200
C	1.28175500	-2.13482700	3.49975100
C	3.59516800	-1.57097200	3.19563300
C	2.58936700	-2.14316600	3.96782500
C	2.30648400	1.35602500	0.14047800
C	3.44038500	1.85884100	-0.51066100
C	1.73679500	2.29633800	1.00399700
C	3.93392800	3.14921400	-0.37187500
C	2.17090100	3.59972300	1.19181800
C	3.28888500	4.03065900	0.48674600
F	0.64367200	1.93044000	1.75001500
F	4.14413700	1.04753700	-1.33283000
F	2.72363500	-3.03187500	-0.14319700
F	1.67707100	0.80593800	-2.72925700
F	-0.29602900	-1.59504900	1.87394700
F	4.26958300	-0.48709600	1.24281700
C	-6.65654300	-0.75866100	-0.15667400
C	-6.95078700	-1.73277800	0.81019700
C	-7.63971500	-0.45356200	-1.11184700
C	-8.18650600	-2.37283900	0.82192700
H	-6.22345200	-1.97066300	1.57504400
C	-8.87425400	-1.09586300	-1.09904700
H	-7.42067300	0.28018600	-1.87914600
C	-9.15201000	-2.05924100	-0.13225600
H	-8.39680300	-3.11552300	1.58323300
H	-9.61659200	-0.84763200	-1.84924000
H	-10.11199800	-2.56244500	-0.12280600
H	4.81922400	3.43119200	-0.92740600
H	1.64617300	4.23807400	1.89115900
H	4.63166100	-1.56564900	3.50763800
H	0.46698400	-2.57642100	4.05930200
H	3.27319200	-4.10467200	-2.34415600
H	2.32193400	-0.61905900	-4.71463700
H	2.82479300	-2.59779200	4.92261400
H	3.65976900	5.04067700	0.61388800
H	3.10122300	-3.00960000	-4.59686300

S 1.3.4 **B5Cl**-NHC TSs

NHC1

C	-3.41483800	0.15506600	-0.27268800
C	-5.57508400	-0.82731600	-0.29383100
C	-5.67784500	0.49531100	-0.36478300
H	-6.54725400	1.12929500	-0.42706000
N	-4.34728100	1.07077000	-0.34997500
C	-4.11066900	-1.19125400	-0.22545600
C	-4.15945900	2.56252400	-0.41929000
C	-4.78848400	3.06153900	-1.73182000
H	-5.86115900	2.86292400	-1.78171900
H	-4.64820900	4.14146100	-1.81170200
H	-4.30948100	2.59122700	-2.59351000
C	-2.66834600	2.89605000	-0.39758200
H	-2.14668200	2.44747800	-1.24392000
H	-2.55278600	3.97994900	-0.45954800
H	-2.19276800	2.55744000	0.52324200
C	-4.85509700	3.18697900	0.80274900
H	-4.42709400	2.80021500	1.73018600
H	-4.71094200	4.26917600	0.78725500
H	-5.93045200	2.99597100	0.81170400
C	-3.67279200	-2.04852500	-1.43865300
H	-2.60183400	-2.25054000	-1.39362100
H	-4.20411600	-3.00331100	-1.42498900
H	-3.89343900	-1.54712400	-2.38338600
C	-3.76031500	-1.91660900	1.09782300
H	-4.31016300	-2.85912700	1.15529900
H	-2.69359600	-2.14027100	1.14154900
H	-4.02801700	-1.31147200	1.96673000
C	-0.55684000	0.02847100	-0.09394700
H	-1.88588300	0.17569500	-0.18901800
H	-0.55276700	-0.33292600	0.92003200
H	-0.44831200	-0.68078300	-0.89655100
H	-0.33760500	1.06381200	-0.28313100
B	1.72855100	-0.06872600	0.08687900
C	2.06708400	-0.73389500	-1.37314000
C	1.49848100	-0.29151200	-2.58806700
C	2.91643700	-1.85429000	-1.50778700
C	1.59211300	-1.00758700	-3.78823700
C	3.03231400	-2.59469900	-2.69154900
C	2.33169500	-2.19255600	-3.83110100

C	1.83880900	-1.03498800	1.40816100
C	1.09383400	-2.22325500	1.57623800
C	2.65559200	-0.70609500	2.51245400
C	1.00250900	-2.90972500	2.79364600
C	2.58829800	-1.36893100	3.74511400
C	1.72344500	-2.45464500	3.90096300
C	2.04183600	1.52994800	0.28828500
C	3.02335900	2.20443500	-0.47070000
C	1.32510900	2.36258000	1.17649100
C	3.15166800	3.59949700	-0.49828600
C	1.42865300	3.75964000	1.17491100
C	2.32062200	4.38739200	0.30165000
Cl	0.00545600	-4.33009800	2.95331800
Cl	0.29142400	-2.97748100	0.20700200
Cl	0.30083300	1.66958000	2.42450900
Cl	0.46396300	4.73460900	2.25085000
Cl	0.69532700	1.26816700	-2.68492300
Cl	2.42486200	6.12085600	0.24329700
Cl	0.80269700	-0.44493800	-5.23604200
Cl	4.23628200	1.29654000	-1.34431700
Cl	4.33323000	4.36985400	-1.51648300
Cl	3.91189000	0.50036200	2.34801300
Cl	2.41453900	-3.12747400	-5.29299100
Cl	3.56745500	-0.86015300	5.08993700
Cl	3.98452500	-2.31060800	-0.19927100
Cl	1.57996600	-3.25548600	5.43582000
Cl	4.03771500	-4.01256100	-2.76549300
H	-6.39433700	-1.53211500	-0.28507900

NHC2

C	-3.40778800	0.14899200	-0.27346200
C	-5.55725400	-0.82450000	-0.28479600
C	-5.66996400	0.50055800	-0.35644200
H	-6.54696600	1.12248900	-0.41539500
N	-4.34240600	1.06509000	-0.34720500
C	-4.09290800	-1.20342900	-0.22208000
C	-4.15291600	2.55889200	-0.41887600
C	-4.78615900	3.05568400	-1.72983300
H	-5.85959600	2.85999900	-1.77512400
H	-4.64384600	4.13509400	-1.81186400
H	-4.31164100	2.58312700	-2.59272000

C	-2.66076500	2.88692200	-0.40285000
H	-2.14323700	2.43650100	-1.25072300
H	-2.54323300	3.97038100	-0.46700600
H	-2.18305100	2.54957300	0.51728300
C	-4.84311300	3.18400400	0.80550500
H	-4.41270300	2.79706900	1.73170100
H	-4.69666000	4.26578400	0.78880000
H	-5.91896600	2.99595200	0.81820800
C	-3.66059500	-2.05366000	-1.44007500
H	-2.59057000	-2.25727400	-1.39277300
H	-4.19723100	-3.00467400	-1.43030900
H	-3.87944000	-1.54480200	-2.38106600
C	-3.73598100	-1.92188600	1.10116800
H	-4.29054100	-2.86028700	1.16666700
H	-2.66980600	-2.14761800	1.13262700
H	-3.99320500	-1.31016700	1.96844000
C	-0.54873300	0.02262800	-0.09480500
H	-1.87905200	0.16959400	-0.19078100
H	-0.55682900	-0.33411200	0.92058000
H	-0.45164500	-0.68911100	-0.89642200
H	-0.34433900	1.05980300	-0.28938600
B	1.70603400	-0.06829000	0.08490000
C	2.05424200	-0.73275500	-1.37512400
C	1.48686300	-0.29250000	-2.59121500
C	2.90747900	-1.85025900	-1.50819900
C	1.58588600	-1.00713700	-3.79178900
C	3.02856800	-2.58981400	-2.69213000
C	2.32959400	-2.18953000	-3.83337800
C	1.82461400	-1.03523400	1.40719800
C	1.08330200	-2.22554600	1.57600600
C	2.64099000	-0.70424800	2.51101100
C	0.99500300	-2.91342200	2.79281600
C	2.57650500	-1.36791000	3.74356300
C	1.71535500	-2.45651500	3.89975300
C	2.02386500	1.53136700	0.28734000
C	3.00685600	2.20548500	-0.46992000
C	1.30604900	2.36460100	1.17389500
C	3.13596400	3.60064100	-0.49691700
C	1.41036000	3.76159700	1.17331800
C	2.30422300	4.38900900	0.30183500
Cl	0.00278000	-4.33702100	2.95222200
Cl	0.28264600	-2.98248800	0.20634400
Cl	0.27971200	1.67177200	2.42123700
Cl	0.44443100	4.73674100	2.24805000

Cl	0.67876300	1.26534900	-2.68954100
Cl	2.40975700	6.12234200	0.24425800
Cl	0.79826200	-0.44620600	-5.24115400
Cl	4.22071500	1.29775900	-1.34201200
Cl	4.31932300	4.37053800	-1.51315200
Cl	3.89352800	0.50599500	2.34683800
Cl	2.41929400	-3.12327200	-5.29543300
Cl	3.55460200	-0.85637700	5.08797300
Cl	3.97397900	-2.30408300	-0.19766300
Cl	1.57562200	-3.25850900	5.43418000
Cl	4.03832200	-4.00449500	-2.76412800
Br	-6.99003900	-2.04854400	-0.26370800

NHC3

C	-3.40560700	0.15692600	-0.27092400
C	-5.53664500	-0.81789400	-0.29869000
C	-5.67890500	0.50229600	-0.36599100
H	-6.56416100	1.11090000	-0.42654100
N	-4.34698300	1.06559400	-0.34644000
C	-4.08751400	-1.19877900	-0.22862500
C	-4.16282300	2.55972100	-0.41032100
C	-4.79247100	3.06077500	-1.72143200
H	-5.86476800	2.86057300	-1.77237200
H	-4.65419500	4.14116300	-1.79728400
H	-4.31213800	2.59454500	-2.58456100
C	-2.67198200	2.89320000	-0.38660100
H	-2.14961900	2.44950000	-1.23502900
H	-2.55831400	3.97743600	-0.44397100
H	-2.19620200	2.55197600	0.53310200
C	-4.86053700	3.17671900	0.81393700
H	-4.43176800	2.78780700	1.74008600
H	-4.71903700	4.25923700	0.80221200
H	-5.93541300	2.98321000	0.82171100
C	-3.66491300	-2.05394500	-1.44745600
H	-2.60180500	-2.28829200	-1.39000900
H	-4.22889100	-2.98929400	-1.44896200
H	-3.85806200	-1.53371400	-2.38791800
C	-3.75828500	-1.93006300	1.09577800
H	-4.34038300	-2.85236000	1.15474400
H	-2.69921100	-2.18576600	1.13402200
H	-4.00325000	-1.31333900	1.96311800

C	-0.54745600	0.03317100	-0.09290400
H	-1.87615100	0.18121900	-0.18689100
H	-0.55116300	-0.32334100	0.92265200
H	-0.44885400	-0.67908700	-0.89392800
H	-0.33685000	1.06920000	-0.28756100
B	1.71571900	-0.06632900	0.08413200
C	2.05730300	-0.73399900	-1.37546800
C	1.48941800	-0.29288800	-2.59108700
C	2.90572100	-1.85518600	-1.50858500
C	1.58324200	-1.00977900	-3.79074700
C	3.02172800	-2.59676100	-2.69173400
C	2.32217300	-2.19518500	-3.83216700
C	1.83033400	-1.03193000	1.40720000
C	1.08378100	-2.21856100	1.57863500
C	2.64948600	-0.70294800	2.50961800
C	0.99327800	-2.90370900	2.79679000
C	2.58335000	-1.36435300	3.74324900
C	1.71705600	-2.44850400	3.90218800
C	2.03739400	1.53221200	0.28397900
C	3.02092300	2.20250500	-0.47601200
C	1.32356400	2.36857900	1.17086200
C	3.15375100	3.59722000	-0.50537900
C	1.43162600	3.76528000	1.16785400
C	2.32551200	4.38896700	0.29368100
Cl	-0.00622200	-4.32194000	2.95992100
Cl	0.27851300	-2.97432900	0.21098200
Cl	0.29757500	1.68043400	2.42087800
Cl	0.47041700	4.74467000	2.24288700
Cl	0.68717700	1.26766100	-2.68991200
Cl	2.43548700	6.12191100	0.23316100
Cl	0.79490900	-0.44784300	-5.23938500
Cl	4.23072400	1.28995400	-1.34884800
Cl	4.33741200	4.36237000	-1.52486200
Cl	3.90709000	0.50147300	2.34190500
Cl	2.40538200	-3.13126700	-5.29314000
Cl	3.56556500	-0.85546800	5.08562100
Cl	3.97248900	-2.31168200	-0.19917800
Cl	1.57511100	-3.24725100	5.43810100
Cl	4.02585400	-4.01546100	-2.76375800
F	-6.51090100	-1.72584300	-0.28992900

NHC4

C	-2.67789600	0.66866800	-0.14335600
C	-4.84123200	0.26456200	-1.13562800
C	-4.92169600	1.12127500	-0.08277100
H	-5.76334700	1.62269800	0.35166900
N	-3.61383600	1.33072500	0.47278000
C	-3.34543400	-0.11452400	-1.26357200
C	-3.43536800	2.24340900	1.65554900
C	-3.92847400	3.64643400	1.26028300
H	-4.99134400	3.65873600	1.01208500
H	-3.77285600	4.33289100	2.09526200
H	-3.36932600	4.02277100	0.40064200
C	-1.95795400	2.30566800	2.04219700
H	-1.34727100	2.68884600	1.22381100
H	-1.84868000	2.97687900	2.89653200
H	-1.57652700	1.32612300	2.33036200
C	-4.25538200	1.67692900	2.82773900
H	-3.91911300	0.66887000	3.08022100
H	-4.11834800	2.31151100	3.70588300
H	-5.32362100	1.63857500	2.60607300
C	-2.69366000	0.36463200	-2.58418400
H	-1.61419400	0.21740600	-2.53306000
H	-3.06354000	-0.18261700	-3.45197100
H	-2.88463500	1.42787500	-2.74657500
C	-3.06125400	-1.61091100	-0.97834700
H	-3.48287000	-2.26537600	-1.74177300
H	-1.98466000	-1.78312700	-0.95312400
H	-3.47951400	-1.90573100	-0.01314600
C	0.13122100	0.18826800	0.12597500
H	-1.17847100	0.47306600	0.05516600
H	0.38221400	0.94952700	0.84321800
H	0.04751100	-0.82997500	0.46692700
H	0.40337600	0.35625000	-0.90296700
B	2.45546400	-0.23380300	0.44928800
C	2.39444300	-1.86631400	0.53306600
C	1.68113500	-2.67782400	-0.37698700
C	3.02778700	-2.58292400	1.57301500
C	1.44304500	-4.04210800	-0.16637900
C	2.80918700	-3.94535500	1.81350100
C	1.97634800	-4.67343200	0.96058600
C	2.64657700	0.59495300	1.84730600
C	1.77577200	0.48169600	2.95484700
C	3.68774200	1.53317600	2.02340500
C	1.81147200	1.35163700	4.05220100
C	3.74864200	2.42195400	3.10471000

C	2.77999100	2.35751400	4.10904900
C	3.01334700	0.43797200	-0.93229500
C	3.92004200	-0.24230200	-1.77585200
C	2.60645400	1.70036700	-1.41919800
C	4.23376700	0.18456600	-3.07241600
C	2.90098700	2.15685000	-2.71045700
C	3.68702000	1.37368500	-3.56036000
N	-5.86641600	-0.17888000	-1.93048800
C	-5.65960500	-1.12464600	-3.05018100
H	-4.59910800	-1.34629400	-3.06838500
C	-7.26386500	0.26982500	-1.71443100
H	-7.83644200	-0.24185200	-2.48859300
C	-6.38805500	-2.45959400	-2.82896200
H	-7.47499400	-2.34408200	-2.83192100
H	-6.13332700	-3.15791300	-3.63063600
H	-6.09479000	-2.91049300	-1.87853200
C	-6.00628900	-0.50212000	-4.41221700
H	-5.74855700	-1.19893500	-5.21431300
H	-7.07201300	-0.27835500	-4.50690800
H	-5.44783100	0.42272400	-4.57213900
C	-7.85729600	-0.20449400	-0.37736100
H	-7.76408100	-1.28791700	-0.27911900
H	-7.37676100	0.24945500	0.48899500
H	-8.92004500	0.04923700	-0.34012500
C	-7.46785100	1.77225100	-1.97103800
H	-7.09957700	2.04479300	-2.96206500
H	-8.53484200	2.00701500	-1.92865700
H	-6.96006700	2.40400500	-1.24249400
Cl	4.24446400	-1.80545600	2.56157200
Cl	0.49302700	-4.97438900	-1.29178300
Cl	1.11146900	-2.02393100	-1.90382300
Cl	4.81123900	-1.62397300	-1.17651900
Cl	5.29693000	-0.74550400	-4.08860700
Cl	4.01698100	1.89389800	-5.18499400
Cl	2.30672100	3.69299500	-3.27868200
Cl	1.76125900	2.83267100	-0.37770000
Cl	5.05360800	1.54588000	0.93064400
Cl	5.01650600	3.60789300	3.21951800
Cl	2.80496200	3.48284400	5.43289600
Cl	0.66936100	1.19718100	5.35979100
Cl	0.62425300	-0.83982200	3.05866900
Cl	3.56130600	-4.74885500	3.16101500
Cl	1.64557100	-6.35058100	1.27133600

NHC5

C	-3.44249700	0.12698100	-0.30694800
C	-5.61161400	-0.89111000	-0.34297900
C	-5.70712700	0.45715600	-0.42176800
H	-6.57070700	1.09352900	-0.48597800
N	-4.38476200	1.02454400	-0.38814100
C	-4.11700000	-1.23604800	-0.27520200
C	-4.20145800	2.51639500	-0.45507100
C	-4.81246100	3.01611300	-1.77590900
H	-5.88315200	2.81373900	-1.84117400
H	-4.67152700	4.09630900	-1.85311100
H	-4.32016800	2.54602400	-2.63025100
C	-2.71209000	2.85706500	-0.41283300
H	-2.17707700	2.41278400	-1.25282900
H	-2.60117500	3.94180300	-0.47016600
H	-2.24704900	2.51754700	0.51301400
C	-4.91380300	3.14134000	0.75715400
H	-4.50057100	2.75090200	1.68982400
H	-4.76537100	4.22315300	0.74556400
H	-5.98889400	2.95158100	0.74977900
C	-3.58324500	-2.02356500	-1.49789000
H	-2.49431000	-2.06148200	-1.45849300
H	-3.95173900	-3.04933300	-1.51024200
H	-3.87453800	-1.54257700	-2.43454800
C	-3.75639700	-1.93683000	1.05563800
H	-4.27800800	-2.89137900	1.14728900
H	-2.68377200	-2.12864600	1.10411300
H	-4.03895200	-1.31889700	1.91072900
C	-0.58957200	0.02424800	-0.11065200
H	-1.92329800	0.15935000	-0.21641800
H	-0.56251500	-0.35728000	0.89618800
H	-0.43771500	-0.66856200	-0.92112600
H	-0.34986400	1.05985100	-0.27473600
B	1.77018400	-0.06532400	0.08410100
C	2.10053800	-0.71398400	-1.38071900
C	1.52998500	-0.26064500	-2.59104300
C	2.95307000	-1.83090800	-1.52605000
C	1.62405700	-0.96712700	-3.79692800
C	3.06979900	-2.56048200	-2.71606600
C	2.36640200	-2.15003600	-3.85093400
C	1.86336200	-1.04227200	1.39365500
C	1.12153800	-2.23514300	1.54333800
C	2.67058900	-0.72120000	2.50760600

C	1.02256500	-2.93215100	2.75412300
C	2.59577900	-1.39547900	3.73322300
C	1.73286300	-2.48511700	3.87164000
C	2.05543800	1.53190200	0.30054100
C	3.03125400	2.22450500	-0.44987100
C	1.32784000	2.34691200	1.19661800
C	3.14471600	3.62068400	-0.46321300
C	1.41625700	3.74499900	1.20798100
C	2.30325700	4.39110900	0.34286700
N	-6.65714400	-1.77062500	-0.20718800
C	-6.56600500	-3.14992800	-0.67562600
H	-7.36884200	-3.72749500	-0.21462200
H	-6.66328000	-3.23419300	-1.76727900
H	-5.62370200	-3.60088700	-0.37543300
C	-7.99732100	-1.20251900	-0.22750100
H	-8.27265400	-0.80734800	-1.21694300
H	-8.71851200	-1.97138700	0.05070400
H	-8.06553300	-0.39079500	0.50063000
Cl	0.02879000	-4.35736500	2.89307500
Cl	0.33267200	-2.97840100	0.16160500
Cl	0.30738000	1.63078900	2.43260400
Cl	0.43840500	4.69895100	2.29064200
Cl	0.72275400	1.29612100	-2.67261000
Cl	2.38871900	6.12619000	0.30197100
Cl	0.83157100	-0.39424000	-5.23918500
Cl	4.25515300	1.33715300	-1.32997400
Cl	4.32069400	4.41395100	-1.47065000
Cl	3.92388800	0.49100600	2.36284700
Cl	2.44942400	-3.07248100	-5.32104000
Cl	3.56328300	-0.89665200	5.09031300
Cl	4.02334200	-2.29458900	-0.22160600
Cl	1.57932200	-3.30054900	5.39800600
Cl	4.07977900	-3.97462200	-2.80369900

NHC6

C	-3.41838300	0.16229000	-0.28534900
C	-5.56790600	-0.82570000	-0.32803100
C	-5.69126200	0.50559700	-0.39613300
H	-6.56478200	1.13210000	-0.46360500
N	-4.35754500	1.06866100	-0.36718600
C	-4.10530800	-1.18970500	-0.24805000

C	-4.17025700	2.56055600	-0.42880200
C	-4.78851500	3.06657000	-1.74376500
H	-5.86115000	2.87062700	-1.80233600
H	-4.64433000	4.14636500	-1.81838900
H	-4.30455000	2.59779600	-2.60349500
C	-2.67911800	2.89357600	-0.39477600
H	-2.15162000	2.44913500	-1.23952500
H	-2.56357400	3.97784000	-0.45031000
H	-2.20998700	2.54993500	0.52738600
C	-4.87377200	3.18100000	0.79071000
H	-4.45348700	2.78851700	1.71925600
H	-4.72698100	4.26293900	0.78127400
H	-5.94934300	2.99159200	0.79089300
C	-3.67499400	-2.04433500	-1.46277300
H	-2.61299100	-2.28265700	-1.39747000
H	-4.24465700	-2.97601400	-1.47173400
H	-3.85669900	-1.52044900	-2.40385300
C	-3.78567800	-1.91918100	1.07807500
H	-4.37373000	-2.83753800	1.13651200
H	-2.72749600	-2.17827800	1.12376600
H	-4.03171800	-1.29820800	1.94248100
C	-0.56415200	0.03402800	-0.09901400
H	-1.89182700	0.18382800	-0.19614200
H	-0.55497400	-0.33394500	0.91272900
H	-0.44617300	-0.67086600	-0.90433400
H	-0.33253300	1.06824400	-0.28040300
B	1.74319100	-0.06965600	0.08927100
C	2.07853100	-0.73082500	-1.37182200
C	1.51343500	-0.28217800	-2.58621200
C	2.92452000	-1.85358800	-1.50871400
C	1.60688400	-0.99489700	-3.78839600
C	3.04003600	-2.59046600	-2.69460800
C	2.34264900	-2.18217100	-3.83394000
C	1.84280000	-1.03911300	1.40736500
C	1.09351700	-2.22557200	1.56950600
C	2.65674300	-0.71543600	2.51537800
C	0.99527500	-2.91406200	2.78526600
C	2.58302700	-1.38091100	3.74608800
C	1.71379900	-2.46394300	3.89621400
C	2.05360100	1.52759600	0.29560500
C	3.03695800	2.20395700	-0.45946000
C	1.33524300	2.35762400	1.18506200
C	3.16563100	3.59894500	-0.48295500
C	1.43901300	3.75467500	1.18706000

C	2.33289300	4.38467500	0.31734500
Cl	0.29396400	-2.97383100	0.19592900
Cl	0.30810200	1.66145400	2.42826900
Cl	0.71497700	1.27966800	-2.67909300
Cl	2.43739800	6.11837300	0.26378200
Cl	4.25139200	1.29775500	-1.33293400
Cl	3.91728600	0.48765200	2.35773800
Cl	2.42494900	-3.11258200	-5.29881400
Cl	3.98883500	-2.31739200	-0.19964700
Cl	1.56204200	-3.26777800	5.42879200
O	-6.49132000	-1.80440500	-0.32092900
H	-7.38005700	-1.43398200	-0.37425800
Cl	-0.00780100	-4.33086600	2.93831800
Cl	3.55950800	-0.87876800	5.09548500
Cl	4.04117200	-4.01127600	-2.77156600
Cl	0.82193200	-0.42499000	-5.23586500
Cl	4.34975100	4.37190000	-1.49639200
Cl	0.47211200	4.72702100	2.26345400

NHC7

C	-2.98212500	0.67371000	-0.30151100
C	-5.27587700	-0.01091900	-0.28167800
C	-5.17147200	1.32252700	-0.29117100
H	-5.94769400	2.07060300	-0.29511200
N	-3.78261500	1.70845800	-0.30884200
C	-3.84957800	-0.56812000	-0.27643800
C	-3.39326100	3.16243000	-0.34037800
C	-3.99187700	3.78755200	-1.61255800
H	-5.08271400	3.73900100	-1.62699400
H	-3.70648500	4.84003400	-1.66697100
H	-3.61251500	3.28486700	-2.50505600
C	-1.87047600	3.28602300	-0.36603400
H	-1.44572700	2.79729800	-1.24379500
H	-1.60566900	4.34475400	-0.40066900
H	-1.41681100	2.85362500	0.52609500
C	-3.95232100	3.83458100	0.92552400
H	-3.54678500	3.36362200	1.82372400
H	-3.66352500	4.88750400	0.93406700
H	-5.04248300	3.78957500	0.97269400
C	-3.49184700	-1.44527600	-1.50087200
H	-2.42336200	-1.66452600	-1.49602600

H	-4.02737400	-2.39460500	-1.45819300
H	-3.73645000	-0.94509700	-2.44053600
C	-3.57624300	-1.35134300	1.03278500
H	-4.24992500	-2.20915700	1.09154500
H	-2.54830400	-1.71535300	1.05176400
H	-3.74295200	-0.72660300	1.91321400
C	-0.16579900	0.17350000	-0.11252200
H	-1.46342800	0.48985000	-0.22058900
H	-0.20241500	-0.18023300	0.90372000
H	-0.14208900	-0.55052800	-0.90891900
H	0.19093700	1.16895400	-0.30736000
B	2.10231100	-0.22186700	0.03808800
C	2.32805200	-0.93402700	-1.42091900
C	1.80653900	-0.42688900	-2.63186100
C	3.02501500	-2.15488600	-1.55860000
C	1.79878400	-1.15192000	-3.83049400
C	3.03516400	-2.90684000	-2.74069800
C	2.38254900	-2.42081800	-3.87605700
C	2.10718100	-1.18200000	1.36718900
C	1.21721200	-2.26168100	1.56002600
C	2.97811500	-0.95158600	2.45510900
C	1.05790400	-2.91920700	2.78640500
C	2.84568800	-1.58855800	3.69597400
C	1.85022100	-2.55146900	3.87727500
C	2.62313800	1.32372400	0.21752400
C	3.67138000	1.85793700	-0.56406800
C	2.03777300	2.24983500	1.10921100
C	3.97871700	3.22423300	-0.60956200
C	2.32103500	3.62158400	1.08990000
C	3.27061500	4.12054800	0.19440800
C	-6.54075600	-0.76227100	-0.17138100
C	-7.48792600	-0.38492500	0.79498800
C	-6.84609100	-1.84337700	-1.01274500
C	-8.69903000	-1.05946000	0.91163600
H	-7.25796200	0.43032300	1.47141600
C	-8.05863300	-2.51598200	-0.89480600
H	-6.14901900	-2.14223900	-1.78402800
C	-8.98886100	-2.12854300	0.06714100
H	-9.41291900	-0.75439800	1.66828200
H	-8.27841600	-3.34256900	-1.56081400
H	-9.93041300	-2.65737300	0.15930200
Cl	0.30124900	-2.91805700	0.21176700
Cl	-0.11271200	-4.19567200	2.97780700
Cl	1.63046000	-3.31311000	5.42294500

Cl	3.90447100	-1.19808700	5.02014100
Cl	4.37763700	0.07992400	2.25824000
Cl	5.23297100	3.82544000	-1.65458500
Cl	4.74420100	0.79243600	-1.44359200
Cl	4.03794300	-2.74164700	-0.25828000
Cl	3.85059200	-4.44175500	-2.81838500
Cl	2.33585800	-3.36071300	-5.33637800
Cl	1.07502900	-0.49710200	-5.27384600
Cl	1.19988300	1.21940300	-2.72732800
Cl	0.95899900	1.70438300	2.38414700
Cl	1.51133700	4.72276600	2.17171600
Cl	3.59657200	5.82540400	0.11396000

S 1.3.5 **B3Cl**-NHC TSs

NHC1

C	-3.42811900	0.15659900	-0.25103300
C	-5.58786400	-0.82941300	-0.29143200
C	-5.69075000	0.49156400	-0.38828800
H	-6.55986600	1.12291400	-0.47700600
N	-4.36130300	1.06883700	-0.36087100
C	-4.12422500	-1.18933800	-0.19188300
C	-4.17387000	2.55900100	-0.45236200
C	-4.77942600	3.03495300	-1.78438700
H	-5.85105700	2.83489200	-1.85015600
H	-4.63777000	4.11338100	-1.88094800
H	-4.28468400	2.54966200	-2.62868800
C	-2.68374700	2.89480500	-0.40879200
H	-2.14606500	2.43814600	-1.24043900
H	-2.56880100	3.97827200	-0.48200200
H	-2.22266700	2.56541400	0.52278600
C	-4.89290400	3.20312300	0.74576900
H	-4.48149600	2.83230700	1.68719300
H	-4.75031600	4.28526700	0.71455600
H	-5.96801500	3.01042200	0.73840700
C	-3.66477200	-2.06795000	-1.38159000
H	-2.59460700	-2.26742100	-1.31461800
H	-4.19582900	-3.02285400	-1.35994000
H	-3.87031500	-1.58360600	-2.33862600
C	-3.79379100	-1.88940500	1.15000100

H	-4.33964100	-2.83400800	1.21406700
H	-2.72630100	-2.10403300	1.21507300
H	-4.08026500	-1.27037000	2.00304500
C	-0.56642900	0.03092600	-0.06320900
H	-1.90294000	0.17811700	-0.15897700
H	-0.57910000	-0.29194500	0.96368000
H	-0.48952500	-0.70622600	-0.84392100
H	-0.37425400	1.06336500	-0.29331500
B	1.64129500	-0.06328400	0.08525700
C	1.98891900	-0.73990000	-1.36305300
C	1.44592400	-0.30859300	-2.59510000
C	2.84042400	-1.85697600	-1.52450000
C	1.59209800	-0.96742000	-3.81044000
C	3.01927800	-2.55585700	-2.71519400
C	2.36221000	-2.11724700	-3.85008500
C	1.79703000	-1.01239400	1.40909100
C	1.09142200	-2.22080200	1.61197100
C	2.63143500	-0.69995700	2.50683100
C	1.08342200	-2.95750600	2.79067000
C	2.65849400	-1.39862300	3.71098200
C	1.85323000	-2.51353200	3.85256400
C	1.99022400	1.52598500	0.26681300
C	2.97285900	2.20590900	-0.48848800
C	1.32461000	2.39014500	1.16660800
C	3.17829200	3.58291700	-0.47170800
C	1.49341500	3.76899900	1.22712400
C	2.40815600	4.36098300	0.37302600
Cl	0.18196000	-3.00491400	0.30436800
Cl	0.23118900	1.77395600	2.42189300
Cl	0.56251800	1.22371000	-2.74438400
Cl	2.62583600	6.10356800	0.40127400
Cl	4.15575400	1.33844700	-1.46902000
Cl	3.84956400	0.57422600	2.41747800
Cl	2.54572600	-2.99159200	-5.36188000
Cl	3.88663200	-2.42536700	-0.22158400
Cl	1.84530100	-3.40288300	5.36649300
H	-6.40646100	-1.53503200	-0.28419400
H	0.50533500	-3.86698400	2.86480800
H	3.31267800	-1.08009000	4.50942300
H	3.93942800	4.02648100	-1.09690500
H	0.93720700	4.35791900	1.94167400
H	3.67422800	-3.41425200	-2.74854800
H	1.12928500	-0.57627400	-4.70460000

NHC2

C	-3.42241600	0.15119400	-0.25230800
C	-5.57156700	-0.82472700	-0.27156400
C	-5.68453000	0.49836300	-0.37224500
H	-6.56145300	1.11769300	-0.45567300
N	-4.35770800	1.06418200	-0.35693300
C	-4.10791400	-1.20037200	-0.18253400
C	-4.16818000	2.55602200	-0.45556300
C	-4.78047400	3.02579600	-1.78628400
H	-5.85295400	2.82800000	-1.84501800
H	-4.63744600	4.10346100	-1.88824700
H	-4.29143800	2.53605700	-2.63127900
C	-2.67670900	2.88576500	-0.42136700
H	-2.14478700	2.42450100	-1.25414900
H	-2.55948500	3.96847700	-0.50030500
H	-2.21189000	2.56033900	0.50972000
C	-4.87926600	3.20471400	0.74443800
H	-4.46435300	2.83581700	1.68502000
H	-4.73326200	4.28616900	0.70893400
H	-5.95516900	3.01627000	0.74298200
C	-3.65926400	-2.07516600	-1.37701100
H	-2.58971600	-2.27575600	-1.31209100
H	-4.19524800	-3.02641700	-1.35428200
H	-3.86760200	-1.58594800	-2.33078100
C	-3.76559800	-1.89041500	1.15956800
H	-4.31671700	-2.83015700	1.23619200
H	-2.69834200	-2.10794300	1.20812900
H	-4.03736300	-1.26245000	2.01068800
C	-0.56032100	0.02528700	-0.06648800
H	-1.89814700	0.17265000	-0.16349100
H	-0.58560100	-0.29385700	0.96121600
H	-0.49477400	-0.71337500	-0.84668900
H	-0.38261200	1.05928700	-0.30074100
B	1.62049200	-0.06342400	0.08241000
C	1.97800100	-0.73750100	-1.36646800
C	1.43640500	-0.30739700	-2.59934200
C	2.83449200	-1.85078900	-1.52723500
C	1.58883400	-0.96312200	-3.81556100
C	3.01934300	-2.54714000	-2.71855700
C	2.36390800	-2.10964000	-3.85483800
C	1.78316100	-1.01484400	1.40577800
C	1.08111100	-2.22541100	1.60713000
C	2.61693200	-0.70219200	2.50382800

C	1.07600700	-2.96530900	2.78380300
C	2.64650400	-1.40345300	3.70649700
C	1.84500300	-2.52129900	3.84630400
C	1.97304300	1.52648100	0.26718400
C	2.95754500	2.20725300	-0.48482500
C	1.30576500	2.38984000	1.16629200
C	3.16356200	3.58422300	-0.46507300
C	1.47535400	3.76843300	1.23041500
C	2.39236900	4.36143000	0.37945700
Cl	0.17332000	-3.01017200	0.29766100
Cl	0.20892300	1.77201100	2.41877600
Cl	0.54683900	1.22224000	-2.74908800
Cl	2.61128200	6.10364200	0.41150300
Cl	4.14207100	1.34160600	-1.46468600
Cl	3.83111200	0.57582000	2.41735500
Cl	2.55559300	-2.98067500	-5.36724700
Cl	3.87953800	-2.41707800	-0.22269900
Cl	1.84080400	-3.41383100	5.35807500
Br	-7.00442400	-2.04951600	-0.24365600
H	0.50112100	-3.87698200	2.85599700
H	3.29994700	-1.08446700	4.50537100
H	0.91846700	4.35625900	1.94534800
H	3.92620700	4.02841700	-1.08799000
H	3.67776800	-3.40290500	-2.75126000
H	1.12719700	-0.57229700	-4.71047300

NHC3

C	-3.42005400	0.15939900	-0.25108200
C	-5.55083600	-0.81808500	-0.28916700
C	-5.69303400	0.50021100	-0.38620000
H	-6.57792400	1.10636700	-0.47230100
N	-4.36183800	1.06492200	-0.35893900
C	-4.10257700	-1.19552200	-0.19106700
C	-4.17740300	2.55715300	-0.44973700
C	-4.78605700	3.03163400	-1.78051400
H	-5.85742100	2.82982400	-1.84467300
H	-4.64659700	4.11033600	-1.87629000
H	-4.29160800	2.54806200	-2.62593100
C	-2.68726100	2.89211100	-0.40813700
H	-2.15061600	2.43685500	-1.24118200
H	-2.57372600	3.97562900	-0.48102800

H	-2.22453300	2.56329400	0.52278100
C	-4.89569200	3.19772400	0.75034800
H	-4.48214900	2.82677200	1.69074500
H	-4.75475700	4.28002000	0.71978600
H	-5.97051900	3.00360900	0.74432800
C	-3.66212000	-2.07519300	-1.38591500
H	-2.59944900	-2.30555700	-1.30946800
H	-4.22479100	-3.01136900	-1.37551700
H	-3.84427200	-1.57472400	-2.33926700
C	-3.78942700	-1.89849700	1.15237700
H	-4.36819800	-2.82235000	1.22121500
H	-2.72921800	-2.14595300	1.20927300
H	-4.04970300	-1.26540500	2.00336000
C	-0.55896700	0.03422300	-0.06377000
H	-1.89472700	0.18367600	-0.15951900
H	-0.58034800	-0.28485200	0.96408600
H	-0.49161400	-0.70494000	-0.84337400
H	-0.37467700	1.06715900	-0.29802200
B	1.62924600	-0.06156900	0.08355700
C	1.98098300	-0.73986400	-1.36428000
C	1.43935300	-0.30977300	-2.59724000
C	2.83267300	-1.85698200	-1.52405300
C	1.58746500	-0.96864200	-3.81230200
C	3.01314000	-2.55635000	-2.71427800
C	2.35785900	-2.11835400	-3.85044800
C	1.78849700	-1.01047900	1.40862800
C	1.08203500	-2.21780100	1.61384300
C	2.62483200	-0.69829000	2.50494300
C	1.07539100	-2.95462000	2.79242000
C	2.65304000	-1.39655000	3.70936000
C	1.84729900	-2.51087200	3.85293000
C	1.98499200	1.52745700	0.26454700
C	2.96998100	2.20425200	-0.49043100
C	1.32110900	2.39417800	1.16298200
C	3.17919400	3.58074900	-0.47408800
C	1.49386200	3.77252700	1.22352600
C	2.41090900	4.36153300	0.36982500
Cl	0.16963200	-3.00255500	0.30741700
Cl	0.22478100	1.78157500	2.41822100
Cl	0.55537000	1.22259400	-2.74852600
Cl	2.63367300	6.10332500	0.39754500
Cl	4.15103300	1.33341200	-1.46998200
Cl	3.84385300	0.57467000	2.41354200
Cl	2.54381600	-2.99309900	-5.36146800

Cl	3.87701900	-2.42517100	-0.21969100
Cl	1.84129600	-3.39954500	5.36696700
F	-6.52507800	-1.72675400	-0.27568400
H	0.49719400	-3.86394800	2.86763700
H	3.30868700	-1.07811800	4.50665000
H	0.93916400	4.36327400	1.93774600
H	3.94193000	4.02185700	-1.09908400
H	3.66811500	-3.41478400	-2.74626700
H	1.12614400	-0.57771900	-4.70733700

NHC4

C	-2.68894000	0.66274200	-0.12384300
C	-4.84434800	0.26767100	-1.13957600
C	-4.93328500	1.12228300	-0.08618300
H	-5.77810700	1.62553000	0.34018000
N	-3.62997200	1.32709600	0.48280200
C	-3.34873400	-0.11613200	-1.25181100
C	-3.46022200	2.23779300	1.66773100
C	-3.95476600	3.64061000	1.27307400
H	-5.01680400	3.65182100	1.02110100
H	-3.80320500	4.32611200	2.10962900
H	-3.39301100	4.01918000	0.41612800
C	-1.98495400	2.30337800	2.06227700
H	-1.37000100	2.68903200	1.24835500
H	-1.88245100	2.97543100	2.91707600
H	-1.60075500	1.32481200	2.34996900
C	-4.28571500	1.66707800	2.83410800
H	-3.94544500	0.66089300	3.08887600
H	-4.15956800	2.30267000	3.71327900
H	-5.35200200	1.62217900	2.60414200
C	-2.68104300	0.36279000	-2.56457600
H	-1.60271900	0.21212300	-2.50214300
H	-3.04384800	-0.18140700	-3.43737000
H	-2.86725500	1.42700200	-2.72668200
C	-3.07261400	-1.61374000	-0.96503700
H	-3.48582300	-2.26548400	-1.73562400
H	-1.99683700	-1.78755800	-0.92445300
H	-3.50568200	-1.90838300	-0.00624900
C	0.11754600	0.15681900	0.17524500
H	-1.19814200	0.45519200	0.09123000
H	0.35204800	0.95931500	0.85184100

H	0.00696800	-0.84043100	0.56661800
H	0.35833300	0.27546500	-0.86769500
B	2.36495600	-0.22349800	0.44791500
C	2.34726200	-1.85133800	0.56118200
C	1.65945700	-2.70954600	-0.32762300
C	3.00394500	-2.57031700	1.58688300
C	1.50254700	-4.08019900	-0.15628000
C	2.87715200	-3.93905600	1.80620700
C	2.09427500	-4.68165200	0.94159800
C	2.61420500	0.62108700	1.82218700
C	1.80523000	0.52370300	2.97860500
C	3.65673700	1.56253700	1.98365700
C	1.90937000	1.34094400	4.09859200
C	3.80302000	2.40780700	3.08024900
C	2.90067400	2.30734800	4.12305600
C	2.91686400	0.42138900	-0.94465300
C	3.82601500	-0.24099700	-1.80179000
C	2.52881100	1.68097100	-1.45698400
C	4.19065700	0.20146500	-3.07001800
C	2.86160700	2.16882100	-2.71574700
C	3.67360500	1.39850300	-3.53070800
N	-5.86233200	-0.17037900	-1.94771000
C	-5.64599900	-1.11676700	-3.06466500
H	-4.58624200	-1.34247500	-3.07034400
C	-7.25988500	0.28445200	-1.74862800
H	-7.82541900	-0.22317000	-2.53069800
C	-6.38210000	-2.44907900	-2.85229000
H	-7.46851600	-2.32936600	-2.86783300
H	-6.12083400	-3.14836800	-3.65108500
H	-6.10168000	-2.90108800	-1.89850700
C	-5.97434600	-0.49341300	-4.43090200
H	-5.70962500	-1.19121900	-5.22989800
H	-7.03811100	-0.26586500	-4.53821100
H	-5.41063100	0.42934600	-4.58411000
C	-7.87275100	-0.18881800	-0.41983400
H	-7.78534900	-1.27276500	-0.32180200
H	-7.40139200	0.26196000	0.45321000
H	-8.93485000	0.06942100	-0.39596900
C	-7.45317800	1.78831700	-2.00520900
H	-7.07342500	2.05986300	-2.99218400
H	-8.51916200	2.02928200	-1.97296800
H	-6.94852500	2.41587400	-1.27090200
Cl	4.18477700	-1.80259100	2.65095800
Cl	0.97568900	-2.12212600	-1.85568300

Cl	4.71180200	-1.67770600	-1.28444200
Cl	4.09163900	1.97196900	-5.13741500
Cl	1.62053700	2.84991400	-0.48127400
Cl	4.98924700	1.68178600	0.83251700
Cl	3.04198400	3.37554700	5.51023700
Cl	0.58668600	-0.75106400	3.16477000
Cl	1.89206500	-6.40629800	1.20484000
H	3.39817700	-4.40887200	2.62762700
H	0.94817900	-4.66251100	-0.87763500
H	1.24251500	1.20694800	4.93772400
H	4.61927900	3.11441800	3.11696500
H	2.50856300	3.13759700	-3.03763100
H	4.87871400	-0.37537800	-3.67061800

NHC5

C	-3.45115600	0.13126300	-0.28480000
C	-5.62107500	-0.88680300	-0.34856400
C	-5.71493000	0.46049700	-0.43866400
H	-6.57744400	1.09640400	-0.52059900
N	-4.39285400	1.02781200	-0.38801500
C	-4.12787600	-1.23102400	-0.25468800
C	-4.20830000	2.51870000	-0.46176400
C	-4.80095000	3.01092400	-1.79381600
H	-5.87098000	2.80942600	-1.87255900
H	-4.65749600	4.09044800	-1.87615800
H	-4.29746200	2.53476500	-2.63820300
C	-2.71956500	2.85915600	-0.40094100
H	-2.17310000	2.41413300	-1.23295400
H	-2.60797100	3.94396200	-0.45936200
H	-2.26543200	2.51918700	0.53017900
C	-4.93761300	3.15105200	0.73654300
H	-4.53624800	2.76692700	1.67704200
H	-4.79078500	4.23309800	0.71965700
H	-6.01229400	2.95962000	0.71642100
C	-3.57437800	-2.02681300	-1.46328300
H	-2.48647100	-2.06661300	-1.40479200
H	-3.94518000	-3.05180700	-1.47625400
H	-3.84917900	-1.55052600	-2.40739200
C	-3.78815700	-1.92285900	1.08621100
H	-4.30587300	-2.88027000	1.17237600
H	-2.71509800	-2.10585600	1.15455500

H	-4.09077000	-1.30228600	1.93253700
C	-0.59375900	0.02702200	-0.07434600
H	-1.93617800	0.16297700	-0.18288900
H	-0.58390000	-0.31281700	0.94744100
H	-0.47493300	-0.69783700	-0.86145900
H	-0.37906400	1.05967100	-0.28375600
B	1.67972800	-0.06420400	0.08275900
C	2.01637000	-0.72947600	-1.36931400
C	1.47211700	-0.28741500	-2.59741500
C	2.86563800	-1.84714500	-1.53959300
C	1.61385200	-0.94035500	-3.81654900
C	3.04056500	-2.53902100	-2.73477600
C	2.38108200	-2.09179700	-3.86493800
C	1.81823500	-1.02100000	1.39828500
C	1.11384100	-2.23274500	1.58646300
C	2.64376400	-0.71425900	2.50463100
C	1.09788200	-2.97611700	2.76085700
C	2.66310100	-1.42064800	3.70422900
C	1.85849800	-2.53772600	3.83170100
C	2.00722000	1.52414000	0.27398200
C	2.98505700	2.21631600	-0.47665900
C	1.33362500	2.37681200	1.17927900
C	3.17899300	3.59463900	-0.45248700
C	1.49015200	3.75685300	1.24539000
C	2.40054800	4.36118700	0.39525600
N	-6.66944500	-1.76549200	-0.22166600
C	-6.57225500	-3.14595000	-0.68496900
H	-7.38257900	-3.72175200	-0.23482900
H	-6.65276400	-3.23336200	-1.77785800
H	-5.63487300	-3.59663500	-0.36927900
C	-8.00850100	-1.19666200	-0.26737800
H	-8.26802300	-0.80812500	-1.26383900
H	-8.73480900	-1.96298800	0.00475400
H	-8.08753000	-0.37966500	0.45373800
Cl	0.21618000	-3.00940500	0.26769500
Cl	0.24549600	1.74471900	2.42882000
Cl	0.59233000	1.24619200	-2.73419000
Cl	2.60254200	6.10566000	0.43239600
Cl	4.17601800	1.36255100	-1.46010200
Cl	3.85979300	0.56304400	2.43159300
Cl	2.55826800	-2.95777700	-5.38274700
Cl	3.91340100	-2.42435900	-0.24155200
Cl	1.84010300	-3.43742500	5.33973900
H	0.52038700	-3.88671200	2.82500100

H	3.31065000	-1.10644900	4.50975000
H	0.92699400	4.33748200	1.96126200
H	3.93719100	4.04807600	-1.07414000
H	3.69400300	-3.39825400	-2.77531300
H	1.14946200	-0.54307400	-4.70718700

NHC6

C	-3.43141100	0.16361000	-0.27126000
C	-5.57999500	-0.82841500	-0.33172900
C	-5.70373700	0.50103400	-0.42721300
H	-6.57699800	1.12463400	-0.52106700
N	-4.37117600	1.06634900	-0.38620000
C	-4.11853200	-1.18815200	-0.22064700
C	-4.18442600	2.55666100	-0.47135300
C	-4.78073900	3.03872600	-1.80534600
H	-5.85226400	2.84116700	-1.87847000
H	-4.63539500	4.11707300	-1.89739600
H	-4.28208900	2.55451500	-2.64794100
C	-2.69439100	2.89204600	-0.41752300
H	-2.15180000	2.43796300	-1.24724700
H	-2.57950900	3.97582700	-0.48632900
H	-2.23894800	2.55925200	0.51549800
C	-4.90977100	3.19761500	0.72461100
H	-4.50473600	2.82187900	1.66682700
H	-4.76486500	4.27961600	0.69847600
H	-5.98492500	3.00613500	0.71004300
C	-3.66656600	-2.06480300	-1.41158900
H	-2.60523800	-2.29866200	-1.32453800
H	-4.23440600	-2.99773700	-1.41230700
H	-3.83461400	-1.55893600	-2.36505400
C	-3.81867300	-1.89162000	1.12399200
H	-4.40301200	-2.81207700	1.18875500
H	-2.75951800	-2.14182600	1.19131500
H	-4.08302700	-1.25608500	1.97231300
C	-0.57363200	0.03635900	-0.06971200
H	-1.90873800	0.18615900	-0.17114600
H	-0.58395600	-0.29075000	0.95594400
H	-0.48548900	-0.69850100	-0.85152300
H	-0.36838800	1.06760000	-0.29428700
B	1.65273400	-0.06328500	0.09292900
C	2.00209900	-0.73970600	-1.35366800

C	1.46683200	-0.30495400	-2.58800900
C	2.85015900	-1.85993500	-1.51178700
C	1.61626600	-0.96390300	-3.80289000
C	3.03214000	-2.55871100	-2.70201700
C	2.38212000	-2.11666700	-3.83962700
C	1.79377700	-1.01253800	1.41684300
C	1.08362300	-2.21935500	1.61412900
C	2.62080600	-0.70206600	2.52075400
C	1.06481100	-2.95538000	2.79314600
C	2.63724900	-1.40056300	3.72512000
C	1.82785800	-2.51323600	3.86067400
C	1.99896600	1.52515000	0.27638000
C	2.98610300	2.20450400	-0.47361900
C	1.32872100	2.38950000	1.17269800
C	3.19192900	3.58138400	-0.45622300
C	1.49743600	3.76838300	1.23307600
C	2.41703700	4.35980200	0.38383100
Cl	0.18210100	-3.00103600	0.30027400
Cl	0.22876900	1.77400500	2.42181000
Cl	0.58991700	1.23025800	-2.74025900
Cl	2.63476600	6.10252500	0.41249100
Cl	4.17411800	1.33586800	-1.44710500
Cl	3.84261300	0.56930800	2.43992800
Cl	2.56948200	-2.99069000	-5.35127700
Cl	3.88777200	-2.43297300	-0.20394800
Cl	1.80624000	-3.40235900	5.37474500
O	-6.50309100	-1.80815200	-0.32173800
H	-7.39062400	-1.43892700	-0.39772800
H	0.48350400	-3.86312200	2.86330400
H	3.28638900	-1.08372900	4.52833200
H	0.93709400	4.35779300	1.94397500
H	3.95672200	4.02454200	-1.07722700
H	3.68396900	-3.41956700	-2.73287100
H	1.15898700	-0.57060600	-4.69894700

NHC7

C	-3.41757800	0.09615600	-0.31276200
C	-5.58392900	-0.92220100	-0.34338600
C	-5.68059800	0.41060000	-0.36936600
H	-6.56032000	1.03282100	-0.40401400
N	-4.36366200	0.99926900	-0.35729700

C	-4.09178600	-1.25998100	-0.28743200
C	-4.19467600	2.49410300	-0.40216600
C	-4.84482700	3.00846500	-1.69840500
H	-5.91545700	2.79757600	-1.73968500
H	-4.71752000	4.09119500	-1.76131800
H	-4.37015500	2.55831300	-2.57314200
C	-2.70742400	2.84478600	-0.39136500
H	-2.18912900	2.41753400	-1.25060600
H	-2.60565100	3.93108300	-0.43672900
H	-2.21647400	2.49445200	0.51686700
C	-4.88335200	3.09016200	0.83794200
H	-4.44066900	2.69217000	1.75374700
H	-4.75104500	4.17408400	0.83939100
H	-5.95641100	2.88742200	0.85507000
C	-3.57679000	-2.10017200	-1.47993400
H	-2.49067400	-2.18432700	-1.42911500
H	-3.99403900	-3.10758400	-1.44163700
H	-3.84316700	-1.64560500	-2.43689600
C	-3.74757000	-1.96960800	1.04749400
H	-4.29254600	-2.91442400	1.10715400
H	-2.67858600	-2.17876800	1.10207100
H	-4.02973900	-1.35802500	1.90760300
C	-0.55757000	0.00942400	-0.09383900
H	-1.89815800	0.13737600	-0.21102000
H	-0.57032000	-0.31423700	0.93285700
H	-0.45318200	-0.72656000	-0.87243800
H	-0.37142500	1.04354300	-0.32153800
B	1.66679500	-0.05473500	0.07760200
C	2.03427500	-0.72680200	-1.36674700
C	1.49625500	-0.30369500	-2.60387500
C	2.90236100	-1.83231400	-1.51951900
C	1.66118100	-0.96263600	-3.81681000
C	3.10032300	-2.53057200	-2.70748200
C	2.44651600	-2.10239500	-3.84825600
C	1.81752600	-1.00130700	1.40246900
C	1.12684100	-2.21991900	1.59604500
C	2.63333500	-0.67707800	2.51074200
C	1.11343800	-2.95589800	2.77515400
C	2.65465700	-1.37502500	3.71536100
C	1.86298100	-2.50087000	3.84683400
C	1.98750400	1.53918100	0.26141700
C	2.96600700	2.23396500	-0.48574700
C	1.30076200	2.39321300	1.15509600
C	3.14959700	3.61401900	-0.46834500

C	1.44725900	3.77458000	1.21565500
C	2.35984000	4.38037900	0.36890100
Cl	0.24665600	-3.01711400	0.27699600
Cl	0.20728300	1.76063900	2.40164500
Cl	0.59470600	1.21650500	-2.76237200
Cl	2.54955200	6.12624400	0.39742600
Cl	4.17100600	1.38434400	-1.45496000
Cl	3.83454000	0.61412700	2.43618400
Cl	2.65365600	-2.97670900	-5.35714700
Cl	3.94570700	-2.38373800	-0.20698100
Cl	1.84749100	-3.38969700	5.36110300
H	0.54670600	-3.87303500	2.84229800
H	3.29402200	-1.04737100	4.52207000
H	3.90907700	4.06903900	-1.08728100
H	0.87558300	4.35516400	1.92480000
H	3.76701900	-3.38010700	-2.73415700
H	1.20071700	-0.57891500	-4.71539300
C	-6.71956900	-1.86165800	-0.26241700
C	-6.86886700	-2.92792400	-1.16264200
C	-7.69326500	-1.69123900	0.73465200
C	-7.95741600	-3.78971000	-1.06895500
H	-6.14890600	-3.06848100	-1.95823800
C	-8.77966400	-2.55606200	0.82788100
H	-7.58189500	-0.88524400	1.45099400
C	-8.91511200	-3.60930600	-0.07320900
H	-8.05950000	-4.60184200	-1.77973500
H	-9.51701800	-2.40961500	1.60901100
H	-9.75950600	-4.28486900	-0.00007100

APPENDIX D. LIST OF PHYSICAL PROPERTIES STUDIED IN CHAPTER 4

Borane	NHC	Ea (kcal/mol)	p (debye)	d	ΔQ (a.u.)	ΔE_{MO} (a.u.)	ΔE_{MO} (kcal/mol)	ΔE_{F} (kcal/mol)
B5F	**NHC1**	47.93	10.0596	27.88	0.36085	0.06731	42.24	6.97
	NHC2	49.63	9.2836	26.37	0.35205	0.07682	48.20	9.67
	NHC3	49.19	9.1357	26.19	0.34878	0.07323	45.95	7.98
	NHC4	45.56	12.451	30.46	0.40881	0.04913	30.83	10.16
	NHC5	46.09	11.6142	29.26	0.39693	0.05682	35.65	6.13
	NHC6	47.09	11.4164	30.93	0.36913	0.06322	39.67	5.81
	NHC7	48.12	10.7708	28.80	0.37403	0.0674	42.29	7.37
B3F	**NHC1**	56.63	7.7611	24.63	0.31517	0.09599	60.23	13.49
	NHC2	57.28	6.9305	22.72	0.30505	0.1055	66.20	15.81
	NHC3	57.48	6.8691	22.69	0.30272	0.10191	63.95	14.15
	NHC4	53.19	9.7946	27.19	0.36029	0.07781	48.83	17.52
	NHC5	53.70	9.0953	26.13	0.34807	0.0855	53.65	13.31
	NHC6	55.82	9.0811	28.13	0.32279	0.0919	57.67	12.62
	NHC7	54.72	8.1372	25.32	0.32139	0.09608	60.29	15.03
B2F	**NHC1**	57.69	5.6455	18.71	0.30178	0.10429	65.44	14.01
	NHC2	58.42	4.8584	16.69	0.2911	0.1138	71.41	16.14
	NHC3	58.37	4.8334	16.72	0.28916	0.11021	69.16	14.49
	NHC4	54.73	7.4784	21.64	0.34552	0.08611	54.03	18.42
	NHC5	55.35	6.8566	20.57	0.33337	0.0938	58.86	14.08
	NHC6	56.86	6.9605	22.51	0.30921	0.1002	62.88	13.26
	NHC7	57.59	5.8769	19.15	0.30692	0.10438	65.50	15.58
B5Cl	**NHC1**	68.01	10.0919	21.10	0.47827	0.06857	43.03	55.19
	NHC2	69.88	9.3063	20.25	0.45959	0.07808	49.00	57.91
	NHC3	69.42	9.127	19.58	0.46618	0.07449	46.74	56.03
	NHC4	64.86	12.0118	23.20	0.51765	0.05039	31.62	58.00
	NHC5	65.83	11.7436	22.74	0.51636	0.05808	36.45	54.10
	NHC6	67.26	11.4979	23.43	0.49079	0.06448	40.46	53.81
	NHC7	68.32	10.8074	21.55	0.50152	0.06866	43.08	57.00
B3Cl	**NHC1**	69.33	8.6836	19.50	0.44533	0.08462	53.10	51.71
	NHC2	71.03	7.8681	18.45	0.42635	0.09413	59.07	54.26
	NHC3	70.56	7.7644	18.05	0.43021	0.09054	56.81	52.32
	NHC4	66.40	10.3811	21.64	0.47976	0.06644	41.69	54.97
	NHC5	67.31	10.5074	20.86	0.50381	0.07413	46.52	50.61
	NHC6	68.58	10.0692	22.21	0.4534	0.08053	50.53	50.51
	NHC7	69.54	9.3485	20.41	0.45804	0.08471	53.16	52.07

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