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C-H on the Oxo Ferryl Wheel: Comparison of Pyridine and Imidazole-Substituted Ligands for C-H Activation and Functionalization

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C–H ON THE OXO FERRYL WHEEL: COMPARISON OF PYRIDINE AND IMIDAZOLE-SUBSTITUTED LIGANDS FOR C–H ACTIVATION AND FUNCTIONALIZATION

By

E. GRACE MILEM, B.S. Chemistry, B.S. Self-Designed

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C–H ON THE OXO FERRYL WHEEL: COMPARISON OF PYRIDINE AND IMIDAZOLE-SUBSTITUTED LIGANDS FOR C–H ACTIVATION AND FUNCTIONALIZATION

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Abstract

The selective and efficient transformation of hydrocarbon feedstocks is of high value for industry and research. While Shilov-type organometallic methods have facilitated this goal, systems designed after nature's use of cheap and abundant iron-based enzymes are desired for wider-scale applications. This work establishes hydrocarbon oxidation efficiency of synthetic pyridine-based ligands (BPMEN, BPMPN) compared to commercially available TPA with *in situ* generated catalysts. Literature studies of traditionally synthesized BPMEN systems and initial *in situ* studies offered evidence for enhanced reactivity (TON) as compared to TPA. Expansion to a propyl backbone to produce BPMPN tested the increased chelate ring size's impact on reactivity as compared to BPMEN. Optimized catalysis yielded higher TON efficiency with BPMEN as well as greater selectivity compared to TPA across all substrates and conditions. Utilization of the BPMPN architecture not only offered lower TON as compared to the BPMEN precursor, but resulted in excessively low product yields below that of TPA, often near or below the limit of quantification. We next turned to addressing the lack of imidazole-substituted models through ligands BItCHEN and ^{nBu}BIMEN. Translating the previously established BItCHEN structure to our simple and modular synthetic approach ultimately proved unsuccessful. Therefore, we focused on ^{nBu}BIMEN, established by our collaborator. Preliminary investigations indicated that while this ligand was less effective for oxidation, epoxidation capability was near or above that of BPMEN. Interestingly, ^{nBu}BIMEN also

showed evidence of a more stable oxo-species intermediate, leading to computational assessment of oxo stability across these scaffolds.

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Abbreviations

TON Turnover Number

CYP450 Cytochrome P450

catA Pyrocatechase

HAT H-Atom Transfer

RM Rebound Mechanism

His Histidine

BPMEN bis-Pyridyl-methylethylenediamine

BPMPN bis-Pyridyl-methylpropylenediamine

TPA tris-(2-Pyridylmethyl)amine

BItCHEN bis-Imidazole-*trans*-cyclohexylmethylethylenediamine

^{nBu}BIMEN *n*-Butyl-bis-imidazole-methylethylenediamine

OTf Triflate

KIE Kinetic Isotope Effect

OAT O-Atom Transfer

DMED N,N'-dimethylethylenediamine

DCM Dichloromethane

DMPD N,N'-dimethyl-1,3-propanediamine

AcOH Acetic acid

CHO (1-butylimidazole)2-carboxaldehyde

^{Me}BPMEN bis-Methylpyridyl-methylethylenediamine

^{Br}BPMEN bis-Bromidepyridyl-methylethylenediamine

BPtCHEN bis-Pyridyl-*trans*-cyclohexylmethylethylenediamine

DMF Dimethylformamide

DCE Dichloroethane

CHAPTER 1

C–H Activation and Functionalization

Functionalization of varying types of chemical bonds is the foundation of modern chemical industry. This is typically introduced within the scope of organic chemistry methodology, utilizing nucleophilic-electrophilic, free radical, carbocation, or functional group interconversion through various synthetic means to achieve a desired organic product.[1,2] While this strategy has been built over time and provides nearly exhaustive ways in which to convert one functional group to another, this method necessitates the use of substrates that contain an existing functionality.

This presents an obvious dilemma when utilizing unactivated and non-functionalized hydrocarbon substrates. These chemical feedstocks, while forming the "building blocks" of organic substrates in nature, are notoriously difficult to transform through these existing methods. Because of the wide prevalence of reduced hydrocarbon substrates and their ability to act as precursors to organic products for industrial synthesis, this introduces the desire for an alternative synthetic strategy to activate and functionalize C–H bonds.

Two main challenges are typically attributed for hydrocarbon activation and functionalization. The first consists of high bond dissociation energies of C–H substrates, with aliphatic ranging from ~95 to ~105 kcal/mol compared to benzene's ~113 kcal/mol.[3]

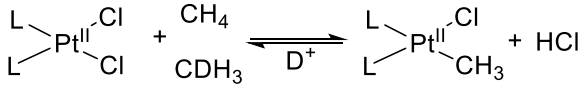
The second difficulty is the high pKa values of these bonds, with aliphatic ranging from ~ 45-60 and benzene's ~ 43.[4,5]

Given these obstacles, achieving selectivity similarly becomes difficult due to the number of C–H bonds and varying bond types, making the utilization of chemical feedstocks in industrial product synthesis more challenging. Natural biochemical pathways, in contrast, are known to oxidize and transform C–H bonds to high selectivity and efficiency with minimal by-products. As such, the ongoing quest is to embody the efficient and selective system in nature through a simple synthetic model.

1.1 Shilov-Type Catalysis

In 1969, Alexander Shilov observed that various alkanes subjected to deuterated acids in the presence of a $PtCl_2$ catalyst produced the deuterated substrate. This deuteration indicated a reversible process, in which substrate C–H bond was broken to produce a Pt–C bond oxidative addition intermediate. In the presence of deuterated acids, the Pt–C can then be protonated by the D^+ source as opposed to H^+ in the reverse reaction, thus identifying the reverse mechanism (Scheme 1.1).[6-8]

Scheme 1.1 Shilov C–H Activation Mechanism.



While use of this system provided an avenue to activate strong C–H bonds, it was impacted heavily by steric accessibility to the C–H bond as evidenced by percent deuteration. Subjecting various alkyl substrates to these conditions indicated that more

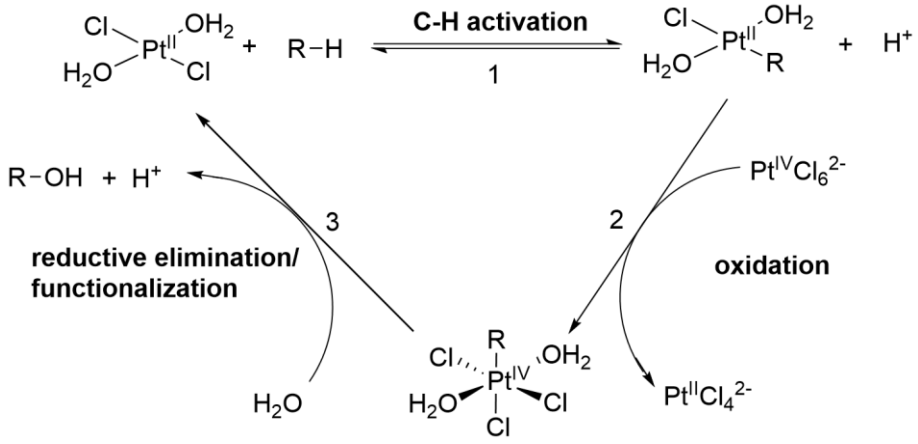
accessible primary positions, out of proximity of other alkyl groups, had deuteration ranging from 53-92%. Accessible secondary positions were slightly less preferred, followed by trace incorporation at tertiary positions. Preference for accessible phenylic C–H bonds containing alkyl substituents and significantly less incorporation for primary positions of a *t*-butyl group similarly indicated steric effects as a driving force for this process.[9]

This regio-preference can be best reasoned through the Pt–C intermediate feasibility. Coordination of substituted alkyl or olefinic substrates to metal centers are generally more stable and subsequently more reactive when the larger metal atom is not in proximity to other bulky substituents.[10] In general, this intermediate is facilitated by the introduction of a more covalent Pt–C bond relative to the weak preceding Pt–Cl bond.[11]

The Shilov mechanism allowed for activation of strong C–H bonds and was adapted for chlorination and hydroxylations utilizing various stoichiometric oxidants, but exhibited poor turnover number (TON) efficiency (<10 TON) (Equation 1.1).[7,8] The subsequent Periana system improved TON (>500 TON) through a catalyst derivative and fuming sulfuric acid.[2,12] The general "Shilov-type" catalytic mechanism (Scheme 1.2) functionalizes the substrate through the reductive elimination step, but presents two key disadvantages.[6,7,10,12]

Equation 1.1 $\text{TON} = \frac{\text{moles oxidation product}}{\text{moles catalyst}}$

Scheme 1.2 Shilov-Type Catalytic Cycle.



The first lies with the dependence on stoichiometric oxidants that preferentially oxidize the Pt^{II}-alkyl intermediate and not the starting species. As a result, one of the few choices is composed of a Pt^{IV} oxidant, making this process highly cost prohibitive. While the Periana system offers a cheaper stoichiometric oxidant species, the catalyst species cannot be isolated outside of the extremely acidic environment. The oxidation conditions also create incompatibility with acid-reactive functional groups.[2] Secondly, the system's regio-preference for C–H bond activation negates selective functionalization at more hindered sites. Compounding this issue, potential for overoxidation in the reaction environment introduces the possibility of subsequent oxidations to an undesired product. Therefore, Shilov-type applications are still impractical in view of industrial application.

1.2 Directing Group Functionalization

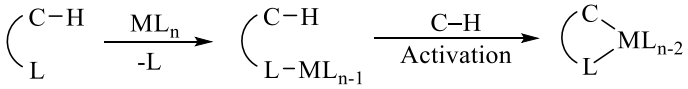
Subsequent C-H functionalization catalyst systems aimed to address lack of selectivity and overoxidation that limited Shilov systems. Preliminary efforts by Sames utilized a Shilov Pt^{II} catalyst with a stoichiometric oxidant Cu^{II} salt. This system allowed for the

regio- and stereo-selective functionalization of valine methyl groups. Subsequently, functionalization was determined to proceed through the formation of a chelate ring from the proximal methyl group to the Pt catalyst center.[13]

Continuing efforts utilizing Pd^{II}, Ru^{II}, and dimeric Rh^{II} carbene catalysts confirmed this selective activation across arene, benzylic, and unactivated sp^3 substrates with chelating functionality.[14-17] This selectivity was further highlighted by the successful oxidation of secondary C–H sites proximal to chelating heteroatoms.[15] Furthermore, manipulation of stoichiometric oxidant equivalents afforded some degree of control for the extent of substrate oxidation.

In essence, these directing group processes are controlled by two main factors. The first is the formation of a stable (typically five or six-membered) palladacycle or rhodacycle intermediate, generally termed the 'chelate effect' for transition metals (Scheme 1.3).[11,18-23] This is achieved through a directing heteroatom or group (typically a sp^2-hybridized nitrogen or carbonyl group) capable of binding to the metal center. This coordination then brings the site of functionalization in proximity to the metal to create the stable metallocycle species. As such, the entropic favorability provided by this cyclic intermediate, through the resulting increased particles, affords near exclusive activation of substrates with chelating ability over those that contain coordination-capable heteroatoms with no chelating functionality.[15]

Scheme 1.3 C–H Activation via Directing Group.



The second driving force for activation is kinetic, resulting from C–H bond proximity after ligand binding. Effectively, substrate concentration is increased through binding to the metal center. This facilitates an intramolecular process, commonly observed to be faster than their intermolecular counterparts.[10] Therefore, activation and varying functionalization through reductive elimination was more successful for these systems as compared to the precedent of the original Shilov systems. However, substrates are still dependent on chelating groups and catalysts are based on relatively rare and expensive noble metals.[24]

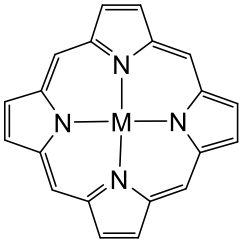
1.3 Nature: Enzymatic Approach

Shilov-type catalysts employ strong, near-covalent bonds between noble metals and carbon, further facilitated by directing group substrates. Translating this approach to abundant 3d metals poses a challenge due to the weaker M–C bonds.[11] However, these metals act as key components in hydrocarbon functionalization within enzyme active sites to a high degree of efficiency and selectivity facilitated by their protein scaffolds. Therefore, mechanistic studies of metabolic C–H bond functionalization and the electronic and structural impacts of the enzyme active site is necessary for these metal sources.

1.3.1 Cytochrome P450 Enzymes

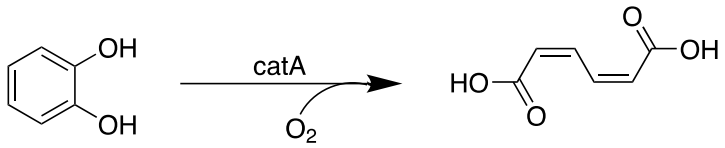
As a counterpoint to the difficulty posed in synthetic production, key metabolic heme enzymes conduct C–H transformations with high selectivity and efficiency. Therefore, these heme enzymes have been the focus of extensive characteristic and mechanistic studies. These heme-containing enzymes are composed of an Fe^{II} center, bound within a protoporphyrin IX architecture, and coordinated to cysteine, tyrosine, or histidine residues (Figure 1.1).[25-27]

Figure 1.1 General metalloporphyrin structure.



Most notable among these are the cytochrome P450 (CYP450) iron-heme enzymes which provide, in a broad definition, the metabolism of xenobiotics and biosynthesis of molecules for organism development.[28,29] The large abundance of these enzymes within animal and plant sources and specifically, the soluble, thermally stable nature of certain CYP450s have lent themselves to useful systems to model for industrial catalysts.[27] These enzymes act as powerful oxidants, first discovered through pyrocatechase (catA), which combine atmospheric O_2 into catechol, thereby cleaving the benzene ring and transforming it into muconic acid (Scheme 1.4).[29,30]

Scheme 1.4 Transformation of catechol into muconic acid by pyrocatechase.



This led to subsequent discoveries for their roles in catalyzing various oxidation reactions for saturated and aromatic substrates. In essence, CYP450s efficiently inserts an oxygen atom from molecular oxygen to the substrate, acting as a monooxygenase. The remaining oxygen is then reduced to water facilitated by two electrons sourced by NADH or NADPH.[31]

Green's kinetic isotope studies of substrate activation indicated that the Fe^{IV}–oxo first proceeds via H-atom transfer (HAT) to produce an alkyl radical, which then quickly recombines with the resultant Fe^{IV}-hydroxide to hydroxylate the substrate.[32,33] This supported the so-called "rebound mechanism" (RM) proposed by Groves and McClusky, contradicting established Fenton mechanisms proceeding through hydroxyl radicals.[34-36]

1.3.2 Non-Heme Iron-Oxo Enzymes

Following CYP450 mechanistic studies, current studies have shown that non-heme iron enzymes catalyze a similarly impressive set of hydrocarbon oxidations that proceed via HAT/RM utilized by CYP450 centers.[37-39] These non-heme species are classified as either mononuclear or binuclear active sites (Table 1.1, Table 1.2).

Table 1.1 Examples of mononuclear non-heme iron enzyme reactions with organic substrates.[28,39-41]

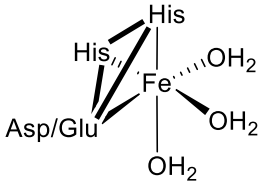
Example enzyme	Substrate	Reaction
Isopenicillin N-synthase	Aliphatic amides	Oxidative ring closure (4 electron)
Phenylalanine hydroxylase	Aromatic rings	Aromatic hydroxylation
Napthalene dioxygenase	Aromatic rings	Extradiol dioxygenation
Clavaminate synthase	Alkanes	Aliphatic hydroxylation
Bleomycin	DNA	H• abstraction
Claviminate synthase	Olefins	Alkene epoxidation
Lipoxygenase	Olefins	Hydroperoxidation
Protocatechuate 3,4-dioxygenase	Substituted aromatic rings	Intradiol dioxygenation

Table 1.2 Examples of binuclear non-heme iron enzyme reactions with organic substrates.[39]

Example enzyme	Substrate	Reaction
Desaturase	Alkanes	Desaturation
Methane monooxygenase	Methane	Alkane oxidation
Ribonucleotide diphosphate reductase	Nucleoside diphosphates	Oxidation (1 electron)
Alkene monooxygenase	Olefins	Alkene epoxidation

Crystal structures of mononuclear iron enzymes in particular have led to the discovery of the '2-His-1-carboxylate facial triad.'[40] The structure of an iron (II) center with facial coordination of two histidine residues and a carboxylate ligand (typically from glutamate or aspartate residues) are similarly utilized for the activation of atmospheric oxygen (Figure 1.2).[40,41]

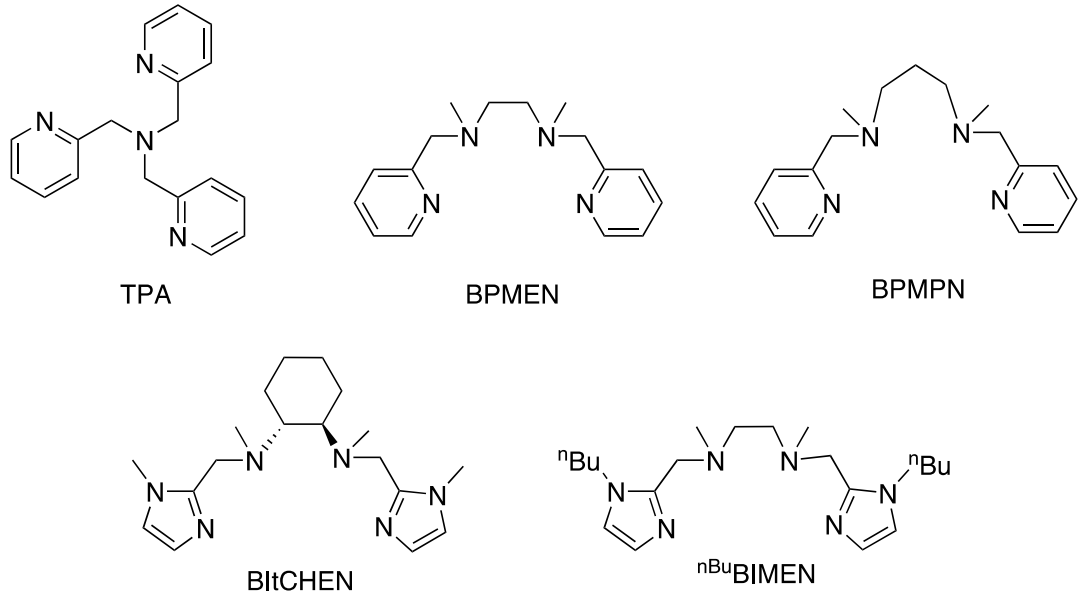
Figure 1.2 Structure of the 2-His-1-carboxylate facial triad.[40,41]



1.4 Project Goal: C-H Activation of Biomimetics vs Shilov-Type

Following biomimetics of non-heme iron oxo enzymes, a simple catalytic method using a "green" oxidant for C–H bond oxidation is desired. In addition, a modular approach with relatively simple conditions (i.e. short reaction times, open air synthesis) is particularly attractive as related to supporting ligand and catalyst synthesis. Therefore, our efforts focused on *in situ* production using commercially available or previously established pyridyl-based tetradentate amine ligand architectures, then expanded our studies to imidazole derivatives (Figure 1.3).

Figure 1.3 Tetradentate amine ligands utilized in catalysis.



Our research goal was to establish hydrocarbon oxidation efficiency of the synthesized pyridine ligands bis-pyridyl-methylethylenediamine (BPMEN) and bis-pyridyl-methylpropylenediamine (BPMPN) as compared to commercially available tris-(2-pyridylmethyl)amine (TPA) through *in situ* generated catalysts. Previous studies of the BPMEN architecture through alternative synthetic methods and initial catalysis conducted by Bailey Jameson offered evidence for enhanced reactivity (TON) as compared to TPA. We then expanded the alkyl backbone to produce BPMPN, supposing that the resulting chelate ring size would impact reactivity as compared to BPMEN.

The BPMEN catalyst scaffold afforded higher oxidation efficiency and selectivity across all substrates and conditions, while BPMPN drastically reduced efficiency as compared to TPA. These findings are highlighted in Chapter 2. While a simple synthetic

approach for bis-imidazole-*trans*-cyclohexylmethylethylenediamine (BItCHEN) was not successful, *n*-butyl-bis-imidazole-methylethylenediamine (^{nBu}BIMEN) showed greater affinity to epoxidation than oxidation reactions compared to pyridyl systems. Preliminary epoxidation catalysis efficiency and oxo stability Density Functional Theory (DFT) calculations are covered in Chapter 3.

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CHAPTER 2

Pyridyl-Based Ligand Architectures for C–H Activation and Epoxidation

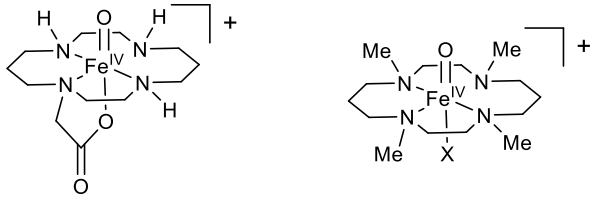
2.1 Background and Significance

Synthetic models of enzymes for catalytic C–H activation first utilized the heme architecture of CYP450s. Groves *et al*. provided the first examples of synthetic, high-valent iron-oxo heme-based systems for C–H hydroxylation and epoxidation.[1,2] Subsequent evidence of similar Fe^{IV}–oxo intermediates within the non-heme TauD enzyme led to further studies with non-heme based architectures.[3,4] Furthermore, kinetic isotope effects (KIE) studies of these non-heme intermediates were found to proceed via HAT, but generally follow radical pathways other than RM following substrate radical formation, or proceed through direct O-atom transfer (OAT).[5-7]

Elucidation of mononuclear active sites of non-heme iron oxo enzymes allowed for an influx of biomimetic catalyst synthesis and study. These studies indicate that analogues with similar reactivity can be produced from tetradentate amine ligands.[6,8-10] The first of these was produced by Wieghardt *et al*., though the Fe^{IV}–oxo exhibited poor stability, preventing full characterization (Figure 2.1, $[(cy\text{-}ac)Fe^{IV}(O)]^{+}$).[11] Following this, an intermediate crystal structure was established by Münck, Nam, and Que utilizing an altered ligand backbone (Figure 2.1, $[(TMC)Fe^{IV}(O)(X)]^{+}$).[12] These tetradentate amine scaffolds

with *cis* coordination sites are proposed to facilitate oxidation of Fe^{II} by hydrogen peroxide systems into an Fe^{III}–OH species. This can then produce the analogous hydroperoxo intermediate, and subsequently Fe^{V}–(O)(OH) or Fe^{V}–(O)(OOCR).[5]

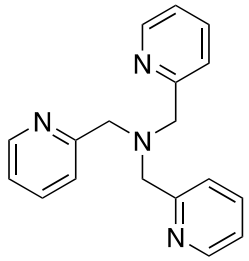
Figure 2.1 First examples of Fe^{IV}–oxo biomimetic intermediates.[11,12]



$[(cy\text{-}ac)Fe^{IV}(O)]^{+}$ $[(TMC)Fe^{IV}(O)(X)]^{+}$

Commonly, ligand architectures introduce pyridine-substituted chelate ligands to the iron center. This is likely due to pyridine's commercial abundance, simplicity in synthesis, and similar basicity to histidine residues contained within the mononuclear non-heme facial triad. Most notable among the pyridine-substituted ligands utilized is tris(2-pyridylmethyl)amine (TPA) (Figure 2.2), a commercially available solid and its associated derivatives.[8,13-16]

Figure 2.2 Structure of ligand TPA.



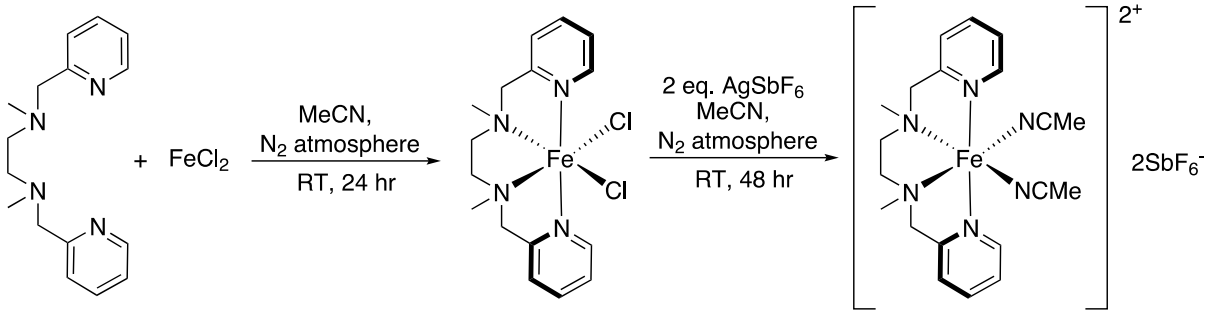
As such, our methodology aimed to utilize commercial TPA to compare to established pyridyl-based ligand architectures within a convenient reaction system. Generation of catalysts *in situ* provided relative ease of synthesis and utilized air-tolerant

materials so that reactions could be conducted on benchtop. Adding to this simplicity, addition of hydrogen peroxide as oxidant source was dropwise via syringe as opposed to syringe-pump methods. Within this system, we were able to show that steric accessibility of the ligand structures within the catalyst systems had a significant effect on TON capability as compared to Fe–TPA.

2.2 Results and Discussion

While Fe–BPMEN has been previously introduced in oxidation studies, the typical synthesis and preparation has two major limitations (Scheme 2.1). This method, relying on Fe (II) chloride, requires a period of approximately three days to complete with a secondary chloride abstraction step to allow for the coordination of acetonitrile. In addition, the constraint of providing an inert N_2 atmosphere for the entirety of the reaction makes the traditional method glovebox dependent.[17]

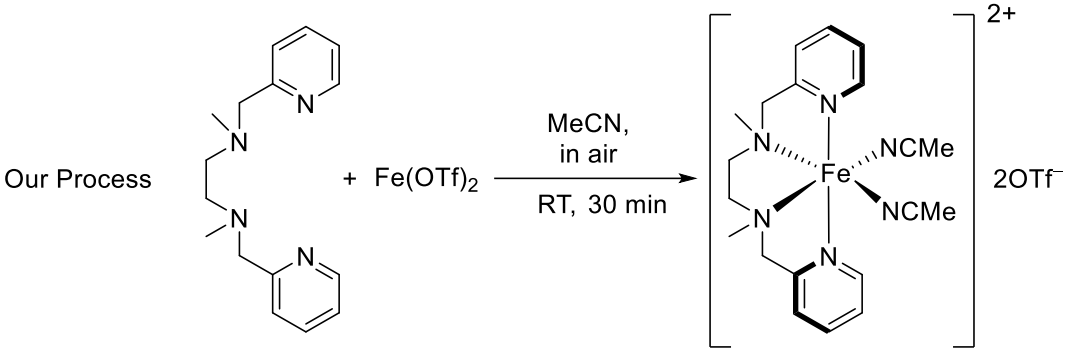
Scheme 2.1 Traditional preparation of Fe–BPMEN catalyst complex.[17]



In contrast, the proposed method utilized for Fe–BPMEN (Scheme 2.2) allowed for catalyst production *in situ*. This was achieved by using the relatively non-coordinating supporting ligand triflate (OTf), that could then exchange with acetonitrile in solution to

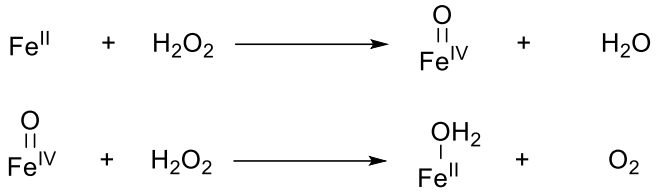
create the same catalyst with a different anion. Furthermore, this *in situ* method was extended to all ligand scaffolds for each Fe–L (where L = TPA, BPMEN, BPMPN) catalyst species. This methodology therefore offered a highly modular system for catalyst production and decreased reaction time to approximately 30 minutes in the presence of air on benchtop.

Scheme 2.2 Method utilized for preparation of Fe–BPMEN catalyst complex.



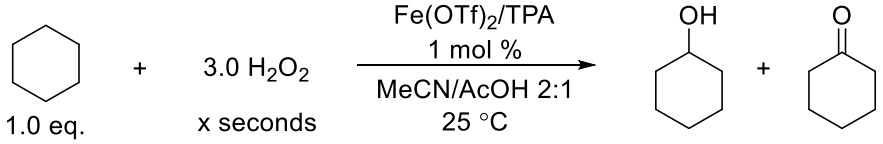
Furthermore, similar catalyst studies utilize syringe pump addition of the oxidant hydrogen peroxide.[18,19] This is likely to create a consistent addition rate as well as to minimize disproportionation of H_2O_2 into water and O_2, to which this oxidant is particularly susceptible in the presence of Fe^{IV}–oxo species (Scheme 2.3). This side reaction, well known through catalase studies and typically observed through the production of "bubbling" solution, can be minimized through slow introduction. While syringe pumps allow for greater control of H_2O_2 disproportionation, they are often slow (over several hours) and cumbersome. Therefore, this method aimed to utilize dropwise addition via syringe for greater convenience.

Scheme 2.3 Disproportionation of H_2O_2.



Varying addition rates had a noticeable effect on oxidation efficiency. Using dropwise addition, we established an addition rate that was relatively convenient while also maximizing TON. Studies using TPA and 1.0 eq. cyclohexane at room temperature with instantaneous, 8-10 second, and 30 second addition rates led to the choice of a 30 second addition rate across all catalysts and reaction conditions (Table 2.1). This addition rate allowed us a relatively simple way to introduce the "green" oxidant, hydrogen peroxide to the catalytic system. The drop in TON efficiency at faster addition rates may result from the disproportionation side reaction. As such, subsequent studies could benefit from the use of oxidants not prone to this degradation to determine the corresponding TON capability.

Table 2.1 Comparison of TPA TON with varying oxidant addition rates for cyclohexane.

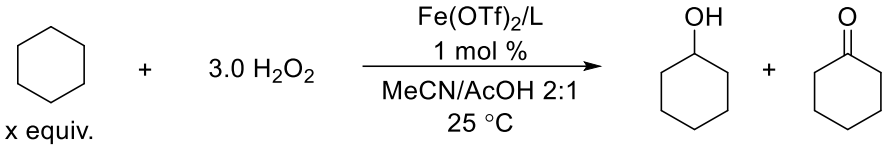


	TPA (TON)		
Addition Rate (s)	Alcohol	Ketone	Total
Instantaneous	4.1	1.6	7.2
8-10	6.1	1.4	9.0
30	8.4	2.6	13.7

While TON efficiency was exhibited for BPMEN for both HAT and OAT processes, catalyst reactivity is somewhat difficult to assess under the established conditions. Preliminary timed reactions yielded negligible differences in product TON, suggesting that the reaction completed essentially upon oxidant addition. This was further supported by the lack of lasting color change across all reaction parameters for the TPA and BPMEN complexes, indicating that the complex intermediate species is short-lived at temperatures of 0ºC or higher (current studied temperature range). As a result, reactivity studies and intermediate characterization should be conducted at lower temperatures for kinetic and catalyst lifetime studies.

Use of the BPMEN system with substrate cyclohexane (Table 2.2) more readily proceeded through the second oxidation of cyclohexanol to produce the cyclohexanone product as compared to TPA. Given BPMEN's dramatically increased TON as compared to TPA, this suggests a more catalytically active system overall, better able to activate the stronger 2° C–H bond to produce the alcohol product. Cyclohexanol's resulting weakened proximal C–H bond is therefore more susceptible to secondary oxidation to produce the ketone under this more effective system. Increasing substrate concentration resulted in higher TON for both, though varying equivalents with BPMEN resulted in a shift in selectivity to favor alcohol under excess conditions and ketone with lower loadings.

Table 2.2 TPA and BPMEN TON for cyclohexane oxidation products.

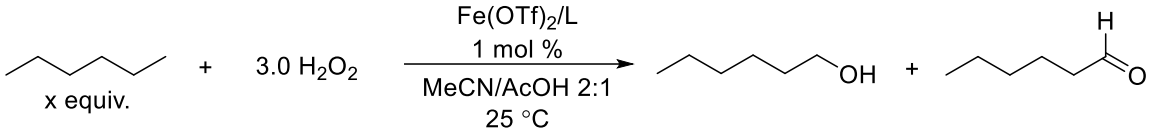


	TPA (TON)			BPMEN (TON)		
Equivalents	Alcohol	Ketone	Total	Alcohol	Ketone	Total
0.5	3.3	1.4	6.1	7.3	11.6	30.5
1.0	6.9	2.2	11.3	16.9	17.2	51.2
2.0	11.3	3.2	17.8	33.4	19.0	71.5
3.0	14.6	3.7	22.1	45.0	18.9	82.8

Following this initial comparison, we then examined the more sterically hindered system BPMPN's impact on reactivity. We suspected that the larger chelate size of the propyl backbone would drop efficiency as compared to BPMEN. Utilizing cyclohexane as substrate not only dropped TON below BPMEN, but yielded products near (at 0.1 TON) or below TON quantification limits. This excessively low reactivity suggested that C–H oxidation was highly sensitive to sterically hindered catalysts within this system.

Enhanced TON efficiency was similarly reflected for BPMEN as compared to TPA with the linear substrate *n*-hexane. Confirming the findings of White *et al.* with analogous systems, 1° products (hexyl alcohol, hexanal) were exceedingly low.[20,21] While TON for these products were quantifiable across TPA and BPMEN, they are difficult to accurately calculate on the extreme low limit of calibration, and thus are likely artificially inflated (Table 2.3). Interestingly, while BPMEN previously favored a second oxidation to ketone using cyclohexane, the aldehyde product was consistently below detection with room temperature and 0°C conditions. Furthermore, there was no evidence of the carboxylic acid product across reaction conditions.

Table 2.3 TPA and BPMEN TON for *n*-hexane 1° oxidation products.

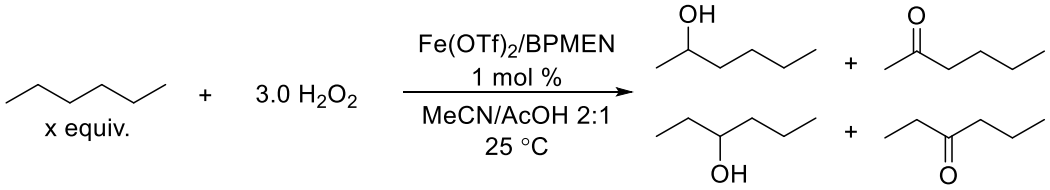


	TPA (TON)		BPMEN (TON)	
Equivalents	Alcohol	Aldehyde	Alcohol	Aldehyde
0.5	0.01	0.11	0.03	BD
1.0	0.03	0.15	0.08	BD
2.0	0.06	0.18	0.21	BD
3.0	0.06	0.19	0.27	BD

BD = below detection

Again confirming previous trends with aliphatic substrates, 2° products at the 2- and 3-positions were much more favored.[20,21] No significant preference for secondary oxidation to ketone was exhibited for either system unless excess BPMEN catalyst was used (Table 2.4).

Table 2.4 BPMEN TON for *n*-hexane 2° oxidation products.

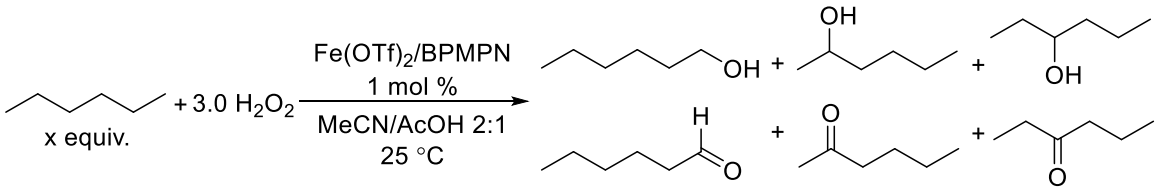


	BPMEN (TON)			
Conditions	2-Alcohol	2-Ketone	3-Alcohol	3-Ketone
0.5 eq.	2.33	3.83	1.99	2.51
1.0 eq.	4.71	6.20	3.73	3.95
2.0 eq.	8.75	8.52	6.57	5.18
3.0 eq.	11.57	9.28	8.62	5.41
1.0 eq. (2.0 mol% cat.)	1.92	4.69	1.74	3.27

As shown for cyclohexane, BPMPN was much less active and yielded product TON's below 1.0 under all conditions (Table 2.5). In particular, no 1-alcohol was detected,

indicating that this system proceeded to create hexanal through the weakened adjacent C–H bond.

Table 2.5 BPMPN TON for *n*-hexane oxidation products.



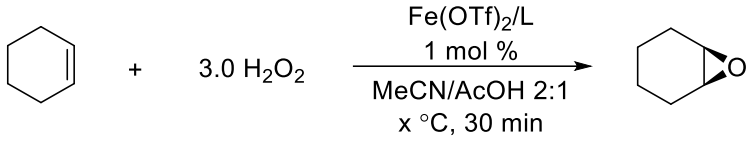
BPMPN (TON)

Conditions	1-Alcohol	1-Aldehyde	2-Alcohol	2-Ketone	3-Alcohol	3-Ketone
0.5 eq.	BD	0.03	0.02	0.58	BD	0.25
1.0 eq.	BD	0.03	0.06	0.61	0.13	0.29
2.0 eq.	BD	0.04	0.09	0.63	0.19	0.30
3.0 eq.	BD	0.05	0.09	0.62	0.19	0.29
1.0 eq (2.0 mol% cat.)	BD	0.03	0.06	0.37	0.14	0.22

BD = below detection

The introduction of the cyclohexene substrate allowed us to probe each catalyst system in terms of their OAT efficiency. Screening reactions for the epoxidation product again showed higher TON for BPMEN as compared to TPA. However, TPA's significantly higher oxide TON under 0°C and higher catalyst loading suggests that indiscriminate oxidation reactions might be occurring to multiple minor oxidation products, evidenced by additional slight spectral peaks observed in GC product traces. The significant drop in oxide TON under BPMEN at 50°C could similarly indicate that HAT is more favorable under higher energy conditions (Table 2.6). BPMPN showed sluggish OAT reactivity, resulting in TON ranging from 0.4-0.6 under all conditions.

Table 2.6 TPA and BPMEN TON for cyclohexene oxide product.



	TPA (TON)	**BPMEN (TON)**
Conditions	Oxide	Oxide
1.0 eq. (0°C)	8.2	57.1
1.0 eq. (50°C)	0.3	1.4
1.0 eq.	0.9	19.3
1.0 eq. (2.0 mol% cat.)	6.3	17.7

2.3 Conclusions

This method allowed for a novel *in situ* generation of catalysts from known ligand architectures. Our modular approach was successfully extended across pyridyl ligand derivative scaffolds to produce catalyst species BPMEN and BPMPN on benchtop over the course of approximately 30 minutes. This provided a much more convenient route to catalyst production compared to analogous synthetic means which require air-free glovebox conditions and reaction times over the course of several days. Methods for ligand synthesis were also relatively simple, corresponding of pyridine-carboxaldehyde and the necessary ethylenediamine derivative backbone to produce both scaffolds. Furthermore, our oxidant introduction was performed via dropwise addition, eliminating the need for syringe-pump techniques.

We suspected that decreased steric accessibility for the catalyst would hinder TON efficiency. We therefore used the extended backbone BPMPN in comparison to BPMEN, proposing that the increased chelate ring size would also increase steric hindrance.

Utilizing commercial TPA as a reference ligand for comparison, our findings demonstrate a marked effect on TON across BPMEN and BPMPN architectures. These findings indicate that steric accessibility plays a large role in efficiency, evidenced by at least a doubling of total TON when comparing BPMEN to TPA, and corresponding fractional or below quantification TON for BPMPN across all substrates.

In addition to overall TON increases when utilizing BPMEN, the shift in alcohol to ketone ratios showed a more catalytically-active system as compared to TPA's. In essence, the first transformation to an alcohol product was preferred in higher substrate concentration or low temperature conditions, but subsequent ketone formation was more facile under low substrate concentration, high temperature, and higher catalyst load conditions. In turn, TPA consistently favored cyclohexanol formation over cyclohexanone, but more readily produced ketone products with *n*-hexane.

While cyclohexane and *n*-hexane gave insight into HAT capability of these systems, cyclohexene was introduced as a function of OAT. TON of the epoxidation product were again higher for BPMEN as compared to TPA. While BPMPN showed slightly higher efficiency for this process as compared to oxidation of cyclohexane, TON were still lower than TPA. Therefore, OAT using these pyridine-based catalyst architectures are similarly sensitive to steric accessibility.

2.4 Experimental Procedures

2.4.1 Instrumentation

Ligand identity was analyzed by ^{1}H-NMR on a JEOL ECS 400 MHz NMR. Reaction products resulting from catalysis reactions were analyzed on a Clarus 590 GC-FID with a 30-meter ZB-5-HT column and quantified through calibration curves established as a ratio of instrument response of substrate and products as compared to a constant 50 µL volume of chlorobenzene as internal standard.

For cyclohexane and cyclohexene substrate reactions, the GC oven temperature was held at 80°C for one minute, then increased at a rate of 15°C per minute until it reached 140 °C. The rate was then increased to 20°C per minute until it reached 220°C, which was held for one minute. For *n*-hexane, the temperature was held at 40°C for five minutes, then ramped at 5°C per minute until it reached 70°C. The rate was then increased to 30°C per minute until reaching 220°C. Both used a helium flow rate of 2 mL per minute.

2.4.2 Ligand Synthesis

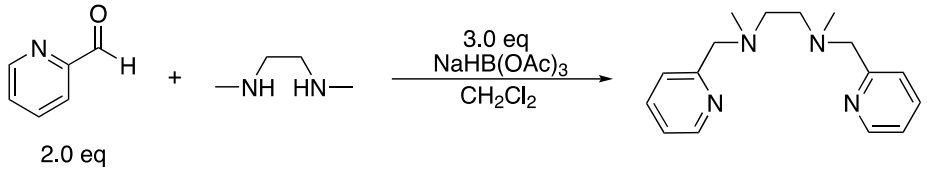
All materials were used as received. TPA was purchased from AK Scientific at 99% purity and, therefore, acted as a reference for the subsequent ligand derivatives. Solvents were HPLC-grade.

2-pyridinecarboxaldehye, N,N'-dimethylethylenediamine (DMED), and sodium triacetoxyborohydride ($NaHB(OAc)_3$) were sourced from AK Scientific at 98%, 95%, and 95% purity, respectively. Anhydrous $MgSO_4$ was sourced from Alfa Aesar at 99.5% purity.

N,N’-dimethyl-1,3-propanediamine (DMPD) was sourced from Acros Organics, at 97% purity.

Bis-pyridyl-methylethylenediamine (BPMEN) (Scheme 2.4)

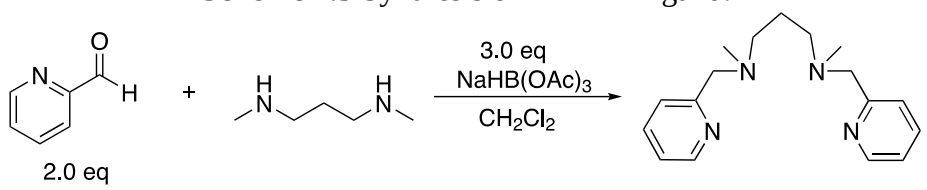
Scheme 2.4 Synthesis of BPMEN ligand.



A volume of 2.52 mL (2.0 eq., 26.49 mmol) of 2-pyridinecarboxaldehyde were combined with 1.42 mL (1.0 eq., 13.21 mmol) of N, N’-dimethylethylenediamine (DMED) and 7.86 g (3.0 eq., 37.09 mmol) of sodium triacetoxyborohydride in 200 mL DCM. The resulting mixture was stirred overnight. This was then added to a saturated aqueous sodium bicarbonate solution and diluted with ethyl acetate. The resulting organic phase product was then dried with anhydrous $MgSO_4$, vacuum filtered, and excess solvent removed through rotary evaporation to produce a dark red oil. The compound was purified using alumina column chromatography with a 0.5-5% gradient MeOH/dichloromethane (DCM) mobile phase and ligand identity confirmed through established ^{1}H-NMR characterization spectra.[22] Yield: 854.0 mg, 24%.

Bis-pyridyl-methylpropylenediamine (BPMPN) (Scheme 2.5)

Scheme 2.5 Synthesis of BPMPN ligand.



Synthesis of BPMPN followed the same procedure as BPMEN, but substituted N, N'-dimethyl-1,3-propanediamine (DMPD) in place of DMED (Scheme 2). DMPD at a volume of 0.79 mL (1.0 eq., 6.14 mmol) was combined with 1.26 mL (2.15 eq., 13.2 mmol) of 2-pyridinecarboxaldehyde and 3.93 g (3.0 eq., 18.5 mmol) of sodium triacetoxyborohydride in 100 mL DCM. Following the extraction and purification method described for BPMEN, this product appeared as a dark brown oil. As with BPMEN, ligand identity was confirmed through established ^{1}H-NMR characterization.[23] Yield: 217.0 mg, 12%.

2.4.3 Catalyst Preparation

Iron (II) triflate was sourced from Strem at 98% purity.

Catalysts using TPA, BPMEN, and BPMEN ligands were produced *in situ* at 5 mM concentration. One equivalent of the target ligand (Scheme 2.2, shown for BPMEN) was mixed with 53.1 mg (1.0 eq., 0.15 mmol) of iron (II) triflate in 30 mL acetonitrile, yielding the corresponding iron-ligand catalyst stock solution. This reaction took approximately 30 minutes, as evidenced by visual decrease of insoluble particles in solution and a gradual color change over the course of mixing.

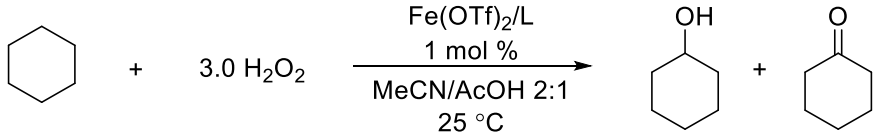
2.4.4 Catalysis

Cyclohexane and cyclohexene were sourced from Sigma-Aldrich at 99.8% and 99% purity, respectively. *n*-hexane was sourced from Thermo Fisher Scientific at 99%

purity, while glacial acetic acid at 99.7% purity and sodium thiosulfate were purchased from Flinn Scientific. Chlorobenzene was sourced from Alfa Aesar at 99% purity.

Catalysis reactions consisted of varying equivalents of substrates (cyclohexane, cyclohexene, *n*-hexane) added to 5 mL of the 1 mol% of the 5 mM Fe–L catalyst complex stock solution in a 2:1 ratio of acetonitrile/glacial acetic acid (AcOH). Then 3.0 equivalents (645 µL) of 35% H_2O_2 (Alfa Aesar) were used as oxidant for the reaction (Scheme 2.6, shown for cyclohexane), added dropwise over approximately 30 seconds. The reaction was quenched with sodium thiosulfate and the organic layer extracted with ethyl acetate. Chlorobenzene at a volume of 50 μL was then added as an internal standard.

Scheme 2.6 Standard catalysis parameters for substrate cyclohexane.



In addition to altering substrate equivalents (0.5, 1.0, 2.0, 3.0) variations in reaction temperature (0, 25, 50°C) and increasing to 2 mol% of catalyst were also investigated (Table 2.7). The standard catalysis method was defined as one equivalent of substrate, three equivalents H_2O_2, and 1 mol% catalyst at 25°C.

Table 2.7 Substrate equivalents and volumes for catalysis reactions.

Reagent	Equivalents	Volume (µL)
Cyclohexane	0.5	135
	1.0	270
	2.0	540
	3.0	810
Cyclohexene	0.5	127.5
	1.0	252.5
	2.0	505
	3.0	760
n-Hexane	0.5	163.75
	1.0	327.5
	2.0	655
	3.0	980

Each reaction was conducted in triplicate and mmols of oxidation products were quantified through calibration curves. Oxidation efficiency of each reaction was evaluated by calculating TON (Equation 1.1). Total TON was calculated for reactions using substrates cyclohexane and n-hexane (Equation 2.1).

Equation 2.1 Total TON = Alcohol TON + 2·Ketone/Aldehyde TON

2.5 References

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CHAPTER 3

Imidazole-Based Ligand Architectures for C–H Activation and Epoxidation

3.1 Background and Significance

This work aimed to use nature's examples of non-heme iron oxo enzymes for oxidation catalysis and investigate the effects of imidazole substitution in model catalyst systems. The common histidine coordination of these systems and their subsequent catalytic efficiency would indicate multidentate imidazole substitution as a viable synthetic model.[1,2] However, as mentioned previously, recent studies have mainly focused on pyridine-based ligands.

Imidazole-substituted ligands feature less prominently in iron oxo enzyme models.[3-6] Due to its basic (protonated pKa approximately 6.99) and electron-donating nature as well as lesser steric encumbrance when compared to pyridine (protonated pKa approximately 5.3), imidazole substitution could present an increase in catalytic oxidation reactivity.[7-11]

Previous work established by Bailey Jameson and Su Sandi, and optimized by these studies, investigated the effect of increased steric hindrance by using the BPMPN catalyst as compared to BPMEN. As seen with pyridyl-substituted scaffolds, total oxidation turnover numbers (total TON) increased from the TPA ligand to BPMEN, while the hindered BPMPN greatly reduced TON (Chapter 2). This observation indicated that steric

effects played a large role in oxidative reactivity, further reinforcing the potential of imidazole as a more effective model.

While iron-based synthetic models are typically employed as a more direct translation from non-heme enzymatic prototypes, varying late transition metals have also been introduced. Recent studies have indicated that Mn^{V}–oxo species with tetradentate amine ligand design are similarly capable of catalyzing HAT and OAT reactions.[12-14] Furthermore, while oxo/oxyl intermediates have been proposed but are less well-characterized, corresponding reactivity studies have also been conducted with analogous high-valent cobalt, nickel, and copper complexes.[12]

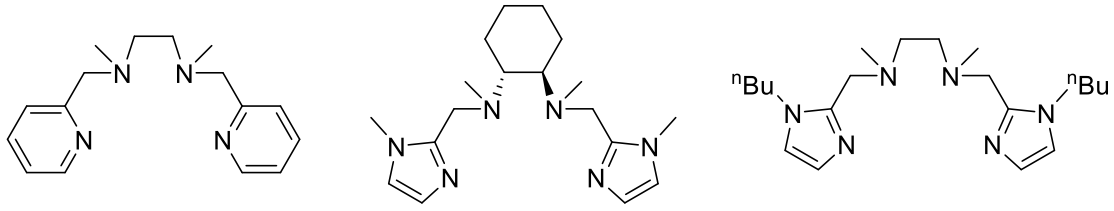
Similar to preceding iron models, other late transition metal derivatives typically employ pyridine or pyridine-type substituents. Some imidazole-based species have been utilized with varying degrees of characterization.[12] A manganese model with an imidazole-substituted tetradentate amine ligand exhibited highest reactivity for alcohol oxidation as compared to pyridyl-based architectures.[14] As such, examining efficiency across HAT and OAT reactions for iron systems with imidazole-substituted scaffolds is desirable.

3.2 Results and Discussion

Direct methylimidazole-substituted derivatives of pyridine ligands (BPMEN, BPMPN) would be desirable as a point of oxidation efficiency comparison. While methylimidazole synthetic procedures have been established, introduction of the imidazole substituent leads to a solubility decrease in organic solvents.[15,16] In light of continuing the

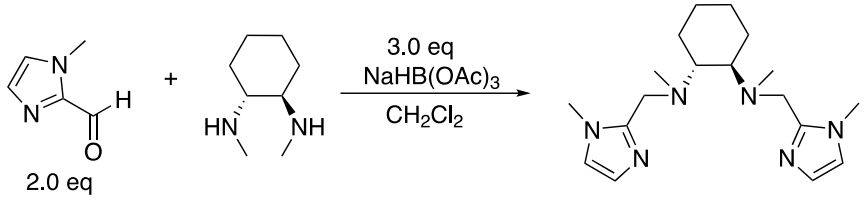
simple modular system approach for ligand and catalyst preparation, derivatives containing soluble alkyl substituents were considered (Figure 3.1).

Figure 3.1 Ligands BPMEN, BItCHEN, and ^{nBu}BIMEN.



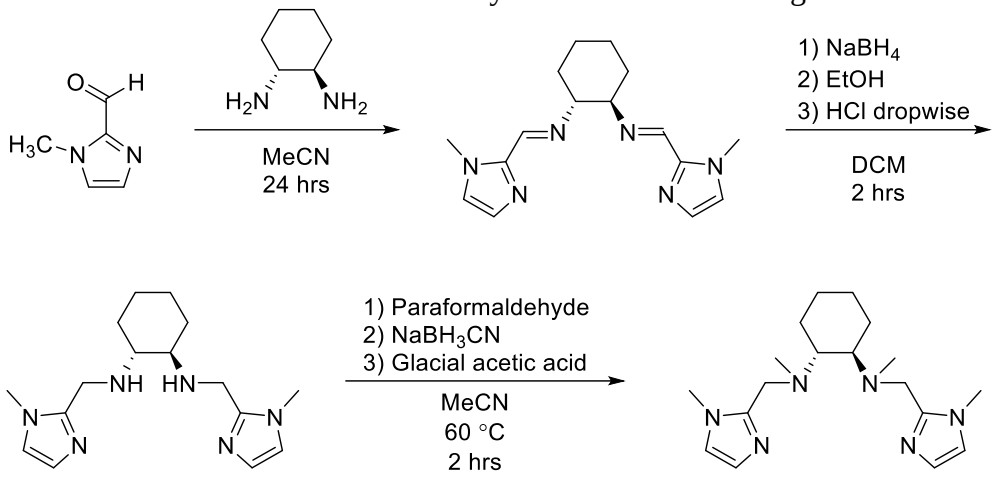
Ligand BItCHEN altered the ethyl backbone of the amine into a cyclohexyl ring (Scheme 3.1). While this offered a promising opportunity to continue the simple synthetic route outlined for pyridyl ligands, our efforts determined that even with an excess of the aldehyde, the reaction was slow to form product and resulted in prohibitively low yields.

Scheme 3.1 Proposed synthesis of BItCHEN ligand.



Alternate synthetic methods for this ligand were significantly more complex and utilized sodium cyanoborohydride in acidic conditions, introducing potential toxicity concerns (Scheme 3.2).[17,18] We therefore turned to alternate alkyl substituent architectures for imidazole-containing ligands.

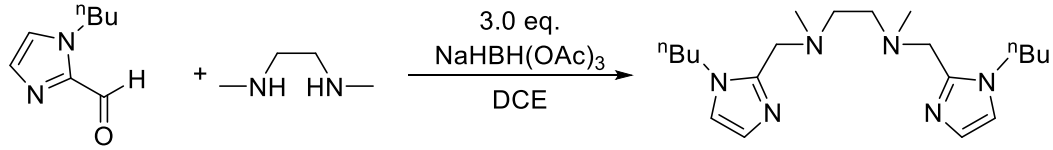
Scheme 3.2 Literature synthesis of BItCHEN ligand.[17,18]



The second route to addressing solubility was provided by our collaborator, Dr. Linus Chiang (University of the Fraser Valley, British Columbia, Canada), through the ^{nBu}BIMEN ligand. (Scheme 3.3, 3.4) As opposed to altering the amine backbone, an aliphatic butyl group was placed onto the imidazole in place of methyl to produce (1-butylimidazole)2-carboxaldehyde (CHO). While this added an alkylation step prior to ligand synthesis, this method was relatively simple and offered appropriate yields of a soluble imidazole BPMEN derivative.

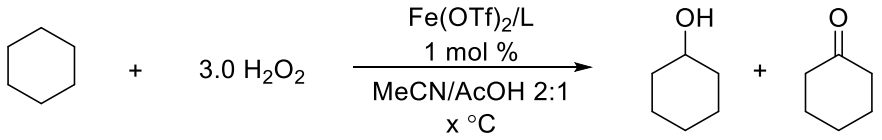
Scheme 3.3 Synthesis of CHO imidazole carboxaldehyde derivative for ^{nBu}BIMEN.

Scheme 3.4 Synthesis of ^{nBu}BIMEN ligand.



Preliminary studies for the ^{nBu}BIMEN catalyst species exhibited poor HAT ability as examined for the cyclohexane substrate. Resulting efficiency was higher than the hindered BPMPN system, but TON for both products were below that of TPA (Table 3.1). While reactivity was impacted by the imidazole substitution, a persistent color change upon oxidant addition within these initial studies suggested the formation of a more stable oxo-type species relative to the previous systems.

Table 3.1 ^{nBu}BIMEN, TPA, and BPMEN TON at varying temperatures for cyclohexane oxidation products.



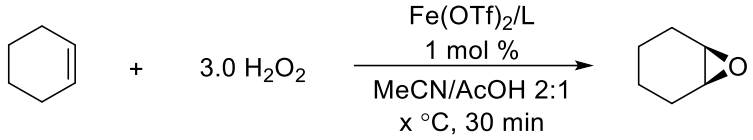
	^{nBu}BIMEN		**TPA**		**BPMEN**	
Conditions	Alcohol	Ketone	Alcohol	Ketone	Alcohol	Ketone
0°C	1.1	BQ	3.6	0.8	15.5	8.7
25°C	1.7	0.4	6.9	2.2	16.9	17.2
50°C	1.8	BQ	7.8	3.2	16.1	9.8

BQ = below quantification

Evidence of a more stable intermediate led us to investigate OAT capability of this system with the cyclohexene substrate and to extend reaction time to 30 minutes. Catalytic activity increased dramatically as compared to initial HAT studies, with oxide TON comparable to that of BPMEN using 1.0 eq. substrate at room temperature (Table 3.2). The lower product TON at higher temperatures could point to subsequent or competing oxidations, while the lower efficiency compared to BPMEN at low temperature could reflect the longer catalyst lifetime. An extended ^{nBu}BIMEN reaction of 1 hour with 1.0 eq

substrate at room temperature dropped TON to 12.8, further emphasizing the likelihood of secondary or competing processes.

Table 3.2 ^{nBu}BIMEN and BPMEN TON for cyclohexene oxide product.



	^{nBu}BIMEN (TON)	BPMEN (TON)
Conditions	Oxide	Oxide
1.0 eq. (0°C)	31.6	57.1
1.0 eq. (50°C)	3.3	1.4
1.0 eq.	20.2	19.3

Following the oxidative reactivity trend exhibited by the pyridyl and imidazoyl catalyst systems, a series of isodesmic reactions were performed on Gaussian 16 utilizing DFT with B3LYP functional and the 6-31G(d) basis set to assess oxo stability among the optimized catalyst systems.[19-23] Hess' Law summations were used to evaluate the stability of the complex for each ligand in terms of Self Consistent Field (SCF) energy compared to TPA (Equation 3.1), with L representing the free ligand.

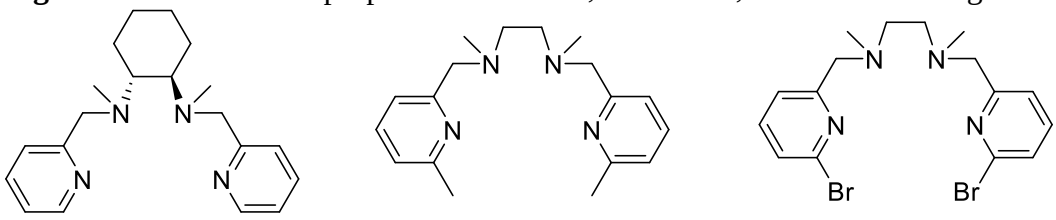
Equation 3.1 $[\mathrm{Fe-TPA(oxo)(MeCN)}]^{2+} + [\mathrm{Fe-L(MeCN)_2}]^{2+} \rightarrow$

$$[\mathrm{Fe-TPA(MeCN)_2}]^{2+} + [\mathrm{Fe-L(oxo)(MeCN)}]^{2+}$$

Further derivatives of BPMEN were investigated based on their establishment in literature and commercial availability of their starting materials in the scope of our synthetic method. The pyridine electronics were altered by substitution of a bromine or methyl group to produce bis-methylpyridyl-methylethylenediamine (^{Me}BPMEN) and bis-bromidepyridyl-methylethylenediamine (^{Br}BPMEN). We also introduced the pyridyl

analogue of BItCHEN to produce bis-pyridyl-*trans*-cyclohexylmethylethylenediamine (BPtCHEN) for comparison (Figure 3.2). Calculations showed that the formation of the Fe^{IV}–oxo with ^{nBu}BIMEN, BPMEN, and BPtCHEN were generally the most thermodynamically favored, closely followed by BItCHEN. ^{Me}BPMEN and BPMPN were thermodynamically unfavorable with respect to TPA, and ^{Br}BPMEN was the least favorable oxo species within the system. These computational findings reinforce the experimental observations of the persistent color change when H_2O_2 is added to the ^{nBu}BIMEN catalyst system, and the lack of long-lasting color change with pyridine-substituted systems.

Figure 3.2 Structures of proposed ^{Me}BPMEN, ^{Br}BPMEN, and BPtCHEN ligands.



BPtCHEN ^{Me}BPMEN ^{Br}BPMEN

3.3 Conclusions

We aimed to create a more efficient catalyst system through replacing pyridine substituents with imidazole as a mimic of the histidine ligation exhibited in the 2-His-1-carboxylate facial triad of non-heme iron oxo enzymes. The translation to a direct imidazole derivative of BPMEN, however, is prohibitively less soluble in organic solvents under our established catalysis procedure. We, therefore, investigated ways to increase alkyl substituents onto the ligand architecture.

The initial approach to altering the ethylenediamine backbone into a cyclic alkyl afforded the established ligand BItCHEN. Under our synthetic method, however, product was sluggish to form even with excessive amounts of imidazolecarboxaldehyde and amine components. While alternate synthetic procedures are available, they are very complex and inconvenient and utilize toxic reaction conditions. ^{nBu}BIMEN, provided by our collaborator, addressed solubility through an *n*-butyl group added to the imidazole substituent. The addition of an alkylation step still afforded a simple and convenient way to produce the beginning imidazolecarboxaldehyde that could be translated to our ligand and catalyst synthetic method used for BPMEN and BPMPN.

Investigations into HAT capability with the ^{nBu}BIMEN catalyst yielded poor TON reactivity below that of both BPMEN and TPA even over extended reaction times. While HAT efficiency was poor, prolonged color change upon oxidant addition led us to believe that ^{nBu}BIMEN had a more stable oxo-type intermediate than its pyridyl counterparts. As such, we performed epoxidation reactions over an extended reaction time to assess OAT capability for this system. In contrast to cyclohexane products, epoxide product TON were comparable to that of BPMEN, suggesting that this catalyst is more favorable for OAT processes. Reduced TON at longer reaction times suggest that subsequent or competing oxidation reactions are susceptible with cyclohexene under this catalyst system.

Evidence of a more stable intermediate led to computational modeling of catalyst and Fe−oxo structures with each ligand and varying derivatives of BPMEN using DFT. Oxo stability was estimated from the resulting optimized structures as compared to the

reference TPA oxo complex, indicating that ^{nBu}BIMEN and BPMEN were the most thermodynamically stable while the hindered BPMPN was relatively unfavorable. Derivative BPtCHEN was similarly favored, followed by BItCHEN, whereas ^{Me}BPMEN was unfavorable. Compared to all other architectures, oxo stability was least favored with the ^{Br}BPMEN ligand.

3.4 Experimental Procedures

3.4.1 Instrumentation

Ligand identity for BItCHEN was analyzed by ^{1}H-NMR on a JEOL ECS 400 MHz NMR. The provided ^{nBu}BIMEN ligand identity was characterized by ^{1}H and ^{13}C-NMR on a Bruker AV 400 MHz NMR with TopSpin software. Reaction products resulting from catalysis reactions were analyzed on a Clarus 590 GC-FID with a 30-meter ZB-5-HT column, using the same ramp and flow rates as outlined in section 2.4.1.

3.4.2 Ligand Synthesis

All materials were used as received. TPA was purchased from AK Scientific at 99% purity and therefore acted as a reference for the subsequent ligand derivatives. Solvents were HPLC-grade.

Bis-imidazole-*trans*-cyclohexylmethylethylenediamine (BItCHEN) (Scheme 3.1)

The initial synthesis of BItCHEN followed our procedure as BPMEN, substituting 2.90 g (2.0 eq., 26.3 mmol) 1-methyl-2-imidazolecarboxaldehyde and 1.88 g (1.0 eq., 13.3 mmol) *trans*-N,N'-dimethylcyclohexane-1,2-diamine mixed with 7.86 g (2.79 eq., 37.1 mmol) sodium triacetoxyborohydride in 200 mL DCM. An alternate, multi-step synthesis

involves the production of the ligand prior to methylation as described by LaRonde and Brook.[17] This derivative is then methylated according to Bennov, *et al*. to produce the desired ligand as a yellow oil.[18] This method involves multiple steps over the period of several days (Scheme 3.2).

(1-butylimidazole)2-carboxaldehyde (CHO) (Scheme 3.3)

1-Bromobutane and 2-imidazolecarboxaldehyde were sourced from AK Scientific at 99% and 98% purity, respectively. Anhydrous $MgSO_4$ was sourced from Alfa Aesar at 99.5% purity.

^{nBu}BIMEN was synthesized and characterized by Dr. Linus Chiang. The imidazole carboxaldehyde derivative (1-butylimidazole)2-carboxaldehyde (CHO) was produced by adding 1.01 g (1.0 eq., 7.3 mmol) K_2CO_3 and 0.79 mL (1.0 eq., 7.3 mmol) 1-bromobutane to a solution of 0.70 g (1.0 eq., 7.3 mmol) 2-imidazolecarboxaldehyde in 10 mL dimethylformamide (DMF). This mixture was then stirred over approximately 16 hours at 70°C, then cooled to room temperature and 20 mL water added. The solution was extracted with hexanes, dried with anhydrous $MgSO_4$, and concentrated using rotary evaporation to produce a yellow oil. Yield: 920 mg, 83%.

^{1}H NMR ($CDCl_3$, 400 MHz): d = 9.60 (s, 1H, CHO), 7.13 (s, 1H, imid-H), 7.05 (s, 1H, imid-H), 4.26 (t, J = 7.3, 2H, C*H*$_2$-$CH_2CH_2CH_3$), 1.64 (quin, J = 7.5, 2H, CH_2-C*H*$_2$-CH_2CH_3), 1.20 (sex, J = 7.5, 2H, CH_2CH_2-C*H*$_2$-CH_3), 0.79 (t, J = 7.3, 3H, $CH_2CH_2CH_2$-C*H*$_3$) (Figure 3.3); ^{13}C NMR ($CDCl_3$, 100 MHz): 182.0, 143.4, 131.6, 126.3, 47.6, 33.1, 19.6, 13.6 (Figure 3.4).

Figure 3.3 ^{1}H-NMR of CHO.

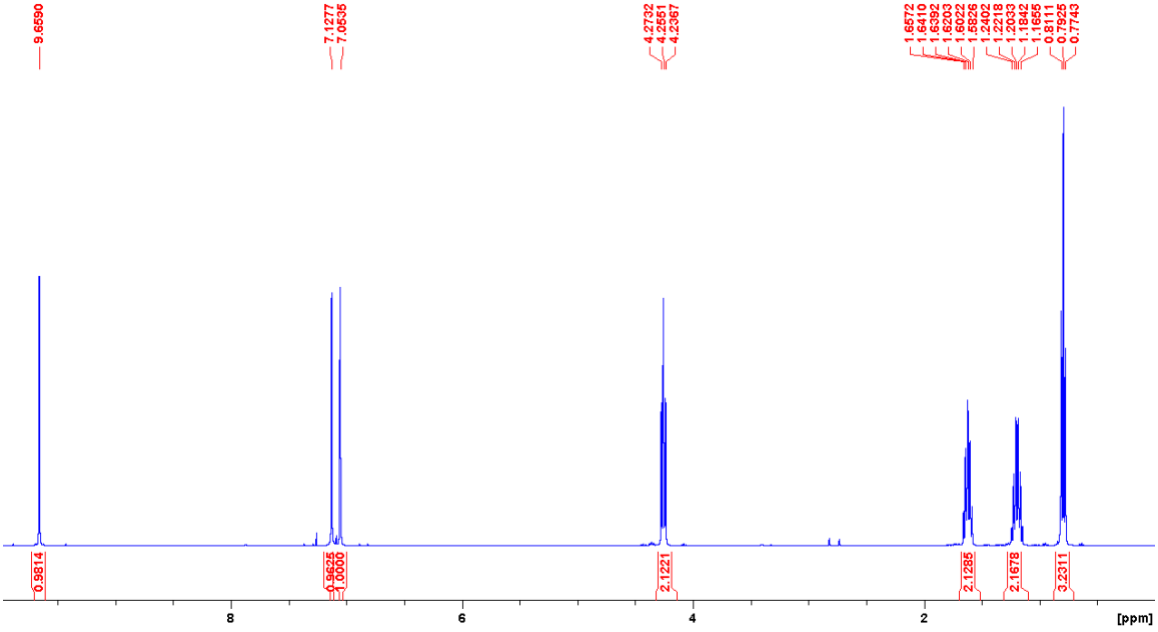
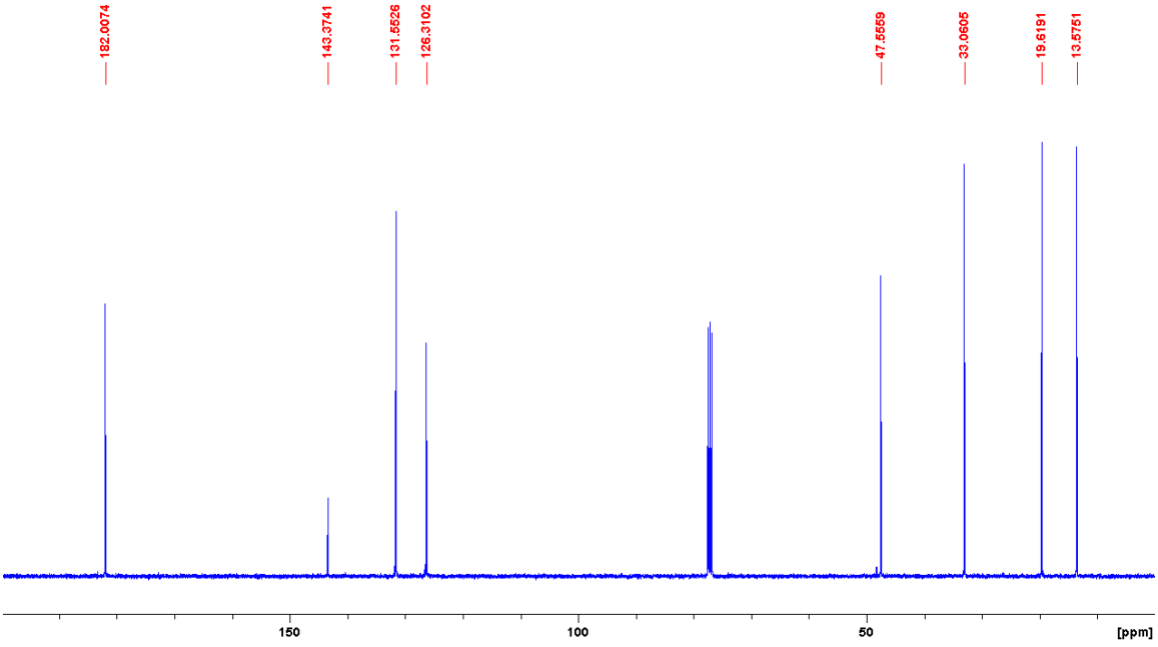


Figure 3.4 ^{13}C-NMR of CHO.



***n*-Butyl-bis-imidazole-methylethylenediamine (^{nBu}BIMEN)** (Scheme 3.4)

Synthesis of ^{nBu}BIMEN followed that of previous ligands, utilizing 248 μL (1.0 eq., 2.3 mmol) DMED and 0.70 g (2.0 eq., 4.6 mmol) CHO for the ethylenediamine and carboxaldehyde derivatives with 10 mL dichloroethane (DCE) as solvent and 1.46 g (3.0 eq., 6.9 mmol) sodium triacetoxyborohydride. Over the course of reaction, 15 mL of water were added. It was then extracted with DCM and purified using alumina column chromatography with a 0.5-5% gradient MeOH/DCM mobile phase. Yield: 450 mg, 54%.

^{1}H NMR ($CDCl_3$, 400 MHz): d = 6.88 (d, J = 1.24, 2H, imid-H), 6.83 (d, J = 1.24, 2H, imid-H), 3.95 (t, J = 7.4, 4H, Ar-H), 3.53 (s, 4H, N-CH_2-imid), 2.47 (s, 4H, N-CH_2-CH_2-N), 2.12 (s, 6H, N-CH_3), 1.67 (m, 4H, CH_2-CH_2-CH_2CH_3), 1.29 (sex, J = 5.0, 4H, CH_2CH_2-CH_2-CH_3), 0.88-0.92 (t, J = 7.3, 3H, $CH_2CH_2CH_2$-CH_3) (Figure 3.5); ^{13}C NMR ($CDCl_3$, 100 MHz): 145.0, 127.2, 120.0, 55.3, 55.1, 45.7, 42.5, 33.0, 20.0, 13.8 (Figure 3.6).

Figure 3.5 ^{1}H-NMR of ^{nBu}BIMEN.

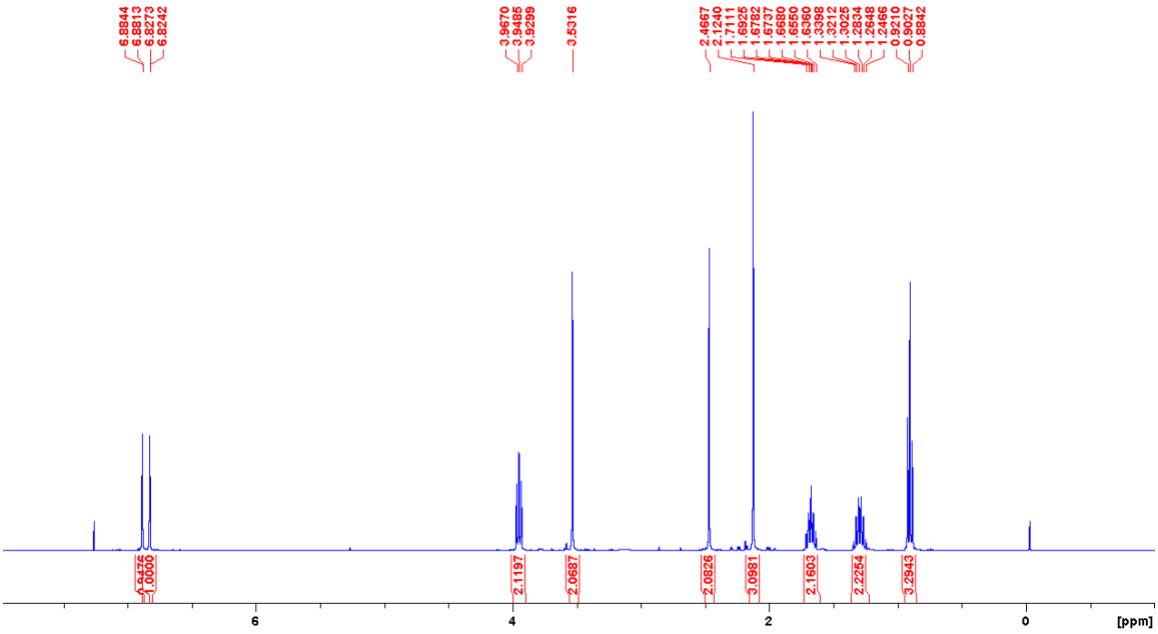
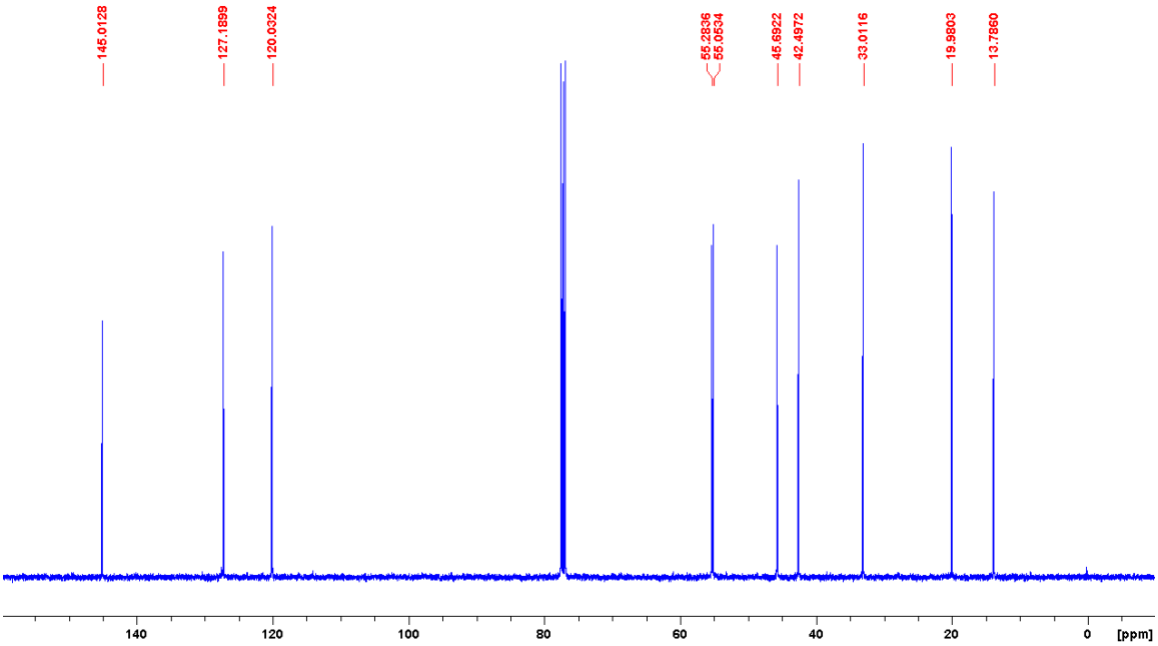


Figure 3.6 ^{13}C-NMR of ^{nBu}BIMEN.



3.4.3 Catalyst Preparation

Iron (II) triflate was sourced from Strem at 98% purity.

The catalyst preparation using ^{nBu}BIMEN as the target ligand was prepared as outlined in section 2.4.3. Reaction time took slightly longer (approximately 1 hour) for this ligand, evidenced by visual decrease of insoluble particles in solution and a gradual color change over the course of mixing.

3.4.4 Catalysis

Cyclohexane and cyclohexene were sourced from Sigma-Aldrich at 99.8% and 99% purity, respectively. Glacial acetic acid at 99.7% purity and sodium thiosulfate were purchased from Flinn Scientific. Chlorobenzene was sourced from Alfa Aesar at 99% purity.

Catalysis reactions, product quantification, and TON calculations were performed as outlined in section 2.4.4 for substrates cyclohexane and cyclohexene.

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CHAPTER 4

Conclusions and Future Prospects

4.1 Conclusions

Transformation of reduced hydrocarbon compounds acts as a starting material for the majority of synthetic materials in modern chemical industry. Therefore, the selective and efficient activation and functionalization of C–H bonds remains an ongoing challenge in catalytic systems. The first major breakthrough for catalytic C–H activation was pioneered by Shilov, then improved upon by Periana and related systems.[1-4] Shilov-type systems, however, were still inhibited by cost-prohibitive oxidants or harsh conditions that made substrates susceptible to over-oxidation. Subsequent studies introduced a ligand-directed approach, in which ligands containing a coordinatively-capable heteroatom brought sites of C–H activation into proximity to the metal center.[5-9] This was a notable improvement on the Shilov system approach, but still requires substrates with chelating ability and catalysts based on relatively noble metals such as Pt, Pd, Ir, and Rh.[10-16]

In an effort to utilize relatively cheap and abundant metal sources, C–H activation and functionalization studies can therefore turn to the elegant iron-based enzymatic systems present in nature. CYP450s presented the first evidence of hydrocarbon oxidation across a wide variety of substrates within metabolic systems through the HAT/RM mechanism with an Fe^{IV}–oxo center.[17-21] Subsequent studies of non-heme iron enzymes

showed similar substrate scope through HAT/RM.[22-,25] Furthermore, crystal structures of mononuclear non-heme species allowed for determination of the protein scaffold in the so-called '2-His-1-carboxylate facial triad.'[26-28]

The subsequent influx of biomimetic studies allowed for synthetic characterization and reactivity studies.[29-31] Tetradentate amine ligand architectures were shown to produce similar reactivity to non-heme models and produce Fe^{IV}–oxo or oxo-type species that reacted via HAT or OAT but generally followed mechanisms other than RM.[32-37] As such, this work aimed to create a simple and modular catalytic method for C–H activation and epoxidation across pyridyl- and imidazole-substituted ligand structures.

The well-studied and commercially available TPA ligand was utilized as a reference, but was generated *in situ* with Fe(II) triflate. This catalyst generation allowed for open-air benchtop synthesis, and was translated across all ligand architectures (BPMEN, BPMPN, ^{nBu}BIMEN) studied. This presented a notable improvement on typical methods, which require air-free glovebox techniques and lengthy multi-step synthesis from the starting Fe(II) chloride.[38] Furthermore, ligand synthesis was optimized by utilizing the pyridine- or imidazole- carboxaldehyde species and ethylenediamine derivative backbones to produce the tetradentate amine ligands for study. We also utilized dropwise addition of H_2O_2 as an oxidant, thereby eliminating the need for syringe pump methods.[39,40]

Ligand BPMEN yielded the most catalytically active system overall across all substrates (cyclohexane, *n*-hexane, cyclohexene). Oxidation studies indicated that BPMEN more readily proceeded to a secondary oxidation for ketone products in 2° C–H substrates

as compared to TPA, but produced no detectable aldehyde products at 1° positions. Oxidation to primary alcohols yielded fractional TON, following established trends across aliphatic substrates.[41,42] OAT assessed through epoxidation reactions similarly afforded higher TON compared to TPA but was susceptible to side oxidation products.

Increasing the ethyl bridge of the BPMEN backbone to produce BPMPN yielded a more sterically-encumbered system. Reactions with this less sterically accessible catalyst resulted in dramatically reduced efficiency across all substrates, often with non-quantifiable TON. Therefore, we determined that steric hindrance played a large role in efficiency across pyridine-substituted structures.

Investigating imidazole substitution necessitated the addition of alkyl substituents to the ligand backbone to increase organic solubility. The introduction of a cyclohexyl ethylenediamine derivative afforded the ligand BItCHEN, which proved to be excessively slow to form under the proposed synthetic method. Therefore, an alternate architecture was created by our collaborator to produce ^{nBu}BIMEN. Adding an alkylation step to the imidazole-carboxaldehyde prior to ligand synthesis successfully created a soluble imidazole-based catalyst.

Preliminary studies on ^{nBu}BIMEN's oxidation capability with cyclohexane showed diminished efficiency below that of the TPA system even across extended reaction times. However, visual evidence of a more stable intermediate upon oxidant addition was observed as compared to the pyridine-substituted systems. OAT capability, in turn, was much more facile, with epoxide TON comparable to that of BPMEN. However, this system

again was prone to side oxidation processes, indicated by a drop in product TON with extended reaction times.

Following the more long-lived observed intermediate with ^{nBu}BIMEN, we calculated oxo stability through DFT calculations. Supporting experimental findings, ranking stability of oxo species resulted in the order ^{nBu}BIMEN, BPMEN, and BPtCHEN (the pyridine analogue of BPMEN), followed by BItCHEN as thermodynamically favored compared to the reference TPA oxo complex, followed by the relatively unfavored ^{Me}BPMEN, BPMPN, and lastly ^{Br}BPMEN.

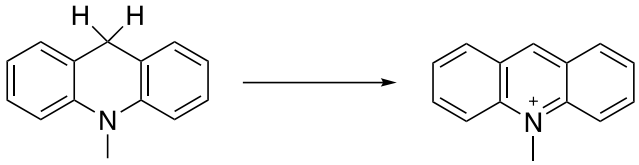
4.2 Future Prospects

While this work offers a highly convenient and modular system for C–H activation and functionalization, there are disadvantages that could be addressed. Use of H_2O_2 is desirable as it is a relatively more "green" oxidant.[43] However, the susceptibility of this species to disproportionation could inhibit TON efficiency, particularly as this method utilizes dropwise syringe addition as opposed to syringe pump. As such, circumventing this side reaction by using alternate oxidant species could provide higher TON efficiency.[43] Therefore, future reactions could use the common *t*-butyl peroxide as an oxidant source for comparison.[44]

Additionally, other substrates would be worthwhile to examine for BPMEN and ^{nBu}BIMEN architectures for processes other than C–H oxidation or OAT. In particular, investigating various anthracene derivatives for isolated HAT studies, substrates capable

of HAT but not RM, could be examined via the weakened doubly benzylic C–H bond (Scheme 4.1).[37]

Scheme 4.1 HAT on an anthracene derivative substrate.



The evidence of an observable longer-lived intermediate with ^{nBu}BIMEN should also be examined to determine whether an active oxo or oxo-type species is present. Characterization studies of this intermediate could similarly provide more information on its reactivity and allow for other similar imidazole-substituted derivatives.

Furthermore, future experimental work should utilize the BPtCHEN, ^{Me}BPMEN, and ^{Br}BPMEN catalyst structures as a comparison to BPMEN.[39] The stable oxo species calculated using BPtCHEN suggests that it might provide an active system similar to BPMEN and ^{nBu}BIMEN across certain reaction mechanisms or substrates. Furthermore, direct BPMEN derivatives (^{Me}BPMEN, ^{Br}BPMEN) could allow for studies on reactivity as influenced by their increased steric bulk and less donating electronic properties. As these substituted pyridine carboxaldehyde derivatives are commercially available, these ligands can easily be produced within the one-step synthetic system utilized for ligand production.

4.3 References

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APPENDIX

XYZ Coordinates – Calculated Structures

TPA (free ligand)

N	-1.042385000	2.671186000	0.412716000
C	-0.380379000	2.754105000	-0.756447000
C	-0.922075000	3.684001000	1.279957000
C	0.406967000	3.863437000	-1.086817000
C	-0.158138000	4.827486000	1.037357000
H	-1.469422000	3.580780000	2.216172000
C	0.519124000	4.916358000	-0.177986000
H	0.924371000	3.895962000	-2.041194000
H	-0.101746000	5.618761000	1.778825000
H	1.125863000	5.786343000	-0.414847000
N	1.824998000	0.530085000	0.918735000
C	2.081049000	0.690898000	-0.393259000
C	2.643902000	1.122179000	1.797031000
C	3.171975000	1.437880000	-0.852998000
C	3.753933000	1.886964000	1.431201000
H	2.405836000	0.973682000	2.849594000
C	4.022897000	2.043485000	0.072439000
H	3.346631000	1.541693000	-1.920039000
H	4.383926000	2.339350000	2.191096000
H	4.875488000	2.628160000	-0.262683000
N	-2.774648000	-0.932676000	-0.110011000
C	-4.046072000	-0.924586000	0.308048000
C	-2.536145000	-0.716533000	-1.417961000
C	-5.139400000	-0.709002000	-0.534701000
H	-4.202581000	-1.104578000	1.370877000
C	-3.568633000	-0.492559000	-2.335868000
C	-4.891154000	-0.489359000	-1.888129000
H	-6.149433000	-0.716974000	-0.136370000
H	-3.335002000	-0.324271000	-3.383188000
H	-5.708158000	-0.317364000	-2.583665000
C	-1.084796000	-0.762651000	-1.860488000
H	-1.040129000	-0.724175000	-2.963573000
H	-0.673821000	-1.731346000	-1.555372000
C	1.170951000	-0.039249000	-1.366223000

H	1.282742000	-1.112017000	-1.169597000
H	1.532512000	0.138319000	-2.395379000
C	-0.590052000	1.617418000	-1.744438000
H	-0.042475000	1.837551000	-2.677369000
H	-1.655613000	1.616212000	-1.998448000
N	-0.256076000	0.279596000	-1.231204000

Fe–TPA 2+ singlet

Fe	-0.380249000	0.276273000	0.304905000
N	-0.632904000	2.243559000	0.289864000
C	-0.462305000	2.828868000	-0.913680000
C	-0.955822000	3.023567000	1.344351000
C	-0.609781000	4.204384000	-1.096583000
C	-1.118534000	4.397911000	1.238415000
H	-1.084793000	2.519261000	2.293330000
C	-0.942466000	5.002885000	-0.007364000
H	-0.463338000	4.630969000	-2.083946000
H	-1.378396000	4.975890000	2.118770000
H	-1.062747000	6.075333000	-0.126955000
N	1.588412000	0.543262000	0.471692000
C	2.242287000	0.409745000	-0.708750000
C	2.288904000	0.896625000	1.565056000
C	3.612394000	0.628993000	-0.819596000
C	3.661825000	1.118658000	1.531932000
H	1.723685000	1.003086000	2.483948000
C	4.336165000	0.983052000	0.318845000
H	4.096935000	0.523237000	-1.784707000
H	4.182588000	1.398505000	2.441433000
H	5.405994000	1.157679000	0.256754000
N	-2.261682000	0.048677000	-0.311251000
C	-3.391064000	0.156157000	0.412657000
C	-2.358793000	-0.174227000	-1.645218000
C	-4.655378000	0.035542000	-0.154896000
H	-3.266181000	0.343527000	1.473091000
C	-3.590330000	-0.291745000	-2.283176000
C	-4.757912000	-0.191601000	-1.526959000
H	-5.535898000	0.125703000	0.472121000
H	-3.625689000	-0.459533000	-3.354695000
H	-5.729501000	-0.283071000	-2.002844000
C	-1.040457000	-0.330779000	-2.363600000
H	-1.121923000	-0.052637000	-3.419119000

H	-0.733673000	-1.379441000	-2.320030000
C	1.380957000	-0.030645000	-1.867134000
H	1.338086000	-1.123192000	-1.884706000
H	1.793999000	0.302129000	-2.824625000
C	-0.100361000	1.928831000	-2.064810000
H	0.855154000	2.249455000	-2.490078000
H	-0.844346000	2.035393000	-2.859829000
N	-0.005549000	0.483825000	-1.659956000
N	-0.736850000	0.094361000	2.187549000
N	-0.127514000	-1.644061000	0.266029000
C	-0.934486000	-0.104098000	3.311716000
C	0.006819000	-2.791685000	0.338736000
C	-1.182796000	-0.343277000	4.723714000
H	-2.011501000	0.285221000	5.065745000
H	-1.440717000	-1.395634000	4.880581000
H	-0.285367000	-0.102656000	5.302997000
C	0.180366000	-4.232562000	0.416645000
H	1.089472000	-4.465845000	0.980332000
H	-0.681101000	-4.682969000	0.920002000
H	0.265720000	-4.648754000	-0.592375000

Fe-TPA 2+ triplet

Fe	-0.456492000	0.248057000	0.295651000
N	-0.658407000	2.424079000	0.271741000
C	-0.405988000	2.953537000	-0.937349000
C	-0.778482000	3.245654000	1.330318000
C	-0.251038000	4.328545000	-1.124379000
C	-0.654898000	4.626715000	1.225700000
H	-0.976683000	2.770339000	2.286037000
C	-0.379516000	5.177426000	-0.027478000
H	-0.037652000	4.717847000	-2.115144000
H	-0.763464000	5.249504000	2.107367000
H	-0.263632000	6.250515000	-0.147787000
N	1.493454000	0.549759000	0.457171000
C	2.142480000	0.569687000	-0.735639000
C	2.193264000	0.805550000	1.580115000
C	3.503309000	0.851436000	-0.823431000
C	3.555945000	1.079834000	1.566300000
H	1.632602000	0.789068000	2.507354000
C	4.224025000	1.106198000	0.342430000
H	3.983584000	0.868641000	-1.796288000

H	4.073122000	1.276031000	2.499399000
H	5.286107000	1.326456000	0.294452000
N	-2.311508000	-0.041570000	-0.334873000
C	-3.445854000	-0.000286000	0.390440000
C	-2.399547000	-0.263072000	-1.673325000
C	-4.702367000	-0.188222000	-0.175178000
H	-3.329522000	0.188851000	1.451369000
C	-3.625255000	-0.446951000	-2.305952000
C	-4.795395000	-0.416225000	-1.547416000
H	-5.584742000	-0.148818000	0.454428000
H	-3.653967000	-0.610024000	-3.378368000
H	-5.761243000	-0.559653000	-2.022172000
C	-1.080910000	-0.330744000	-2.411235000
H	-1.208802000	-0.088017000	-3.471825000
H	-0.688901000	-1.350404000	-2.348708000
C	1.316917000	0.200220000	-1.947795000
H	1.359032000	-0.886279000	-2.075859000
H	1.730518000	0.652396000	-2.855198000
C	-0.380114000	2.001588000	-2.115142000
H	0.344898000	2.340117000	-2.862146000
H	-1.364950000	2.042555000	-2.591840000
N	-0.107574000	0.580034000	-1.746239000
N	-0.853748000	0.056750000	2.306476000
N	-0.106947000	-1.897619000	0.224537000
C	-1.082269000	-0.140391000	3.425077000
C	0.079905000	-3.034745000	0.346730000
C	-1.369867000	-0.387834000	4.826540000
H	-2.227480000	0.217611000	5.137206000
H	-1.606094000	-1.447497000	4.968266000
H	-0.498639000	-0.125551000	5.435191000
C	0.313841000	-4.461151000	0.494421000
H	1.224951000	-4.628231000	1.077555000
H	-0.535756000	-4.922945000	1.007242000
H	0.429105000	-4.916619000	-0.494421000

Fe-TPA 2+ quintet

Fe	-0.562640000	0.210163000	0.507351000
N	-0.708240000	2.380510000	0.391896000
C	-0.440057000	2.909784000	-0.816578000
C	-0.866672000	3.205245000	1.445479000
C	-0.308110000	4.289291000	-0.998307000

C	-0.767948000	4.586777000	1.341277000
H	-1.074781000	2.728536000	2.397945000
C	-0.476977000	5.138323000	0.091571000
H	-0.080913000	4.682349000	-1.984517000
H	-0.907496000	5.210108000	2.218065000
H	-0.380123000	6.213122000	-0.030853000
N	1.626073000	0.513242000	0.475236000
C	2.181969000	0.575168000	-0.752495000
C	2.383688000	0.796096000	1.550484000
C	3.517816000	0.932365000	-0.935192000
C	3.726003000	1.146295000	1.450179000
H	1.888580000	0.741200000	2.514572000
C	4.301908000	1.218247000	0.181326000
H	3.928435000	0.982890000	-1.938498000
H	4.297523000	1.364545000	2.345979000
H	5.344277000	1.498577000	0.061823000
N	-2.496878000	-0.069235000	-0.527945000
C	-3.697076000	-0.052761000	0.078822000
C	-2.429522000	-0.268759000	-1.858814000
C	-4.886168000	-0.241749000	-0.617268000
H	-3.690175000	0.117385000	1.151635000
C	-3.578753000	-0.454975000	-2.626977000
C	-4.822448000	-0.447170000	-1.996542000
H	-5.833764000	-0.222783000	-0.089790000
H	-3.492717000	-0.602807000	-3.698750000
H	-5.729855000	-0.592693000	-2.575162000
C	-1.038604000	-0.323617000	-2.451725000
H	-1.066689000	-0.066512000	-3.518148000
H	-0.668960000	-1.351399000	-2.373345000
C	1.300088000	0.167313000	-1.911338000
H	1.338457000	-0.924575000	-1.991658000
H	1.692201000	0.576241000	-2.850491000
C	-0.363424000	1.983906000	-2.015626000
H	0.391444000	2.356089000	-2.717812000
H	-1.325139000	2.056952000	-2.535472000
N	-0.112606000	0.552289000	-1.696616000
N	-0.683727000	0.069563000	2.652592000
N	-0.290482000	-1.942331000	0.430759000
C	-0.828275000	-0.071347000	3.793713000
C	-0.126699000	-3.088392000	0.481062000
C	-1.001149000	-0.241435000	5.225143000

H	-1.897214000	0.295503000	5.552714000
H	-1.106762000	-1.304967000	5.461578000
H	-0.127724000	0.161569000	5.748043000
C	0.082340000	-4.524795000	0.539242000
H	1.001129000	-4.738750000	1.094855000
H	-0.764054000	-4.999328000	1.045805000
H	0.170245000	-4.927112000	-0.474900000

Fe-TPA 3+ doublet

Fe	-0.379435000	0.324963000	0.261035000
N	-0.630462000	2.254302000	0.266412000
C	-0.461020000	2.836851000	-0.941049000
C	-0.952999000	3.012242000	1.339828000
C	-0.613327000	4.211120000	-1.108303000
C	-1.117807000	4.383186000	1.236303000
H	-1.077203000	2.499052000	2.282836000
C	-0.945669000	4.994399000	-0.008322000
H	-0.471203000	4.646481000	-2.091744000
H	-1.376952000	4.955728000	2.119692000
H	-1.070163000	6.067008000	-0.118416000
N	1.564819000	0.584986000	0.436896000
C	2.231556000	0.397997000	-0.731786000
C	2.237336000	0.947493000	1.547959000
C	3.608614000	0.566019000	-0.807983000
C	3.613968000	1.121063000	1.536786000
H	1.651436000	1.099733000	2.445599000
C	4.309647000	0.926152000	0.342439000
H	4.114601000	0.419741000	-1.755994000
H	4.123527000	1.409682000	2.449163000
H	5.385604000	1.063672000	0.303887000
N	-2.246828000	0.099888000	-0.320502000
C	-3.352535000	0.224864000	0.440993000
C	-2.359317000	-0.169071000	-1.647033000
C	-4.622172000	0.067700000	-0.096293000
H	-3.200337000	0.454043000	1.488293000
C	-3.603841000	-0.322796000	-2.245321000
C	-4.749717000	-0.209947000	-1.458392000
H	-5.489884000	0.168998000	0.545632000
H	-3.665269000	-0.526888000	-3.308746000
H	-5.731500000	-0.329054000	-1.905719000
C	-1.055104000	-0.328608000	-2.381577000

H	-1.138047000	-0.032196000	-3.430063000
H	-0.750917000	-1.378095000	-2.353818000
C	1.378941000	-0.032176000	-1.894910000
H	1.340051000	-1.123944000	-1.933630000
H	1.780809000	0.323021000	-2.846913000
C	-0.104151000	1.940901000	-2.090870000
H	0.852721000	2.254204000	-2.515507000
H	-0.851942000	2.041866000	-2.881669000
N	-0.011300000	0.488041000	-1.679515000
N	-0.733206000	0.129183000	2.169772000
N	-0.124439000	-1.613349000	0.217828000
C	-0.915724000	-0.125273000	3.282366000
C	0.013039000	-2.754847000	0.334775000
C	-1.147431000	-0.430393000	4.679824000
H	-1.995857000	0.157141000	5.045354000
H	-1.367204000	-1.497544000	4.787224000
H	-0.252293000	-0.180879000	5.258957000
C	0.191764000	-4.184919000	0.468920000
H	0.726726000	-4.397365000	1.400478000
H	-0.789234000	-4.670765000	0.491090000
H	0.768688000	-4.561460000	-0.381942000

Fe-TPA 3+ quartet

Fe	-0.455165000	0.320716000	0.268002000
N	-0.634239000	2.447191000	0.280003000
C	-0.433777000	2.975741000	-0.940338000
C	-0.751477000	3.256086000	1.351943000
C	-0.332074000	4.352032000	-1.132100000
C	-0.676885000	4.637076000	1.234904000
H	-0.901605000	2.773785000	2.311403000
C	-0.458355000	5.192450000	-0.028288000
H	-0.161947000	4.747228000	-2.128122000
H	-0.778930000	5.258978000	2.117272000
H	-0.382736000	6.268391000	-0.151314000
N	1.498698000	0.554091000	0.454667000
C	2.159925000	0.546258000	-0.733829000
C	2.171655000	0.772457000	1.603978000
C	3.531060000	0.765889000	-0.789416000
C	3.542367000	0.984086000	1.610294000
H	1.589752000	0.777723000	2.516642000
C	4.231293000	0.983765000	0.396293000

H	4.033780000	0.764198000	-1.750216000
H	4.051812000	1.153064000	2.552206000
H	5.302408000	1.157408000	0.371594000
N	-2.302078000	-0.001333000	-0.348949000
C	-3.421387000	0.052632000	0.402487000
C	-2.385292000	-0.268182000	-1.682274000
C	-4.673978000	-0.170949000	-0.150921000
H	-3.295491000	0.280346000	1.453213000
C	-3.613050000	-0.490654000	-2.291595000
C	-4.771332000	-0.447651000	-1.515241000
H	-5.552192000	-0.123444000	0.482858000
H	-3.652510000	-0.690688000	-3.356690000
H	-5.740031000	-0.619738000	-1.973687000
C	-1.067095000	-0.339667000	-2.401753000
H	-1.157549000	-0.070443000	-3.457544000
H	-0.672885000	-1.357891000	-2.343348000
C	1.332142000	0.214976000	-1.944217000
H	1.377590000	-0.864456000	-2.117029000
H	1.708928000	0.711041000	-2.841475000
C	-0.406387000	2.013831000	-2.101871000
H	0.318069000	2.330255000	-2.855412000
H	-1.392853000	2.025449000	-2.573869000
N	-0.106001000	0.583920000	-1.705532000
N	-0.841917000	0.099532000	2.213569000
N	-0.093218000	-1.847123000	0.203401000
C	-1.067117000	-0.112870000	3.328375000
C	0.084837000	-2.983734000	0.338792000
C	-1.348608000	-0.376416000	4.722999000
H	-2.210349000	0.221406000	5.037844000
H	-1.576082000	-1.440411000	4.848574000
H	-0.474213000	-0.113102000	5.326999000
C	0.306990000	-4.406898000	0.502343000
H	1.261799000	-4.571510000	1.012002000
H	-0.504974000	-4.836100000	1.098150000
H	0.330029000	-4.886592000	-0.481450000

Fe-TPA 3+ sextet

Fe	-0.599056000	0.275385000	0.500893000
N	-0.733398000	2.356561000	0.344183000
C	-0.468816000	2.883801000	-0.866948000

C	-1.048593000	3.163548000	1.382768000
C	-0.505169000	4.263788000	-1.069856000
C	-1.109322000	4.540265000	1.244348000
H	-1.250171000	2.677415000	2.330589000
C	-0.829534000	5.099343000	-0.005878000
H	-0.286196000	4.665001000	-2.054043000
H	-1.367556000	5.156632000	2.098072000
H	-0.865140000	6.174761000	-0.149264000
N	1.556473000	0.540580000	0.499808000
C	2.185931000	0.437418000	-0.691982000
C	2.263611000	0.905272000	1.589347000
C	3.547406000	0.694031000	-0.825177000
C	3.626302000	1.166804000	1.530326000
H	1.717520000	0.994461000	2.519695000
C	4.280066000	1.058842000	0.302529000
H	4.013923000	0.611448000	-1.800891000
H	4.155032000	1.457177000	2.431418000
H	5.342419000	1.267025000	0.221404000
N	-2.432582000	0.068240000	-0.568578000
C	-3.607400000	0.153610000	0.086606000
C	-2.400892000	-0.171522000	-1.893507000
C	-4.816585000	-0.005464000	-0.576444000
H	-3.555594000	0.354776000	1.151967000
C	-3.576596000	-0.327753000	-2.621857000
C	-4.797429000	-0.248820000	-1.952198000
H	-5.747844000	0.065328000	-0.025781000
H	-3.527974000	-0.510376000	-3.689975000
H	-5.726640000	-0.371450000	-2.499910000
C	-1.021716000	-0.308953000	-2.473262000
H	-0.991405000	-0.007140000	-3.524984000
H	-0.715941000	-1.357949000	-2.419324000
C	1.329098000	-0.008828000	-1.841704000
H	1.290906000	-1.102376000	-1.855067000
H	1.742580000	0.322966000	-2.799246000
C	-0.164873000	1.957437000	-2.020987000
H	0.765187000	2.276448000	-2.500027000
H	-0.956309000	2.076642000	-2.766599000
N	-0.059590000	0.498912000	-1.667245000
N	-0.555369000	0.058399000	2.600459000
N	-0.338348000	-1.825022000	0.401396000
C	-0.619387000	-0.165738000	3.735189000

C	-0.174419000	-2.969416000	0.471783000
C	-0.675683000	-0.441057000	5.153821000
H	-1.482791000	0.144410000	5.606187000
H	-0.863905000	-1.508732000	5.308277000
H	0.280133000	-0.165945000	5.612450000
C	0.038398000	-4.398533000	0.554996000
H	0.972283000	-4.594674000	1.092306000
H	-0.797559000	-4.860462000	1.090171000
H	0.101871000	-4.814368000	-0.455924000

Fe-TPA oxo (*trans*-py) 2+ triplet

Fe	-0.322527000	0.215740000	0.326334000
N	-0.625637000	2.269847000	0.303023000
C	-0.463909000	2.818631000	-0.915428000
C	-0.969911000	3.061295000	1.340758000
C	-0.645053000	4.183985000	-1.137575000
C	-1.165274000	4.426956000	1.195572000
H	-1.088612000	2.577186000	2.301852000
C	-1.000757000	4.999023000	-0.067972000
H	-0.507373000	4.588931000	-2.134859000
H	-1.441388000	5.024253000	2.057557000
H	-1.148209000	6.064342000	-0.216494000
N	1.622834000	0.603272000	0.499654000
C	2.283897000	0.438568000	-0.671917000
C	2.289619000	1.007181000	1.594913000
C	3.649549000	0.680749000	-0.771814000
C	3.657420000	1.253620000	1.565966000
H	1.708438000	1.134472000	2.500212000
C	4.347378000	1.087491000	0.365294000
H	4.149293000	0.551700000	-1.725779000
H	4.162135000	1.575017000	2.470291000
H	5.414237000	1.280639000	0.311175000
N	-2.211929000	0.046813000	-0.275340000
C	-3.326478000	0.181333000	0.464077000
C	-2.307048000	-0.214575000	-1.601393000
C	-4.592161000	0.044573000	-0.094190000
H	-3.189732000	0.403837000	1.515487000
C	-3.542925000	-0.348808000	-2.224414000
C	-4.701864000	-0.224743000	-1.458324000
H	-5.468598000	0.154793000	0.534646000
H	-3.587648000	-0.547941000	-3.289773000

H	-5.677230000	-0.329689000	-1.923107000
C	-0.988832000	-0.391452000	-2.306975000
H	-1.051580000	-0.132000000	-3.366928000
H	-0.674207000	-1.434991000	-2.224777000
C	1.434459000	-0.056714000	-1.811841000
H	1.399874000	-1.149029000	-1.789202000
H	1.825854000	0.258463000	-2.782578000
C	-0.069556000	1.897977000	-2.038592000
H	0.892651000	2.216013000	-2.448172000
H	-0.798122000	1.973414000	-2.849929000
N	0.038084000	0.451503000	-1.611599000
N	-0.696643000	0.118767000	2.249029000
C	-0.891413000	-0.060765000	3.373772000
C	-1.135979000	-0.279541000	4.786224000
H	-2.039797000	0.259317000	5.088224000
H	-1.270737000	-1.350477000	4.969769000
H	-0.281490000	0.085281000	5.365176000
O	-0.074792000	-1.396411000	0.253642000

Fe-TPA oxo (*trans*-py) 2+ quintet

Fe	-0.359808000	0.222864000	0.473559000
N	-0.649545000	2.269586000	0.331705000
C	-0.476185000	2.809297000	-0.893133000
C	-1.015089000	3.066865000	1.360400000
C	-0.664665000	4.173922000	-1.117289000
C	-1.216529000	4.429576000	1.205729000
H	-1.144710000	2.586581000	2.321696000
C	-1.037727000	4.994611000	-0.058632000
H	-0.517609000	4.574568000	-2.115054000
H	-1.508100000	5.028873000	2.061117000
H	-1.188338000	6.058147000	-0.216428000
N	1.701013000	0.632795000	0.478683000
C	2.310086000	0.442529000	-0.709646000
C	2.412045000	1.032672000	1.547664000
C	3.677499000	0.658703000	-0.860154000
C	3.781930000	1.254114000	1.470570000
H	1.861965000	1.179342000	2.471001000
C	4.423639000	1.062745000	0.246114000
H	4.140286000	0.510209000	-1.830192000
H	4.325180000	1.575842000	2.352248000
H	5.491378000	1.234703000	0.151009000

N	-2.287537000	0.037491000	-0.332161000
C	-3.432337000	0.146762000	0.365039000
C	-2.319997000	-0.202708000	-1.658990000
C	-4.673446000	0.012030000	-0.245599000
H	-3.338839000	0.349728000	1.426619000
C	-3.530072000	-0.333350000	-2.336094000
C	-4.721292000	-0.230602000	-1.619079000
H	-5.577031000	0.104883000	0.346637000
H	-3.528430000	-0.514358000	-3.405860000
H	-5.674921000	-0.332056000	-2.127854000
C	-0.978211000	-0.368243000	-2.334511000
H	-1.043349000	-0.116718000	-3.397954000
H	-0.671290000	-1.415359000	-2.255053000
C	1.426821000	-0.053158000	-1.830948000
H	1.385607000	-1.145906000	-1.793018000
H	1.832684000	0.237547000	-2.805307000
C	-0.060638000	1.907484000	-2.030327000
H	0.905019000	2.249091000	-2.415655000
H	-0.776360000	2.014319000	-2.851243000
N	0.045333000	0.464612000	-1.650852000
N	-0.725827000	0.218583000	2.543436000
C	-0.903751000	-0.015539000	3.663299000
C	-1.125691000	-0.300297000	5.066373000
H	-1.965335000	0.299419000	5.432327000
H	-1.351771000	-1.364360000	5.190171000
H	-0.222863000	-0.049785000	5.633248000
O	-0.114879000	-1.380208000	0.446062000

Fe-TPA oxo (*trans*-amine) 2+ triplet

Fe	-0.409382000	0.271893000	0.331282000
N	-0.642828000	2.221522000	0.278227000
C	-0.463727000	2.827398000	-0.911613000
C	-0.965137000	2.955491000	1.365035000
C	-0.604529000	4.208302000	-1.047716000
C	-1.120757000	4.331035000	1.295830000
H	-1.093030000	2.402837000	2.287368000
C	-0.936974000	4.970030000	0.067357000
H	-0.453293000	4.665093000	-2.020305000
H	-1.380461000	4.884868000	2.191206000
H	-1.051998000	6.046020000	-0.019163000
N	1.553498000	0.519333000	0.454640000

C	2.222401000	0.396548000	-0.717033000
C	2.217237000	0.826392000	1.583893000
C	3.598365000	0.592463000	-0.780998000
C	3.592545000	1.022761000	1.587636000
H	1.617430000	0.910609000	2.482339000
C	4.293088000	0.905817000	0.386746000
H	4.108288000	0.499752000	-1.733857000
H	4.096011000	1.267629000	2.516324000
H	5.366786000	1.063001000	0.357173000
N	-2.256559000	0.037613000	-0.345961000
C	-3.364564000	0.110930000	0.413723000
C	-2.357328000	-0.181489000	-1.678942000
C	-4.632337000	-0.036323000	-0.134722000
H	-3.207467000	0.288894000	1.470936000
C	-3.599116000	-0.324351000	-2.290063000
C	-4.751227000	-0.255408000	-1.507499000
H	-5.503691000	0.025375000	0.507734000
H	-3.652372000	-0.488428000	-3.361043000
H	-5.729235000	-0.366679000	-1.965297000
C	-1.046604000	-0.309182000	-2.416028000
H	-1.142072000	-0.001275000	-3.461119000
H	-0.732807000	-1.356745000	-2.406891000
C	1.382110000	-0.009251000	-1.902572000
H	1.344807000	-1.101011000	-1.956450000
H	1.808604000	0.356981000	-2.840554000
C	-0.109913000	1.952084000	-2.082275000
H	0.841072000	2.281524000	-2.509797000
H	-0.863772000	2.070661000	-2.865740000
N	-0.009477000	0.499267000	-1.706022000
N	-0.140995000	-1.673022000	0.228333000
C	0.003822000	-2.817558000	0.282576000
C	0.189977000	-4.254391000	0.343066000
H	1.105042000	-4.480400000	0.899921000
H	-0.667024000	-4.712650000	0.846728000
H	0.272599000	-4.653752000	-0.672852000
O	-0.734512000	0.188495000	1.925082000

Fe-TPA oxo (*trans*-amine) 2+ quintet

Fe	-0.525114000	0.313670000	0.373498000
N	-0.665069000	2.408308000	0.322276000
C	-0.442302000	2.963373000	-0.884334000

C	-0.803573000	3.190807000	1.410524000
C	-0.336604000	4.344730000	-1.038076000
C	-0.725957000	4.573864000	1.328978000
H	-0.972781000	2.674646000	2.348960000
C	-0.482560000	5.158452000	0.083343000
H	-0.148441000	4.765527000	-2.020321000
H	-0.845220000	5.175274000	2.223413000
H	-0.404378000	6.237087000	-0.012658000
N	1.525698000	0.502036000	0.491289000
C	2.157046000	0.526596000	-0.704910000
C	2.219303000	0.693539000	1.629118000
C	3.526782000	0.759371000	-0.788673000
C	3.589809000	0.916039000	1.616320000
H	1.646864000	0.666868000	2.549513000
C	4.251195000	0.953447000	0.387230000
H	4.010307000	0.784883000	-1.759275000
H	4.120433000	1.064138000	2.550301000
H	5.320401000	1.136570000	0.343537000
N	-2.391875000	-0.066660000	-0.392007000
C	-3.532736000	-0.075367000	0.322960000
C	-2.422989000	-0.274183000	-1.730926000
C	-4.764694000	-0.296077000	-0.278822000
H	-3.431907000	0.098776000	1.388531000
C	-3.625663000	-0.491092000	-2.395388000
C	-4.810136000	-0.505530000	-1.658307000
H	-5.665659000	-0.298253000	0.324412000
H	-3.627019000	-0.645056000	-3.469103000
H	-5.759249000	-0.673459000	-2.157958000
C	-1.076704000	-0.307038000	-2.410634000
H	-1.147403000	-0.013445000	-3.461960000
H	-0.685842000	-1.327488000	-2.372928000
C	1.303661000	0.207043000	-1.906448000
H	1.338093000	-0.874021000	-2.071856000
H	1.688730000	0.689754000	-2.808460000
C	-0.397774000	2.023486000	-2.059124000
H	0.342233000	2.349372000	-2.794349000
H	-1.374140000	2.059748000	-2.551955000
N	-0.128254000	0.589333000	-1.671120000
N	-0.138454000	-1.855766000	0.175508000
C	0.029224000	-2.993271000	0.313118000
C	0.240995000	-4.419674000	0.477271000

H	1.150485000	-4.589411000	1.062397000
H	-0.614787000	-4.858518000	1.000033000
H	0.347517000	-4.889568000	-0.505622000
O	-0.870997000	0.205849000	1.951327000

BPMEN (free ligand)

C	2.989793000	-0.143640000	0.312869000
C	2.440383000	1.206522000	0.794726000
H	2.662288000	-0.900743000	1.033592000
H	4.095952000	-0.103845000	0.370874000
H	3.010045000	1.449987000	1.697820000
H	2.657878000	2.012444000	0.069925000
N	0.809335000	0.732401000	4.130822000
C	1.274333000	0.424317000	5.347928000
C	1.257732000	1.861201000	3.547369000
C	2.194687000	1.207018000	6.049159000
H	0.888975000	-0.493580000	5.790160000
C	2.179632000	2.706701000	4.175753000
C	2.655227000	2.375889000	5.445934000
H	2.533141000	0.905160000	7.035721000
H	2.516554000	3.608627000	3.672887000
H	3.371920000	3.018182000	5.950709000
N	1.356378000	0.371150000	-3.628859000
C	0.794784000	0.213283000	-4.834225000
C	2.622961000	-0.052870000	-3.456631000
C	1.450219000	-0.360826000	-5.925503000
H	-0.229946000	0.568076000	-4.935994000
C	3.356412000	-0.640662000	-4.493975000
C	2.762556000	-0.795808000	-5.747497000
H	0.943401000	-0.459450000	-6.880634000
H	4.375876000	-0.970580000	-4.316404000
H	3.314178000	-1.250024000	-6.566205000
C	0.691809000	2.189825000	2.177710000
H	1.019357000	3.203412000	1.880682000
H	-0.401107000	2.221412000	2.263586000
C	3.235610000	0.162346000	-2.084527000
H	3.159390000	1.228538000	-1.847752000
H	4.313039000	-0.085342000	-2.125671000
C	2.779273000	-2.027385000	-1.173291000
H	2.215979000	-2.569983000	-0.406701000
H	2.425754000	-2.361021000	-2.154087000

H	3.845887000	-2.311719000	-1.082747000
C	0.147529000	1.360694000	-0.009538000
H	0.402776000	0.619960000	-0.769162000
H	-0.899478000	1.221772000	0.285118000
H	0.242272000	2.365908000	-0.466308000
N	2.558452000	-0.590543000	-1.020701000
N	1.014757000	1.185040000	1.155039000

Fe-BPMEN 2+ singlet

C	3.581768000	1.427242000	0.152965000
C	2.460050000	2.246102000	-0.446038000
H	3.613399000	1.559424000	1.237114000
H	4.550231000	1.751326000	-0.246022000
H	2.571513000	3.303822000	-0.178640000
H	2.477917000	2.179052000	-1.536107000
Fe	1.318297000	-0.340853000	0.017389000
N	1.364157000	-0.136723000	2.000956000
C	1.573023000	-1.116719000	2.906366000
C	1.206638000	1.128009000	2.447428000
C	1.650580000	-0.873676000	4.271247000
H	1.688566000	-2.118099000	2.510687000
C	1.294106000	1.451487000	3.802007000
C	1.519599000	0.438565000	4.729280000
H	1.819139000	-1.699100000	4.954508000
H	1.176382000	2.484425000	4.113736000
H	1.588239000	0.666970000	5.788587000
N	1.398884000	-0.389366000	-1.976776000
C	0.350888000	-0.447343000	-2.826040000
C	2.644191000	-0.320090000	-2.496208000
C	0.501209000	-0.424178000	-4.206579000
H	-0.631255000	-0.505679000	-2.373521000
C	2.871683000	-0.271911000	-3.871797000
C	1.786450000	-0.324886000	-4.741845000
H	-0.376170000	-0.474061000	-4.842459000
H	3.888925000	-0.201676000	-4.243366000
H	1.940293000	-0.291657000	-5.816164000
C	0.834591000	2.158788000	1.417593000
H	1.307162000	3.123505000	1.634940000
H	-0.246970000	2.313297000	1.490733000
C	3.777291000	-0.394753000	-1.510380000
H	4.627699000	0.215542000	-1.835472000

H	4.120650000	-1.434525000	-1.488001000
C	4.241938000	-0.794034000	0.815033000
H	4.012667000	-0.518781000	1.844197000
H	4.076530000	-1.863778000	0.682314000
H	5.296560000	-0.566378000	0.614715000
C	0.088400000	2.324653000	-0.864059000
H	0.295903000	2.078244000	-1.905187000
H	-0.891296000	1.932830000	-0.588979000
H	0.082402000	3.416406000	-0.754044000
N	3.368196000	-0.029856000	-0.117788000
N	1.133266000	1.729007000	0.014519000
C	-1.715050000	-0.792910000	0.275647000
C	1.612053000	-3.404485000	-0.041167000
C	1.707819000	-4.852814000	-0.121747000
H	1.259074000	-5.304034000	0.769073000
H	1.178080000	-5.209854000	-1.010917000
H	2.759130000	-5.151649000	-0.185725000
C	-3.136123000	-1.043006000	0.453346000
H	-3.445251000	-1.885657000	-0.173553000
H	-3.341709000	-1.281074000	1.501991000
H	-3.707255000	-0.153477000	0.168162000
N	1.541934000	-2.250394000	0.029250000
N	-0.584941000	-0.586701000	0.127202000

Fe-BPMEN 2+ triplet

C	3.624158000	1.473334000	0.165148000
C	2.503659000	2.299950000	-0.448099000
H	3.635145000	1.599793000	1.250780000
H	4.590225000	1.832916000	-0.213520000
H	2.653450000	3.358244000	-0.194231000
H	2.528652000	2.220697000	-1.537811000
Fe	1.307630000	-0.358746000	0.019876000
N	1.309467000	-0.087522000	1.981103000
C	1.493540000	-1.071032000	2.890259000
C	1.195564000	1.186701000	2.422357000
C	1.580939000	-0.827747000	4.253748000
H	1.578110000	-2.075862000	2.495314000
C	1.293926000	1.504987000	3.777821000
C	1.488216000	0.488822000	4.708236000
H	1.727185000	-1.656101000	4.938539000
H	1.210230000	2.541762000	4.087910000

H	1.564280000	0.718482000	5.766753000
N	1.455615000	-0.439420000	-1.953619000
C	0.407804000	-0.532467000	-2.802382000
C	2.698690000	-0.310575000	-2.474309000
C	0.552325000	-0.492725000	-4.182426000
H	-0.568834000	-0.635237000	-2.345592000
C	2.914610000	-0.244578000	-3.851246000
C	1.830976000	-0.337370000	-4.719710000
H	-0.324273000	-0.573455000	-4.816111000
H	3.926549000	-0.128333000	-4.225859000
H	1.981124000	-0.290335000	-5.794021000
C	0.866164000	2.248679000	1.402710000
H	1.368949000	3.191238000	1.654306000
H	-0.210101000	2.439701000	1.475523000
C	3.854455000	-0.335901000	-1.506012000
H	4.672218000	0.302508000	-1.863645000
H	4.238426000	-1.362088000	-1.491462000
C	4.333337000	-0.740405000	0.826657000
H	4.072524000	-0.480814000	1.853850000
H	4.180815000	-1.811771000	0.680651000
H	5.393648000	-0.504517000	0.660904000
C	0.131683000	2.436413000	-0.891645000
H	0.343123000	2.162199000	-1.926389000
H	-0.854424000	2.056230000	-0.616911000
H	0.126913000	3.532382000	-0.811715000
N	3.471012000	0.016834000	-0.112659000
N	1.157987000	1.846164000	0.000981000
C	-1.896940000	-0.862478000	0.343607000
C	1.588121000	-3.623765000	-0.094029000
C	1.633634000	-5.064356000	-0.276556000
H	1.161389000	-5.560065000	0.577450000
H	1.101767000	-5.336186000	-1.193963000
H	2.675696000	-5.390847000	-0.353427000
C	-3.298870000	-1.131670000	0.613313000
H	-3.629393000	-1.991052000	0.021207000
H	-3.435158000	-1.349429000	1.677405000
H	-3.897425000	-0.255431000	0.343837000
N	1.552974000	-2.475124000	0.056160000
N	-0.780036000	-0.646112000	0.123349000

Fe-BPMEN 2+ quintet

C	3.604313000	1.403431000	0.148673000
C	2.477003000	2.261212000	-0.408802000
H	3.630963000	1.484536000	1.238373000
H	4.564354000	1.785005000	-0.226505000
H	2.661751000	3.311641000	-0.142742000
H	2.466115000	2.203622000	-1.500245000
Fe	1.207122000	-0.457356000	0.019042000
N	1.319107000	-0.066704000	2.146766000
C	1.541494000	-1.015904000	3.079641000
C	1.254846000	1.224571000	2.525066000
C	1.711643000	-0.717425000	4.424477000
H	1.586634000	-2.038446000	2.719895000
C	1.435506000	1.602824000	3.858327000
C	1.663448000	0.622073000	4.818837000
H	1.884713000	-1.514101000	5.139831000
H	1.389977000	2.653105000	4.128551000
H	1.802853000	0.896960000	5.860190000
N	1.452945000	-0.435886000	-2.134306000
C	0.429519000	-0.477072000	-3.012166000
C	2.706582000	-0.251690000	-2.591684000
C	0.613282000	-0.334085000	-4.380848000
H	-0.558731000	-0.623722000	-2.588384000
C	2.966424000	-0.081209000	-3.954021000
C	1.909391000	-0.125393000	-4.858624000
H	-0.238732000	-0.376400000	-5.050753000
H	3.986224000	0.078080000	-4.289793000
H	2.092644000	0.003107000	-5.921354000
C	0.887474000	2.253264000	1.477582000
H	1.389279000	3.204948000	1.697277000
H	-0.187813000	2.436425000	1.582489000
C	3.839240000	-0.328932000	-1.591502000
H	4.666744000	0.317236000	-1.913188000
H	4.215003000	-1.357974000	-1.623976000
C	4.322127000	-0.833994000	0.713832000
H	4.055769000	-0.629937000	1.752471000
H	4.177959000	-1.898066000	0.514600000
H	5.383172000	-0.584895000	0.567509000
C	0.095936000	2.436286000	-0.793024000
H	0.267582000	2.138909000	-1.829270000
H	-0.889314000	2.081606000	-0.482114000

H	0.113904000	3.534245000	-0.734946000
N	3.454597000	-0.039050000	-0.186903000
N	1.135699000	1.834905000	0.074513000
C	-2.058220000	-0.966865000	0.249006000
C	1.526557000	-3.747988000	0.043111000
C	1.624500000	-5.193856000	-0.051174000
H	1.175101000	-5.649950000	0.836727000
H	1.091558000	-5.539511000	-0.942859000
H	2.676060000	-5.490153000	-0.118975000
C	-3.472865000	-1.241262000	0.430006000
H	-3.739043000	-2.161123000	-0.100600000
H	-3.687715000	-1.364787000	1.496407000
H	-4.064484000	-0.409165000	0.035322000
N	1.451383000	-2.594114000	0.121754000
N	-0.930132000	-0.746458000	0.100887000

Fe-BPMEN 3+ doublet

C	3.584770000	1.470122000	0.116957000
C	2.448341000	2.258679000	-0.488070000
H	3.652031000	1.643044000	1.192414000
H	4.540453000	1.761025000	-0.328883000
H	2.537492000	3.320517000	-0.239225000
H	2.440455000	2.170598000	-1.575486000
Fe	1.348700000	-0.289991000	0.024395000
N	1.401369000	-0.100024000	1.988780000
C	1.612748000	-1.109356000	2.865236000
C	1.202937000	1.153667000	2.449939000
C	1.646256000	-0.891829000	4.233082000
H	1.761194000	-2.096497000	2.448111000
C	1.250739000	1.442395000	3.811828000
C	1.473289000	0.407758000	4.715193000
H	1.814606000	-1.728378000	4.901743000
H	1.104164000	2.464050000	4.145627000
H	1.509139000	0.610626000	5.780898000
N	1.416800000	-0.366657000	-1.958564000
C	0.356798000	-0.399669000	-2.796966000
C	2.670167000	-0.372254000	-2.466126000
C	0.516747000	-0.431899000	-4.173659000
H	-0.625948000	-0.395767000	-2.344734000
C	2.897512000	-0.381021000	-3.840151000
C	1.807945000	-0.413219000	-4.705390000

H	-0.359838000	-0.461455000	-4.810949000
H	3.916336000	-0.368439000	-4.211804000
H	1.963111000	-0.423284000	-5.779582000
C	0.852163000	2.190494000	1.427523000
H	1.371536000	3.134014000	1.619886000
H	-0.220649000	2.389213000	1.507466000
C	3.786899000	-0.447697000	-1.468712000
H	4.654361000	0.136687000	-1.789155000
H	4.103153000	-1.493047000	-1.397469000
C	4.222487000	-0.742738000	0.889673000
H	4.017920000	-0.390796000	1.898603000
H	4.031531000	-1.812855000	0.818629000
H	5.272106000	-0.544029000	0.648420000
C	0.052377000	2.307957000	-0.850635000
H	0.244086000	2.063654000	-1.894095000
H	-0.916601000	1.915083000	-0.545744000
H	0.055409000	3.396904000	-0.734727000
N	3.363332000	-0.007307000	-0.092177000
N	1.128114000	1.734635000	0.017958000
C	-1.695739000	-0.787750000	0.307998000
C	1.618835000	-3.375910000	-0.127437000
C	1.664511000	-4.817329000	-0.260235000
H	1.185312000	-5.276343000	0.610667000
H	1.133228000	-5.115340000	-1.169994000
H	2.707505000	-5.144628000	-0.319454000
C	-3.098682000	-1.081254000	0.511319000
H	-3.362371000	-1.994775000	-0.031327000
H	-3.288120000	-1.220475000	1.580864000
H	-3.700170000	-0.244887000	0.139887000
N	1.589972000	-2.226047000	-0.013982000
N	-0.579364000	-0.543661000	0.134044000

Fe-BPMEN 3+ quartet

C	3.656382000	1.451556000	0.261952000
C	2.549412000	2.288416000	-0.350397000
H	3.633745000	1.503437000	1.352239000
H	4.627430000	1.838451000	-0.068270000
H	2.624213000	3.325815000	-0.009954000
H	2.624700000	2.290428000	-1.439015000
Fe	1.317662000	-0.300391000	0.004253000
N	1.345900000	-0.100713000	1.968006000

C	1.590555000	-1.097315000	2.851547000
C	1.140767000	1.162710000	2.416890000
C	1.648710000	-0.859690000	4.215013000
H	1.748086000	-2.086351000	2.442888000
C	1.205621000	1.465154000	3.773312000
C	1.461589000	0.442981000	4.683503000
H	1.846423000	-1.683501000	4.891254000
H	1.050148000	2.487791000	4.099336000
H	1.515091000	0.659464000	5.745775000
N	1.493319000	-0.374223000	-1.986286000
C	0.424959000	-0.525612000	-2.803334000
C	2.736106000	-0.276740000	-2.504533000
C	0.564077000	-0.569260000	-4.180506000
H	-0.544645000	-0.603204000	-2.328152000
C	2.934203000	-0.298620000	-3.885737000
C	1.841625000	-0.446116000	-4.732458000
H	-0.316240000	-0.692173000	-4.801186000
H	3.942698000	-0.207130000	-4.275203000
H	1.982900000	-0.468075000	-5.808376000
C	0.752523000	2.172752000	1.383652000
H	1.150351000	3.164888000	1.614673000
H	-0.339810000	2.247324000	1.381944000
C	3.904094000	-0.216152000	-1.555489000
H	4.620544000	0.544148000	-1.885281000
H	4.418598000	-1.180243000	-1.610086000
C	4.365292000	-0.827622000	0.749179000
H	4.105354000	-0.649621000	1.793128000
H	4.206494000	-1.879599000	0.507082000
H	5.422326000	-0.576862000	0.597985000
C	0.197705000	2.355353000	-0.967896000
H	0.514463000	2.145808000	-1.988109000
H	-0.792260000	1.935827000	-0.787857000
H	0.167904000	3.439877000	-0.815854000
N	3.515289000	0.017772000	-0.132632000
N	1.176498000	1.765395000	-0.001813000
C	-1.958244000	-0.803028000	0.382407000
C	1.511837000	-3.438077000	-0.094259000
C	1.559294000	-4.879870000	-0.207545000
H	1.094280000	-5.329131000	0.675924000
H	1.020432000	-5.191325000	-1.108345000
H	2.603897000	-5.201463000	-0.276036000

C	-3.340188000	-1.099088000	0.703279000
H	-3.666074000	-1.976460000	0.135195000
H	-3.428496000	-1.304335000	1.775175000
H	-3.966615000	-0.239878000	0.442507000
N	1.475798000	-2.286466000	0.008308000
N	-0.855269000	-0.562499000	0.120608000

Fe-BPMEN 3+ sextet

C	3.629812000	1.426591000	0.228758000
C	2.521838000	2.280529000	-0.355870000
H	3.622176000	1.460359000	1.319858000
H	4.603192000	1.800264000	-0.107771000
H	2.647210000	3.322423000	-0.041821000
H	2.557554000	2.258077000	-1.447084000
Fe	1.336600000	-0.424901000	0.049283000
N	1.371603000	-0.054521000	2.120967000
C	1.606719000	-1.014296000	3.046556000
C	1.182982000	1.223811000	2.511914000
C	1.665681000	-0.725305000	4.400072000
H	1.753954000	-2.021606000	2.673783000
C	1.248076000	1.583611000	3.856984000
C	1.489832000	0.599251000	4.810943000
H	1.853370000	-1.520613000	5.112449000
H	1.103949000	2.620966000	4.140076000
H	1.542305000	0.860665000	5.863250000
N	1.471709000	-0.400027000	-2.054158000
C	0.409340000	-0.520573000	-2.885481000
C	2.709274000	-0.243742000	-2.570329000
C	0.548363000	-0.479977000	-4.262790000
H	-0.560235000	-0.643505000	-2.418269000
C	2.915167000	-0.176772000	-3.947998000
C	1.824562000	-0.296977000	-4.803306000
H	-0.326670000	-0.582199000	-4.894683000
H	3.920830000	-0.039603000	-4.331278000
H	1.966354000	-0.249126000	-5.878476000
C	0.809867000	2.222341000	1.450236000
H	1.255710000	3.199791000	1.662680000
H	-0.276788000	2.347799000	1.489721000
C	3.870455000	-0.226230000	-1.611722000
H	4.606538000	0.525224000	-1.914808000
H	4.364282000	-1.200481000	-1.676354000

C	4.339467000	-0.864659000	0.686015000
H	4.081806000	-0.703039000	1.732600000
H	4.188303000	-1.913236000	0.426298000
H	5.392251000	-0.600279000	0.531569000
C	0.144878000	2.373047000	-0.869358000
H	0.397728000	2.118481000	-1.898024000
H	-0.841680000	1.978885000	-0.623299000
H	0.135901000	3.464247000	-0.763295000
N	3.480242000	-0.008338000	-0.183045000
N	1.161347000	1.795769000	0.058854000
C	-1.888063000	-0.864055000	0.302217000
C	1.514137000	-3.688972000	-0.072498000
C	1.551413000	-5.129732000	-0.196434000
H	1.072154000	-5.580970000	0.678564000
H	1.016792000	-5.429135000	-1.104041000
H	2.593275000	-5.461061000	-0.257227000
C	-3.292622000	-1.135008000	0.519093000
H	-3.569727000	-2.051979000	-0.011677000
H	-3.476669000	-1.260862000	1.591264000
H	-3.886110000	-0.296492000	0.139882000
N	1.486201000	-2.535339000	0.029582000
N	-0.765186000	-0.644005000	0.120036000

Fe-BPMEN oxo 2+ triplet

C	3.587579000	1.446886000	0.136555000
C	2.474378000	2.275009000	-0.463420000
H	3.619395000	1.564124000	1.221720000
H	4.559872000	1.756826000	-0.258862000
H	2.590357000	3.328766000	-0.185028000
H	2.493827000	2.218119000	-1.553808000
Fe	1.376022000	-0.394754000	-0.025080000
N	1.382192000	-0.146764000	1.948380000
C	1.567466000	-1.165703000	2.815309000
C	1.195965000	1.104460000	2.415042000
C	1.595208000	-0.963629000	4.186484000
H	1.702390000	-2.144212000	2.371082000
C	1.234562000	1.378256000	3.782762000
C	1.436773000	0.333988000	4.679262000
H	1.746192000	-1.808345000	4.849415000
H	1.096009000	2.398334000	4.125513000
H	1.466484000	0.527449000	5.747106000

N	1.417913000	-0.357218000	-2.008255000
C	0.350685000	-0.405486000	-2.833122000
C	2.660045000	-0.281870000	-2.531640000
C	0.488880000	-0.365919000	-4.213111000
H	-0.623612000	-0.468721000	-2.366961000
C	2.868369000	-0.218588000	-3.908077000
C	1.768992000	-0.262104000	-4.760523000
H	-0.395147000	-0.407763000	-4.839565000
H	3.880205000	-0.145642000	-4.292244000
H	1.908372000	-0.217686000	-5.836164000
C	0.853672000	2.166020000	1.407004000
H	1.357016000	3.109268000	1.645966000
H	-0.222347000	2.351404000	1.484506000
C	3.790870000	-0.371591000	-1.551249000
H	4.640068000	0.247528000	-1.856349000
H	4.132494000	-1.411207000	-1.534172000
C	4.229871000	-0.803118000	0.781359000
H	4.008863000	-0.523807000	1.810365000
H	4.033594000	-1.865197000	0.636050000
H	5.282752000	-0.586470000	0.569787000
C	0.093066000	2.361857000	-0.876514000
H	0.301252000	2.131331000	-1.921211000
H	-0.884122000	1.962828000	-0.602799000
H	0.085678000	3.451037000	-0.749595000
N	3.373149000	-0.013935000	-0.152878000
N	1.144469000	1.762054000	-0.006011000
C	-1.697808000	-0.793821000	0.273892000
C	-3.110907000	-1.046052000	0.481350000
H	-3.414353000	-1.919274000	-0.105139000
H	-3.295055000	-1.237966000	1.543280000
H	-3.688522000	-0.172503000	0.162448000
N	-0.574152000	-0.590474000	0.098527000
O	1.626387000	-2.001749000	0.043241000

Fe-BPMEN oxo 2+ quintet

C	3.587904000	1.446091000	0.137716000
C	2.474977000	2.275004000	-0.461652000
H	3.619786000	1.562502000	1.222963000
H	4.560295000	1.756029000	-0.257478000
H	2.591351000	3.328532000	-0.182542000
H	2.494467000	2.218900000	-1.552092000

Fe	1.375771000	-0.394701000	-0.024427000
N	1.382932000	-0.147236000	1.949027000
C	1.568859000	-1.166304000	2.815645000
C	1.196838000	1.103897000	2.416058000
C	1.597418000	-0.964482000	4.186852000
H	1.703615000	-2.144720000	2.371160000
C	1.236236000	1.377434000	3.783790000
C	1.439128000	0.333010000	4.679974000
H	1.748950000	-1.809316000	4.849504000
H	1.097803000	2.397431000	4.126823000
H	1.469488000	0.526287000	5.747833000
N	1.416842000	-0.356522000	-2.007730000
C	0.349346000	-0.404490000	-2.832265000
C	2.658761000	-0.280744000	-2.531544000
C	0.487022000	-0.364173000	-4.212282000
H	-0.624792000	-0.468137000	-2.365841000
C	2.866577000	-0.216678000	-3.908027000
C	1.766914000	-0.259880000	-4.760119000
H	-0.397247000	-0.405810000	-4.838408000
H	3.878269000	-0.143404000	-4.292509000
H	1.905898000	-0.214861000	-5.835784000
C	0.853817000	2.165574000	1.408388000
H	1.356530000	3.109088000	1.647638000
H	-0.222334000	2.350175000	1.485923000
C	3.790063000	-0.370975000	-1.551749000
H	4.638978000	0.248525000	-1.856834000
H	4.131903000	-1.410535000	-1.535670000
C	4.229980000	-0.804664000	0.780242000
H	4.009714000	-0.526129000	1.809622000
H	4.033212000	-1.866553000	0.634209000
H	5.282831000	-0.588269000	0.568243000
C	0.093808000	2.362760000	-0.875164000
H	0.302151000	2.132654000	-1.919921000
H	-0.883553000	1.963908000	-0.601830000
H	0.086742000	3.451882000	-0.747725000
N	3.373038000	-0.014451000	-0.152860000
N	1.144847000	1.762225000	-0.004736000
C	-1.698272000	-0.793559000	0.272730000
C	-3.111759000	-1.046769000	0.476061000
H	-3.397387000	-1.959466000	-0.056933000
H	-3.310580000	-1.171147000	1.545377000

H	-3.693082000	-0.202374000	0.092094000
N	-0.574362000	-0.589794000	0.099484000
O	1.625613000	-2.001790000	0.043394000

BPMPN (free ligand)

C	-0.943333000	-0.498207000	-0.101856000
C	-0.891353000	2.064861000	0.130328000
C	-1.755145000	0.800027000	0.018278000
H	-1.545482000	2.957459000	0.128187000
H	-0.278953000	2.121078000	-0.774280000
H	-2.416034000	0.926519000	-0.846532000
H	-2.413282000	0.699986000	0.888637000
H	-1.632305000	-1.364023000	-0.095370000
H	-0.326186000	-0.580341000	0.797454000
N	-0.992736000	0.380495000	3.547634000
C	-1.523919000	1.570074000	3.206007000
C	-1.772619000	-0.497932000	4.191303000
C	-2.846851000	1.908848000	3.516043000
C	-3.101962000	-0.248001000	4.537786000
H	-1.310065000	-1.449757000	4.449305000
C	-3.647546000	0.987749000	4.192514000
H	-3.239492000	2.879069000	3.225788000
H	-3.683500000	-0.999514000	5.063094000
H	-4.677246000	1.230592000	4.441072000
N	-1.034769000	1.168318000	-3.527432000
C	-1.595304000	-0.002611000	-3.168640000
C	-1.798962000	2.065830000	-4.163427000
C	-2.933114000	-0.303156000	-3.453079000
C	-3.141183000	1.854034000	-4.484835000
H	-1.312529000	3.001591000	-4.435907000
C	-3.717576000	0.637611000	-4.121547000
H	-3.349500000	-1.259337000	-3.149632000
H	-3.708994000	2.619470000	-5.005023000
H	-4.758412000	0.424600000	-4.350275000
C	-0.692556000	-1.020624000	-2.492606000
H	0.101691000	-1.267520000	-3.207955000
H	-1.267393000	-1.949840000	-2.321388000
C	1.122325000	-1.407588000	-0.970930000
H	1.815890000	-1.391361000	-1.819137000
H	1.648985000	-1.018898000	-0.093094000
H	0.858533000	-2.464003000	-0.769554000

N	-0.036677000	-0.562757000	-1.261789000
C	-0.603212000	2.566126000	2.521400000
C	1.208505000	2.905708000	0.984456000
H	1.909222000	2.863903000	1.825871000
H	1.714728000	2.505742000	0.099668000
H	0.975194000	3.970701000	0.790764000
H	0.205047000	2.790813000	3.228362000
H	-1.155715000	3.510357000	2.359127000
N	0.026985000	2.095117000	1.282222000

Fe-BPMPN 2+ singlet

C	-3.171845000	-0.328551000	-0.433681000
C	-3.185500000	2.104629000	0.197919000
C	-3.597166000	0.698853000	0.606456000
Fe	-0.325813000	0.783533000	-0.016168000
H	-3.717916000	2.854705000	0.795225000
H	-3.488593000	2.249870000	-0.842665000
H	-4.692950000	0.691943000	0.652494000
H	-3.247182000	0.435063000	1.609678000
H	-3.304166000	0.105039000	-1.429427000
H	-3.803808000	-1.224148000	-0.384432000
N	-0.379649000	0.726868000	1.995268000
C	-0.994859000	1.782014000	2.575453000
C	0.122450000	-0.233999000	2.798737000
C	-1.168926000	1.877768000	3.955252000
C	0.007965000	-0.197111000	4.183319000
H	0.630430000	-1.055157000	2.310933000
C	-0.662906000	0.872562000	4.775498000
H	-1.685953000	2.737305000	4.369311000
H	0.433294000	-0.999713000	4.776249000
H	-0.784350000	0.926312000	5.853148000
N	-0.368473000	0.803881000	-2.024195000
C	-0.934578000	-0.289813000	-2.587072000
C	0.128120000	1.755408000	-2.841362000
C	-1.054857000	-0.436759000	-3.967498000
C	0.061588000	1.668752000	-4.227242000
H	0.591750000	2.608328000	-2.362946000
C	-0.550006000	0.556173000	-4.804064000
H	-1.533061000	-1.323927000	-4.369834000
H	0.478675000	2.465794000	-4.833394000
H	-0.630420000	0.461693000	-5.882741000

C	-1.352184000	-1.363580000	-1.623326000
H	-0.504247000	-2.034207000	-1.455494000
H	-2.168976000	-1.969680000	-2.032111000
C	-1.698001000	-1.854453000	0.704555000
H	-0.674536000	-2.206977000	0.829190000
H	-2.073317000	-1.486079000	1.659299000
H	-2.324408000	-2.695512000	0.380475000
N	-1.744503000	-0.769477000	-0.311436000
C	-1.374810000	2.894649000	1.645950000
C	-1.501821000	3.563533000	-0.650004000
H	-0.462119000	3.887733000	-0.617274000
H	-1.758996000	3.269742000	-1.667694000
H	-2.143657000	4.403677000	-0.353822000
H	-0.507355000	3.556705000	1.558379000
H	-2.193153000	3.494421000	2.058921000
N	-1.713455000	2.410027000	0.271315000
C	2.060070000	2.727543000	0.189034000
C	2.006954000	-1.227321000	-0.195396000
N	1.075974000	-0.543771000	-0.110772000
N	1.111738000	2.069378000	0.096018000
C	3.241031000	3.567754000	0.299666000
H	3.808026000	3.293550000	1.195151000
H	3.874678000	3.433296000	-0.582895000
H	2.941544000	4.618411000	0.371235000
C	3.166374000	-2.097988000	-0.296980000
H	3.745438000	-1.839823000	-1.189521000
H	3.797952000	-1.977957000	0.589123000
H	2.840519000	-3.140703000	-0.368635000

Fe-BPMPN 2+ triplet

C	-3.205685000	-0.254127000	-0.476629000
C	-3.301417000	2.205151000	0.220216000
C	-3.654236000	0.761707000	0.577667000
Fe	-0.381678000	0.771268000	-0.030454000
H	-3.875877000	2.899322000	0.850728000
H	-3.615953000	2.378398000	-0.813332000
H	-4.749079000	0.714976000	0.623674000
H	-3.302199000	0.490053000	1.578019000
H	-3.262439000	0.212047000	-1.464672000
H	-3.883704000	-1.117505000	-0.488302000
N	-0.445547000	0.782510000	1.969101000

C	-1.072855000	1.823893000	2.564713000
C	0.074696000	-0.186816000	2.752282000
C	-1.235412000	1.888358000	3.948781000
C	-0.029653000	-0.174634000	4.137134000
H	0.586536000	-0.992046000	2.240641000
C	-0.710762000	0.877334000	4.749340000
H	-1.761020000	2.732866000	4.382537000
H	0.409752000	-0.980690000	4.714783000
H	-0.826860000	0.912739000	5.828342000
N	-0.389550000	0.726513000	-2.016181000
C	-0.952339000	-0.374118000	-2.571308000
C	0.095306000	1.683873000	-2.834763000
C	-1.053820000	-0.535853000	-3.950625000
C	0.039742000	1.583494000	-4.219727000
H	0.538115000	2.548071000	-2.355572000
C	-0.548054000	0.454693000	-4.790493000
H	-1.522533000	-1.429020000	-4.350566000
H	0.446959000	2.381718000	-4.830886000
H	-0.614625000	0.348158000	-5.868934000
C	-1.397586000	-1.421139000	-1.590486000
H	-0.555921000	-2.088488000	-1.379858000
H	-2.209690000	-2.033184000	-2.000749000
C	-1.835049000	-1.845513000	0.737725000
H	-0.826517000	-2.231326000	0.892573000
H	-2.213499000	-1.439443000	1.675757000
H	-2.487951000	-2.669168000	0.419738000
N	-1.811799000	-0.787871000	-0.304741000
C	-1.481185000	2.970937000	1.678131000
C	-1.620253000	3.716352000	-0.601478000
H	-0.570299000	4.013297000	-0.560474000
H	-1.868870000	3.431588000	-1.625835000
H	-2.241101000	4.578647000	-0.315581000
H	-0.612649000	3.635174000	1.601774000
H	-2.282366000	3.552444000	2.152839000
N	-1.853847000	2.565114000	0.301983000
C	2.149312000	2.679356000	0.218474000
C	2.348416000	-1.415876000	-0.263750000
N	1.342486000	-0.852631000	-0.135959000
N	1.193288000	2.036704000	0.102306000
C	3.346338000	3.488876000	0.359856000
H	3.892963000	3.184235000	1.258091000

H	3.986389000	3.357551000	-0.518365000
H	3.065237000	4.543324000	0.448450000
C	3.608894000	-2.125127000	-0.416985000
H	4.136272000	-1.754409000	-1.301640000
H	4.232130000	-1.965112000	0.468575000
H	3.417095000	-3.196436000	-0.534708000

Fe-BPMPN 2+ quintet

C	-3.200314000	-0.307805000	-0.528173000
C	-3.253409000	2.129777000	0.326479000
C	-3.587040000	0.660212000	0.600259000
Fe	-0.316144000	0.819459000	-0.013633000
H	-3.845488000	2.771441000	0.993845000
H	-3.572064000	2.356947000	-0.695248000
H	-4.678901000	0.615613000	0.697126000
H	-3.190659000	0.330703000	1.566026000
H	-3.297231000	0.210012000	-1.487784000
H	-3.899256000	-1.156854000	-0.550370000
N	-0.374490000	0.830020000	2.177722000
C	-1.066235000	1.847643000	2.730843000
C	0.102708000	-0.145056000	2.975369000
C	-1.313435000	1.904654000	4.103103000
C	-0.089290000	-0.148622000	4.352093000
H	0.651115000	-0.940508000	2.483314000
C	-0.817692000	0.894858000	4.925159000
H	-1.883442000	2.732915000	4.511546000
H	0.316656000	-0.954936000	4.953464000
H	-0.999094000	0.920839000	5.995598000
N	-0.364484000	0.730414000	-2.209338000
C	-0.975330000	-0.353604000	-2.730883000
C	0.113930000	1.675973000	-3.040898000
C	-1.130901000	-0.513059000	-4.108607000
C	0.008634000	1.580007000	-4.423459000
H	0.593215000	2.528246000	-2.571991000
C	-0.629487000	0.463496000	-4.966391000
H	-1.637619000	-1.392483000	-4.493068000
H	0.411766000	2.365604000	-5.053495000
H	-0.739620000	0.357380000	-6.041584000
C	-1.419266000	-1.418007000	-1.754455000
H	-0.576987000	-2.098955000	-1.587563000
H	-2.233722000	-2.014693000	-2.186809000

C	-1.767918000	-1.930909000	0.570451000
H	-0.746260000	-2.303145000	0.667312000
H	-2.095217000	-1.548954000	1.538374000
H	-2.426234000	-2.763262000	0.281583000
N	-1.812980000	-0.853051000	-0.443069000
C	-1.471366000	2.972397000	1.809607000
C	-1.597965000	3.682687000	-0.484198000
H	-0.563671000	4.022745000	-0.414050000
H	-1.799359000	3.368954000	-1.510555000
H	-2.263889000	4.521507000	-0.234040000
H	-0.611827000	3.648506000	1.734905000
H	-2.292257000	3.549264000	2.254636000
N	-1.814086000	2.535623000	0.433025000
C	2.304486000	2.880085000	0.069997000
C	2.237613000	-1.341137000	-0.112413000
N	1.294977000	-0.675176000	-0.004989000
N	1.316472000	2.281499000	-0.026097000
C	3.540265000	3.635491000	0.183499000
H	4.085870000	3.314120000	1.076548000
H	4.160104000	3.457515000	-0.701177000
H	3.315671000	4.704016000	0.260593000
C	3.413194000	-2.185193000	-0.240497000
H	3.972935000	-1.903737000	-1.138141000
H	4.052922000	-2.057585000	0.638607000
H	3.108148000	-3.233684000	-0.316935000

Fe-BPMPN 3+ doublet

C	-3.205445000	-0.347501000	-0.410237000
C	-3.185298000	2.095521000	0.126746000
C	-3.630482000	0.718337000	0.583706000
Fe	-0.395952000	0.786521000	-0.014449000
H	-3.720931000	2.880175000	0.669202000
H	-3.429491000	2.200781000	-0.932691000
H	-4.726387000	0.732700000	0.594074000
H	-3.319094000	0.484770000	1.606750000
H	-3.358920000	0.029183000	-1.424364000
H	-3.805306000	-1.256026000	-0.300397000
N	-0.415467000	0.727663000	1.983144000
C	-1.010549000	1.790890000	2.571487000
C	0.127706000	-0.235081000	2.762998000
C	-1.135581000	1.887774000	3.954326000

C	0.061355000	-0.185195000	4.146777000
H	0.628726000	-1.051539000	2.263841000
C	-0.595469000	0.885447000	4.754972000
H	-1.639742000	2.746805000	4.383408000
H	0.515025000	-0.979620000	4.728493000
H	-0.678133000	0.942486000	5.835732000
N	-0.398921000	0.801170000	-2.005703000
C	-0.936119000	-0.311704000	-2.564547000
C	0.112536000	1.761479000	-2.808083000
C	-1.016299000	-0.467434000	-3.944449000
C	0.082779000	1.654990000	-4.190575000
H	0.557183000	2.622053000	-2.328717000
C	-0.500750000	0.528097000	-4.770670000
H	-1.473328000	-1.362395000	-4.352378000
H	0.507728000	2.449802000	-4.793091000
H	-0.551287000	0.424889000	-5.849948000
C	-1.364024000	-1.376557000	-1.602538000
H	-0.529407000	-2.062204000	-1.432871000
H	-2.195890000	-1.965911000	-1.998986000
C	-1.696065000	-1.844524000	0.745082000
H	-0.673942000	-2.200431000	0.856985000
H	-2.075493000	-1.470444000	1.694704000
H	-2.322426000	-2.679549000	0.414439000
N	-1.759552000	-0.767112000	-0.290221000
C	-1.416594000	2.894475000	1.651025000
C	-1.473584000	3.561927000	-0.660048000
H	-0.441222000	3.899793000	-0.594520000
H	-1.712179000	3.272552000	-1.681968000
H	-2.134594000	4.382848000	-0.361569000
H	-0.581255000	3.599369000	1.590921000
H	-2.276672000	3.447140000	2.037927000
N	-1.709431000	2.401859000	0.260201000
C	2.030845000	2.709288000	0.235001000
C	1.985248000	-1.198052000	-0.247321000
N	1.026174000	-0.563599000	-0.129032000
N	1.063520000	2.088501000	0.112899000
C	3.232144000	3.505188000	0.378439000
H	3.779187000	3.177964000	1.268777000
H	3.862051000	3.373236000	-0.507304000
H	2.959296000	4.560371000	0.482575000
C	3.177078000	-2.008570000	-0.388041000

H	3.725936000	-1.693917000	-1.281733000
H	3.810134000	-1.876921000	0.495610000
H	2.892683000	-3.061550000	-0.482619000

Fe-BPMPN 3+ quartet

C	-3.208433000	-0.238118000	-0.482298000
C	-3.267794000	2.220621000	0.187900000
C	-3.660155000	0.792157000	0.550377000
Fe	-0.441386000	0.782889000	-0.055601000
H	-3.842321000	2.934805000	0.789448000
H	-3.528202000	2.390650000	-0.859648000
H	-4.756085000	0.769905000	0.548050000
H	-3.361502000	0.519016000	1.567305000
H	-3.266871000	0.199727000	-1.481691000
H	-3.863814000	-1.114880000	-0.465195000
N	-0.453295000	0.764742000	1.974710000
C	-1.048663000	1.813284000	2.588609000
C	0.098591000	-0.216808000	2.723557000
C	-1.157431000	1.867557000	3.977129000
C	0.045985000	-0.204058000	4.108787000
H	0.593763000	-1.018913000	2.193967000
C	-0.608446000	0.848763000	4.748758000
H	-1.661550000	2.712915000	4.432914000
H	0.506127000	-1.013207000	4.664522000
H	-0.683798000	0.878894000	5.831143000
N	-0.412432000	0.717289000	-2.039922000
C	-0.935767000	-0.414729000	-2.575613000
C	0.089202000	1.677600000	-2.849059000
C	-0.976972000	-0.607075000	-3.951671000
C	0.082665000	1.537971000	-4.228342000
H	0.495358000	2.559411000	-2.371709000
C	-0.459004000	0.379644000	-4.788550000
H	-1.410315000	-1.517727000	-4.350173000
H	0.494581000	2.328792000	-4.844907000
H	-0.481212000	0.247334000	-5.865576000
C	-1.391702000	-1.440154000	-1.585439000
H	-0.568629000	-2.127004000	-1.368729000
H	-2.227549000	-2.032298000	-1.970014000
C	-1.825298000	-1.818463000	0.768100000
H	-0.822140000	-2.215322000	0.919505000
H	-2.211958000	-1.398896000	1.694926000

H	-2.482611000	-2.631810000	0.440546000
N	-1.801753000	-0.777158000	-0.300819000
C	-1.480891000	2.963832000	1.728288000
C	-1.547866000	3.741491000	-0.552072000
H	-0.502758000	4.041065000	-0.472035000
H	-1.776595000	3.476944000	-1.585296000
H	-2.185384000	4.581711000	-0.249293000
H	-0.643071000	3.668474000	1.689848000
H	-2.322179000	3.495160000	2.185057000
N	-1.810100000	2.569166000	0.330349000
C	2.059443000	2.691350000	0.210138000
C	2.242001000	-1.336426000	-0.299557000
N	1.261063000	-0.734846000	-0.162014000
N	1.111265000	2.045018000	0.066569000
C	3.242142000	3.508086000	0.381846000
H	3.696001000	3.291167000	1.354322000
H	3.956365000	3.285136000	-0.417307000
H	2.959638000	4.565149000	0.335988000
C	3.467931000	-2.094496000	-0.463968000
H	4.003319000	-1.736260000	-1.349141000
H	4.098350000	-1.963344000	0.421428000
H	3.228193000	-3.155515000	-0.587275000

Fe-BPMPN 3+ sextet

C	-3.199244000	-0.299597000	-0.567328000
C	-3.290754000	2.151763000	0.276173000
C	-3.651491000	0.682727000	0.524153000
Fe	-0.460093000	0.888044000	-0.028556000
H	-3.913604000	2.791694000	0.910997000
H	-3.529302000	2.390022000	-0.762914000
H	-4.747232000	0.654694000	0.521808000
H	-3.348758000	0.351910000	1.523060000
H	-3.265541000	0.187047000	-1.544197000
H	-3.867040000	-1.169033000	-0.584886000
N	-0.390895000	0.870388000	2.128018000
C	-1.062780000	1.865578000	2.750074000
C	0.171273000	-0.110496000	2.869862000
C	-1.196319000	1.896415000	4.136795000
C	0.088995000	-0.131080000	4.253930000
H	0.687541000	-0.892624000	2.328854000
C	-0.612323000	0.888943000	4.899545000

H	-1.749199000	2.706312000	4.600681000
H	0.558000000	-0.937161000	4.806948000
H	-0.706517000	0.896950000	5.980991000
N	-0.355677000	0.720378000	-2.179619000
C	-0.888492000	-0.408878000	-2.696508000
C	0.140723000	1.667683000	-3.002450000
C	-0.937765000	-0.618717000	-4.072587000
C	0.134845000	1.514846000	-4.381816000
H	0.546256000	2.554735000	-2.530884000
C	-0.415139000	0.351952000	-4.924962000
H	-1.380931000	-1.530078000	-4.459657000
H	0.547405000	2.295499000	-5.011164000
H	-0.442367000	0.205145000	-6.000223000
C	-1.357202000	-1.447638000	-1.711892000
H	-0.529102000	-2.130742000	-1.497906000
H	-2.173208000	-2.043890000	-2.134534000
C	-1.773089000	-1.881688000	0.642485000
H	-0.751881000	-2.235510000	0.787667000
H	-2.151694000	-1.466823000	1.575926000
H	-2.409174000	-2.721594000	0.337928000
N	-1.796383000	-0.842011000	-0.423775000
C	-1.569846000	2.991730000	1.893466000
C	-1.596803000	3.740324000	-0.424149000
H	-0.585082000	4.114751000	-0.272656000
H	-1.717715000	3.413357000	-1.457860000
H	-2.313159000	4.543557000	-0.211928000
H	-0.786150000	3.756830000	1.863804000
H	-2.455763000	3.453035000	2.340903000
N	-1.857559000	2.588170000	0.489693000
C	2.184101000	2.850122000	0.088111000
C	2.087315000	-1.246242000	-0.185309000
N	1.189484000	-0.528459000	-0.042598000
N	1.179535000	2.285405000	-0.029936000
C	3.442374000	3.553352000	0.227595000
H	3.965987000	3.185019000	1.116069000
H	4.057227000	3.373172000	-0.660466000
H	3.252775000	4.626494000	0.332201000
C	3.202417000	-2.154606000	-0.358781000
H	3.759059000	-1.881139000	-1.260997000
H	3.862307000	-2.092671000	0.512585000
H	2.823700000	-3.177161000	-0.458613000

Fe-BPMPN oxo 2+ triplet

C	-3.184345000	-0.307425000	-0.406848000
C	-3.046074000	2.136087000	0.158988000
C	-3.549152000	0.770833000	0.601565000
Fe	-0.242129000	0.787445000	0.049746000
H	-3.558305000	2.934466000	0.705805000
H	-3.285012000	2.259631000	-0.900090000
H	-4.642914000	0.839457000	0.630074000
H	-3.232845000	0.510146000	1.616745000
H	-3.318729000	0.095591000	-1.414330000
H	-3.846751000	-1.176061000	-0.313738000
N	-0.370690000	0.664606000	2.039942000
C	-0.951922000	1.739505000	2.616735000
C	0.088483000	-0.332265000	2.824523000
C	-1.142350000	1.820488000	3.993560000
C	-0.050598000	-0.307389000	4.205636000
H	0.575889000	-1.161091000	2.331178000
C	-0.689338000	0.780417000	4.801098000
H	-1.628097000	2.694416000	4.413987000
H	0.333720000	-1.133323000	4.793747000
H	-0.825281000	0.821865000	5.877303000
N	-0.287906000	0.751204000	-1.956599000
C	-0.899508000	-0.304151000	-2.541162000
C	0.312699000	1.679083000	-2.728917000
C	-0.981618000	-0.417716000	-3.927422000
C	0.283003000	1.615250000	-4.115413000
H	0.826667000	2.475110000	-2.206305000
C	-0.387772000	0.555810000	-4.726885000
H	-1.497071000	-1.267957000	-4.361211000
H	0.777408000	2.386396000	-4.695740000
H	-0.440168000	0.483844000	-5.808830000
C	-1.386896000	-1.377575000	-1.611052000
H	-0.574223000	-2.093898000	-1.454949000
H	-2.226070000	-1.930645000	-2.046621000
C	-1.758310000	-1.897292000	0.715647000
H	-0.747628000	-2.285619000	0.838903000
H	-2.129531000	-1.525913000	1.671218000
H	-2.409070000	-2.712999000	0.377280000
N	-1.770540000	-0.800192000	-0.291081000
C	-1.252187000	2.870346000	1.687978000

C	-1.264000000	3.538666000	-0.616424000
H	-0.209895000	3.801159000	-0.541303000
H	-1.509655000	3.263062000	-1.641074000
H	-1.877014000	4.398769000	-0.323978000
H	-0.351617000	3.489395000	1.626768000
H	-2.063457000	3.500605000	2.062178000
N	-1.563745000	2.394282000	0.298120000
C	1.979321000	-1.393373000	-0.167853000
N	1.082147000	-0.674136000	-0.055333000
C	3.099386000	-2.304033000	-0.306642000
H	3.661094000	-2.053590000	-1.212384000
H	3.754321000	-2.212732000	0.565673000
H	2.728966000	-3.331517000	-0.379572000
O	0.977698000	1.860905000	0.108383000

Fe-BPMPN oxo 2+ quintet

C	-3.156904000	-0.194921000	-0.496392000
C	-3.151122000	2.215442000	0.308222000
C	-3.572325000	0.780837000	0.603566000
Fe	-0.259214000	0.766644000	-0.008846000
H	-3.662864000	2.910721000	0.984316000
H	-3.470075000	2.457338000	-0.708834000
H	-4.668160000	0.782361000	0.635563000
H	-3.243387000	0.448977000	1.593279000
H	-3.211805000	0.310296000	-1.464767000
H	-3.844488000	-1.048141000	-0.533382000
N	-0.398883000	0.666592000	2.088938000
C	-0.958453000	1.753841000	2.660510000
C	0.044986000	-0.336791000	2.872921000
C	-1.134600000	1.840170000	4.040540000
C	-0.079441000	-0.306304000	4.255529000
H	0.509474000	-1.176401000	2.372159000
C	-0.691474000	0.797446000	4.850013000
H	-1.604553000	2.722520000	4.461954000
H	0.292633000	-1.137262000	4.844573000
H	-0.817233000	0.847824000	5.927186000
N	-0.250770000	0.700221000	-2.059260000
C	-0.882577000	-0.352556000	-2.625770000
C	0.341260000	1.629539000	-2.837524000
C	-0.965457000	-0.484981000	-4.009176000
C	0.303769000	1.551044000	-4.222299000

H	0.846386000	2.435682000	-2.319383000
C	-0.365797000	0.479511000	-4.817036000
H	-1.488045000	-1.334324000	-4.435904000
H	0.788623000	2.317226000	-4.816897000
H	-0.419228000	0.395097000	-5.898060000
C	-1.398593000	-1.384326000	-1.666630000
H	-0.606852000	-2.117746000	-1.484661000
H	-2.256933000	-1.923163000	-2.081185000
C	-1.816759000	-1.857852000	0.656612000
H	-0.823764000	-2.288002000	0.784652000
H	-2.175565000	-1.473117000	1.610218000
H	-2.502320000	-2.639821000	0.309030000
N	-1.769369000	-0.763174000	-0.355389000
C	-1.273419000	2.910304000	1.751878000
C	-1.381355000	3.619633000	-0.548746000
H	-0.321543000	3.868902000	-0.497195000
H	-1.638407000	3.324229000	-1.567162000
H	-1.975142000	4.500656000	-0.273123000
H	-0.358768000	3.505069000	1.659738000
H	-2.039078000	3.553139000	2.199021000
N	-1.677962000	2.495156000	0.381139000
C	2.154884000	-1.559268000	-0.127218000
N	1.213114000	-0.894487000	-0.013082000
C	3.327831000	-2.402580000	-0.265309000
H	3.879233000	-2.116533000	-1.166775000
H	3.972853000	-2.276805000	0.610145000
H	3.019208000	-3.449893000	-0.343592000
O	0.946815000	1.849974000	0.042924000

BItCHEN (free ligand)

C	-2.195596000	2.478246000	-0.073252000
C	-0.644565000	2.409909000	0.002841000
C	-0.118849000	3.675713000	0.726845000
C	-0.543706000	4.965271000	0.009614000
C	-2.066872000	5.030239000	-0.153593000
C	-2.605482000	3.764086000	-0.835886000
N	-0.500945000	-1.615605000	1.431176000
C	-0.484538000	-2.751135000	2.214531000
C	-0.442274000	-0.597562000	2.277173000
C	-0.419104000	-2.414718000	3.541980000
H	-0.520046000	-3.741251000	1.777468000

H	-0.391308000	-3.000526000	4.449400000
N	-2.869542000	-1.562776000	-1.439099000
C	-3.009894000	-2.688888000	-2.223842000
C	-2.736135000	-0.551789000	-2.285648000
C	-2.957081000	-2.354797000	-3.552353000
H	-3.140924000	-3.670858000	-1.786730000
H	-3.022258000	-2.935907000	-4.460851000
C	-0.463564000	0.873132000	1.933295000
C	1.278893000	0.919140000	0.256691000
H	1.541318000	-0.121226000	0.472965000
H	1.473720000	1.099776000	-0.806383000
H	1.957719000	1.566728000	0.842719000
H	0.211780000	1.404956000	2.629723000
H	-1.468392000	1.260087000	2.138060000
C	-2.522451000	0.906448000	-1.952374000
H	-3.114340000	1.513317000	-2.663748000
H	-1.473042000	1.152571000	-2.151564000
C	-4.252783000	1.174070000	-0.281304000
H	-4.618155000	0.158742000	-0.461456000
H	-4.427312000	1.412121000	0.773980000
H	-4.862552000	1.865980000	-0.891917000
N	-2.822145000	1.234617000	-0.564233000
N	-0.136277000	1.133045000	0.537137000
N	-0.388509000	-1.033852000	3.575895000
H	-0.259813000	2.455210000	-1.025239000
H	-2.571075000	2.591224000	0.952842000
H	-0.499895000	3.691156000	1.757854000
H	0.975113000	3.630367000	0.793110000
H	-0.178600000	5.841886000	0.560870000
H	-0.070780000	4.998859000	-0.983070000
H	-2.533703000	5.132617000	0.837290000
H	-2.353972000	5.920242000	-0.728979000
H	-2.223851000	3.716590000	-1.865646000
H	-3.698865000	3.816259000	-0.904555000
C	-2.667022000	-0.170973000	-4.790559000
H	-2.731921000	-0.826556000	-5.660416000
H	-3.474894000	0.565750000	-4.840555000
H	-1.706035000	0.351991000	-4.811984000
N	-2.785413000	-0.984423000	-3.585990000
C	-0.325467000	-0.214048000	4.780416000
H	-0.300656000	-0.874155000	5.648994000

H	0.576812000	0.405211000	4.779830000
H	-1.203395000	0.435058000	4.853977000

Fe-BItCHEN 2+ singlet

C	-2.237756000	1.926613000	0.181383000
C	-0.749191000	1.929242000	-0.192336000
C	-0.062162000	3.211543000	0.321796000
C	-0.756754000	4.478572000	-0.195188000
C	-2.231206000	4.475385000	0.217104000
C	-2.924950000	3.214980000	-0.316905000
Fe	-1.492142000	-0.893360000	-0.025173000
N	-1.597256000	-0.808188000	1.948991000
C	-2.354366000	-1.322605000	2.982022000
C	-0.671027000	-0.033999000	2.501994000
C	-1.866356000	-0.839267000	4.167299000
H	-3.193281000	-1.979438000	2.806862000
H	-2.174585000	-0.989796000	5.190932000
N	-1.387259000	-0.776911000	-1.997665000
C	-0.629768000	-1.274651000	-3.038522000
C	-2.316624000	0.001903000	-2.538786000
C	-1.120924000	-0.776806000	-4.216441000
H	0.211405000	-1.931185000	-2.873439000
H	-0.813544000	-0.912338000	-5.242418000
C	0.387120000	0.589552000	1.658520000
C	1.156711000	0.471611000	-0.618856000
H	1.612190000	-0.497004000	-0.412665000
H	0.885658000	0.518206000	-1.672753000
H	1.889636000	1.257047000	-0.403437000
H	1.279617000	-0.043912000	1.693506000
H	0.690882000	1.569633000	2.030089000
C	-3.375572000	0.610132000	-1.685088000
H	-4.265771000	-0.026154000	-1.727152000
H	-3.683708000	1.594190000	-2.042390000
C	-4.141317000	0.461454000	0.591773000
H	-4.596860000	-0.504380000	0.372952000
H	-3.868277000	0.493366000	1.645687000
H	-4.875087000	1.249439000	0.388882000
N	-2.921116000	0.635705000	-0.248905000
N	-0.065115000	0.633497000	0.222019000
N	-0.799640000	-0.016976000	3.850130000
C	0.590911000	-3.145381000	0.188099000

C	-3.571850000	-3.144534000	-0.277459000
C	1.537780000	-4.243516000	0.300594000
H	1.339242000	-4.812461000	1.214711000
H	1.440135000	-4.908579000	-0.563525000
H	2.559276000	-3.851284000	0.337273000
C	-4.515458000	-4.243050000	-0.411241000
H	-4.305894000	-4.802446000	-1.328794000
H	-4.426125000	-4.916604000	0.447196000
H	-5.537215000	-3.852245000	-0.455238000
N	-0.156920000	-2.265424000	0.095789000
N	-2.825945000	-2.264802000	-0.168833000
H	-0.679732000	1.931986000	-1.284511000
H	-2.307577000	1.915971000	1.273494000
H	-0.098560000	3.241952000	1.417019000
H	0.993846000	3.209485000	0.031567000
H	-0.243082000	5.361336000	0.204284000
H	-0.679612000	4.531107000	-1.290308000
H	-2.308432000	4.513114000	1.312830000
H	-2.745345000	5.363154000	-0.170497000
H	-2.887527000	3.259400000	-1.411632000
H	-3.981194000	3.208772000	-0.027597000
C	-3.061768000	0.729315000	-4.833306000
H	-3.951132000	0.128229000	-5.045584000
H	-3.364920000	1.692454000	-4.418058000
H	-2.507757000	0.896721000	-5.758223000
N	-2.189939000	0.037584000	-3.886803000
C	0.068790000	0.665403000	4.806363000
H	-0.487661000	0.822111000	5.731665000
H	0.958407000	0.063185000	5.014360000
H	0.371775000	1.633263000	4.402130000

Fe-BItCHEN 2+ triplet

C	-2.297373000	2.100006000	0.195950000
C	-0.826867000	2.023392000	-0.275556000
C	0.022072000	3.315752000	-0.069433000
C	-0.794608000	4.567626000	0.288868000
C	-2.092769000	4.600533000	-0.516557000
C	-3.016400000	3.462395000	-0.059088000
Fe	-1.502720000	-0.838951000	0.051071000
N	-1.492038000	-0.906243000	2.021332000
C	-2.033023000	-1.678622000	3.033469000

C	-0.675165000	-0.028335000	2.599095000
C	-1.530533000	-1.242855000	4.227032000
H	-2.734906000	-2.474007000	2.834057000
H	-1.696602000	-1.566575000	5.243384000
N	-1.458607000	-0.720688000	-1.974073000
C	-0.812373000	-1.417236000	-2.977749000
C	-2.344257000	0.073645000	-2.565791000
C	-1.316854000	-1.019007000	-4.185335000
H	-0.038849000	-2.138448000	-2.762231000
H	-1.084472000	-1.310194000	-5.198643000
C	0.080463000	0.982429000	1.807485000
C	1.103241000	0.509096000	-0.353479000
H	1.545053000	-0.394665000	0.066936000
H	0.918609000	0.353581000	-1.417248000
H	1.806210000	1.339214000	-0.226246000
H	1.154081000	0.895977000	2.002492000
H	-0.208239000	1.988386000	2.125858000
C	-3.267020000	0.992702000	-1.822586000
H	-4.304989000	0.715766000	-2.037701000
H	-3.145672000	2.014947000	-2.200046000
C	-4.295723000	0.688897000	0.367660000
H	-4.754240000	-0.236780000	0.011764000
H	-4.085579000	0.584875000	1.435547000
H	-5.012666000	1.509563000	0.227107000
N	-3.028514000	0.914845000	-0.356804000
N	-0.190805000	0.784103000	0.334052000
N	-0.670612000	-0.194146000	3.938100000
C	0.789537000	-3.516354000	0.122657000
C	-3.495817000	-3.163063000	-0.201663000
C	1.575240000	-4.729856000	0.288376000
H	1.042585000	-5.430048000	0.939679000
H	1.738520000	-5.199640000	-0.686789000
H	2.543481000	-4.486419000	0.737152000
C	-4.435432000	-4.264239000	-0.333277000
H	-4.219662000	-4.826943000	-1.247403000
H	-4.346811000	-4.932938000	0.529025000
H	-5.458207000	-3.876772000	-0.383458000
N	0.165480000	-2.548097000	-0.014251000
N	-2.745656000	-2.286466000	-0.096757000
H	-0.835299000	1.814616000	-1.346624000
H	-2.300026000	1.937770000	1.277429000

H	0.793205000	3.159635000	0.690846000
H	0.559174000	3.507736000	-1.004945000
H	-1.035790000	4.574674000	1.361465000
H	-0.183893000	5.457891000	0.097021000
H	-2.611879000	5.558546000	-0.392458000
H	-1.859455000	4.502612000	-1.586479000
H	-3.829126000	3.333803000	-0.781263000
H	-3.495412000	3.762780000	0.879898000
C	-3.105195000	0.633329000	-4.895459000
H	-2.872663000	0.236743000	-5.884290000
H	-4.166876000	0.477880000	-4.685601000
H	-2.883217000	1.704076000	-4.873847000
N	-2.289193000	-0.074869000	-3.912036000
C	0.110570000	0.575425000	4.904982000
H	-0.218465000	0.302880000	5.908108000
H	1.175179000	0.349137000	4.797724000
H	-0.054028000	1.644506000	4.749136000

Fe-BItCHEN 2+ quintet

C	-2.269597000	2.163561000	-0.099560000
C	-0.731570000	2.019573000	-0.206821000
C	-0.038986000	3.366223000	0.099107000
C	-0.566053000	4.510503000	-0.776639000
C	-2.084596000	4.646023000	-0.633337000
C	-2.771825000	3.320461000	-0.985610000
Fe	-1.544484000	-0.918334000	0.113801000
N	-1.383664000	-1.073095000	2.233165000
C	-1.643943000	-2.019683000	3.204963000
C	-0.708003000	-0.091685000	2.825726000
C	-1.117298000	-1.591323000	4.391929000
H	-2.176857000	-2.932815000	2.983091000
H	-1.100100000	-2.029323000	5.378603000
N	-1.407829000	-0.688756000	-2.012552000
C	-0.601528000	-1.081642000	-3.062130000
C	-2.375002000	0.062918000	-2.534486000
C	-1.096967000	-0.554143000	-4.223019000
H	0.271738000	-1.698785000	-2.910852000
H	-0.763949000	-0.615923000	-5.248129000
C	-0.301279000	1.156650000	2.101828000
C	1.152088000	0.504021000	0.274793000
H	1.446564000	-0.372652000	0.856644000

H	1.188843000	0.247032000	-0.786594000
H	1.872087000	1.308219000	0.473432000
H	0.653399000	1.538148000	2.483551000
H	-1.048215000	1.930174000	2.300709000
C	-3.484902000	0.607441000	-1.691166000
H	-4.270515000	-0.153795000	-1.625591000
H	-3.947110000	1.486142000	-2.148425000
C	-4.168236000	0.799845000	0.616177000
H	-4.677876000	-0.159648000	0.501240000
H	-3.815785000	0.884863000	1.646434000
H	-4.888781000	1.606662000	0.420514000
N	-3.007318000	0.855586000	-0.304630000
N	-0.229556000	0.887910000	0.640960000
N	-0.521222000	-0.366956000	4.137897000
C	0.612861000	-3.504874000	-0.118975000
C	-3.866224000	-3.291348000	-0.060413000
C	1.490229000	-4.662116000	-0.183324000
H	1.353224000	-5.277811000	0.711310000
H	1.249291000	-5.256688000	-1.070348000
H	2.532907000	-4.334122000	-0.240461000
C	-4.857379000	-4.348007000	-0.169278000
H	-4.645898000	-4.958814000	-1.052838000
H	-4.820033000	-4.980689000	0.723222000
H	-5.856596000	-3.910837000	-0.262080000
N	-0.087912000	-2.583346000	-0.068250000
N	-3.076898000	-2.447428000	0.027808000
H	-0.481678000	1.732758000	-1.233113000
H	-2.493651000	2.441961000	0.935186000
H	-0.202407000	3.630302000	1.151975000
H	1.042336000	3.258757000	-0.039117000
H	-0.064698000	5.445500000	-0.497580000
H	-0.315270000	4.317327000	-1.829527000
H	-2.334613000	4.933266000	0.397916000
H	-2.465676000	5.440458000	-1.286782000
H	-2.566805000	3.099543000	-2.040844000
H	-3.859245000	3.413710000	-0.878194000
C	-3.100888000	0.874768000	-4.810823000
H	-2.543121000	1.070066000	-5.727760000
H	-3.977985000	0.263292000	-5.041728000
H	-3.422083000	1.824511000	-4.378996000
N	-2.221524000	0.175402000	-3.874688000

C	0.148867000	0.478669000	5.124716000
H	0.330795000	-0.115613000	6.020849000
H	1.103884000	0.828972000	4.726546000
H	-0.477362000	1.338350000	5.380153000

Fe-BItCHEN 3+ doublet

C	-2.249939000	1.941892000	0.188880000
C	-0.762034000	1.962243000	-0.175966000
C	-0.089494000	3.218441000	0.410312000
C	-0.774890000	4.496041000	-0.095847000
C	-2.263648000	4.477620000	0.261466000
C	-2.938084000	3.224915000	-0.316988000
Fe	-1.494826000	-0.820148000	-0.035471000
N	-1.596236000	-0.739276000	1.899239000
C	-2.396223000	-1.226838000	2.917558000
C	-0.615570000	-0.032411000	2.465155000
C	-1.872801000	-0.795200000	4.102568000
H	-3.270442000	-1.830035000	2.728621000
H	-2.188265000	-0.947330000	5.123540000
N	-1.386689000	-0.749847000	-1.967025000
C	-0.593488000	-1.262570000	-2.978445000
C	-2.338440000	-0.010904000	-2.540171000
C	-1.092775000	-0.814197000	-4.167461000
H	0.260024000	-1.892257000	-2.781864000
H	-0.773956000	-0.976293000	-5.185873000
C	0.445588000	0.555933000	1.607942000
C	1.134360000	0.501394000	-0.704408000
H	1.591659000	-0.475243000	-0.552204000
H	0.837736000	0.608867000	-1.745349000
H	1.864390000	1.277195000	-0.456624000
H	1.311814000	-0.112451000	1.603559000
H	0.795986000	1.523037000	1.967443000
C	-3.391474000	0.614206000	-1.698975000
H	-4.294374000	-0.002252000	-1.740793000
H	-3.670198000	1.609262000	-2.046012000
C	-4.156862000	0.455978000	0.583428000
H	-4.612166000	-0.507254000	0.359938000
H	-3.895164000	0.502305000	1.638121000
H	-4.875322000	1.248251000	0.356247000
N	-2.928367000	0.639570000	-0.257523000
N	-0.064482000	0.642667000	0.186297000

N	-0.752774000	-0.033526000	3.800961000
C	0.573552000	-3.116666000	0.196422000
C	-3.559946000	-3.119474000	-0.263921000
C	1.465003000	-4.251033000	0.333296000
H	1.383640000	-4.653855000	1.348111000
H	1.185142000	-5.023705000	-0.389790000
H	2.495359000	-3.930887000	0.148213000
C	-4.456290000	-4.250480000	-0.395764000
H	-4.212592000	-4.802245000	-1.309508000
H	-4.340000000	-4.909649000	0.470492000
H	-5.489686000	-3.893296000	-0.448158000
N	-0.129045000	-2.205702000	0.089177000
N	-2.855477000	-2.209842000	-0.157975000
H	-0.679887000	2.013325000	-1.264709000
H	-2.336024000	1.921459000	1.278427000
H	-0.169148000	3.209107000	1.503272000
H	0.974787000	3.227255000	0.154603000
H	-0.280411000	5.366388000	0.350608000
H	-0.654540000	4.580121000	-1.184473000
H	-2.383417000	4.496816000	1.353246000
H	-2.767733000	5.367419000	-0.132837000
H	-2.866738000	3.281578000	-1.408997000
H	-4.000259000	3.207862000	-0.054453000
C	-3.056132000	0.638209000	-4.857090000
H	-3.878817000	-0.026841000	-5.133163000
H	-3.454592000	1.559653000	-4.429910000
H	-2.460937000	0.874377000	-5.739901000
N	-2.189873000	-0.016301000	-3.874949000
C	0.140887000	0.592948000	4.776908000
H	-0.441124000	0.850563000	5.662591000
H	0.941899000	-0.099308000	5.049546000
H	0.567947000	1.499732000	4.345997000

Fe-BItCHEN 3+ quartet

C	-2.244871000	2.141172000	0.020232000
C	-0.734313000	2.005202000	-0.256939000
C	0.005971000	3.326278000	0.043020000
C	-0.612101000	4.499311000	-0.732819000
C	-2.106062000	4.632579000	-0.425219000
C	-2.835998000	3.326342000	-0.765216000
Fe	-1.439882000	-0.809219000	0.130710000

N	-1.454033000	-0.973680000	2.026780000
C	-1.948401000	-1.886553000	2.944891000
C	-0.684327000	-0.100785000	2.694824000
C	-1.465723000	-1.539118000	4.170689000
H	-2.586108000	-2.707705000	2.658549000
H	-1.602805000	-1.979807000	5.146462000
N	-1.381410000	-0.601036000	-1.839661000
C	-0.560562000	-1.043860000	-2.859695000
C	-2.407147000	0.044128000	-2.399475000
C	-1.111482000	-0.643213000	-4.044599000
H	0.347661000	-1.594936000	-2.673029000
H	-0.787309000	-0.774614000	-5.065730000
C	-0.073471000	1.053728000	1.987510000
C	1.199281000	0.467660000	-0.020930000
H	1.566915000	-0.416717000	0.499757000
H	1.145106000	0.273689000	-1.091942000
H	1.886781000	1.296279000	0.166189000
H	0.968828000	1.207258000	2.278520000
H	-0.617356000	1.961630000	2.255163000
C	-3.508195000	0.590556000	-1.555488000
H	-4.305267000	-0.156248000	-1.478988000
H	-3.957260000	1.486829000	-1.987137000
C	-4.111140000	0.741278000	0.793253000
H	-4.600445000	-0.229515000	0.697255000
H	-3.724364000	0.850021000	1.807112000
H	-4.846471000	1.531625000	0.601095000
N	-2.983825000	0.825823000	-0.174686000
N	-0.164935000	0.808171000	0.495333000
N	-0.668053000	-0.413868000	3.996811000
C	0.679610000	-3.385361000	-0.020009000
C	-3.593515000	-3.084173000	-0.275445000
C	1.499235000	-4.581554000	-0.012560000
H	1.498776000	-5.018161000	0.991246000
H	1.093722000	-5.305759000	-0.726386000
H	2.524243000	-4.323083000	-0.297449000
C	-4.537413000	-4.159487000	-0.497436000
H	-4.280001000	-4.683685000	-1.423530000
H	-4.499883000	-4.857715000	0.344983000
H	-5.546439000	-3.742416000	-0.581632000
N	0.029534000	-2.426891000	-0.030913000
N	-2.841474000	-2.223728000	-0.098837000

H	-0.578815000	1.768544000	-1.311375000
H	-2.369516000	2.359785000	1.084788000
H	-0.042265000	3.557713000	1.113069000
H	1.062628000	3.222010000	-0.220939000
H	-0.077287000	5.419022000	-0.468721000
H	-0.471596000	4.345416000	-1.811575000
H	-2.247569000	4.875626000	0.636908000
H	-2.546594000	5.452898000	-1.003761000
H	-2.733903000	3.150938000	-1.842601000
H	-3.905648000	3.410781000	-0.543227000
C	-3.206910000	0.609916000	-4.715211000
H	-3.999292000	-0.110227000	-4.935916000
H	-3.643766000	1.526356000	-4.315832000
H	-2.654539000	0.839615000	-5.627160000
N	-2.272119000	0.045932000	-3.739483000
C	0.011855000	0.319419000	5.067386000
H	0.172602000	-0.364536000	5.900982000
H	0.973708000	0.683649000	4.702816000
H	-0.605246000	1.160940000	5.393182000

Fe-BItCHEN 3+ sextet

C	-2.243303000	2.009446000	0.168039000
C	-0.743376000	2.011421000	-0.177907000
C	-0.062578000	3.301584000	0.327168000
C	-0.757590000	4.563738000	-0.198578000
C	-2.227773000	4.560996000	0.224154000
C	-2.923461000	3.306747000	-0.319194000
Fe	-1.494360000	-0.922907000	-0.021852000
N	-1.568992000	-0.800638000	2.007195000
C	-2.305773000	-1.353753000	3.041498000
C	-0.663491000	0.015480000	2.561403000
C	-1.827682000	-0.856356000	4.217899000
H	-3.116030000	-2.043514000	2.862373000
H	-2.120930000	-1.023431000	5.243281000
N	-1.414747000	-0.775421000	-2.049165000
C	-0.678254000	-1.318979000	-3.088747000
C	-2.321041000	0.045000000	-2.595536000
C	-1.157367000	-0.811585000	-4.260430000
H	0.132601000	-2.009684000	-2.916153000
H	-0.864620000	-0.969406000	-5.287421000
C	0.367586000	0.712319000	1.738470000

C	1.191031000	0.528089000	-0.536382000
H	1.637383000	-0.434256000	-0.283614000
H	0.927174000	0.538751000	-1.593405000
H	1.921843000	1.318710000	-0.338475000
H	1.304850000	0.151251000	1.808632000
H	0.575245000	1.712525000	2.119030000
C	-3.351787000	0.734862000	-1.765999000
H	-4.290458000	0.177244000	-1.844736000
H	-3.555974000	1.739955000	-2.135524000
C	-4.179454000	0.523212000	0.504977000
H	-4.623883000	-0.437342000	0.242162000
H	-3.917376000	0.523659000	1.562535000
H	-4.911282000	1.314447000	0.313350000
N	-2.949230000	0.740418000	-0.317792000
N	-0.037706000	0.735704000	0.290962000
N	-0.791424000	0.011665000	3.898679000
C	0.681917000	-3.376980000	0.058156000
C	-3.668506000	-3.376622000	-0.148738000
C	1.565438000	-4.519487000	0.161003000
H	1.317694000	-5.089791000	1.062261000
H	1.441384000	-5.155177000	-0.721700000
H	2.602195000	-4.172585000	0.220229000
C	-4.551317000	-4.516609000	-0.281439000
H	-4.295284000	-5.069878000	-1.190994000
H	-4.436013000	-5.169178000	0.590021000
H	-5.587348000	-4.168103000	-0.343868000
N	-0.021805000	-2.460999000	-0.027142000
N	-2.965709000	-2.462304000	-0.040849000
H	-0.645581000	1.985663000	-1.267167000
H	-2.341431000	1.968732000	1.256766000
H	-0.102628000	3.342414000	1.421061000
H	0.992672000	3.294085000	0.036666000
H	-0.239216000	5.445563000	0.195585000
H	-0.685336000	4.609917000	-1.293884000
H	-2.299812000	4.591467000	1.320035000
H	-2.745888000	5.448573000	-0.157236000
H	-2.884027000	3.362765000	-1.412460000
H	-3.978501000	3.295787000	-0.028107000
C	-3.031543000	0.773804000	-4.893749000
H	-3.928890000	0.191335000	-5.119684000
H	-3.315283000	1.741439000	-4.477191000

H	-2.453769000	0.927246000	-5.805650000
N	-2.194054000	0.052809000	-3.932988000
C	0.044675000	0.725563000	4.865963000
H	-0.534397000	0.872372000	5.778116000
H	0.941653000	0.141401000	5.088953000
H	0.329059000	1.696139000	4.456728000

Fe-BItCHEN oxo 2+ triplet

C	-2.222067000	1.932219000	0.176071000
C	-0.734308000	1.862547000	-0.193929000
C	0.001570000	3.135554000	0.273270000
C	-0.643723000	4.402318000	-0.305934000
C	-2.120587000	4.474320000	0.090223000
C	-2.856535000	3.217811000	-0.393561000
Fe	-1.458966000	-0.959783000	0.035050000
N	-1.662493000	-0.845303000	1.968857000
C	-2.449438000	-1.388846000	2.964459000
C	-0.751185000	-0.075813000	2.555511000
C	-1.993256000	-0.919417000	4.165202000
H	-3.279293000	-2.045006000	2.752333000
H	-2.330784000	-1.085953000	5.176899000
N	-1.433214000	-0.778154000	-1.920200000
C	-0.675001000	-1.304975000	-2.944871000
C	-2.381221000	-0.024887000	-2.469338000
C	-1.182538000	-0.842353000	-4.127932000
H	0.169656000	-1.949987000	-2.758390000
H	-0.880315000	-1.002237000	-5.151795000
C	0.323444000	0.548703000	1.740287000
C	1.153944000	0.325692000	-0.516121000
H	1.540025000	-0.665353000	-0.281042000
H	0.920879000	0.381060000	-1.577914000
H	1.906278000	1.080422000	-0.269971000
H	1.226468000	-0.064426000	1.817157000
H	0.587837000	1.546359000	2.090421000
C	-3.439665000	0.582527000	-1.616311000
H	-4.314447000	-0.076053000	-1.627756000
H	-3.775825000	1.550702000	-1.989788000
C	-4.158735000	0.526679000	0.682757000
H	-4.631872000	-0.441843000	0.516998000
H	-3.862852000	0.605044000	1.727880000
H	-4.884849000	1.315328000	0.457520000

N	-2.957171000	0.651213000	-0.194408000
N	-0.089054000	0.558285000	0.285129000
N	-0.920477000	-0.085504000	3.892538000
C	-3.664433000	-3.136040000	-0.264610000
C	-4.636384000	-4.200406000	-0.428804000
H	-4.429300000	-4.743315000	-1.356616000
H	-4.570640000	-4.889760000	0.418987000
H	-5.643144000	-3.772964000	-0.473443000
N	-2.893768000	-2.285909000	-0.132866000
H	-0.653604000	1.810985000	-1.282887000
H	-2.294455000	1.980337000	1.266696000
H	-0.040979000	3.214109000	1.365362000
H	1.056788000	3.081456000	-0.012226000
H	-0.098754000	5.279895000	0.061310000
H	-0.553703000	4.403264000	-1.401002000
H	-2.208139000	4.566458000	1.181656000
H	-2.596264000	5.360752000	-0.345747000
H	-2.803724000	3.206623000	-1.488305000
H	-3.915068000	3.261511000	-0.116625000
C	-3.140264000	0.630665000	-4.776135000
H	-3.993194000	-0.011962000	-5.012320000
H	-3.496948000	1.573118000	-4.357441000
H	-2.571499000	0.832199000	-5.684960000
N	-2.258993000	-0.029502000	-3.813431000
C	-0.082158000	0.584034000	4.886960000
H	-0.685946000	0.782756000	5.773347000
H	0.766368000	-0.051605000	5.155344000
H	0.281974000	1.528209000	4.478523000
O	-0.304666000	-2.104965000	0.077354000

Fe-BItCHEN oxo 2+ quintet

C	-2.137879000	2.012938000	0.065049000
C	-0.633954000	1.900260000	-0.245730000
C	0.102031000	3.231060000	0.031345000
C	-0.556394000	4.419266000	-0.682357000
C	-2.035860000	4.522291000	-0.303663000
C	-2.761326000	3.218656000	-0.662663000
Fe	-1.452945000	-0.979635000	0.005770000
N	-1.581754000	-0.982281000	2.022977000
C	-2.183761000	-1.783943000	2.974070000
C	-0.777258000	-0.140000000	2.663351000

C	-1.737726000	-1.392061000	4.204787000
H	-2.885465000	-2.559599000	2.709416000
H	-1.963773000	-1.745485000	5.199425000
N	-1.459965000	-0.731160000	-1.959022000
C	-0.703470000	-1.180734000	-3.023359000
C	-2.456190000	0.008546000	-2.455877000
C	-1.260326000	-0.691815000	-4.169867000
H	0.171144000	-1.797401000	-2.884446000
H	-0.980500000	-0.794588000	-5.207331000
C	0.044379000	0.895732000	1.963670000
C	1.299973000	0.376253000	-0.066616000
H	1.644882000	-0.548576000	0.397090000
H	1.221600000	0.225818000	-1.145060000
H	2.025082000	1.171608000	0.135778000
H	1.088467000	0.830468000	2.284924000
H	-0.305779000	1.888097000	2.258900000
C	-3.491394000	0.545900000	-1.531288000
H	-4.300201000	-0.187804000	-1.451437000
H	-3.941107000	1.473317000	-1.886455000
C	-4.004703000	0.618082000	0.827392000
H	-4.516852000	-0.339397000	0.729584000
H	-3.602857000	0.706369000	1.835674000
H	-4.722259000	1.427229000	0.651293000
N	-2.887135000	0.690361000	-0.161509000
N	-0.040138000	0.718868000	0.479788000
N	-0.850466000	-0.349937000	3.994770000
C	-3.878032000	-3.286631000	-0.280263000
C	-4.770504000	-4.410921000	-0.496347000
H	-4.509048000	-4.909394000	-1.435331000
H	-4.671044000	-5.120960000	0.330873000
H	-5.804262000	-4.055141000	-0.548337000
N	-3.170868000	-2.385618000	-0.106969000
H	-0.509694000	1.668197000	-1.307211000
H	-2.242244000	2.189242000	1.139458000
H	0.108609000	3.441129000	1.107260000
H	1.146046000	3.135064000	-0.283482000
H	-0.021337000	5.338950000	-0.417292000
H	-0.465484000	4.298993000	-1.770939000
H	-2.133114000	4.724290000	0.772137000
H	-2.513798000	5.356306000	-0.831041000
H	-2.683094000	3.083303000	-1.747866000

H	-3.826098000	3.290055000	-0.414326000
C	-3.290667000	0.716406000	-4.723351000
H	-4.080252000	0.020847000	-5.020252000
H	-3.732291000	1.590109000	-4.242599000
H	-2.729243000	1.032283000	-5.603754000
N	-2.366976000	0.060309000	-3.796011000
C	-0.104763000	0.369700000	5.026875000
H	-0.533691000	0.118628000	5.997259000
H	0.948572000	0.076590000	5.006259000
H	-0.189599000	1.446286000	4.861915000
O	-0.332600000	-2.152525000	-0.043849000

BIMEN (free ligand)

C	0.318865000	1.427258000	0.343745000
C	-0.717882000	0.613474000	-0.442411000
H	-0.241233000	2.146585000	0.951041000
H	0.928676000	2.012685000	-0.363680000
H	-1.443383000	0.176650000	0.263073000
H	-1.270346000	1.326327000	-1.064475000
N	-0.894268000	0.502134000	3.268088000
C	-1.679810000	0.769797000	4.370613000
C	0.210594000	1.215319000	3.435686000
C	-1.041984000	1.647262000	5.208952000
H	-2.655861000	0.317580000	4.493936000
H	-1.315387000	2.091756000	6.154999000
C	1.413998000	1.261193000	2.527259000
H	2.242497000	0.731238000	3.017535000
H	1.752660000	2.311241000	2.427233000
N	0.540831000	1.473385000	-3.409778000
C	0.451997000	2.315660000	-4.498817000
C	-0.477909000	0.632639000	-3.525089000
C	-0.624806000	1.977154000	-5.277355000
H	1.165267000	3.114894000	-4.656513000
H	-1.024546000	2.382050000	-6.195797000
C	-0.813523000	-0.518128000	-2.609898000
H	-0.492823000	-1.453591000	-3.089431000
H	-1.913748000	-0.596194000	-2.512948000
C	-0.167210000	-1.742161000	-0.649067000
H	0.392544000	-2.472175000	-1.245348000
H	0.306114000	-1.653215000	0.331183000
H	-1.191599000	-2.134936000	-0.497851000

C	2.464983000	0.318469000	0.585631000
H	3.027923000	-0.399152000	1.193824000
H	2.272881000	-0.126223000	-0.393307000
H	3.099503000	1.213371000	0.434214000
N	-0.152964000	-0.437203000	-1.310207000
N	1.189111000	0.631064000	1.229894000
N	0.166214000	1.932007000	4.603037000
N	-1.218514000	0.901191000	-4.646568000
C	-2.401085000	0.185294000	-5.112257000
H	-3.197305000	0.228291000	-4.362945000
H	-2.754312000	0.656610000	-6.030732000
H	-2.162869000	-0.862310000	-5.320272000
C	1.200907000	2.811690000	5.134216000
H	1.426126000	3.612971000	4.424047000
H	0.838041000	3.254014000	6.063289000
H	2.117753000	2.250996000	5.341844000

Fe-BIMEN 2+ singlet

C	-0.355640000	2.540175000	-0.272335000
C	-1.547794000	1.713466000	0.161653000
H	-0.453447000	3.570441000	0.091326000
H	-0.296798000	2.581383000	-1.362058000
H	-1.625114000	1.697986000	1.250825000
H	-2.476078000	2.149489000	-0.227355000
Fe	0.645110000	-0.150693000	-0.017510000
N	0.472230000	-0.111314000	1.950598000
C	0.173080000	-0.982605000	2.979138000
C	0.704851000	1.071974000	2.507635000
C	0.225208000	-0.298256000	4.164280000
H	-0.067647000	-2.019688000	2.799406000
H	0.053657000	-0.605410000	5.184937000
C	1.127330000	2.240536000	1.682127000
H	2.193402000	2.431306000	1.843248000
H	0.594038000	3.156070000	1.964062000
N	0.695619000	-0.014142000	-1.987859000
C	1.632517000	-0.049061000	-3.001424000
C	-0.488054000	0.154879000	-2.566710000
C	0.989330000	0.107300000	-4.200269000
H	2.687046000	-0.168409000	-2.802697000
H	1.352281000	0.143798000	-5.216294000
C	-1.742842000	0.168016000	-1.759198000

H	-2.276388000	-0.776916000	-1.904976000
H	-2.423187000	0.968596000	-2.072191000
C	-2.364453000	-0.536924000	0.470375000
H	-2.271864000	-1.579365000	0.163604000
H	-2.144899000	-0.456234000	1.535142000
H	-3.393282000	-0.199633000	0.289324000
C	2.043033000	2.537138000	-0.537043000
H	2.985992000	2.100858000	-0.205734000
H	1.910714000	2.338185000	-1.600539000
H	2.073473000	3.622491000	-0.375688000
N	-1.402193000	0.297076000	-0.298632000
N	0.917754000	1.931023000	0.223978000
N	0.558779000	1.007614000	3.852255000
N	-0.357157000	0.241236000	-3.911899000
C	0.189272000	-3.180541000	-0.240404000
C	3.644900000	-0.754820000	0.252956000
C	5.056662000	-1.076536000	0.389590000
H	5.198320000	-1.782602000	1.214214000
H	5.426201000	-1.528580000	-0.536523000
H	5.626698000	-0.164882000	0.596444000
C	0.007082000	-4.618396000	-0.360714000
H	0.529559000	-4.985585000	-1.250038000
H	0.411039000	-5.119865000	0.524694000
H	-1.059124000	-4.851206000	-0.449472000
N	2.522432000	-0.491723000	0.140410000
N	0.325230000	-2.034250000	-0.143556000
C	-1.434542000	0.383665000	-4.888202000
H	-2.184990000	1.080057000	-4.507806000
H	-1.014409000	0.779330000	-5.813926000
H	-1.903781000	-0.584854000	-5.086118000
C	0.773784000	2.092493000	4.806662000
H	0.372397000	3.023609000	4.400681000
H	0.250092000	1.850088000	5.732477000
H	1.841200000	2.215582000	5.013722000

Fe-BIMEN 2+ triplet

C	-0.399861000	2.597803000	-0.272000000
C	-1.596878000	1.762536000	0.160463000
H	-0.539045000	3.633330000	0.068137000
H	-0.331035000	2.621297000	-1.362455000
H	-1.660959000	1.730903000	1.250921000

H	-2.519052000	2.234068000	-0.206312000
Fe	0.665603000	-0.186452000	-0.012265000
N	0.541263000	-0.082774000	1.943979000
C	0.287454000	-0.969347000	2.973068000
C	0.713876000	1.113940000	2.502449000
C	0.309309000	-0.286055000	4.158639000
H	0.101858000	-2.017100000	2.790926000
H	0.158706000	-0.603687000	5.179360000
C	1.054858000	2.331396000	1.702041000
H	2.099830000	2.603307000	1.887218000
H	0.448089000	3.192314000	2.011728000
N	0.648853000	-0.081339000	-1.971736000
C	1.590137000	-0.161055000	-2.980148000
C	-0.523029000	0.156317000	-2.558314000
C	0.965624000	0.033957000	-4.182074000
H	2.634398000	-0.340014000	-2.773087000
H	1.336930000	0.053215000	-5.195500000
C	-1.799631000	0.258292000	-1.783909000
H	-2.399606000	-0.641097000	-1.960670000
H	-2.403198000	1.109755000	-2.123937000
C	-2.466558000	-0.479073000	0.434364000
H	-2.383065000	-1.517190000	0.106470000
H	-2.231366000	-0.425217000	1.499087000
H	-3.500019000	-0.137824000	0.279883000
C	2.007893000	2.653987000	-0.509859000
H	2.951010000	2.230273000	-0.158484000
H	1.892754000	2.427327000	-1.571430000
H	2.036037000	3.745123000	-0.379347000
N	-1.506636000	0.357331000	-0.322225000
N	0.884786000	2.052028000	0.244511000
N	0.576653000	1.034465000	3.847696000
N	-0.372877000	0.239391000	-3.902056000
C	0.181551000	-3.403012000	-0.214265000
C	3.849330000	-0.826494000	0.233177000
C	5.250555000	-1.179004000	0.387699000
H	5.362770000	-1.888635000	1.213651000
H	5.622247000	-1.634765000	-0.535448000
H	5.832380000	-0.277622000	0.605904000
C	0.029058000	-4.840146000	-0.365570000
H	0.559457000	-5.175235000	-1.262641000
H	0.440038000	-5.350675000	0.511119000

H	-1.033328000	-5.086698000	-0.461542000
N	2.733119000	-0.542808000	0.106584000
N	0.298081000	-2.256651000	-0.092774000
C	-1.431993000	0.448043000	-4.886409000
H	-2.123186000	1.214198000	-4.528245000
H	-0.976609000	0.783648000	-5.819077000
H	-1.979826000	-0.482516000	-5.063152000
C	0.734063000	2.128473000	4.803198000
H	0.174273000	3.002628000	4.462138000
H	0.341191000	1.804357000	5.767562000
H	1.790352000	2.392149000	4.911557000

Fe-BIMEN 2+ quintet

C	-0.403121000	2.584825000	-0.277439000
C	-1.621447000	1.743353000	0.081165000
H	-0.581783000	3.624282000	0.033300000
H	-0.254375000	2.594690000	-1.359906000
H	-1.730536000	1.691302000	1.167854000
H	-2.524457000	2.233525000	-0.309829000
Fe	0.698330000	-0.248420000	0.004912000
N	0.538422000	-0.084465000	2.103845000
C	0.371668000	-0.949255000	3.170502000
C	0.677469000	1.134878000	2.618181000
C	0.410960000	-0.230600000	4.332331000
H	0.234390000	-2.010762000	3.025808000
H	0.321137000	-0.520335000	5.368525000
C	0.900426000	2.369537000	1.797411000
H	1.881933000	2.789531000	2.043300000
H	0.163591000	3.138367000	2.064326000
N	0.674965000	-0.042863000	-2.099625000
C	1.600911000	-0.092716000	-3.125472000
C	-0.507379000	0.196132000	-2.662472000
C	0.958256000	0.122687000	-4.312069000
H	2.649713000	-0.268172000	-2.936952000
H	1.311519000	0.167666000	-5.331281000
C	-1.789758000	0.277248000	-1.888524000
H	-2.383319000	-0.619352000	-2.098869000
H	-2.389766000	1.133749000	-2.224070000
C	-2.502910000	-0.502865000	0.296695000
H	-2.420533000	-1.532450000	-0.058326000
H	-2.276732000	-0.481327000	1.365227000

H	-3.535554000	-0.155522000	0.145517000
C	2.020669000	2.655113000	-0.340779000
H	2.935645000	2.256422000	0.103008000
H	1.997142000	2.384377000	-1.398679000
H	2.031274000	3.751496000	-0.254351000
N	-1.530774000	0.347406000	-0.425201000
N	0.846025000	2.067074000	0.340391000
N	0.604952000	1.091576000	3.968717000
N	-0.379329000	0.309660000	-4.005354000
C	0.191823000	-3.527212000	-0.128846000
C	3.944274000	-0.936282000	0.147015000
C	5.345513000	-1.302159000	0.263580000
H	5.470793000	-2.019006000	1.081437000
H	5.683254000	-1.760233000	-0.671557000
H	5.945994000	-0.410076000	0.467892000
C	-0.009824000	-4.960689000	-0.252113000
H	0.521190000	-5.331203000	-1.134850000
H	0.378115000	-5.464185000	0.639135000
H	-1.078111000	-5.176764000	-0.354183000
N	2.826740000	-0.644443000	0.052225000
N	0.348303000	-2.383054000	-0.031855000
C	-1.452391000	0.531222000	-4.972606000
H	-2.137830000	1.294374000	-4.597686000
H	-1.008769000	0.876040000	-5.907427000
H	-2.003323000	-0.396894000	-5.151878000
C	0.719833000	2.229151000	4.879268000
H	-0.070726000	2.956505000	4.675689000
H	0.618804000	1.863416000	5.901387000
H	1.695346000	2.709067000	4.762147000

Fe-BIMEN 3+ doublet

C	-0.360560000	2.573407000	-0.289531000
C	-1.559401000	1.761474000	0.145230000
H	-0.437679000	3.600951000	0.078720000
H	-0.288025000	2.612371000	-1.377590000
H	-1.659564000	1.762825000	1.231780000
H	-2.479615000	2.179015000	-0.274137000
Fe	0.599008000	-0.076558000	-0.016314000
N	0.425917000	-0.076055000	1.910878000
C	0.114567000	-0.983991000	2.907962000
C	0.724252000	1.082646000	2.502471000

C	0.234196000	-0.342514000	4.107312000
H	-0.156348000	-2.006272000	2.695900000
H	0.088538000	-0.683741000	5.120886000
C	1.123628000	2.263419000	1.690156000
H	2.183844000	2.480957000	1.849024000
H	0.559301000	3.161161000	1.961732000
N	0.681334000	0.056154000	-1.945933000
C	1.652364000	0.032356000	-2.932268000
C	-0.504132000	0.131384000	-2.553628000
C	1.020054000	0.092929000	-4.141020000
H	2.705186000	-0.030521000	-2.706328000
H	1.401403000	0.095368000	-5.150661000
C	-1.758536000	0.155738000	-1.755490000
H	-2.291542000	-0.791852000	-1.875349000
H	-2.434902000	0.954740000	-2.074351000
C	-2.371085000	-0.501554000	0.498203000
H	-2.278576000	-1.548331000	0.211215000
H	-2.165468000	-0.389083000	1.561294000
H	-3.389265000	-0.156650000	0.287782000
C	2.054285000	2.544843000	-0.534214000
H	2.990543000	2.104298000	-0.194114000
H	1.922321000	2.361365000	-1.599074000
H	2.074464000	3.624766000	-0.352323000
N	-1.408560000	0.326243000	-0.292509000
N	0.911185000	1.949043000	0.223923000
N	0.617279000	0.962655000	3.836080000
N	-0.341925000	0.157646000	-3.886450000
C	0.165750000	-3.129840000	-0.270748000
C	3.610306000	-0.732420000	0.266336000
C	5.001667000	-1.108724000	0.415271000
H	5.100020000	-1.811223000	1.249291000
H	5.349571000	-1.585925000	-0.506617000
H	5.601686000	-0.215216000	0.615551000
C	0.038176000	-4.565656000	-0.417545000
H	0.568412000	-4.886099000	-1.320362000
H	0.473656000	-5.060884000	0.456291000
H	-1.020609000	-4.831464000	-0.500263000
N	2.504493000	-0.421042000	0.144761000
N	0.255300000	-1.983997000	-0.153627000
C	-1.404974000	0.261742000	-4.888724000
H	-1.809236000	1.277356000	-4.901416000

H	-0.978981000	0.024945000	-5.863662000
H	-2.199093000	-0.450668000	-4.655572000
C	0.827120000	2.021323000	4.826293000
H	-0.037204000	2.690423000	4.848736000
H	0.955484000	1.554333000	5.802990000
H	1.726596000	2.585774000	4.572346000

Fe-BIMEN 3+ quartet

C	-0.405954000	2.599197000	-0.290438000
C	-1.628917000	1.808356000	0.139249000
H	-0.485687000	3.634988000	0.054743000
H	-0.312224000	2.617342000	-1.377221000
H	-1.719817000	1.793185000	1.227423000
H	-2.531257000	2.284401000	-0.261589000
Fe	0.649451000	-0.077639000	0.029489000
N	0.494121000	-0.060964000	1.928766000
C	0.254259000	-0.995766000	2.924219000
C	0.701862000	1.123382000	2.526778000
C	0.318146000	-0.348148000	4.121555000
H	0.056921000	-2.033643000	2.707868000
H	0.191760000	-0.699709000	5.134182000
C	1.028631000	2.331287000	1.724172000
H	2.067435000	2.624612000	1.903540000
H	0.396014000	3.183001000	1.992725000
N	0.631207000	0.034811000	-1.935654000
C	1.599031000	-0.082978000	-2.917857000
C	-0.548138000	0.165911000	-2.545833000
C	0.974888000	-0.009310000	-4.130716000
H	2.645128000	-0.202640000	-2.684443000
H	1.359955000	-0.050970000	-5.138149000
C	-1.830778000	0.266837000	-1.789812000
H	-2.420696000	-0.640134000	-1.956041000
H	-2.434588000	1.112320000	-2.139276000
C	-2.491810000	-0.452475000	0.444377000
H	-2.392365000	-1.491910000	0.127765000
H	-2.266221000	-0.374328000	1.508717000
H	-3.522087000	-0.118665000	0.268824000
C	2.021206000	2.579892000	-0.492444000
H	2.948543000	2.147758000	-0.117229000
H	1.912833000	2.361876000	-1.553959000
H	2.037670000	3.665035000	-0.342703000

N	-1.542488000	0.392286000	-0.326605000
N	0.864342000	2.002525000	0.257042000
N	0.603704000	0.985789000	3.854707000
N	-0.377286000	0.145991000	-3.881359000
C	0.235921000	-3.190530000	-0.242094000
C	3.883839000	-0.810782000	0.204907000
C	5.259144000	-1.237366000	0.372737000
H	5.321282000	-1.946720000	1.204446000
H	5.605656000	-1.720708000	-0.546405000
H	5.886868000	-0.366569000	0.587785000
C	0.073715000	-4.618689000	-0.416612000
H	0.612090000	-4.938966000	-1.314512000
H	0.471970000	-5.141028000	0.459178000
H	-0.991377000	-4.848884000	-0.526575000
N	2.787300000	-0.464992000	0.064075000
N	0.359990000	-2.049501000	-0.102040000
C	-1.432554000	0.282050000	-4.887446000
H	-1.812627000	1.306944000	-4.896203000
H	-1.007435000	0.041591000	-5.861878000
H	-2.245904000	-0.412069000	-4.664466000
C	0.740906000	2.050211000	4.853101000
H	-0.158475000	2.671234000	4.860370000
H	0.875620000	1.585137000	5.829578000
H	1.613902000	2.661497000	4.615836000

Fe-BIMEN 3+ sextet

C	-0.450888000	2.647978000	-0.139457000
C	-1.628284000	1.758647000	0.216033000
H	-0.588091000	3.641681000	0.300753000
H	-0.381918000	2.776119000	-1.221970000
H	-1.709863000	1.620030000	1.295756000
H	-2.559351000	2.224347000	-0.127061000
Fe	0.656964000	-0.136963000	-0.033395000
N	0.459371000	-0.073675000	1.995463000
C	0.174446000	-0.974150000	3.009810000
C	0.688117000	1.111568000	2.576994000
C	0.234046000	-0.310072000	4.199176000
H	-0.057357000	-2.008706000	2.809160000
H	0.076733000	-0.636632000	5.216014000
C	1.083723000	2.314869000	1.786347000
H	2.148821000	2.512147000	1.942860000

H	0.537039000	3.205924000	2.114527000
N	0.662710000	-0.009679000	-2.061891000
C	1.595645000	-0.185196000	-3.071785000
C	-0.520817000	0.198848000	-2.653399000
C	0.952886000	-0.076880000	-4.269388000
H	2.636925000	-0.375175000	-2.862367000
H	1.306523000	-0.148935000	-5.286728000
C	-1.773625000	0.437810000	-1.877934000
H	-2.512872000	-0.331363000	-2.120339000
H	-2.216673000	1.401201000	-2.152663000
C	-2.431689000	-0.544576000	0.259098000
H	-2.340325000	-1.529763000	-0.199780000
H	-2.191850000	-0.611270000	1.320953000
H	-3.460471000	-0.184105000	0.141282000
C	1.965886000	2.693422000	-0.451549000
H	2.917642000	2.268790000	-0.129541000
H	1.818747000	2.495358000	-1.513849000
H	1.975788000	3.776628000	-0.281238000
N	-1.489254000	0.400609000	-0.404223000
N	0.856043000	2.070492000	0.325449000
N	0.555759000	1.009461000	3.909640000
N	-0.385661000	0.163799000	-3.988766000
C	0.238276000	-3.382824000	-0.093681000
C	3.853794000	-0.803519000	0.123720000
C	5.249631000	-1.165669000	0.249618000
H	5.398571000	-1.720229000	1.181931000
H	5.539916000	-1.791338000	-0.600768000
H	5.860190000	-0.256860000	0.261868000
C	0.136666000	-4.824427000	-0.179073000
H	0.668861000	-5.173442000	-1.070138000
H	0.582249000	-5.273597000	0.714422000
H	-0.918177000	-5.110378000	-0.246658000
N	2.738189000	-0.510908000	0.018171000
N	0.315191000	-2.229512000	-0.021567000
C	-1.444114000	0.380086000	-4.977160000
H	-1.691087000	1.443629000	-5.035126000
H	-1.082860000	0.034407000	-5.945661000
H	-2.331611000	-0.190818000	-4.695804000
C	0.766957000	2.069370000	4.897720000
H	0.398708000	3.017317000	4.501731000
H	0.211122000	1.813641000	5.800248000

H	1.831333000	2.155849000	5.132806000

Fe-BIMEN-oxo 2+ triplet

C	-0.242765000	2.504819000	-0.272861000
C	-1.486570000	1.755494000	0.156453000
H	-0.278509000	3.541952000	0.075898000
H	-0.154109000	2.522414000	-1.360392000
H	-1.588442000	1.765152000	1.243492000
H	-2.378720000	2.236717000	-0.261244000
Fe	0.728728000	-0.193247000	0.055512000
N	0.429733000	-0.148506000	1.978670000
C	0.071402000	-1.025634000	2.983535000
C	0.689124000	1.025270000	2.548309000
C	0.111729000	-0.347107000	4.169921000
H	-0.198502000	-2.051399000	2.785977000
H	-0.104096000	-0.654875000	5.181752000
C	1.189036000	2.162367000	1.729170000
H	2.259531000	2.299526000	1.910038000
H	0.690887000	3.105492000	1.975536000
N	0.711717000	-0.083851000	-1.902523000
C	1.679395000	-0.207470000	-2.878571000
C	-0.454717000	0.095275000	-2.515081000
C	1.069979000	-0.087532000	-4.096755000
H	2.719698000	-0.356091000	-2.633934000
H	1.460501000	-0.114303000	-5.102655000
C	-1.726188000	0.187378000	-1.742164000
H	-2.303235000	-0.731328000	-1.887114000
H	-2.353264000	1.017499000	-2.087242000
C	-2.415508000	-0.458465000	0.491157000
H	-2.359708000	-1.508393000	0.200479000
H	-2.207952000	-0.367759000	1.557446000
H	-3.426194000	-0.082458000	0.288899000
C	2.174389000	2.369792000	-0.478618000
H	3.072872000	1.862731000	-0.127774000
H	2.043357000	2.185887000	-1.543924000
H	2.260212000	3.448068000	-0.303080000
N	-1.413573000	0.326616000	-0.279685000
N	0.994509000	1.840696000	0.265431000
N	0.499444000	0.951198000	3.880047000
N	-0.279236000	0.108461000	-3.853370000
C	0.078095000	-3.224237000	-0.180924000

C	-0.159969000	-4.648933000	-0.317165000
H	0.372752000	-5.024444000	-1.196770000
H	0.201388000	-5.167349000	0.576665000
H	-1.232916000	-4.831047000	-0.435737000
N	0.265590000	-2.089890000	-0.072336000
C	-1.324691000	0.241243000	-4.867733000
H	-2.072049000	0.961975000	-4.530013000
H	-0.867451000	0.601536000	-5.790132000
H	-1.802852000	-0.725632000	-5.049142000
C	0.722034000	2.020051000	4.853678000
H	0.428798000	2.976541000	4.416308000
H	0.108122000	1.821002000	5.732918000
H	1.776315000	2.055280000	5.142179000
O	2.322639000	-0.490579000	0.156064000

Fe-BIMEN oxo 2+ quintet

C	-0.281127000	2.597835000	-0.214284000
C	-1.492912000	1.770377000	0.171326000
H	-0.403409000	3.624119000	0.154131000
H	-0.178164000	2.650155000	-1.300595000
H	-1.595712000	1.719612000	1.256659000
H	-2.404828000	2.234255000	-0.221442000
Fe	0.715088000	-0.237339000	0.002769000
N	0.422017000	-0.111929000	2.005495000
C	0.109360000	-0.999148000	3.018340000
C	0.685212000	1.062588000	2.573723000
C	0.176048000	-0.329048000	4.207358000
H	-0.149310000	-2.027720000	2.819834000
H	-0.003348000	-0.645582000	5.223697000
C	1.131136000	2.255673000	1.788612000
H	2.188566000	2.446201000	1.999438000
H	0.577941000	3.154753000	2.086635000
N	0.718459000	-0.137133000	-1.966064000
C	1.676908000	-0.312468000	-2.947641000
C	-0.445953000	0.094838000	-2.578774000
C	1.065998000	-0.179434000	-4.160347000
H	2.708535000	-0.516626000	-2.706070000
H	1.444856000	-0.241156000	-5.169165000
C	-1.703125000	0.297668000	-1.807590000
H	-2.382272000	-0.540907000	-1.990923000
H	-2.224444000	1.206198000	-2.127352000

C	-2.394502000	-0.467603000	0.393611000
H	-2.349703000	-1.495552000	0.034408000
H	-2.177110000	-0.446855000	1.461576000
H	-3.400690000	-0.066539000	0.222309000
C	2.147204000	2.535536000	-0.406850000
H	3.052391000	2.051807000	-0.036447000
H	2.035674000	2.319137000	-1.470527000
H	2.228704000	3.621321000	-0.266762000
N	-1.390165000	0.360211000	-0.335197000
N	0.973622000	2.001616000	0.326341000
N	0.537260000	0.974525000	3.912216000
N	-0.276740000	0.075138000	-3.911622000
C	0.002478000	-3.502511000	-0.124174000
C	-0.133315000	-4.938813000	-0.284134000
H	0.406757000	-5.258513000	-1.181186000
H	0.285371000	-5.445786000	0.591024000
H	-1.191949000	-5.198745000	-0.384061000
N	0.102043000	-2.355771000	0.003852000
C	-1.311919000	0.304338000	-4.920941000
H	-1.568143000	1.366484000	-4.962152000
H	-0.923785000	-0.015757000	-5.887942000
H	-2.200793000	-0.280896000	-4.675460000
C	0.760857000	2.045191000	4.883761000
H	0.269786000	2.959698000	4.543574000
H	0.331272000	1.737619000	5.837478000
H	1.832197000	2.227106000	5.006675000
O	2.298437000	-0.572266000	0.101452000

BPtCHEN (free ligand)

C	-1.478901000	1.888876000	0.008489000
C	0.072234000	1.995078000	-0.042869000
C	0.521215000	3.303228000	0.657757000
C	-0.111434000	4.551531000	0.028025000
C	-1.640333000	4.449868000	0.039661000
C	-2.104394000	3.152575000	-0.635741000
N	0.238836000	-1.883647000	1.780317000
C	1.008573000	-0.892975000	2.269426000
C	0.520174000	-3.142728000	2.140487000
C	2.078969000	-1.147520000	3.135418000
C	1.565331000	-3.487984000	2.999326000
H	-0.126494000	-3.915126000	1.726581000

C	2.361914000	-2.462671000	3.506678000
H	2.678668000	-0.322897000	3.509758000
H	1.742618000	-4.527356000	3.258490000
H	3.189068000	-2.680306000	4.177041000
N	-2.393641000	-1.277633000	-3.609149000
C	-1.832729000	-1.008649000	-2.416456000
C	-2.340316000	-2.539503000	-4.063156000
C	-1.209793000	-1.996869000	-1.642160000
C	-1.743366000	-3.587552000	-3.364461000
H	-2.804792000	-2.719368000	-5.031937000
C	-1.167211000	-3.303524000	-2.124277000
H	-0.776689000	-1.732514000	-0.682747000
H	-1.734931000	-4.591276000	-3.778744000
H	-0.690415000	-4.088498000	-1.542618000
C	-1.865724000	0.447972000	-1.976496000
C	-3.353799000	0.316308000	-0.079580000
H	-3.620217000	-0.706047000	-0.370747000
H	-3.401032000	0.375709000	1.013473000
H	-4.127605000	0.989340000	-0.493763000
H	-2.667027000	0.946694000	-2.549541000
H	-0.924954000	0.911759000	-2.296058000
C	0.645619000	0.529996000	1.874918000
H	-0.396541000	0.699428000	2.163977000
H	1.265954000	1.219015000	2.474760000
C	2.156915000	0.716137000	-0.008179000
H	2.569192000	-0.276077000	0.206132000
H	2.204117000	0.870917000	-1.091683000
H	2.820734000	1.459130000	0.472239000
N	-2.000413000	0.617834000	-0.532549000
N	0.767939000	0.780128000	0.435708000
H	0.360901000	2.085429000	-1.098859000
H	-1.775074000	1.889833000	1.066025000
H	-1.832715000	3.187265000	-1.700104000
H	-3.197914000	3.077777000	-0.590985000
H	-1.997737000	4.468375000	1.079932000
H	-2.089286000	5.316958000	-0.462614000
H	0.219952000	5.451470000	0.562777000
H	0.238743000	4.654755000	-1.009749000
H	0.242955000	3.260776000	1.719981000
H	1.614860000	3.379138000	0.620115000

Fe-BPtCHEN 2+ singlet

C	-1.207758000	1.271030000	0.219301000
C	0.261258000	1.280977000	-0.213106000
C	0.968271000	2.543172000	0.320004000
C	0.263290000	3.821543000	-0.155521000
C	-1.205949000	3.812383000	0.277006000
C	-1.913830000	2.557501000	-0.254357000
Fe	-0.478396000	-1.533232000	-0.008426000
N	-0.520694000	-1.413273000	1.984706000
C	0.430114000	-0.607517000	2.507616000
C	-1.395358000	-2.004315000	2.824304000
C	0.504715000	-0.337585000	3.873325000
C	-1.368579000	-1.801703000	4.199049000
H	-2.138149000	-2.648085000	2.369289000
C	-0.408243000	-0.942446000	4.734275000
H	1.275526000	0.328920000	4.246454000
H	-2.095443000	-2.303033000	4.829143000
H	-0.368557000	-0.750009000	5.802169000
N	-0.426242000	-1.465501000	-2.002039000
C	-1.328907000	-0.623446000	-2.550943000
C	0.428794000	-2.113692000	-2.819927000
C	-1.369231000	-0.370716000	-3.921888000
C	0.431267000	-1.932717000	-4.197610000
H	1.131948000	-2.786285000	-2.344383000
C	-0.475799000	-1.033497000	-4.759846000
H	-2.100471000	0.327223000	-4.316675000
H	1.140103000	-2.480657000	-4.809156000
H	-0.490169000	-0.855457000	-5.830869000
C	-2.361207000	-0.077647000	-1.607529000
C	-3.113428000	-0.177286000	0.664299000
H	-3.546098000	-1.165033000	0.505787000
H	-2.852406000	-0.064839000	1.715751000
H	-3.863293000	0.578111000	0.406073000
H	-3.207029000	-0.773428000	-1.629169000
H	-2.747383000	0.884103000	-1.949968000
C	1.465038000	-0.123477000	1.534273000
H	1.924704000	0.808680000	1.867499000
H	2.263419000	-0.873407000	1.519964000
C	2.133304000	-0.173951000	-0.766450000
H	2.567135000	-1.166520000	-0.643887000
H	1.831609000	-0.040716000	-1.804455000

H	2.895773000	0.573982000	-0.523102000
N	-1.894191000	-0.024498000	-0.184584000
N	0.948736000	-0.031351000	0.131523000
H	0.287857000	1.322753000	-1.306602000
H	-1.235719000	1.261659000	1.313471000
H	-1.906037000	2.605816000	-1.349755000
H	-2.961057000	2.549647000	0.065063000
H	-1.267113000	3.839363000	1.374041000
H	-1.724270000	4.704849000	-0.093755000
H	0.782176000	4.695936000	0.255349000
H	0.325198000	3.897650000	-1.250187000
H	0.956228000	2.541067000	1.416492000
H	2.017202000	2.546873000	0.005017000
C	-2.542776000	-3.805688000	-0.256962000
C	1.583137000	-3.801598000	0.307373000
N	0.854164000	-2.916431000	0.142909000
N	-1.812114000	-2.917256000	-0.120011000
C	-3.465796000	-4.916421000	-0.423771000
H	-3.669535000	-5.072166000	-1.488143000
H	-3.027240000	-5.827738000	-0.004659000
H	-4.405555000	-4.698728000	0.094184000
C	2.504225000	-4.908201000	0.508335000
H	2.602619000	-5.118823000	1.578204000
H	2.126099000	-5.800938000	-0.000248000
H	3.487199000	-4.651384000	0.100266000

Fe-BPtCHEN 2+ triplet

C	-1.201613000	1.340028000	0.221256000
C	0.273736000	1.334028000	-0.230348000
C	0.980212000	2.619663000	0.251053000
C	0.272759000	3.886389000	-0.247801000
C	-1.187842000	3.892512000	0.211225000
C	-1.901609000	2.624014000	-0.273933000
Fe	-0.471447000	-1.574754000	0.006358000
N	-0.447254000	-1.452408000	1.981956000
C	0.446525000	-0.580468000	2.505467000
C	-1.296906000	-2.086217000	2.818303000
C	0.482983000	-0.296600000	3.870331000
C	-1.300507000	-1.869270000	4.190354000
H	-1.992818000	-2.777921000	2.359508000
C	-0.401065000	-0.947790000	4.727393000

H	1.205291000	0.420493000	4.246679000
H	-2.004075000	-2.407302000	4.816535000
H	-0.386336000	-0.742103000	5.793429000
N	-0.495253000	-1.463292000	-1.969975000
C	-1.387083000	-0.591858000	-2.497821000
C	0.352493000	-2.103544000	-2.803271000
C	-1.423553000	-0.315195000	-3.864114000
C	0.356006000	-1.893869000	-4.176498000
H	1.046878000	-2.794583000	-2.341170000
C	-0.541446000	-0.973141000	-4.718072000
H	-2.144245000	0.401698000	-4.243933000
H	1.058009000	-2.436928000	-4.800088000
H	-0.556128000	-0.773067000	-5.785176000
C	-2.411815000	-0.031838000	-1.548206000
C	-3.111710000	-0.088070000	0.752773000
H	-3.543920000	-1.081190000	0.614257000
H	-2.804714000	0.021846000	1.793352000
H	-3.883139000	0.660261000	0.533240000
H	-3.249916000	-0.738175000	-1.541690000
H	-2.813421000	0.912980000	-1.922216000
C	1.473700000	-0.027880000	1.554026000
H	1.874768000	0.919486000	1.922272000
H	2.311573000	-0.734541000	1.554761000
C	2.179054000	-0.106494000	-0.744383000
H	2.605805000	-1.100721000	-0.597115000
H	1.875755000	-0.003098000	-1.786749000
H	2.953785000	0.639454000	-0.528440000
N	-1.932934000	0.065090000	-0.140485000
N	0.998687000	0.059391000	0.144350000
H	0.283914000	1.340177000	-1.325312000
H	-1.211907000	1.357566000	1.316091000
H	-1.908951000	2.641886000	-1.370529000
H	-2.945807000	2.625326000	0.057125000
H	-1.229176000	3.949186000	1.308197000
H	-1.712488000	4.775399000	-0.173900000
H	0.801797000	4.770805000	0.127690000
H	0.314289000	3.930892000	-1.345331000
H	0.988004000	2.649279000	1.347399000
H	2.024240000	2.612072000	-0.080404000
C	-2.646984000	-3.992513000	-0.345838000
C	1.689418000	-4.001498000	0.367540000

N	0.991310000	-3.105245000	0.138554000
N	-1.944950000	-3.098896000	-0.118464000
C	-3.530654000	-5.111014000	-0.625601000
H	-3.487904000	-5.358038000	-1.691142000
H	-3.219990000	-5.981172000	-0.038505000
H	-4.557449000	-4.842392000	-0.357235000
C	2.568313000	-5.123315000	0.648894000
H	2.516448000	-5.375485000	1.712822000
H	2.260538000	-5.989874000	0.054982000
H	3.597806000	-4.855614000	0.390102000

Fe-BPtCHEN 2+ quintet

C	-1.232068000	1.282209000	0.195823000
C	0.266393000	1.294398000	-0.183262000
C	0.944610000	2.556386000	0.392897000
C	0.265747000	3.848361000	-0.078622000
C	-1.216224000	3.835805000	0.304844000
C	-1.902476000	2.592027000	-0.273887000
Fe	-0.510354000	-1.696219000	0.002494000
N	-0.479930000	-1.404823000	2.154197000
C	0.443688000	-0.514445000	2.570657000
C	-1.355962000	-1.910394000	3.043137000
C	0.496115000	-0.084959000	3.897260000
C	-1.351934000	-1.545849000	4.384781000
H	-2.077378000	-2.622051000	2.654598000
C	-0.411803000	-0.608688000	4.816171000
H	1.244054000	0.641330000	4.198292000
H	-2.073308000	-1.981622000	5.067578000
H	-0.385537000	-0.289932000	5.853932000
N	-0.494789000	-1.497641000	-2.159836000
C	-1.320067000	-0.543040000	-2.634496000
C	0.358391000	-2.109336000	-3.004362000
C	-1.290818000	-0.154206000	-3.975232000
C	0.428254000	-1.792437000	-4.355518000
H	1.001575000	-2.867413000	-2.569708000
C	-0.407430000	-0.787424000	-4.846625000
H	-1.959079000	0.626955000	-4.323007000
H	1.127440000	-2.314279000	-5.000013000
H	-0.371444000	-0.501381000	-5.893647000
C	-2.362612000	-0.001839000	-1.684449000
C	-3.181777000	-0.143680000	0.568944000

H	-3.620927000	-1.120745000	0.356269000
H	-2.925182000	-0.096908000	1.628329000
H	-3.932319000	0.628203000	0.355987000
H	-3.215886000	-0.687115000	-1.746427000
H	-2.725687000	0.966951000	-2.037111000
C	1.484754000	-0.100481000	1.558699000
H	1.996323000	0.807335000	1.889691000
H	2.241400000	-0.893901000	1.552114000
C	2.158801000	-0.144402000	-0.740327000
H	2.606397000	-1.129125000	-0.589123000
H	1.839792000	-0.059940000	-1.779899000
H	2.923727000	0.618542000	-0.545299000
N	-1.955315000	0.032390000	-0.253079000
N	0.986140000	0.008245000	0.160136000
H	0.324636000	1.355265000	-1.275300000
H	-1.295766000	1.253856000	1.288563000
H	-1.854219000	2.660422000	-1.367598000
H	-2.962444000	2.581533000	0.002539000
H	-1.313229000	3.841467000	1.399834000
H	-1.721301000	4.736755000	-0.064603000
H	0.775230000	4.711939000	0.366366000
H	0.363459000	3.946519000	-1.169112000
H	0.895965000	2.530963000	1.488535000
H	2.005090000	2.561766000	0.117159000
C	-2.701948000	-4.181786000	-0.178831000
C	1.726244000	-4.121378000	0.231441000
N	1.001032000	-3.231655000	0.070349000
N	-1.992082000	-3.277059000	-0.034905000
C	-3.595315000	-5.312700000	-0.359129000
H	-3.816073000	-5.437356000	-1.424200000
H	-3.120404000	-6.222649000	0.021048000
H	-4.528567000	-5.134566000	0.184680000
C	2.639839000	-5.232733000	0.430092000
H	2.748300000	-5.429880000	1.501530000
H	2.246618000	-6.126643000	-0.064364000
H	3.618724000	-4.984394000	0.007533000

Fe-BPtCHEN 3+ doublet

C	-1.209857000	1.308140000	0.240259000
C	0.243813000	1.334926000	-0.215300000
C	0.963495000	2.579037000	0.337315000

C	0.241926000	3.859578000	-0.109139000
C	-1.219432000	3.836127000	0.348556000
C	-1.938626000	2.592823000	-0.197884000
Fe	-0.476745000	-1.464414000	-0.021436000
N	-0.491086000	-1.371710000	1.963546000
C	0.482395000	-0.592122000	2.484716000
C	-1.358943000	-1.997348000	2.787669000
C	0.587033000	-0.377623000	3.855746000
C	-1.297780000	-1.839504000	4.164902000
H	-2.116377000	-2.616392000	2.324276000
C	-0.316814000	-1.008057000	4.707704000
H	1.374287000	0.263274000	4.237558000
H	-2.015294000	-2.356302000	4.792238000
H	-0.253818000	-0.856397000	5.780642000
N	-0.445772000	-1.456543000	-2.002683000
C	-1.335365000	-0.612800000	-2.569712000
C	0.385233000	-2.178019000	-2.786913000
C	-1.380499000	-0.423101000	-3.948442000
C	0.375249000	-2.051934000	-4.168027000
H	1.072309000	-2.848777000	-2.288316000
C	-0.511019000	-1.148972000	-4.758289000
H	-2.098599000	0.272768000	-4.368580000
H	1.059792000	-2.647102000	-4.761761000
H	-0.529468000	-1.017658000	-5.835560000
C	-2.344786000	-0.020382000	-1.638519000
C	-3.102807000	-0.194816000	0.641346000
H	-3.522689000	-1.181917000	0.454328000
H	-2.855711000	-0.088076000	1.695532000
H	-3.847001000	0.559256000	0.372487000
H	-3.227794000	-0.666704000	-1.667803000
H	-2.667578000	0.968694000	-1.962094000
C	1.493699000	-0.100839000	1.498729000
H	1.951352000	0.837561000	1.809325000
H	2.297356000	-0.843188000	1.456137000
C	2.084484000	-0.155594000	-0.837746000
H	2.512612000	-1.151551000	-0.732236000
H	1.755484000	0.000842000	-1.862736000
H	2.849250000	0.585732000	-0.590724000
N	-1.874977000	0.003443000	-0.204281000
N	0.925891000	0.002798000	0.107024000
H	0.263566000	1.391855000	-1.307016000

H	-1.233729000	1.265467000	1.332691000
H	-1.950077000	2.663301000	-1.291063000
H	-2.976875000	2.572423000	0.146438000
H	-1.263248000	3.840473000	1.446191000
H	-1.747402000	4.731967000	0.002325000
H	0.763953000	4.726899000	0.310914000
H	0.288103000	3.954134000	-1.202532000
H	0.961200000	2.556971000	1.432765000
H	2.006365000	2.588829000	0.005361000
C	-2.501983000	-3.801100000	-0.323192000
C	1.545225000	-3.789639000	0.398000000
N	0.853610000	-2.888363000	0.185395000
N	-1.796570000	-2.900598000	-0.158218000
C	-3.397551000	-4.921486000	-0.523047000
H	-3.480970000	-5.132794000	-1.594147000
H	-3.003452000	-5.801015000	-0.003978000
H	-4.385128000	-4.670606000	-0.121832000
C	2.419421000	-4.914237000	0.659256000
H	2.298163000	-5.231443000	1.700257000
H	2.159317000	-5.741149000	-0.009181000
H	3.458324000	-4.614495000	0.487295000

Fe-BPtCHEN 3+ quartet

C	-1.214988000	1.361112000	0.206224000
C	0.254501000	1.306963000	-0.244411000
C	0.996003000	2.582340000	0.205147000
C	0.314946000	3.841815000	-0.349802000
C	-1.147914000	3.900810000	0.097358000
C	-1.889388000	2.633339000	-0.347057000
Fe	-0.429665000	-1.516554000	0.022961000
N	-0.481954000	-1.449643000	1.993260000
C	0.409809000	-0.592447000	2.549213000
C	-1.348141000	-2.126764000	2.782664000
C	0.427177000	-0.360155000	3.921029000
C	-1.361613000	-1.955274000	4.157503000
H	-2.035599000	-2.801092000	2.289697000
C	-0.469174000	-1.049046000	4.734749000
H	1.142749000	0.341898000	4.334662000
H	-2.068647000	-2.516730000	4.757542000
H	-0.470109000	-0.882961000	5.807376000
N	-0.474613000	-1.353612000	-1.974510000

C	-1.450711000	-0.568074000	-2.482512000
C	0.393762000	-1.976508000	-2.801266000
C	-1.550606000	-0.351765000	-3.855602000
C	0.328333000	-1.817715000	-4.177260000
H	1.148978000	-2.598557000	-2.336898000
C	-0.653610000	-0.982580000	-4.712962000
H	-2.333727000	0.296670000	-4.233484000
H	1.043158000	-2.334549000	-4.807563000
H	-0.720514000	-0.826580000	-5.785053000
C	-2.473488000	-0.043768000	-1.514989000
C	-3.121994000	-0.066180000	0.807695000
H	-3.547978000	-1.064846000	0.699470000
H	-2.797801000	0.081581000	1.837283000
H	-3.894362000	0.673037000	0.569618000
H	-3.288744000	-0.775326000	-1.486784000
H	-2.908624000	0.890678000	-1.872734000
C	1.433433000	-0.029136000	1.617004000
H	1.786571000	0.950014000	1.939832000
H	2.297631000	-0.701412000	1.640681000
C	2.175634000	-0.172354000	-0.673113000
H	2.575911000	-1.175143000	-0.524317000
H	1.922280000	-0.024724000	-1.721222000
H	2.936678000	0.557151000	-0.382762000
N	-1.960380000	0.079716000	-0.117536000
N	0.959071000	0.010224000	0.185781000
H	0.281332000	1.268447000	-1.336407000
H	-1.230844000	1.416951000	1.298690000
H	-1.886048000	2.607011000	-1.442858000
H	-2.933960000	2.664457000	-0.020754000
H	-1.198350000	4.001504000	1.190145000
H	-1.647787000	4.778032000	-0.329514000
H	0.864201000	4.723888000	-0.000856000
H	0.368017000	3.842573000	-1.447066000
H	0.990483000	2.650203000	1.298687000
H	2.039245000	2.541222000	-0.121699000
C	-2.489172000	-3.869991000	-0.365074000
C	1.747977000	-4.027175000	0.389740000
N	1.074469000	-3.114240000	0.153486000
N	-1.779828000	-2.982803000	-0.145793000
C	-3.380467000	-4.979378000	-0.627815000
H	-3.716703000	-4.937314000	-1.668685000

H	-2.846282000	-5.919106000	-0.451486000
H	-4.243579000	-4.918278000	0.043185000
C	2.597853000	-5.164968000	0.678668000
H	2.488648000	-5.442470000	1.732140000
H	2.304641000	-6.009070000	0.046184000
H	3.640963000	-4.900794000	0.476702000

Fe-BPtCHEN 3+ sextet

C	-1.202846000	1.320951000	0.187595000
C	0.283703000	1.308756000	-0.202850000
C	0.973193000	2.591569000	0.306358000
C	0.290643000	3.850307000	-0.246806000
C	-1.191820000	3.862388000	0.134438000
C	-1.882072000	2.588176000	-0.371604000
Fe	-0.465071000	-1.599686000	0.017352000
N	-0.470508000	-1.418330000	2.113012000
C	0.436284000	-0.549444000	2.610879000
C	-1.334071000	-2.041316000	2.945936000
C	0.479584000	-0.250535000	3.970674000
C	-1.327946000	-1.806240000	4.312358000
H	-2.037256000	-2.729110000	2.491344000
C	-0.412588000	-0.886754000	4.830959000
H	1.209790000	0.461397000	4.340088000
H	-2.033092000	-2.326268000	4.950978000
H	-0.393548000	-0.669348000	5.894370000
N	-0.471108000	-1.424370000	-2.080975000
C	-1.394709000	-0.571197000	-2.575690000
C	0.394060000	-2.039253000	-2.917802000
C	-1.454159000	-0.280199000	-3.936378000
C	0.373257000	-1.810920000	-4.285463000
H	1.110260000	-2.715322000	-2.465796000
C	-0.559668000	-0.907658000	-4.800966000
H	-2.197555000	0.419375000	-4.303072000
H	1.080629000	-2.323773000	-4.927412000
H	-0.590521000	-0.695704000	-5.865207000
C	-2.420118000	-0.060157000	-1.602555000
C	-3.117698000	-0.128569000	0.706970000
H	-3.566914000	-1.109785000	0.550406000
H	-2.814418000	-0.027888000	1.748012000
H	-3.861032000	0.640776000	0.475774000
H	-3.243851000	-0.782323000	-1.599665000

H	-2.839964000	0.889656000	-1.934422000
C	1.465043000	-0.028658000	1.646386000
H	1.855243000	0.936409000	1.970526000
H	2.306051000	-0.729979000	1.670039000
C	2.204619000	-0.157530000	-0.646707000
H	2.648213000	-1.135109000	-0.455147000
H	1.921716000	-0.084065000	-1.695835000
H	2.945402000	0.615836000	-0.421517000
N	-1.926864000	0.027054000	-0.188088000
N	0.997477000	0.024369000	0.220956000
H	0.347614000	1.302786000	-1.294685000
H	-1.265302000	1.354965000	1.278962000
H	-1.823492000	2.585464000	-1.466035000
H	-2.941773000	2.592786000	-0.097287000
H	-1.294123000	3.935806000	1.225774000
H	-1.695702000	4.736080000	-0.294983000
H	0.800534000	4.736153000	0.149345000
H	0.392953000	3.881987000	-1.340140000
H	0.918942000	2.631996000	1.400200000
H	2.031611000	2.577959000	0.027856000
C	-2.657061000	-4.005002000	-0.298959000
C	1.706375000	-4.024076000	0.307553000
N	0.998379000	-3.124239000	0.130059000
N	-1.941150000	-3.115336000	-0.102819000
C	-3.557001000	-5.111644000	-0.541009000
H	-3.908876000	-5.071664000	-1.577050000
H	-3.026854000	-6.054146000	-0.368379000
H	-4.410787000	-5.040172000	0.141019000
C	2.597041000	-5.143639000	0.523117000
H	2.824038000	-5.226014000	1.591219000
H	2.112761000	-6.063019000	0.177785000
H	3.523193000	-4.982004000	-0.038469000

Fe-BPtCHEN oxo 2+ triplet

C	-1.226719000	1.266202000	0.236612000
C	0.238537000	1.266126000	-0.205355000
C	0.964849000	2.511642000	0.339457000
C	0.271369000	3.799323000	-0.128634000
C	-1.195887000	3.805087000	0.309622000
C	-1.922156000	2.562448000	-0.225936000
Fe	-0.431112000	-1.573046000	0.008747000

N	-0.531013000	-1.411219000	1.986752000
C	0.433280000	-0.621368000	2.506863000
C	-1.424880000	-1.997630000	2.808254000
C	0.506050000	-0.361512000	3.872926000
C	-1.397137000	-1.798030000	4.182108000
H	-2.173844000	-2.626447000	2.344637000
C	-0.422604000	-0.957974000	4.722834000
H	1.286588000	0.288544000	4.253374000
H	-2.134218000	-2.288932000	4.807794000
H	-0.384289000	-0.772872000	5.791832000
N	-0.454267000	-1.489860000	-1.977929000
C	-1.358980000	-0.660531000	-2.537145000
C	0.387501000	-2.193045000	-2.763500000
C	-1.408514000	-0.469959000	-3.917851000
C	0.372958000	-2.068834000	-4.145067000
H	1.077723000	-2.849608000	-2.248211000
C	-0.531056000	-1.180740000	-4.731922000
H	-2.136761000	0.217047000	-4.335757000
H	1.065323000	-2.651761000	-4.742297000
H	-0.555685000	-1.048631000	-5.809196000
C	-2.377408000	-0.067117000	-1.608334000
C	-3.153497000	-0.174535000	0.662033000
H	-3.580413000	-1.165086000	0.504635000
H	-2.903795000	-0.050053000	1.714933000
H	-3.901829000	0.575634000	0.387221000
H	-3.251737000	-0.726209000	-1.638706000
H	-2.715167000	0.908627000	-1.960807000
C	1.468590000	-0.161508000	1.529041000
H	1.945798000	0.766882000	1.842154000
H	2.249053000	-0.928733000	1.500676000
C	2.098577000	-0.220131000	-0.787959000
H	2.505574000	-1.223467000	-0.666463000
H	1.786818000	-0.071599000	-1.820120000
H	2.867216000	0.516866000	-0.538310000
N	-1.926803000	-0.018625000	-0.178881000
N	0.927565000	-0.057875000	0.130727000
H	0.266331000	1.312689000	-1.297627000
H	-1.253172000	1.247788000	1.330120000
H	-1.921403000	2.616631000	-1.320706000
H	-2.965925000	2.561665000	0.103431000
H	-1.253148000	3.827093000	1.406712000

H	-1.705193000	4.704529000	-0.055808000
H	0.802970000	4.663371000	0.286917000
H	0.332186000	3.880398000	-1.222674000
H	0.950781000	2.500261000	1.435349000
H	2.012448000	2.504402000	0.021919000
C	-2.570009000	-3.821056000	-0.270842000
N	-1.837119000	-2.942587000	-0.109128000
O	0.746326000	-2.697828000	0.067432000
C	-3.493473000	-4.921854000	-0.467237000
H	-3.244478000	-5.444475000	-1.396449000
H	-3.416315000	-5.617570000	0.374447000
H	-4.515722000	-4.535306000	-0.528799000

Fe-BPtCHEN oxo 2+ quintet

C	-1.174452000	1.276990000	0.196039000
C	0.304129000	1.268408000	-0.216953000
C	0.999578000	2.558405000	0.266228000
C	0.298152000	3.813258000	-0.271241000
C	-1.176624000	3.816622000	0.139714000
C	-1.870486000	2.538760000	-0.353434000
Fe	-0.460361000	-1.638479000	0.015668000
N	-0.517722000	-1.446189000	2.084855000
C	0.404352000	-0.602875000	2.588373000
C	-1.379574000	-2.072167000	2.911576000
C	0.459218000	-0.326364000	3.954595000
C	-1.362814000	-1.861725000	4.283230000
H	-2.094590000	-2.742284000	2.449292000
C	-0.433415000	-0.963723000	4.812138000
H	1.202380000	0.369859000	4.328914000
H	-2.071375000	-2.385046000	4.915620000
H	-0.403118000	-0.765298000	5.879085000
N	-0.488554000	-1.493989000	-2.030683000
C	-1.399394000	-0.635298000	-2.538251000
C	0.374650000	-2.127647000	-2.850653000
C	-1.446163000	-0.356682000	-3.902251000
C	0.367537000	-1.911645000	-4.221220000
H	1.073189000	-2.805644000	-2.374096000
C	-0.550882000	-1.003020000	-4.752778000
H	-2.178978000	0.346809000	-4.282589000
H	1.073891000	-2.438277000	-4.853248000
H	-0.570776000	-0.801505000	-5.819423000

C	-2.411642000	-0.114275000	-1.561526000
C	-3.079999000	-0.156295000	0.748792000
H	-3.527294000	-1.142615000	0.627343000
H	-2.776712000	-0.018880000	1.785380000
H	-3.825547000	0.603544000	0.494888000
H	-3.238390000	-0.832659000	-1.545843000
H	-2.833592000	0.835725000	-1.889809000
C	1.445140000	-0.073643000	1.634949000
H	1.830264000	0.886735000	1.982067000
H	2.285387000	-0.775149000	1.668644000
C	2.203592000	-0.228518000	-0.646554000
H	2.600433000	-1.225468000	-0.451730000
H	1.925591000	-0.151305000	-1.697558000
H	2.977393000	0.515284000	-0.428010000
N	-1.890556000	-0.031381000	-0.153554000
N	1.003495000	-0.007733000	0.210223000
H	0.350397000	1.252898000	-1.310368000
H	-1.218664000	1.320488000	1.288015000
H	-1.830588000	2.537445000	-1.448901000
H	-2.925731000	2.541828000	-0.061940000
H	-1.256935000	3.888176000	1.233230000
H	-1.693338000	4.689006000	-0.277397000
H	0.809650000	4.703903000	0.112545000
H	0.376294000	3.845308000	-1.366805000
H	0.977747000	2.602178000	1.361406000
H	2.050307000	2.547464000	-0.041287000
C	-2.776252000	-3.988909000	-0.294583000
N	-2.088277000	-3.082641000	-0.077609000
O	0.684276000	-2.788845000	0.041424000
C	-3.645573000	-5.118381000	-0.563824000
H	-3.568516000	-5.391678000	-1.621233000
H	-3.340911000	-5.968917000	0.054360000
H	-4.680567000	-4.848306000	-0.331333000

^{Me}BPMEN (free ligand)

C	3.781533000	1.682090000	0.217402000
C	2.663433000	2.511280000	-0.424170000
H	3.733484000	1.791744000	1.305726000
H	4.734833000	2.153497000	-0.098788000
H	2.887733000	3.570719000	-0.182910000
H	2.730875000	2.425836000	-1.513415000

N	0.709707000	0.064254000	1.940381000
C	0.859689000	-0.996803000	2.753118000
C	1.229343000	1.247097000	2.304956000
C	1.523041000	-0.902673000	3.983912000
C	1.905111000	1.422800000	3.519082000
C	2.047398000	0.329247000	4.372350000
H	1.621629000	-1.778090000	4.618951000
H	2.309212000	2.395780000	3.783447000
H	2.565179000	0.433910000	5.322357000
N	1.790323000	-0.974308000	-1.889935000
C	0.686596000	-1.147840000	-2.638483000
C	2.774987000	-0.184909000	-2.349313000
C	0.537231000	-0.545350000	-3.894991000
C	2.701535000	0.451367000	-3.594933000
C	1.564635000	0.262451000	-4.379722000
H	-0.365529000	-0.711086000	-4.475385000
H	3.518989000	1.080362000	-3.935640000
H	1.478264000	0.742045000	-5.351372000
C	0.986881000	2.424555000	1.370548000
H	1.528012000	3.308162000	1.752160000
H	-0.080896000	2.665303000	1.441577000
C	4.027458000	-0.068658000	-1.490637000
H	4.721749000	0.651799000	-1.957942000
H	4.525501000	-1.044985000	-1.531938000
C	4.764268000	-0.429391000	0.784084000
H	4.519857000	-0.239647000	1.834882000
H	4.722132000	-1.510839000	0.616453000
H	5.807558000	-0.097400000	0.615267000
C	0.342976000	2.867390000	-0.917768000
H	0.544945000	2.604637000	-1.961782000
H	-0.679620000	2.554417000	-0.681496000
H	0.391312000	3.970776000	-0.832104000
N	3.792162000	0.244318000	-0.075751000
N	1.287676000	2.172439000	-0.044407000
C	0.277415000	-2.300069000	2.265430000
H	0.728348000	-2.581332000	1.305774000
H	0.445396000	-3.110915000	2.980652000
H	-0.802409000	-2.203371000	2.097110000
C	-0.387751000	-2.029001000	-2.051642000
H	-1.254805000	-2.104968000	-2.714631000
H	-0.001936000	-3.039568000	-1.867850000

H	-0.719890000	-1.630822000	-1.085025000

Fe-^{Me}BPMEN 2+ singlet

C	3.540671000	1.368008000	0.206763000
C	2.439596000	2.201564000	-0.410396000
H	3.555533000	1.493442000	1.291273000
H	4.520184000	1.681277000	-0.173740000
H	2.535062000	3.251324000	-0.107442000
H	2.497509000	2.167953000	-1.500208000
Fe	1.267167000	-0.400785000	0.014135000
N	1.344498000	-0.168868000	2.089354000
C	1.554417000	-1.069908000	3.091056000
C	1.232686000	1.138634000	2.433488000
C	1.737872000	-0.651262000	4.414115000
C	1.424450000	1.610950000	3.729664000
C	1.698266000	0.698790000	4.741234000
H	1.910861000	-1.401176000	5.178354000
H	1.343325000	2.674338000	3.928891000
H	1.857023000	1.028797000	5.763581000
N	1.376810000	-0.403699000	-2.073102000
C	0.405134000	-0.467762000	-3.027841000
C	2.658293000	-0.246232000	-2.489955000
C	0.709009000	-0.288711000	-4.382450000
C	3.013695000	-0.045600000	-3.821631000
C	2.016636000	-0.051986000	-4.789189000
H	-0.095820000	-0.338068000	-5.107926000
H	4.057628000	0.097024000	-4.080596000
H	2.253870000	0.103968000	-5.837383000
C	0.748375000	2.084784000	1.372759000
H	1.093381000	3.106485000	1.567835000
H	-0.345015000	2.099449000	1.437777000
C	3.738405000	-0.429605000	-1.462670000
H	4.643525000	0.123126000	-1.738953000
H	4.000173000	-1.493475000	-1.465385000
C	4.177117000	-0.865159000	0.849500000
H	3.939634000	-0.606620000	1.880627000
H	4.012402000	-1.931818000	0.694448000
H	5.233603000	-0.634923000	0.661362000
C	0.083873000	2.268670000	-0.917264000
H	0.329742000	2.039062000	-1.953220000
H	-0.901853000	1.868202000	-0.678990000

H	0.068383000	3.358799000	-0.790924000
N	3.314782000	-0.083966000	-0.079377000
N	1.100017000	1.667477000	-0.010403000
C	-1.717498000	-0.785730000	0.647198000
C	1.556672000	-3.429369000	-0.436901000
C	1.658731000	-4.843909000	-0.755900000
H	1.294659000	-5.440006000	0.087540000
H	1.057600000	-5.070942000	-1.642240000
H	2.703308000	-5.104587000	-0.954977000
C	-3.096383000	-0.985548000	1.062396000
H	-3.544520000	-1.797597000	0.480483000
H	-3.132119000	-1.243779000	2.125656000
H	-3.669354000	-0.067299000	0.896817000
N	1.479653000	-2.308085000	-0.158874000
N	-0.626138000	-0.622643000	0.296611000
C	1.569478000	-2.545073000	2.803616000
H	2.441606000	-2.835761000	2.212175000
H	1.600116000	-3.099060000	3.745351000
H	0.675161000	-2.849986000	2.254007000
C	-1.019947000	-0.760807000	-2.650147000
H	-1.614933000	-0.907976000	-3.555213000
H	-1.088421000	-1.667267000	-2.043025000
H	-1.468072000	0.057366000	-2.080690000

Fe-^{Me}BPMEN 2+ quintet

C	3.539430000	1.323999000	0.215093000
C	2.434392000	2.172911000	-0.400108000
H	3.541763000	1.439913000	1.300765000
H	4.510404000	1.689924000	-0.148433000
H	2.595705000	3.223584000	-0.118967000
H	2.485221000	2.123345000	-1.489677000
Fe	1.126329000	-0.564535000	0.060897000
N	1.327982000	-0.027072000	2.228455000
C	1.595997000	-0.884926000	3.244253000
C	1.222556000	1.291390000	2.488656000
C	1.809697000	-0.418619000	4.543694000
C	1.440596000	1.818684000	3.762340000
C	1.743813000	0.948327000	4.804348000
H	2.025412000	-1.128268000	5.335342000
H	1.361423000	2.888884000	3.923638000
H	1.918577000	1.327407000	5.807120000

N	1.504366000	-0.425441000	-2.204372000
C	0.558154000	-0.418388000	-3.174554000
C	2.795140000	-0.235283000	-2.536580000
C	0.896333000	-0.165950000	-4.506960000
C	3.194064000	0.037521000	-3.846260000
C	2.225670000	0.079546000	-4.844675000
H	0.118525000	-0.161680000	-5.263268000
H	4.243472000	0.203043000	-4.067782000
H	2.502689000	0.291308000	-5.873422000
C	0.734753000	2.188419000	1.376051000
H	1.081600000	3.217224000	1.542724000
H	-0.358853000	2.208502000	1.450071000
C	3.831905000	-0.451068000	-1.459541000
H	4.753467000	0.091594000	-1.710639000
H	4.079354000	-1.519157000	-1.476941000
C	4.265686000	-0.886722000	0.850304000
H	3.996359000	-0.652123000	1.880708000
H	4.135934000	-1.958378000	0.681593000
H	5.324730000	-0.630856000	0.698407000
C	0.082721000	2.344150000	-0.919313000
H	0.315926000	2.059125000	-1.945766000
H	-0.919013000	1.988444000	-0.667309000
H	0.096764000	3.441700000	-0.848161000
N	3.396288000	-0.128517000	-0.079580000
N	1.070090000	1.738442000	0.004870000
C	-2.075773000	-1.026381000	0.958705000
C	1.312768000	-3.813379000	-0.735390000
C	1.440886000	-5.201865000	-1.144082000
H	1.009304000	-5.853214000	-0.377469000
H	0.911596000	-5.357537000	-2.089538000
H	2.498646000	-5.450803000	-1.276799000
C	-3.434046000	-1.289421000	1.403144000
H	-3.831118000	-2.161819000	0.874235000
H	-3.436274000	-1.488559000	2.479533000
H	-4.065998000	-0.420391000	1.194501000
N	1.212205000	-2.705620000	-0.411124000
N	-0.993576000	-0.818286000	0.600852000
C	1.633314000	-2.354273000	2.934888000
H	2.362687000	-2.576925000	2.150866000
H	1.896686000	-2.929393000	3.826346000
H	0.654436000	-2.698259000	2.580678000

C	-0.862615000	-0.712268000	-2.779205000
H	-1.516367000	-0.692997000	-3.655311000
H	-0.936408000	-1.702496000	-2.315828000
H	-1.235258000	0.017923000	-2.054968000

Fe-^{Me}BPMEN 3+ doublet

C	3.568584000	1.396394000	0.232620000
C	2.490555000	2.226959000	-0.415222000
H	3.568615000	1.516342000	1.316857000
H	4.559447000	1.679402000	-0.134226000
H	2.557859000	3.274474000	-0.106948000
H	2.565643000	2.193465000	-1.503200000
Fe	1.311000000	-0.351166000	0.009970000
N	1.342005000	-0.127477000	2.058096000
C	1.511380000	-1.060658000	3.041860000
C	1.225101000	1.179001000	2.411865000
C	1.668535000	-0.653079000	4.370748000
C	1.386833000	1.626511000	3.716744000
C	1.634033000	0.692140000	4.715584000
H	1.814325000	-1.414659000	5.128351000
H	1.300581000	2.685885000	3.931619000
H	1.772663000	1.003187000	5.746305000
N	1.413493000	-0.398683000	-2.043747000
C	0.414878000	-0.511739000	-2.969484000
C	2.690334000	-0.230868000	-2.476969000
C	0.702248000	-0.346820000	-4.328549000
C	3.015864000	-0.048086000	-3.814695000
C	1.997144000	-0.086913000	-4.759586000
H	-0.111467000	-0.428120000	-5.040383000
H	4.052669000	0.101794000	-4.095097000
H	2.211024000	0.057713000	-5.813994000
C	0.756800000	2.119673000	1.348513000
H	1.108956000	3.139647000	1.523882000
H	-0.337051000	2.137729000	1.389147000
C	3.771192000	-0.402031000	-1.457802000
H	4.665028000	0.174360000	-1.711786000
H	4.050614000	-1.460628000	-1.456486000
C	4.161358000	-0.865642000	0.872951000
H	3.924900000	-0.599564000	1.901220000
H	3.985531000	-1.927835000	0.707061000
H	5.214698000	-0.637718000	0.677161000

C	0.127507000	2.258436000	-0.969302000
H	0.409461000	2.045529000	-1.998373000
H	-0.855515000	1.842644000	-0.751007000
H	0.103460000	3.343542000	-0.822623000
N	3.323912000	-0.057347000	-0.070990000
N	1.142186000	1.680553000	-0.028912000
C	-1.674966000	-0.795894000	0.716165000
C	1.527711000	-3.403364000	-0.503150000
C	1.597266000	-4.807408000	-0.851800000
H	1.198545000	-5.406654000	-0.026608000
H	1.005705000	-4.988337000	-1.755184000
H	2.640039000	-5.084934000	-1.036870000
C	-3.034130000	-1.015870000	1.166253000
H	-3.479630000	-1.836010000	0.593973000
H	-3.028355000	-1.272027000	2.230700000
H	-3.618267000	-0.102378000	1.013766000
N	1.477303000	-2.289857000	-0.200087000
N	-0.599461000	-0.616596000	0.334731000
C	1.502848000	-2.531557000	2.743175000
H	2.380891000	-2.840848000	2.170531000
H	1.503836000	-3.086149000	3.684033000
H	0.608768000	-2.813376000	2.180781000
C	-0.994089000	-0.841318000	-2.570677000
H	-1.584151000	-1.032991000	-3.469629000
H	-1.026914000	-1.735563000	-1.943170000
H	-1.468809000	-0.020773000	-2.027052000

Fe-^{Me}BPMEN 3+ quartet

C	3.550590000	1.454233000	0.200354000
C	2.429804000	2.224028000	-0.470192000
H	3.539030000	1.608954000	1.280240000
H	4.514012000	1.820005000	-0.173515000
H	2.483401000	3.282511000	-0.196183000
H	2.498593000	2.159047000	-1.556593000
Fe	1.175739000	-0.354276000	-0.083006000
N	1.279652000	-0.146422000	1.990719000
C	1.498632000	-1.084757000	2.959045000
C	1.192341000	1.161781000	2.355043000
C	1.714061000	-0.686446000	4.282418000
C	1.416336000	1.599866000	3.654008000
C	1.699442000	0.657162000	4.635666000

H	1.893058000	-1.452395000	5.028359000
H	1.353864000	2.658920000	3.878220000
H	1.886471000	0.961458000	5.660764000
N	1.555991000	-0.370655000	-2.117467000
C	0.585165000	-0.476754000	-3.070807000
C	2.854365000	-0.257981000	-2.480610000
C	0.928047000	-0.378241000	-4.420412000
C	3.233384000	-0.148191000	-3.815395000
C	2.253719000	-0.194660000	-4.800112000
H	0.139478000	-0.451170000	-5.161113000
H	4.284770000	-0.040764000	-4.059276000
H	2.519105000	-0.105538000	-5.848964000
C	0.703280000	2.117372000	1.315859000
H	1.059282000	3.135284000	1.498549000
H	-0.389988000	2.135036000	1.370925000
C	3.899876000	-0.383112000	-1.409419000
H	4.794228000	0.192124000	-1.673224000
H	4.192276000	-1.438521000	-1.376329000
C	4.239233000	-0.757702000	0.941856000
H	3.955527000	-0.461895000	1.951031000
H	4.080528000	-1.829340000	0.811449000
H	5.302488000	-0.530473000	0.792314000
C	0.058492000	2.306610000	-0.999835000
H	0.321991000	2.087969000	-2.033196000
H	-0.930153000	1.910707000	-0.767603000
H	0.059736000	3.392062000	-0.850379000
N	3.424834000	-0.010789000	-0.052979000
N	1.069272000	1.704956000	-0.075844000
C	-2.063669000	-0.876207000	1.061901000
C	1.423307000	-3.419327000	-0.610306000
C	1.497483000	-4.814784000	-0.985051000
H	1.185907000	-5.435462000	-0.138425000
H	0.838460000	-4.997058000	-1.840147000
H	2.528680000	-5.059454000	-1.260842000
C	-3.357998000	-1.105774000	1.678157000
H	-3.853775000	-1.950324000	1.189442000
H	-3.222678000	-1.328489000	2.741457000
H	-3.977475000	-0.209599000	1.570597000
N	1.364977000	-2.312892000	-0.279708000
N	-1.029625000	-0.687021000	0.574765000
C	1.489499000	-2.551870000	2.646197000

H	2.353907000	-2.840515000	2.042699000
H	1.527598000	-3.117646000	3.579720000
H	0.581151000	-2.836113000	2.108919000
C	-0.838395000	-0.746345000	-2.677455000
H	-1.474800000	-0.744762000	-3.564770000
H	-0.920527000	-1.728077000	-2.196229000
H	-1.221460000	-0.003844000	-1.974230000

Fe-^{Me}BPMEN 3+ sextet

C	3.523210000	1.367035000	0.235554000
C	2.427511000	2.180742000	-0.423995000
H	3.513979000	1.501581000	1.317700000
H	4.498901000	1.709991000	-0.127189000
H	2.541114000	3.237251000	-0.155747000
H	2.489636000	2.111778000	-1.510562000
Fe	1.141143000	-0.517541000	0.036267000
N	1.327147000	-0.002969000	2.159745000
C	1.577464000	-0.909392000	3.141197000
C	1.185552000	1.303825000	2.457736000
C	1.752880000	-0.478860000	4.457269000
C	1.363039000	1.785393000	3.751674000
C	1.661227000	0.877307000	4.763641000
H	1.960169000	-1.212514000	5.228410000
H	1.257633000	2.846397000	3.950798000
H	1.810026000	1.220368000	5.782981000
N	1.562767000	-0.408260000	-2.149056000
C	0.597150000	-0.458966000	-3.105914000
C	2.854869000	-0.253048000	-2.496912000
C	0.936349000	-0.274201000	-4.447668000
C	3.243372000	-0.049368000	-3.818341000
C	2.263200000	-0.047832000	-4.806515000
H	0.153922000	-0.310194000	-5.197759000
H	4.292347000	0.091431000	-4.055405000
H	2.530645000	0.112872000	-5.846510000
C	0.703362000	2.197300000	1.351965000
H	1.062921000	3.222560000	1.488852000
H	-0.389788000	2.223220000	1.410822000
C	3.870705000	-0.446805000	-1.409645000
H	4.789772000	0.108338000	-1.625366000
H	4.128180000	-1.511605000	-1.399136000
C	4.221319000	-0.853477000	0.927192000

H	3.939157000	-0.593219000	1.946087000
H	4.094723000	-1.924347000	0.762930000
H	5.275512000	-0.590231000	0.774521000
C	0.063394000	2.305773000	-0.961571000
H	0.317657000	2.033116000	-1.984783000
H	-0.933550000	1.938267000	-0.714766000
H	0.077637000	3.398578000	-0.870012000
N	3.381923000	-0.098724000	-0.043124000
N	1.059648000	1.720807000	-0.018412000
C	-1.996921000	-0.934355000	1.045133000
C	1.273168000	-3.721517000	-0.830818000
C	1.379682000	-5.096295000	-1.274761000
H	1.149901000	-5.768647000	-0.442064000
H	0.673034000	-5.269456000	-2.092841000
H	2.399480000	-5.284044000	-1.626644000
C	-3.313653000	-1.207681000	1.583497000
H	-3.758026000	-2.052327000	1.047077000
H	-3.226491000	-1.453629000	2.646939000
H	-3.947320000	-0.323110000	1.462728000
N	1.189586000	-2.620875000	-0.480843000
N	-0.943340000	-0.715271000	0.617235000
C	1.627125000	-2.366161000	2.783091000
H	2.364815000	-2.569096000	2.003616000
H	1.882808000	-2.962427000	3.662250000
H	0.650781000	-2.700337000	2.413074000
C	-0.820661000	-0.753989000	-2.703865000
H	-1.467592000	-0.751264000	-3.584290000
H	-0.888466000	-1.740011000	-2.230436000
H	-1.205213000	-0.017443000	-1.993978000

Fe-^{Me}BPMEN oxo 2+ triplet

C	3.530454000	1.409154000	0.151394000
C	2.430322000	2.245746000	-0.459817000
H	3.547886000	1.517895000	1.237008000
H	4.510300000	1.716376000	-0.227578000
H	2.523912000	3.290030000	-0.139347000
H	2.486480000	2.229151000	-1.549843000
Fe	1.314250000	-0.446777000	-0.087527000
N	1.337859000	-0.244847000	1.952456000
C	1.504262000	-1.221804000	2.892635000
C	1.223345000	1.045151000	2.358140000

C	1.654519000	-0.875705000	4.239814000
C	1.385656000	1.431699000	3.684917000
C	1.623438000	0.454060000	4.642751000
H	1.794577000	-1.669482000	4.964996000
H	1.306569000	2.481292000	3.946993000
H	1.758903000	0.719618000	5.686748000
N	1.399070000	-0.346827000	-2.148785000
C	0.413932000	-0.401107000	-3.090633000
C	2.680744000	-0.181702000	-2.562989000
C	0.717731000	-0.198102000	-4.441719000
C	3.027620000	0.040821000	-3.891008000
C	2.022467000	0.048091000	-4.850355000
H	-0.089505000	-0.238024000	-5.164584000
H	4.069938000	0.187215000	-4.152670000
H	2.252375000	0.221087000	-5.897229000
C	0.765547000	2.057640000	1.346358000
H	1.147331000	3.054581000	1.590328000
H	-0.325927000	2.105777000	1.423264000
C	3.752656000	-0.387064000	-1.538334000
H	4.660586000	0.169407000	-1.789289000
H	4.006359000	-1.451925000	-1.545400000
C	4.162643000	-0.843808000	0.781916000
H	3.922168000	-0.587421000	1.812219000
H	3.987495000	-1.905068000	0.610133000
H	5.215833000	-0.608581000	0.591777000
C	0.060505000	2.323344000	-0.936319000
H	0.298372000	2.132872000	-1.982359000
H	-0.918563000	1.905848000	-0.700197000
H	0.039788000	3.407213000	-0.769142000
N	3.314101000	-0.047460000	-0.152913000
N	1.094530000	1.702010000	-0.061978000
C	-1.704341000	-0.808367000	0.570264000
C	-3.069753000	-1.025858000	1.008666000
H	-3.564655000	-1.723982000	0.325669000
H	-3.068355000	-1.444328000	2.020115000
H	-3.609146000	-0.073292000	1.009409000
N	-0.625595000	-0.633268000	0.196479000
O	1.574221000	-2.048166000	-0.170106000
C	-1.007877000	-0.708575000	-2.718234000
H	-1.599639000	-0.834556000	-3.627939000
H	-1.071002000	-1.633295000	-2.138468000

H	-1.459281000	0.094590000	-2.130916000
C	1.501588000	-2.678910000	2.523833000
H	2.392846000	-2.960904000	1.957732000
H	1.473952000	-3.276770000	3.438422000
H	0.632994000	-2.933068000	1.911772000

Fe-^{Me}BPMEN oxo 2+ quintet

C	3.560345000	1.356616000	0.167336000
C	2.457500000	2.206012000	-0.426752000
H	3.562520000	1.429003000	1.256459000
H	4.537436000	1.704022000	-0.188321000
H	2.554017000	3.244464000	-0.089899000
H	2.513610000	2.208095000	-1.516908000
Fe	1.208526000	-0.465697000	-0.130699000
N	1.304894000	-0.237599000	2.030503000
C	1.508676000	-1.190169000	2.982737000
C	1.218311000	1.061937000	2.400968000
C	1.693855000	-0.820108000	4.318581000
C	1.414906000	1.480886000	3.713989000
C	1.667754000	0.520886000	4.688095000
H	1.857515000	-1.596034000	5.058330000
H	1.353190000	2.536260000	3.956892000
H	1.826803000	0.810986000	5.722339000
N	1.435558000	-0.340539000	-2.270956000
C	0.465836000	-0.372943000	-3.223973000
C	2.723996000	-0.164191000	-2.634265000
C	0.791156000	-0.152778000	-4.564966000
C	3.095579000	0.078428000	-3.954504000
C	2.109491000	0.095598000	-4.934704000
H	-0.000574000	-0.177101000	-5.305718000
H	4.141845000	0.234167000	-4.195314000
H	2.365285000	0.283536000	-5.973077000
C	0.755059000	2.047062000	1.363065000
H	1.122215000	3.053951000	1.586652000
H	-0.337868000	2.081986000	1.423494000
C	3.789735000	-0.373471000	-1.588455000
H	4.686702000	0.203901000	-1.837301000
H	4.065818000	-1.432424000	-1.629736000
C	4.193639000	-0.923595000	0.717723000
H	3.933039000	-0.709986000	1.753747000
H	4.009067000	-1.976364000	0.502054000

H	5.256959000	-0.701202000	0.564361000
C	0.092572000	2.322002000	-0.934881000
H	0.342678000	2.124772000	-1.976641000
H	-0.897001000	1.923539000	-0.710806000
H	0.093277000	3.405582000	-0.766602000
N	3.370292000	-0.082586000	-0.191043000
N	1.104058000	1.680648000	-0.044122000
C	-1.957339000	-0.824584000	0.682436000
C	-3.299832000	-1.122356000	1.143916000
H	-3.515102000	-2.182855000	0.977689000
H	-3.377713000	-0.897923000	2.212570000
H	-4.020940000	-0.512417000	0.590256000
N	-0.889647000	-0.584900000	0.305492000
O	1.393828000	-2.071200000	-0.207912000
C	-0.953117000	-0.668873000	-2.832301000
H	-1.572148000	-0.760219000	-3.728045000
H	-1.015885000	-1.607963000	-2.273139000
H	-1.372951000	0.124220000	-2.207399000
C	1.510896000	-2.646492000	2.611745000
H	2.354534000	-2.899561000	1.964204000
H	1.576902000	-3.253934000	3.517908000
H	0.596731000	-2.916874000	2.075427000

^{Br}BPMEN (free ligand)

C	3.637814000	1.521625000	0.438718000
C	2.505042000	2.295246000	-0.248573000
H	3.497121000	1.568321000	1.521828000
H	4.578173000	2.067960000	0.225760000
H	2.626309000	3.361074000	0.029494000
H	2.643737000	2.246293000	-1.331651000
N	0.842877000	0.011264000	2.392718000
C	1.144553000	-0.771755000	3.405757000
C	1.093297000	1.331573000	2.519173000
C	1.705399000	-0.359326000	4.615326000
C	1.651462000	1.861771000	3.686281000
C	1.959880000	1.004473000	4.744383000
H	1.926217000	-1.062716000	5.409109000
H	1.842571000	2.927705000	3.760866000
H	2.396012000	1.391423000	5.660967000
N	2.294674000	-0.774013000	-2.398458000
C	1.498196000	-0.753528000	-3.445222000

C	3.401221000	-0.001049000	-2.432137000
C	1.691796000	0.003166000	-4.601759000
C	3.701346000	0.797630000	-3.539841000
C	2.835278000	0.798360000	-4.634967000
H	0.992014000	-0.031524000	-5.428029000
H	4.598463000	1.408647000	-3.540429000
H	3.045925000	1.411030000	-5.506969000
C	0.663193000	2.226831000	1.370628000
H	0.939489000	3.269347000	1.610400000
H	-0.432758000	2.191580000	1.346663000
C	4.354683000	-0.104155000	-1.254029000
H	5.208270000	0.574821000	-1.430477000
H	4.757154000	-1.124100000	-1.273608000
C	4.536929000	-0.615749000	1.085267000
H	4.060664000	-0.500887000	2.064036000
H	4.561349000	-1.683589000	0.842809000
H	5.582342000	-0.261814000	1.173446000
C	0.213819000	2.302091000	-0.988475000
H	0.548278000	1.956073000	-1.971541000
H	-0.784254000	1.889901000	-0.804987000
H	0.125122000	3.405006000	-1.029493000
N	3.762458000	0.103899000	0.072438000
N	1.141276000	1.830443000	0.041578000
Br	0.752587000	-2.658201000	3.186622000
Br	-0.065087000	-1.897911000	-3.365462000

Fe-^{Br}BPMEN 2+ singlet

C	3.512258000	1.324322000	0.222166000
C	2.419510000	2.153045000	-0.418101000
H	3.517949000	1.462734000	1.304927000
H	4.495849000	1.630880000	-0.152336000
H	2.500557000	3.202296000	-0.110294000
H	2.504354000	2.123993000	-1.506035000
Fe	1.248237000	-0.449160000	0.019808000
N	1.309680000	-0.159080000	2.116504000
C	1.543146000	-0.964534000	3.169270000
C	1.160755000	1.164203000	2.406165000
C	1.719764000	-0.521878000	4.478635000
C	1.334916000	1.694189000	3.681491000
C	1.634029000	0.840914000	4.736576000
H	1.915086000	-1.234630000	5.269707000

H	1.223070000	2.762314000	3.832315000
H	1.779331000	1.219945000	5.743182000
N	1.391190000	-0.476585000	-2.090911000
C	0.490917000	-0.523262000	-3.090168000
C	2.688909000	-0.306123000	-2.470173000
C	0.792627000	-0.316592000	-4.434788000
C	3.078026000	-0.079575000	-3.787183000
C	2.113481000	-0.066756000	-4.787681000
H	0.007894000	-0.356381000	-5.179770000
H	4.128086000	0.072011000	-4.011933000
H	2.380729000	0.111469000	-5.824433000
C	0.660959000	2.049574000	1.303609000
H	0.952974000	3.090599000	1.477241000
H	-0.433165000	2.011050000	1.341617000
C	3.736546000	-0.502827000	-1.414643000
H	4.658677000	0.027392000	-1.676286000
H	3.971891000	-1.572886000	-1.402531000
C	4.131141000	-0.906894000	0.906611000
H	3.902478000	-0.609444000	1.928912000
H	3.940684000	-1.973089000	0.782279000
H	5.191973000	-0.705139000	0.713079000
C	0.076323000	2.180955000	-1.006544000
H	0.377478000	1.967265000	-2.030968000
H	-0.906188000	1.749823000	-0.813212000
H	0.022946000	3.269270000	-0.878898000
N	3.287522000	-0.132864000	-0.047324000
N	1.070763000	1.609269000	-0.054350000
C	-1.718261000	-0.850783000	0.719372000
C	1.504989000	-3.473425000	-0.465610000
C	1.577440000	-4.877640000	-0.832868000
H	1.121406000	-5.492068000	-0.049303000
H	1.041941000	-5.043527000	-1.773306000
H	2.623954000	-5.173862000	-0.958364000
C	-3.076553000	-1.062338000	1.190930000
H	-3.546649000	-1.869945000	0.620074000
H	-3.063400000	-1.334140000	2.251355000
H	-3.659617000	-0.144484000	1.062515000
N	1.453753000	-2.361192000	-0.150256000
N	-0.645544000	-0.677547000	0.321329000
Br	1.608189000	-2.859312000	2.950263000
Br	-1.335401000	-0.944904000	-2.731353000

Fe-^{Br}BPMEN 2+ triplet

C	3.455767000	1.251278000	0.161718000
C	2.327647000	2.095127000	-0.387124000
H	3.518889000	1.356085000	1.246294000
H	4.417651000	1.567360000	-0.257128000
H	2.434500000	3.139795000	-0.073241000
H	2.331387000	2.077772000	-1.478431000
Fe	1.181025000	-0.509831000	0.041180000
N	1.287941000	-0.104404000	2.442602000
C	1.611888000	-0.827632000	3.510271000
C	1.242199000	1.238333000	2.590251000
C	1.957194000	-0.299984000	4.752423000
C	1.582663000	1.868943000	3.786288000
C	1.952991000	1.087002000	4.878807000
H	2.215755000	-0.946430000	5.582180000
H	1.546215000	2.950701000	3.857116000
H	2.224303000	1.547882000	5.823666000
N	1.412439000	-0.486700000	-2.403008000
C	0.584700000	-0.408622000	-3.440347000
C	2.726062000	-0.270957000	-2.638109000
C	0.965413000	-0.076261000	-4.738527000
C	3.210679000	0.084404000	-3.896441000
C	2.314700000	0.189040000	-4.958719000
H	0.237484000	-0.028834000	-5.539185000
H	4.271026000	0.265484000	-4.036366000
H	2.660230000	0.463459000	-5.950720000
C	0.661400000	2.031372000	1.446771000
H	0.929182000	3.088617000	1.542249000
H	-0.427308000	1.961829000	1.540604000
C	3.681629000	-0.568527000	-1.510547000
H	4.652667000	-0.100032000	-1.702593000
H	3.838978000	-1.652417000	-1.509754000
C	4.045665000	-1.000519000	0.814142000
H	3.792931000	-0.730193000	1.838176000
H	3.865218000	-2.064326000	0.658468000
H	5.107863000	-0.786529000	0.644905000
C	-0.048098000	2.097137000	-0.838009000
H	0.179729000	1.826046000	-1.867767000
H	-1.021104000	1.693430000	-0.558355000
H	-0.075164000	3.190582000	-0.758606000

N	3.213859000	-0.200957000	-0.136096000
N	1.005257000	1.551842000	0.070310000
C	-1.826445000	-1.012130000	0.601379000
C	1.385814000	-3.582848000	-0.362474000
C	1.434654000	-5.009889000	-0.622632000
H	0.982937000	-5.552381000	0.214372000
H	0.879478000	-5.234347000	-1.539330000
H	2.475359000	-5.327828000	-0.741989000
C	-3.216056000	-1.288312000	0.917138000
H	-3.567657000	-2.136033000	0.319898000
H	-3.309412000	-1.532378000	1.980413000
H	-3.826813000	-0.407712000	0.693120000
N	1.352178000	-2.445905000	-0.152435000
N	-0.721798000	-0.787632000	0.342365000
Br	1.571078000	-2.737925000	3.337833000
Br	-1.267170000	-0.810399000	-3.136696000

Fe-^{Br}BPMEN 2+ quintet

C	3.497469000	1.312195000	0.200605000
C	2.383453000	2.144448000	-0.418284000
H	3.507068000	1.439255000	1.284924000
H	4.465608000	1.669388000	-0.175002000
H	2.522062000	3.198010000	-0.141250000
H	2.432290000	2.090235000	-1.507649000
Fe	1.139489000	-0.575640000	0.027949000
N	1.246272000	-0.046505000	2.285156000
C	1.516949000	-0.819949000	3.339764000
C	1.177764000	1.289702000	2.493243000
C	1.780616000	-0.346468000	4.620590000
C	1.442786000	1.861352000	3.737702000
C	1.755343000	1.033463000	4.811847000
H	1.996908000	-1.029146000	5.433055000
H	1.392875000	2.938483000	3.854662000
H	1.966864000	1.450680000	5.791542000
N	1.486770000	-0.491454000	-2.260204000
C	0.624941000	-0.476383000	-3.281293000
C	2.794636000	-0.284818000	-2.547889000
C	0.968999000	-0.213790000	-4.603219000
C	3.234785000	0.000816000	-3.840338000
C	2.309746000	0.044167000	-4.879028000
H	0.217694000	-0.212552000	-5.383222000

H	4.289823000	0.176672000	-4.020232000
H	2.623820000	0.264885000	-5.894510000
C	0.675521000	2.148412000	1.358151000
H	1.000809000	3.185939000	1.503262000
H	-0.418086000	2.143152000	1.428642000
C	3.802432000	-0.497227000	-1.443821000
H	4.732461000	0.032391000	-1.685552000
H	4.036193000	-1.568394000	-1.441400000
C	4.185516000	-0.903724000	0.883829000
H	3.906128000	-0.638281000	1.903918000
H	4.036302000	-1.975335000	0.735420000
H	5.249516000	-0.669258000	0.741267000
C	0.020533000	2.243163000	-0.942005000
H	0.278001000	1.970224000	-1.965620000
H	-0.967146000	1.846204000	-0.698727000
H	-0.006389000	3.339132000	-0.869781000
N	3.344444000	-0.146452000	-0.076828000
N	1.026704000	1.679304000	-0.006184000
C	-1.995134000	-1.015056000	0.857995000
C	1.409018000	-3.795583000	-0.621219000
C	1.486507000	-5.196960000	-0.989452000
H	1.074792000	-5.810045000	-0.181115000
H	0.911312000	-5.368769000	-1.904845000
H	2.531879000	-5.474045000	-1.159297000
C	-3.344505000	-1.244502000	1.342138000
H	-3.799438000	-2.066709000	0.780265000
H	-3.315995000	-1.504657000	2.405010000
H	-3.943178000	-0.338292000	1.204767000
N	1.348578000	-2.680681000	-0.314676000
N	-0.922152000	-0.829408000	0.463711000
Br	1.509510000	-2.714396000	3.076713000
Br	-1.209565000	-0.872552000	-2.913174000

Fe-^{Br}BPMEN 3+ doublet

C	3.531518000	1.357420000	0.236126000
C	2.457416000	2.177358000	-0.432808000
H	3.528666000	1.498178000	1.317609000
H	4.523421000	1.632285000	-0.133437000
H	2.513729000	3.227002000	-0.129953000
H	2.549190000	2.138566000	-1.518802000
Fe	1.286033000	-0.390709000	0.015772000

N	1.309424000	-0.116455000	2.080785000
C	1.507469000	-0.962699000	3.118394000
C	1.140411000	1.199673000	2.391318000
C	1.630347000	-0.538706000	4.437665000
C	1.261379000	1.697611000	3.683072000
C	1.526766000	0.817911000	4.724196000
H	1.798029000	-1.266407000	5.221510000
H	1.132023000	2.760488000	3.853576000
H	1.631603000	1.171138000	5.744718000
N	1.422141000	-0.453550000	-2.059240000
C	0.492163000	-0.536978000	-3.038902000
C	2.718911000	-0.317842000	-2.456607000
C	0.792737000	-0.397473000	-4.390284000
C	3.092438000	-0.157779000	-3.785250000
C	2.112802000	-0.180600000	-4.769659000
H	0.001946000	-0.463448000	-5.127088000
H	4.141735000	-0.033922000	-4.028049000
H	2.367088000	-0.055366000	-5.817027000
C	0.672096000	2.093322000	1.290284000
H	0.997391000	3.124804000	1.445338000
H	-0.422662000	2.084821000	1.308853000
C	3.763865000	-0.494309000	-1.403409000
H	4.677983000	0.053753000	-1.646460000
H	4.013561000	-1.560120000	-1.373453000
C	4.103621000	-0.896525000	0.943150000
H	3.872893000	-0.581407000	1.958240000
H	3.910088000	-1.960487000	0.812409000
H	5.161896000	-0.696235000	0.744820000
C	0.101613000	2.172900000	-1.041507000
H	0.427389000	1.973954000	-2.060169000
H	-0.877444000	1.734778000	-0.852187000
H	0.043044000	3.256838000	-0.897869000
N	3.290387000	-0.105826000	-0.039091000
N	1.101399000	1.628113000	-0.063611000
C	-1.665754000	-0.867978000	0.815283000
C	1.480847000	-3.424656000	-0.565400000
C	1.530165000	-4.807312000	-0.990740000
H	1.047829000	-5.441288000	-0.239213000
H	1.004773000	-4.910369000	-1.946046000
H	2.575148000	-5.110582000	-1.113730000
C	-2.989308000	-1.112095000	1.348105000

H	-3.449342000	-1.950652000	0.814841000
H	-2.911785000	-1.353480000	2.413510000
H	-3.601516000	-0.213085000	1.220168000
N	1.451075000	-2.328471000	-0.200475000
N	-0.620574000	-0.669188000	0.363666000
Br	1.590463000	-2.843046000	2.865664000
Br	-1.328926000	-0.907223000	-2.648296000

Fe-^{Br}BPMEN 3+ quartet

C	3.499636000	1.309384000	0.214640000
C	2.412071000	2.139155000	-0.416514000
H	3.517642000	1.428246000	1.298164000
H	4.483448000	1.594145000	-0.169775000
H	2.481983000	3.185495000	-0.103520000
H	2.472120000	2.111772000	-1.505134000
Fe	1.231391000	-0.453988000	0.017927000
N	1.309380000	-0.104082000	2.277055000
C	1.560632000	-0.884333000	3.339381000
C	1.172500000	1.225494000	2.496270000
C	1.754300000	-0.398255000	4.627525000
C	1.364178000	1.801945000	3.748265000
C	1.671289000	0.977799000	4.826674000
H	1.960657000	-1.076101000	5.446502000
H	1.259798000	2.874667000	3.866927000
H	1.829706000	1.394010000	5.816375000
N	1.422341000	-0.454923000	-2.258461000
C	0.546616000	-0.460194000	-3.275614000
C	2.733257000	-0.298863000	-2.562997000
C	0.901411000	-0.243872000	-4.602448000
C	3.177881000	-0.063786000	-3.860594000
C	2.245644000	-0.022795000	-4.892838000
H	0.149544000	-0.251721000	-5.381914000
H	4.237116000	0.072222000	-4.048405000
H	2.557224000	0.161667000	-5.915899000
C	0.655219000	2.056057000	1.355682000
H	0.952705000	3.101103000	1.470314000
H	-0.437362000	2.015244000	1.395401000
C	3.726695000	-0.533102000	-1.458978000
H	4.664243000	-0.009109000	-1.663969000
H	3.941734000	-1.606092000	-1.439821000
C	4.080084000	-0.961923000	0.884761000

H	3.848416000	-0.665943000	1.905585000
H	3.887894000	-2.023443000	0.733985000
H	5.137935000	-0.755216000	0.689109000
C	0.033247000	2.143877000	-0.965478000
H	0.322813000	1.927740000	-1.991110000
H	-0.943593000	1.719566000	-0.737206000
H	-0.006628000	3.230379000	-0.832978000
N	3.264541000	-0.153811000	-0.078619000
N	1.058703000	1.598386000	-0.018310000
C	-1.751730000	-0.936396000	0.769780000
C	1.436968000	-3.516238000	-0.517866000
C	1.461818000	-4.913189000	-0.889264000
H	1.026500000	-5.510485000	-0.080554000
H	0.873400000	-5.052618000	-1.802506000
H	2.496626000	-5.224936000	-1.064249000
C	-3.082845000	-1.218571000	1.258209000
H	-3.509330000	-2.051087000	0.688509000
H	-3.024185000	-1.491955000	2.317412000
H	-3.709347000	-0.328266000	1.141038000
N	1.426004000	-2.402010000	-0.207526000
N	-0.692269000	-0.702529000	0.368661000
Br	1.616526000	-2.773510000	3.099633000
Br	-1.286953000	-0.830364000	-2.910932000

Fe-^{Br}BPMEN 3+ sextet

C	3.513537000	1.322282000	0.252291000
C	2.429291000	2.153028000	-0.407679000
H	3.503316000	1.449322000	1.335320000
H	4.495352000	1.648310000	-0.106786000
H	2.518198000	3.196205000	-0.085157000
H	2.529163000	2.135973000	-1.493556000
Fe	1.198915000	-0.530227000	0.010378000
N	1.300539000	-0.085563000	2.181833000
C	1.550863000	-0.884142000	3.235544000
C	1.114164000	1.238231000	2.422380000
C	1.691466000	-0.419682000	4.536524000
C	1.253904000	1.785956000	3.694087000
C	1.556351000	0.948549000	4.762558000
H	1.897043000	-1.108759000	5.346253000
H	1.112596000	2.851897000	3.833276000
H	1.672405000	1.347062000	5.765242000

N	1.496491000	-0.460655000	-2.178458000
C	0.603352000	-0.480109000	-3.185267000
C	2.805820000	-0.290435000	-2.497327000
C	0.939324000	-0.262776000	-4.514775000
C	3.223594000	-0.052869000	-3.803320000
C	2.277550000	-0.025051000	-4.822591000
H	0.177425000	-0.281897000	-5.284263000
H	4.278270000	0.095617000	-4.006176000
H	2.573335000	0.161271000	-5.849930000
C	0.610168000	2.084523000	1.287884000
H	0.882712000	3.133088000	1.437953000
H	-0.483291000	2.023834000	1.306603000
C	3.817224000	-0.504602000	-1.406763000
H	4.742900000	0.035161000	-1.628784000
H	4.052919000	-1.574716000	-1.398239000
C	4.185482000	-0.917443000	0.934911000
H	3.935986000	-0.626118000	1.953882000
H	4.021335000	-1.986054000	0.791652000
H	5.241934000	-0.689016000	0.753657000
C	0.078466000	2.224736000	-1.050392000
H	0.405994000	2.014283000	-2.066904000
H	-0.912449000	1.805058000	-0.872636000
H	0.036662000	3.311399000	-0.914157000
N	3.349237000	-0.145152000	-0.032413000
N	1.051380000	1.650171000	-0.072768000
C	-1.871431000	-0.932964000	0.928566000
C	1.413032000	-3.678181000	-0.673215000
C	1.460835000	-5.061615000	-1.088106000
H	1.666825000	-5.692014000	-0.216109000
H	0.496367000	-5.340748000	-1.525689000
H	2.254156000	-5.188810000	-1.832361000
C	-3.191202000	-1.145974000	1.477490000
H	-3.675124000	-1.973302000	0.947657000
H	-3.105467000	-1.389360000	2.541928000
H	-3.783594000	-0.232880000	1.354316000
N	1.380633000	-2.574491000	-0.321089000
N	-0.818990000	-0.755413000	0.476833000
Br	1.678419000	-2.759701000	2.950705000
Br	-1.213780000	-0.870593000	-2.784499000

Fe-^{Br}BPMEN oxo 2+ triplet

C	3.501030000	1.370056000	0.136047000
C	2.408988000	2.210761000	-0.484701000
H	3.518631000	1.489302000	1.220535000
H	4.483935000	1.664773000	-0.244348000
H	2.501041000	3.253603000	-0.160285000
H	2.475628000	2.197989000	-1.573992000
Fe	1.270248000	-0.466911000	-0.119254000
N	1.283083000	-0.275693000	1.925471000
C	1.453694000	-1.207002000	2.890126000
C	1.169955000	1.021696000	2.323778000
C	1.613813000	-0.885944000	4.235126000
C	1.333559000	1.415522000	3.648053000
C	1.576526000	0.450740000	4.617325000
H	1.758895000	-1.674056000	4.963176000
H	1.254932000	2.467033000	3.900927000
H	1.712862000	0.725453000	5.658324000
N	1.395993000	-0.373466000	-2.201875000
C	0.481773000	-0.381389000	-3.194022000
C	2.696140000	-0.216342000	-2.576821000
C	0.792083000	-0.142491000	-4.530787000
C	3.085250000	0.035387000	-3.887523000
C	2.116166000	0.093152000	-4.881362000
H	0.006803000	-0.150210000	-5.276192000
H	4.137377000	0.171986000	-4.110794000
H	2.382163000	0.293349000	-5.914190000
C	0.720065000	2.027386000	1.301941000
H	1.097757000	3.024678000	1.548838000
H	-0.372229000	2.071713000	1.369595000
C	3.731441000	-0.455647000	-1.523993000
H	4.663619000	0.066448000	-1.758037000
H	3.944137000	-1.529796000	-1.520723000
C	4.096737000	-0.887232000	0.804195000
H	3.875206000	-0.585819000	1.826404000
H	3.882930000	-1.946564000	0.666626000
H	5.156170000	-0.694773000	0.602405000
C	0.040204000	2.285783000	-0.989734000
H	0.305397000	2.116018000	-2.032799000
H	-0.937453000	1.852123000	-0.778547000
H	0.001063000	3.366719000	-0.810368000
N	3.272586000	-0.089628000	-0.153606000

N	1.066454000	1.668399000	-0.101137000
C	-1.730694000	-0.793237000	0.600176000
C	-3.075805000	-0.988816000	1.105249000
H	-3.550262000	-1.818070000	0.570209000
H	-3.035150000	-1.222141000	2.174070000
H	-3.658901000	-0.074737000	0.952814000
N	-0.670913000	-0.632659000	0.169434000
O	1.516410000	-2.070644000	-0.209834000
Br	-1.343144000	-0.794525000	-2.853697000
Br	1.431071000	-3.066949000	2.492497000

Fe-^{Br}BPMEN oxo 2+ quintet

C	3.491012000	1.315437000	0.148108000
C	2.389431000	2.165485000	-0.444677000
H	3.506551000	1.396586000	1.236095000
H	4.468203000	1.643484000	-0.221921000
H	2.482342000	3.202715000	-0.104507000
H	2.446154000	2.170594000	-1.534768000
Fe	1.182476000	-0.501516000	-0.155403000
N	1.245986000	-0.248176000	2.079475000
C	1.470779000	-1.125555000	3.069897000
C	1.164486000	1.065378000	2.406572000
C	1.691968000	-0.753147000	4.392511000
C	1.387646000	1.526087000	3.701631000
C	1.666626000	0.603569000	4.705375000
H	1.874981000	-1.504161000	5.150902000
H	1.329849000	2.588473000	3.911047000
H	1.847229000	0.929561000	5.724830000
N	1.424289000	-0.340100000	-2.370771000
C	0.548671000	-0.309933000	-3.386464000
C	2.736822000	-0.194558000	-2.670597000
C	0.904870000	-0.069936000	-4.709249000
C	3.181082000	0.062528000	-3.965355000
C	2.251293000	0.137395000	-4.996859000
H	0.150761000	-0.050242000	-5.486296000
H	4.242187000	0.188425000	-4.150266000
H	2.565569000	0.337691000	-6.016187000
C	0.678518000	2.010291000	1.341615000
H	1.020065000	3.030158000	1.543663000
H	-0.414751000	2.017115000	1.403059000
C	3.738796000	-0.456857000	-1.577048000

H	4.674078000	0.071651000	-1.786483000
H	3.955708000	-1.529786000	-1.599855000
C	4.084609000	-0.973043000	0.741612000
H	3.842257000	-0.710936000	1.770289000
H	3.862865000	-2.024804000	0.560454000
H	5.150900000	-0.785831000	0.570621000
C	0.019704000	2.262879000	-0.954643000
H	0.285350000	2.088236000	-1.996325000
H	-0.965045000	1.846593000	-0.742565000
H	0.001174000	3.343800000	-0.774088000
N	3.282834000	-0.131936000	-0.194239000
N	1.036929000	1.630004000	-0.061046000
C	-1.896089000	-0.864974000	0.636713000
C	-3.222628000	-1.135899000	1.152061000
H	-3.708733000	-1.892321000	0.527100000
H	-3.142716000	-1.507887000	2.178853000
H	-3.814157000	-0.214837000	1.141595000
N	-0.842556000	-0.641004000	0.214345000
O	1.402511000	-2.101554000	-0.251802000
Br	-1.291725000	-0.656160000	-3.033064000
Br	1.448105000	-2.993653000	2.690771000

VITA

Upon completing her studies at Nacogdoches High School, Nacogdoches, Texas, in 2013, and a following exchange year abroad, E. Grace Milem entered Antioch College. She received a Self-Designed Bachelor of Science from this institution in 2018. Following this degree, she attended Stephen F. Austin State University to obtain a Bachelor of Science in Chemistry in 2020. She entered the Graduate Program of Natural and Applied Sciences in 2020 to receive the Master of Science in Natural and Applied Science with Chemistry Focus in 2022.

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This thesis was typed by E. Grace Milem.