SYNTHESIS AND ELECTROCHEMICAL CHARACTERIZATION OF NOVEL BRIDGED DIFERROCENE TAGGED ALKANETHIOL SELF-ASSEMBLED MONOLAYERS

by

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Abstract

A diferrocene tagged alkanethiol monolayer was synthesized via a four part reaction procedure to produce 6-(diferrocenylhexanylcarbonyl)pentanethiol. Monolayers were adsorbed onto a polycrystalline gold electrode by soaking in a solution of the thiol. Cyclic voltammetric experiments were done to determine the heterogeneous electron transfer rate constant, k°. Formal potentials, surface coverages and FWHM values were investigated to determine the thermodynamic properties of the thiol monolayer.

Single crystal X-ray crystallography was performed on three compounds synthesized throughout the reaction pathway. These experiments provided information regarding symmetry and unit cell packing of the molecules, as well as the relative positions of the ferrocenes with respect to one another.

This research provides preliminary voltammetric data on alkanethiol monolayers tagged with dimeric ferrocenes. Introduction of another electroactive moiety within the monolayer can dramatically alter the shape of the voltammograms. Formal potentials, FWHM data and electrochemical kinetics were similar to those reported in the literature. Analysis of surface coverages indicates that only 40% of the outer ferrocenes are electrochemically accessible. A possible explanation for this unusual phenomenon is suggested.

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Table of Contents

LIST OF TABLES

LIST OF FIGURES

CHAPTER ONE

INTRODUCTION

Introduction to Self-Assembled Monolayers

Self-assembled monolayers (SAMs) have become a popular and convenient method for studying the chemistry of interfaces at the molecular level. The term self-assembly arises from the fact that molecules or atoms will assemble themselves in an ordered fashion, without machine or human manipulation. SAMs have potential applications in a variety of areas such as chemical and biochemical sensors, protective coatings, and molecular scale electronics.[1] Devices constructed using SAM technology could allow the machines and computers of the future to be drastically reduced in size while becoming increasingly more complex because of microscale electronics.

Although self-assembly has gained much attention recently, it is a phenomenon that nature has inspired. Simple, or thermodynamic self-assembly, can be exemplified in a raindrop. The drop takes a spherical shape because of the instability of the molecules on the exterior of the sphere in contact with air, while those on the interior exhibit more stability. The laws of thermodynamics govern that to keep the drop stable, the exterior surface area needs to be minimal. The water molecules will therefore assemble themselves into a spherical shape to minimize the surface area in contact with the air. Monolayer chemistry has the same fundamental principles as that of simple self-assembly, but the breadth of SAM chemistry is much more extensive. [2]

Another type of self-assembly, which pertains to more complicated situations, i.e. living organisms, is called coded self-assembly. Coded designates that self-assembly occurs through a set of instructions contained within the system. For example, cell reproduction is based on the genetic code of DNA within the cell. The cell will "follow" the instructions encoded on the DNA and reproduce to form another fully functioning cell without external manipulation. The ability of a system, as simple as a raindrop or as complex as a human cell, to "build" itself into an energetically stable state presents many advantages. [2]

Self-Assembled Monolayer Formation

Formation of self-assembled monolayers occurs spontaneously when a surface is exposed to a solution containing the species that will be adsorbed onto the substrate. The part of the molecule that adsorbs onto the surface is referred to as the head group (see Figure 1.1) and this generally occurs through an exothermic chemisorption process, producing strong interactions between the head group and the surface. The energy evolved during chemisorption lies in the tens of kilocalories per mole.[3] Thermodynamics usually dictates that the head group molecules will "assemble" themselves at all available sites on the substrate, forming a close packed monolayer. The majority of monolayer systems contain an alkyl chain attached to the head group to promote close packing and order within the monolayer. As a result of close packing of the adsorbate molecules, van der Waals interactions occur between neighboring molecules. The van der Waals energies are slightly less than ten kilocalories per mole, and contribute to the overall stability of the monolayer.[3] These van der Waals interactions between neighboring molecules become a driving force for monolayer

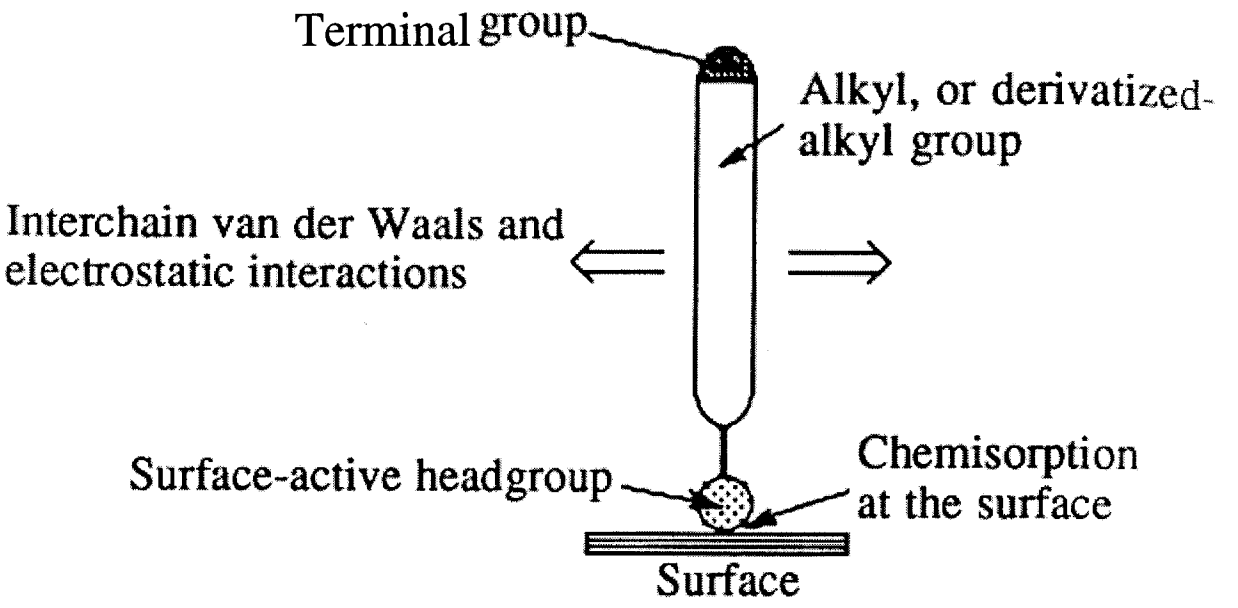


Figure 1.1: Schematic representation of the components of a self-assembled monolayer and the interactions involved. Reprinted from reference 3.

ordering on a surface.

The choice of head and terminal groups for the monolayer is limitless and is usually based on the desired properties that are to be investigated. The stability of the monolayer is usually determined by the strength of head group-substrate bond. The size of head and terminal groups can drastically affect the extent of ordering within the monolayer. Groups larger in size attached to a small alkyl chain do not pack as efficiently on the surface and van der Waals forces between adjacent chains are less effective, therefore the ordering of the monolayer is poor. Larger functionalities allow room for more defects, which translates into poor ordering. Defects associated with large head and terminal groups are corrected for by including molecules similar in nature to the alkyl chain connecting both groups. Smaller functionalities allow for more ordered monolayers because the molecules can pack on the surface much more efficiently, thereby increasing lateral van der Waals interactions.

The polarity of the terminal group can alter the chemical and physical properties of the monolayer. The polarity will dictate the type of surface, i.e. hydrophobic or hydrophilic, that will be constructed. For example, a methyl terminal group produces a hydrophobic surface, while a hydroxyl group produces a hydrophilic one. The desired chemical and physical properties depend on the application, i.e. sensing of hydronium ions may entail a pyridine group. The choice of head and terminal groups and the length of the alkyl chain allows the ability to tailor properties of the interface that is to be studied.

There are various ways to prepare self-assembled monolayers, each having inherent advantages and disadvantages.[3] Some of the techniques can be used to form multilayer assemblies, but the focus will remain on the formation of monolayers. The three most

common methods used to prepare monolayers are Langmuir-Blodgett techniques and adsorption of organosilanes and alkanethiols to substrates.

Langmuir-Blodgett (LB) Films

The oldest and most studied process of monolayer preparation is that of Langmuir-Blogdett techniques.[3] Although LB film preparation is not necessarily a self-assembly technique, it was the first technique that allowed the study and construction of ordered molecular assemblies. LB films usually consist of amphiphilic molecules in solution that are transferred to a solid substrate, from the solvent-air interface. The hydrophilic portion of the molecule resides at the water interface while the hydrophobic portion resides at the air interface. Experimentally, the conditions are controlled to the highest degree of sensitivity. The most common film preparation technique is called vertical deposition. The substrate, commonly glass, quartz, or silicon wafers, is placed into the amphiphilic solution, usually water, and moved through it, creating a film on the substrate surface. The film is then compressed in a Langmuir trough creating the solvent-air interface (see Figure 1.2). The monolayer is relatively unstable due to the absence of a chemical bond between the head group and the surface. Thus the absorbate molecules are mobile on the surface. The motion causes instability and defect sites to be introduced, which can ultimately affect the overall properties of the monolayer. Another drawback to this technique is that the same surface is not created each time the process is performed. This process however, will form a film on a surface that is one molecule thick. Film instability and poor reproducibility are major disadvantages, thus LB techniques are rarely used for real devices.[3]

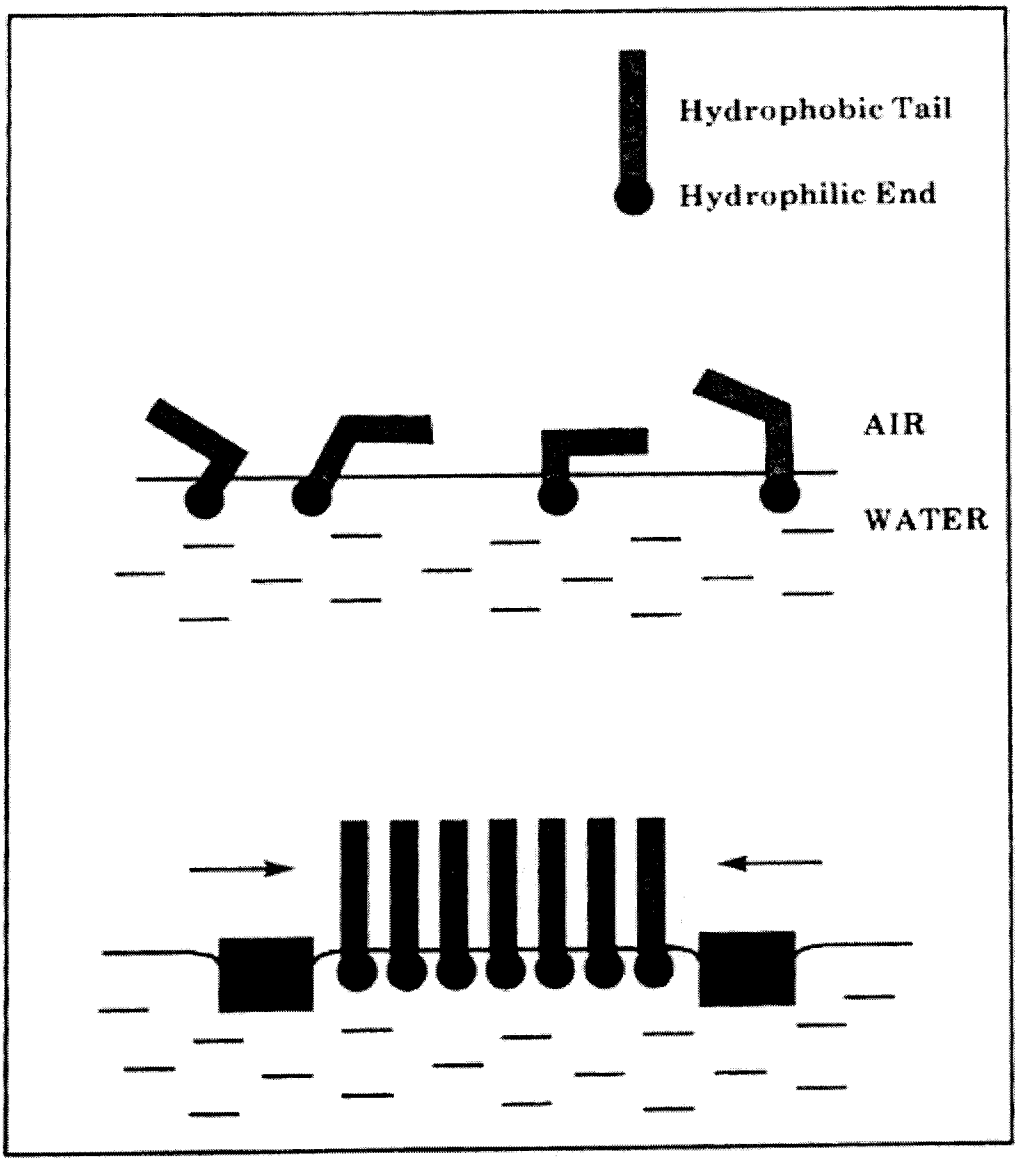


Figure 1.2: The formation of a monolayer through Langmuir-Blodgett techniques. Reprinted from reference 4.

Organosilanes

Monolayer preparation can also take place through a reaction involving trichloroalkylsilanes or triethoxyalkylsilanes with a hydroxylated surface, usually silica, or platinum.[3] The chlorine-silicon or ethoxy-silicon bond reacts with free hydroxyls on the surface, creating a complex silicon-oxygen bond network. A robust monolayer is formed due to the silanes covalently bonding to the hydroxylated surface, as well as Si-O-Si crosslinking between neighboring alkylsilanes (see Figure 1.3). A polymer network is created, producing a strong monolayer, but due to the large head group, the alkyl chains have some degree of movement and the films are disordered. Disorder is also introduced when the siloxanes cross link with a contaminant or bond to different points on the surface. Water sensitivity is also a problem during film preparation that can cause disorder. LB films do not possess this degree of order or strength, so organosilanes have the potential for more applications. The organosilane molecules, due to the size of their head group, cannot close pack on the substrate surface, and therefore van der Waals forces between the alkyl chains are less effective. Reproducibility, as with LB films, is also a problem because the same surface is not produced each time. Murray[4] demonstrated that alkylsilane films are disordered by constructing a ferrocene terminated alkylsilane monolayer. The results of the study demonstrated that electron transfer between the ferrocene and a platinum electrode was rapid on the voltammetric time scale, indicating extensive disorder in the film. Although organosilanes form a more robust monolayer than LB techniques, the poor ordering is a major disadvantage.

Alkanethiol SAMs

SAMs formed from alkanethiols offer significant advantages over other monolayer

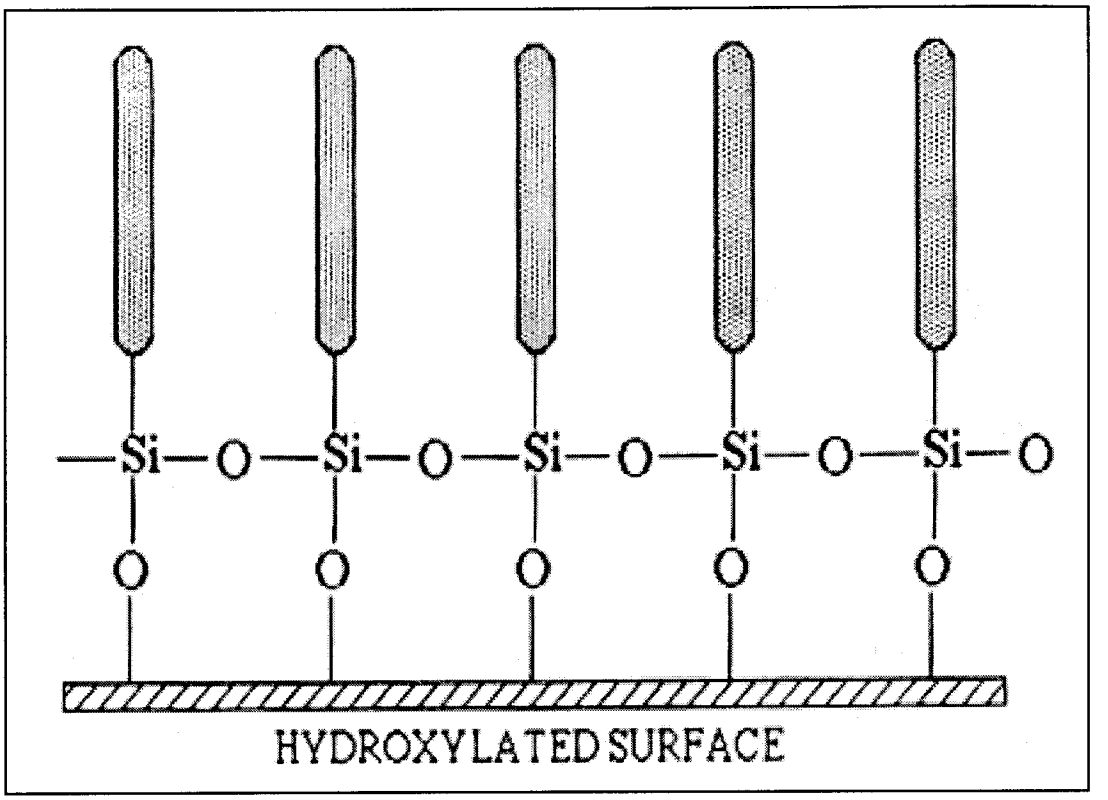


Figure 1.3: An organosilane self-assembled monolayer. Reprinted from reference 3.

systems in terms of stability, ease of preparation, and order on the molecular level. Unlike organosilanes, alkanethiols are not water sensitive and polymeric in nature. Alkanethiols form a stronger covalent bond to the adsorbing surface (30-40 kcal/mol), than the Si-O-Si bond network, thereby creating a much more stable monolayer.[3] Self-assembled monolayers formed from alkanethiols are quite advantageous, not only in ease of construction and stability, but are excellent systems for studying a species in a well-defined environment.

Alkanethiol self-assembled monolayers consist of an alkane chain of variable length connected to a thiol head group, which is commonly bound to a gold surface, with the terminal group pointing away from the surface (see Figure1.4). Nuzzo and Allara found that the primary driving force for alkanethiol monolayer formation is a strong gold-sulfur covalent bond, 30-40 kcal/mol, as stated previously.[3,5] A secondary driving force for the formation of highly ordered monolayers occurs via van der Waals interactions between adjacent alkyl chains. Alkanethiols tend to close pack on the gold surface and will "assemble" themselves on the surface until all available sites are occupied. This will form, in some cases, a crystalline monolayer. The alkyl chains become extremely close to one another and the van der Waals interactions between them hold the monolayer together in an extended all *trans* configuration. Longer alkyl chains yield more van der Waals forces between them, resulting in more highly ordered structures. Monolayers containing less than eight methylene units are disordered, eight to twelve methylene units are somewhat ordered, and chains containing twelve or more methylene units are crystalline. The extent of ordering in SAMs has been studied via x-ray and neutron diffraction, ellipsometry, STM (scanning tunneling microscopy), contact angle

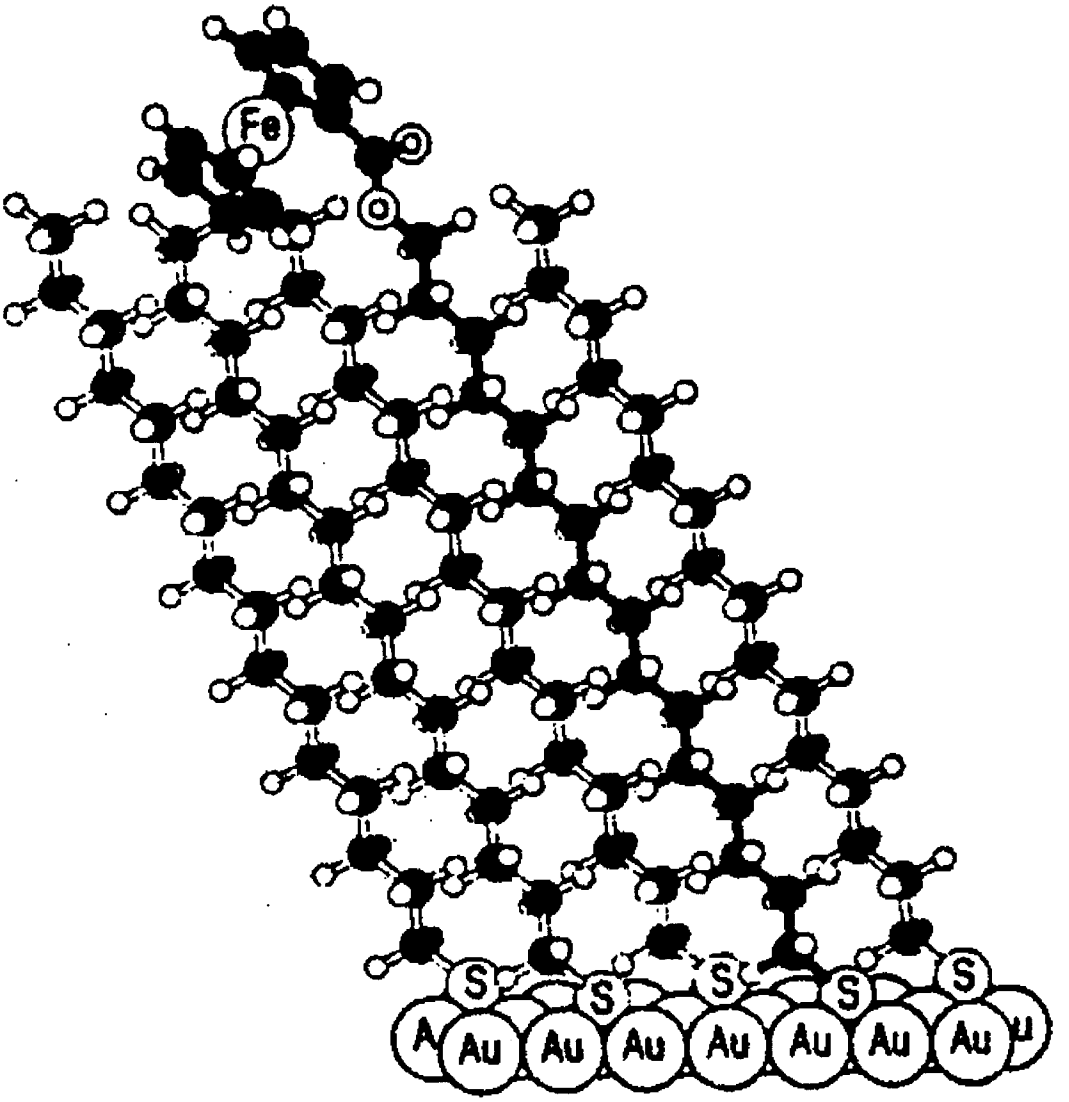


Figure 1.4: An alkanethiol self-assembled monolayer on gold. Reprinted from reference 6.

measurements, surface IR, and electrochemical methods.[1,3,7-11]

As stated previously, the choice of the head group can effect the extent of ordering and stability in the monolayer. Bain [3] studied various head groups such as sulfur, phosphorous, mercury, amines, and cyano functionalities adsorbed onto a gold surface. The study concluded that sulfur and phosphorous produced the strongest covalent bond with gold. However, sulfur created a more closely packed and better ordered monolayer than phosphorous. Sulfur also produces strong bonds to silver, copper, and platinum, but gold is commonly chosen because it exhibits only one stable oxidation state.

The biggest advantage of alkanethiols is that synthetically they are easily attached to a variety of terminal groups. However, the size of the terminal group effects the ordering, i.e. large terminal groups translate into less order. The polarity of the head group can also effect the properties displayed by the monolayer. The physical nature of the film dictates the type of surface that is constructed. Chidsey [6] demonstrated that a polar, ester linked ferrocene terminated alkanethiol, produced better electrochemical data than a non-polar linked alkanethiol.

The attachment of an electroactive molecule ω to the thiol head group allows for the electrochemical study of alkanethiol monolayers. An electroactive molecule is one that is capable of undergoing either oxidation or reduction. Attachment of such a molecule can provide information on the relationship between the structure and properties of the monolayer. Examples of typical electroactive molecules used in alkanethiol SAMs are ferrocenes, ruthenium pentaamines, anthroquinones, and porphyrins. Ideally, the electroactive molecule should be synthetically easy to couple to an alkanethiol and be both chemically and electrochemically reversible. Monolayers can also be constructed of

electroinactive functionalities such as methyl, hydroxyl, and acetyl groups. Electroactive monolayers, however, are more commonly studied because the insulating alkane chain separates the electroactive portion of the molecule from the electrode surface at a fixed distance. This characteristic of the monolayer allows the study of electrochemical kinetics and thermodynamics as a function of alkane chain length in a well-defined environment.

Electrochemistry

Electrochemistry is a discipline of chemistry that can encompass a variety of applications such as electrophoresis, batteries, digital displays and fuel cells.[12] Although each of these applications is quite different, the fundamental principles of electrochemistry are the same throughout. Electrochemistry probes the relationship between the electronic structure and the physical and chemical properties of a molecule. The majority of electrochemical studies are done to obtain thermodynamic and kinetic information on electron transfer. Thermodynamic studies typically yield information regarding the formal potential, $E^{\circ'}$, of an electroactive species and ion-pairing effects. Determination of heterogeneous electron transfer rate constants, k°'s, or the rate of coupled homogeneous chemical reactions, are examples of kinetic parameters obtained via electrochemical methods.

Electrochemical reactions occur when one molecule is oxidized and another is reduced. Electrochemical experiments occur in cells in which two electrodes are required, one for the oxidation reaction and the other for the reduction. The two electrodes are the cathode, at which a species is reduced and the anode, where oxidation occurs. During a typical electrochemical experiment, only one reaction, either oxidation

or reduction, is of interest. The working electrode detects the half reaction of interest, while the other half reaction occurs at the counter electrode. Thus, current flows between the working and counter electrodes. The working and counter electrodes are generally made of inert metals such as platinum, gold, mercury, or glassy carbon. Both the working and counter electrodes can be made of the same material while performing the experiment. A reference electrode is used to control the potential of the working electrode. A high input impedance is placed between the working and reference electrodes so that just enough current flows between them to measure the potential difference. The reference electrode has a potential that is constant, allowing the potential of the working electrode to be accurately known at all times during the experiment. Common reference electrodes include the standard calomel (SCE), silver/silver chloride, and nonaqueous silver/silver nitrate electrodes. Typically this three-electrode arrangement is used because a two-electrode arrangement would not allow for the potential of the working electrode to be accurately known.[12]

Cyclic Voltammetry

Cyclic voltammetry is the most common linear sweep technique in electrochemistry. A typical CV experiment involves the application of a linear potential ramp to an electrode at a given scan rate, ν. The potential of the electrode is increased to a predetermined switching potential, E_λ, at which point the electrode potential is decreased (see Figure 1.5) back to the initial potential. A current response is observed as a result of analyte oxidation or reduction during the potential sweep.

Solution electrochemistry is much more complicated than monolayer electrochemistry due to mass transport effects. Mass transport deals with the delivery of

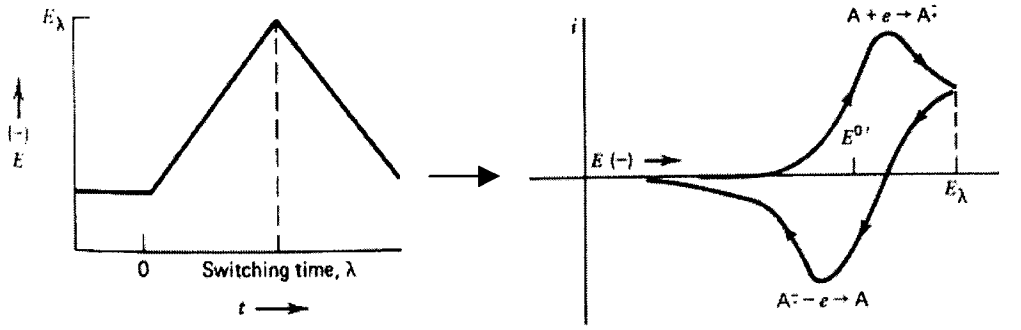


Figure 1.5: Potential versus time profile and the resulting voltammogram for a reversible redox couple. Reprinted from reference 12.

analyte molecules to the electrode/solution surface, which must be considered in solution voltammetry experiments. Mass transport affects the current drawn in response to a changing electrode potential and affects the overall shape of the voltammogram. There are three types of mass transport: diffusion, migration and hydrodynamic. Hydrodynamic mass transport results from stirring the solution or rotating the electrode throughout the experiment. Solution electrochemistry is typically done in a quiescent environment to remove effects due to hydrodynamic mass transport. Migrational mass transport deals with the motion of ions under the influence of a potential gradient. Ions will migrate in response to a change in electrode potential, which gives rise to non-faradaic currents. Solutions are generally prepared with a large excess of non-electroactive supporting electrolyte. A large excess of electrolyte supplies charge-compensating ions, which migrate in response to a change in the electrode potential. Since there are many more electrolyte ions, migration of the analyte is minimized. Data from a CV experiment where migrational mass transport is not minimized is more difficult to analyze because of the analyte molecules acting as charge carriers.

Diffusional mass transport is defined as the motion of a species under the influence of a concentration gradient. A concentration gradient is generated at the electrode surface as a result of oxidation and reduction of the analyte. Diffusion is a relatively slow process, which is responsible for delivering more analyte to the electrode surface to undergo electron transfer. When electron transfer is fast with respect to diffusion, concentration polarization is observed. This affects the shape of the voltammogram by causing peak tailing. However, if the electron transfer is slow with respect to diffusion, kinetic polarization predominates and the rate of electron transfer can be determined. A graphical representation of diffusion controlled electron transfer is demonstrated by plotting the peak currents, i_p, (cathodic or anodic) versus the square root of scan rate, $\nu^{1/2}$. If the electron transfer is diffusion controlled, the plot will be linear.

There are two types of currents encountered in an electrochemical experiment, non-faradaic and faradaic. Non-faradaic currents are generated from the motion of charge compensating ions migrating toward the electrode due to the potential gradient generated at the working electrode. Non-faradaic currents limit the sensitivity and time scale of the experiment. Faradaic currents arise from electron transfer and are therefore associated with oxidation and/or reduction of the analyte. Typically, these are the focus of a cyclic voltammetry experiment, because faradaic currents can be analyzed to obtain thermodynamic and kinetic information. Faradaic and non-faradaic are terms derived from Faraday's Law, which explains that the amount of electricity generated is directly proportional to the number of electrons transferred.

A CV experiment begins at a potential that is not sufficient to reduce the analyte in solution. Thus, only non-faradaic currents are observed. As the potential is made more

negative, the energy of the electrons in the metal increases until the potential becomes sufficiently negative for electron transfer from the electrode to the analyte to be energetically favorable (see Figure 1.6). As the analyte is reduced, an increase in current occurs, i.e. faradaic currents and the current increases until the surface concentration of the analyte is driven to zero, at which point it reaches a maximum. The current then decreases due to concentration polarization, until the switching potential is reached. The scan is then reversed and the energy of electrons in the metal decreases until it is energetically favorable for an electron to be transferred from the analyte to the electrode. Thus, the analyte is oxidized and an increase in faradaic current is observed. The current continues to increase until the surface concentration of the reduced form of the analyte reaches zero. At this point, the current reaches a maximum and subsequently decreases due to concentration polarization.

Cyclic voltammetry is commonly performed on electroactive substances to determine the formal potential, $E^{\circ\prime}$, a thermodynamic property that is characteristic of the analyte. The formal potential is the potential at which electron transfer occurs. This provides information concerning the electronic structure of the analyte. The formal potential is experimentally determined as:

$$E^{\circ\prime} = (E_{p,a} + E_{p,c})/2$$

The formal potential of an electroactive molecule, $E^{\circ\prime}$, can be used to calculate the relative amounts of oxidized and reduced species. For $O + ne^- \rightarrow R$, the Nernst equation. states that:

$$E = E^{\circ\prime} + (RT)/(nF) \ln [O]/[R]$$

where E is the potential of the cell, $E^{\circ\prime}$,is the formal potential, R is the ideal gas constant

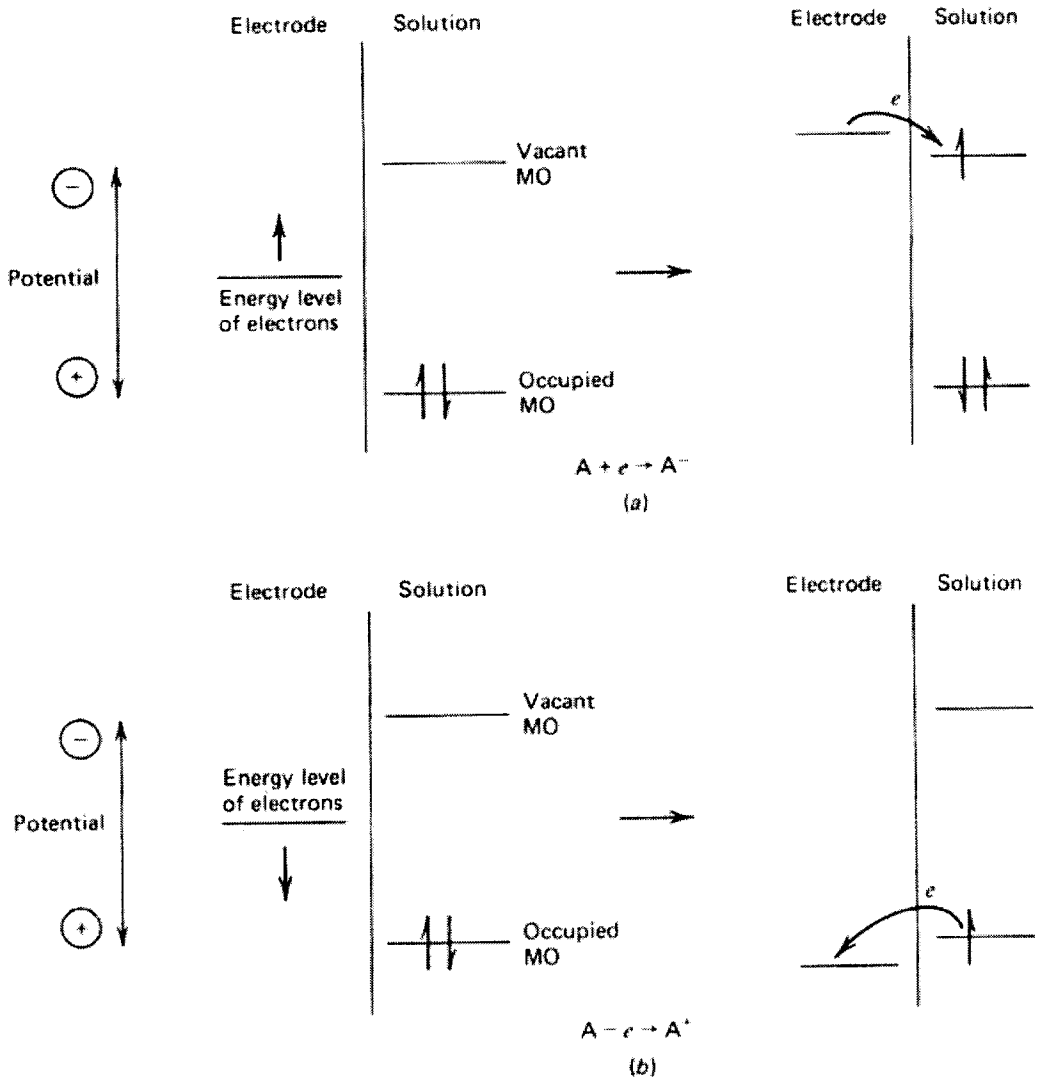


Figure 1.6: Representation of (a) reduction and (b) oxidation process of a species in solution. Reprinted from reference 12.

(8.314 J/mol·K), T is the temperature in Kelvin, n is the number of electrons transferred, F is Faraday's constant, [O] is the surface concentration of the oxidized species and [R] is the surface concentration of the reduced form of molecule. The Nernst equation can be used to relate the kinetics of a system to the relative concentrations of the oxidized or reduced forms of the analyte.

Electron transfer kinetics are generally investigated using cyclic voltammetric methods. There are two very distinct areas in the study of electron transfer kinetics, reversible and irreversible. A grey area exists, known as quasi-reversible electron transfer, but the focus will remain on systems that are purely reversible or totally irreversible. CV is used to investigate the reversibility or irreversibility of an electron transfer, both chemically and electrochemically. Each of these areas has different criteria in data analysis to determine if the electron transfer is reversible or irreversible and of what type, chemical or electrochemical.

In an electrochemically reversible system, electron transfer is rapid on the voltammetric time scale. Thus, the Nernst equation is obeyed at all potentials. Electrochemical reversibility is indicated in a cyclic voltammetry experiment when ΔE_p, ($E_{p,a}$-$E_{p,c}$), is equal to 57/n mV and is independent of scan rate. Another test for electrochemical reversibility is a Nernst plot of log ($i_{p,c}$ –i)/i in the rising portion of the cathodic wave versus potential. If the slope is equal to 57/n mV and the y intercept is equal to the formal potential of the analyte, the electron transfer is electrochemically reversible. In practice, ΔE_p for a reversible couple is typically about 70/n mV and independent of scan rate, due to problems with solution resistance.

An irreversible system is one in which heterogeneous electron transfer kinetics are slow. Due to slow charge transfer kinetics, an overpotential must be applied in the cathodic and anodic directions in order to induce electron transfer. The overpotential is the amount of extra potential needed to observe a current response equal to that of a reversible electron transfer. ΔE_p values increase with increasing scan rate for electrochemically irreversible systems. The rate constant is obtained based on how ΔE_p increases with increasing scan rate. For a totally irreversible electron transfer, k° can be obtained from the Butler-Volmer equation. The Bulter-Volmer equation is stated as follows:

$$i = nFAk^\circ[C_o e^{-\alpha nf\eta} - C_R e^{-(1-\alpha)nf\eta}]$$

where i is the current, n is the number of electrons transferred, F is Faraday's constant, A is the electrode surface area, k° is the heterogeneous electron transfer rate constant, C_O, is the surface concentration of oxidized form of the analyte, C_R is the surface concentration of reduced form of the analyte, α is the electron transfer coefficient (usually 0.5), f is F/RT, and η is the overpotential.

Chemical reversibility deals with the chemical stability of the analyte. For example, if ten molecules are oxidized in the forward sweep of the experiment and all ten are re-oxidized in the reverse sweep, this is a chemically reversible couple. Chemically reversible systems are observed when small deviations from $E^{\circ\prime}$ drives the forward or reverse reaction, and only that reaction. The test for chemical reversibility is that the ratio of the peak currents, i.e. $i_{p,a}/i_{p,c}$, should be equal to one at all scan rates.

If the analyte molecules cannot be re-oxidized in the reverse sweep, due for example to a homogeneous decomposition reaction, then this is referred to as a chemically

irreversible process. A decomposition reaction may produce another species from the unstable reduced analyte, which may or may not be electroactive, i.e. $O + ne^- \rightarrow R \rightarrow Z$. Rate constants for the decomposition reaction, as well as mechanistic information can be determined with CV.

Cyclic voltammetry is a very powerful tool for obtaining k_{chem}, the rate constant for a homogeneous chemical reaction, as well as providing mechanistic information. Cyclic voltammetry provides two different methods of obtaining the value of k_{chem}. The first method involves decreasing the time scale of the experiment by increasing the scan rate. Increasing the scan rate allows less time for the decomposition reaction to occur, thereby altering the shape of the voltammogram. Ideally, the time scale of the experiment is adjusted to the same range as that of k_{chem}. To obtain the value of k_{chem}, a working curve of $i_{p,a}/i_{p,c}$ versus log $\nu^{1/2}$ as a function of k_{chem} is constructed. When the working curve matches the data from the CV experiment, k_{chem} is determined. The mechanism of the chemical reaction can be obtained by proposing a reasonable pathway, and using digital methods to simulate the CV experiment. When the digital simulation matches the experimental CV, the proposed mechanism may be the correct one. The proposed mechanism must be checked with an independent method because two different mechanisms may give rise to the same simulated CV. It is, however, unlikely to produce the same simulation for an independent experiment, i.e., chronoamperometry or rotated ring disk electrochemistry. The main disadvantage of performing high scan rate voltammetry is that high-speed electronics are required, which tend to be expensive.

Another method of acquiring k_{chem} is to perform low temperature electrochemistry. Running the CV experiment at low temperatures slows the kinetics of the chemical step

down until k_{chem} decreases into a measurable range. An advantage to low temperature CV is that the experiment need not be as sophisticated and commercially available potentiostats can be used. A major disadvantage to this technique is high iR drop at low temperatures, which makes it difficult to accurately know the potential of the working electrode. In addition, the presence of a large solution iR can mimic slow electron transfer kinetics, making it impossible to extract k_{chem}. Other problems include the solubility of the analyte, a decrease in the diffusion coefficient, and aqueous solutions generally cannot be used.

Both of the described methods are useful in acquiring k_{chem}. Generally, with either technique, the shape of the voltammogram changes in a similar fashion, with increasing scan rates or decreasing temperatures. At low scan rates or high temperature, the cathodic wave is present, but no anodic wave. This is because upon reduction, the analyte quickly decomposes to Z and cannot be re-oxidized back to O. At intermediate scan rates or temperatures, some of R decomposes to Z, but a small portion is also re-oxidized, as evident from a small anodic peak. At high scan rates or low temperatures, the analyte appears to be reversible because there is not sufficient time for R to decompose to Z.

The basic principles of solution electrochemistry and cyclic voltammetry have been presented. The majority of studies done on electroactive molecules concentrate on the kinetics and thermodynamics of a system. Monolayers are model systems for exploring such areas. The responses generated from electrochemical experiments, typically cyclic voltammetry, on monolayer systems are quite different and will be discussed.

Monolayer Electrochemistry

Electrochemistry performed on self-assembled monolayers produces different responses than when the analyte is dissolved in solution. The largest difference is the fact that the analyte molecules are surface confined, so diffusional mass transport has no effect on the voltammetry. The absence of diffusion is indicated by a linear plot of i_p versus scan rate, providing evidence that the species is adsorbed to the electrode surface. Cyclic voltammetry is a common technique used to study SAMs, but other methods, i.e. chronoamperometry, are used as well. The potential versus time profile for a surface confined species is the same as solution CV, but data analysis is quite different.

A linear potential ramp is applied to the working electrode and the current is measured as a function of the applied potential (see Figure 1.5). The voltammogram generated from a monolayer has observable differences when compared to one generated from a solution experiment (see Figure 1.7). One distinct feature is that peak tailing does not occur due to the absence of diffusional mass transport. The result is a voltammogram which closely resembles that observed in a thin layer electrochemical cell.

The terminal groups used in SAMs are generally chosen so that they are chemically reversible, resulting in symmetric peak shapes. Chemically reversible monolayers produce $i_{p,a}/i_{p,c}$ equal to one, as in solution electrochemistry. Deviation from unity suggests chemical irreversibility due to a homogeneous reaction taking place.

Electrochemically reversible monolayers usually produce symmetric peaks on the voltammogram and ΔE_p should theoretically be 0 mV and independent of scan rate. In practice, ΔE_p is usually ten to twenty mV for a reversible couple due to the effects of solution iR. For a reversible reaction, the rate at which electron transfer occurs is too

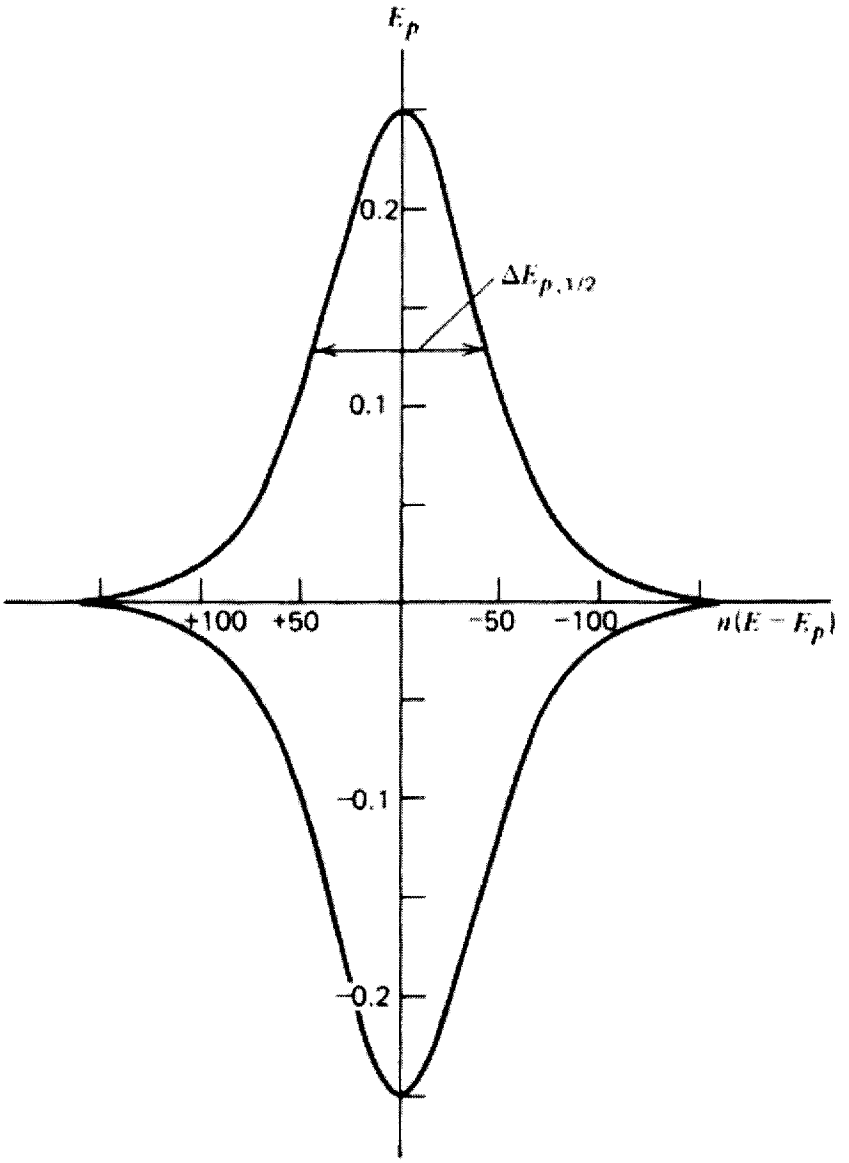
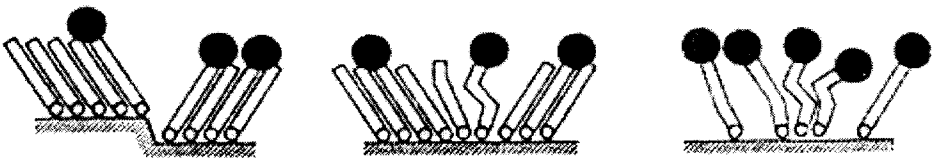


Figure 1.7: Theoretical cyclic voltammogram of a reversible surface confined species. Reprinted from reference 7.

rapid to be measured on the voltammetric time scale and k° cannot be extracted. Rapid electron transfer kinetics can be an indication of defect sites embedded within the monolayer (see Figure 1.8). The monolayer may contain functionalities that can be folded over on themselves because they are located at step or other defect sites. Therefore, a small portion of the electroactive groups are closer to the electrode surface, resulting in a more rapid electron transfer. Electrons in more ordered regions of the monolayer can "hop" to this defect site, rather than tunneling through the insulating alkane chain. Collard and Fox[13] demonstrated that defect sites in ferrocene alkanethiol monolayers, could be eliminated by soaking the electrode in a solution of electroinactive alkanethiols. The electroactive alkanethiols located at defect sites are replaced by the electroinactive species, resulting in decreased faradaic currents and more order. Under the appropriate conditions, k° can be measured for diluted electroactive SAMs. This process of exchanging sites is known as dilution and is a common method to introduce more order into the monolayer. Fully loaded films are generally reversible because of disorder, but dilution isolates the redox sites so that a single rate constant can be calculated.

Electrochemically irreversible monolayers provide information regarding heterogeneous electron transfer kinetics. Electron transfers in monolayers containing long alkane chains or films that are diluted with electroinactive alkanethiol, are typically kinetically slow due to the insulating alkane chain. For an irreversible electron transfer, ΔE_p increases with increasing scan rate. In order to extract a rate constant, electron transfer should occur to and from isolated, independent molecules. Interactions between the redox active groups, gives rise to a broad distribution of rate constants and a single



A: Impurities or crystal defects (boundaries, steps) on a gold surface

B: Alkanethiol two-dimensional crystal domain boundary

C: Steric interactions between ferrocene-substituted alkanethiols in neighboring monolayer lattice sites

Figure 1.8: Possible self-assembled monolayer defects. Reprinted from reference 13.

rate constant cannot be extracted.

As with solution voltammetry, the Butler-Volmer equation can be used to determine the value of k°. However, the equation is rearranged to neglect effects from diffusion and the equation is based on monolayer surface coverage, Γ, instead of concentration. Laviron[14] developed a mathematical model based on the Butler-Volmer equation, which established the relationship of how ΔE_p increases with increasing scan rate. A plot of how ΔE_p varies with scan rate demonstrates that the rate constant, k°, is inversely proportional to the slope of the curve. The rate constant is solved for with the following equation:

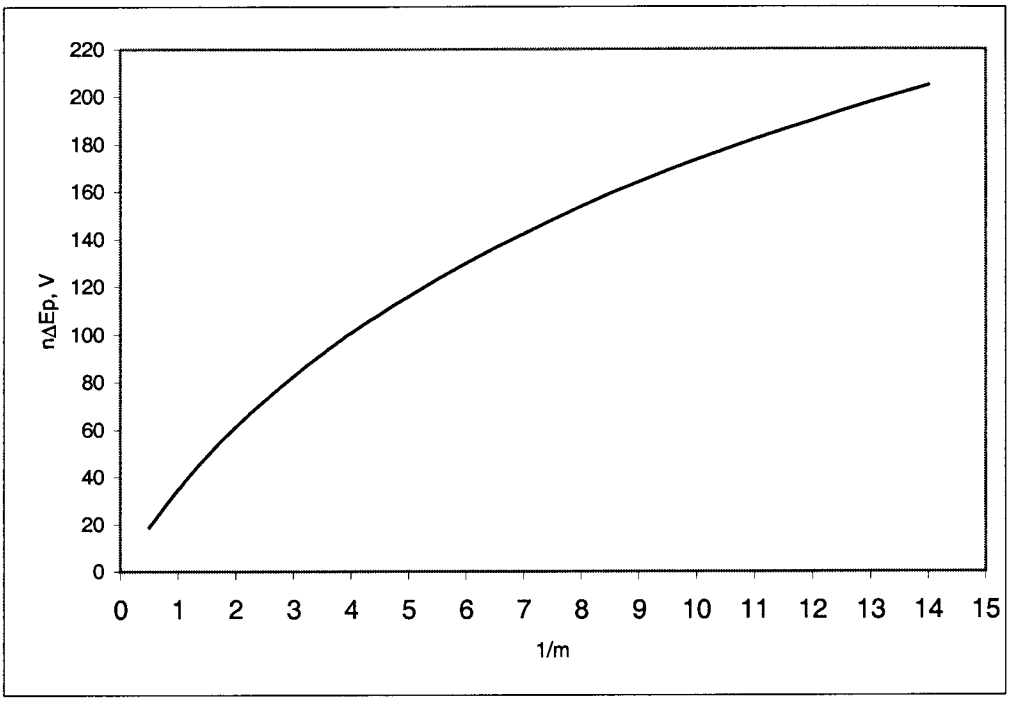
$$1/m = (nF\nu)/(RTk^\circ)$$

Laviron tabulated the values for 1/m and $n\Delta E_p$ at various scan rates, so that rate constants could be easily extracted (see Figure 1.9) by measuring ΔE_p as a function of scan rate.[14]

Surface coverage of the monolayer is also an important factor, which can be calculated from the voltammogram. The surface coverage is defined as:

$$\Gamma = Q/(nFA)$$

where Q is the charge passed during oxidation or reduction. The extent of coverage can affect the overall thermodynamic and kinetic properties of the monolayer. Surface coverage is determined by integrating the peak areas of the cathodic and anodic waves and dividing by the scan rate, number of electrons transferred and Faraday's constant. The charge passed is directly proportional to the number of sites occupied on the substrate surface. The value obtained indicates if the monolayer is close packed on the surface. If the coverage is too low, the possibility of disorder is higher. If the surface coverage is too high, this indicates the presence of multi-layers or non-specific adsorption



1/m	0.5	0.8	1	1.5	2	2.5	3	3.5	4	5
$n\Delta E_p$ (mV)	19	27	34.8	48.8	61.2	72.2	82.4	91.8	100.6	116

1/m	6	7	8	9	10	11	12	13	14
$n\Delta E_p$ (mV)	130	142	154	164	173.4	182	190	197.6	204.6

Figure 1.9: Plot of $n\Delta E_p$ versus 1/m based on Laviron's tabulated values to determine the rate constant of a redox couple. Reprinted from reference 14.

of redox active molecules. Thus, at high or low surface coverages, the voltammogram displays broad peaks, due to the presence of defect sites, and calculation of a rate constant is difficult.

The ordering of the monolayer, a thermodynamic property, can be quantified on the voltammogram using full width at half-maximum values (FWHM). Theoretical values for FWHM are 90/n mV and values above this indicate that the species within the monolayer are disordered or are interacting with one another. Undiluted films usually produce broadened peaks on the voltammogram and FWHM values much greater than 90/n mV, complicating the task of extracting a rate constant. Dilution of the monolayer with electroinactive alkanethiols, removes electroactive molecules from defect sites, resulting in voltammetric waves displaying FWHM values of 90/n mV.

Self-assembled monolayer studies provide fundamental information regarding electron transfer in a well-defined environment. Monolayers used to study electron transfer rates are typically constructed of ferrocene linked to the electrode surface via an alkanethiol. Ferrocene is commonly chosen because it is a reversible, outer sphere redox couple. Another advantage of using ferrocene is that synthetically it is easy to attach to the alkanethiol chain. Although SAMs can be constructed from a variety of redoxactive molecules, i.e. ruthenium pentaamine, anthroquinones, porphyrins and viologens, the focus throughout will remain on those constructed of ferrocene alkanethiols.

Monomeric Ferrocene Alkanethiol Monolayers

Ferrocene terminated alkanethiol SAMs are widely studied to determine the rate of electron transfer. Chidsey[15] constructed the first ferrocene terminated alkanethiol monolayer. Shown in Figure 1.10 is a voltammogram of monomeric ferrocene

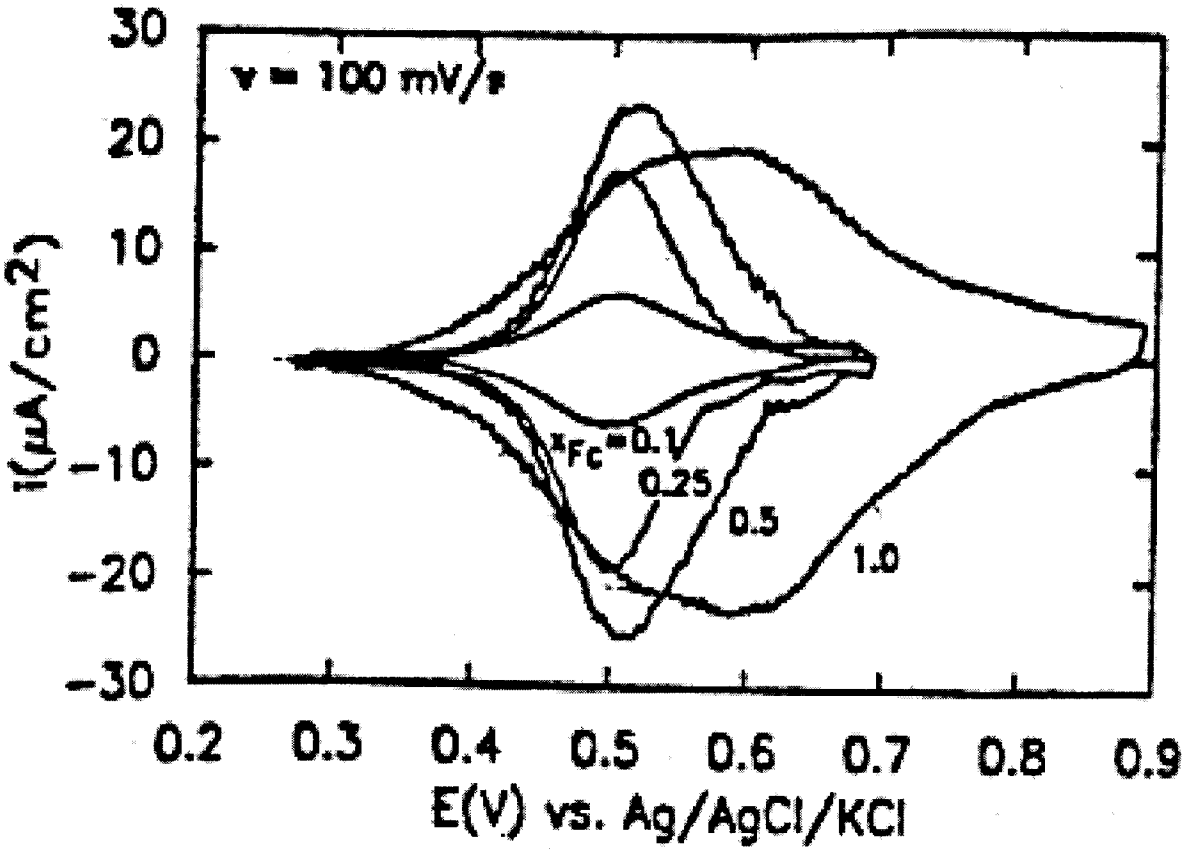


Figure 1.10: Voltammogram for mixed monolayers of $FcCO_2(CH_2)_{11}SH$ and $CH_3(CH_2)_{15}SH$. Reprinted from reference 15. The broadened outer wave represents the undiluted film.

alkanethiols diluted with unsubstituted alkanethiols. The broadened peaks displayed by the fully loaded films demonstrate that there are many defect sites present in the monolayer. As the film is diluted, the peaks narrow, as evident from the voltammograms. The peaks on the voltammogram are also symmetrical, which is typical for monolayer chemistry. Ferrocene containing SAMs are typically chemically reversible as demonstrated by Chidsey.[15] The ratio of the peak currents for the voltammograms shown in Figure 1.10 is equal to one for fully loaded and diluted films, confirming that the reaction is chemically reversible.

The CV's for the fully loaded and partially diluted films displayed ΔE_p values which were independent of scan rate, indicating electrochemical reversibility. A rate constant could not be extracted because of the presence of defect sites in the films. When the ratio of $Cp_2FcCO_2(CH_2)_{11}SH$ to undecanethiol was1:15, ΔE_p increased with increasing scan rate, indicating an electrochemically irreversible electron transfer. Using the method of Laviron[14], a heterogeneous electron transfer rate constant of 5.2 s^{-1} was obtained. This indicated the effectiveness of monolayer dilution for slowing electron transfer kinetics into a measurable range.

In a separate study, Chidsey[6] constructed diluted films having a longer alkane chain of sixteen methylene units. The ferrocene was connected to the alkanethiol via an ester group. The results of this study demonstrated that the currents obtained at high overpotentials were lower than those predicted by Butler-Volmer theory. Thus, the more general Marcus-Hush theory, in conjunction with the density of states in the metal, was needed to provide an accurate rate constant. Using this method, Chidsey obtained a heterogeneous electron transfer rate constant of 1.3 s^{-1} for the ferrocenes in the

monolayer. Thus, the rate of electron transfer was shown to decrease with an increase in alkane chain length. Although this research does not provide extensive information on the distance dependence of electron transfer, it does demonstrate that separating a reversible redox couple from an electrode with an insulator slows the electron transfer kinetics into a measurable range.

Finklea[16] et al. also investigated the distance dependence of electron transfer in SAMs by attaching ruthenium pentaamine to alkyl chains of ten, eleven, and fifteen methylene units. The results demonstrated that the electron transfer rate between the electrode and the ruthenium decreased exponentially with increasing distance. Based on Tafel plots, the mechanism of electron transfer was found to occur through bond tunneling, i.e. through the alkyl chain, rather than through space.

The surface coverage for SAMs constructed from ferrocene alkanethiols was also calculated for Chidsey's fully loaded films. He obtained a value of 5.8×10^{-10} mol/cm^2. This value is typical for ferrocene containing monolayers and indicates close packing of the molecules on the surface. The value is somewhat high due to the broad peaks on the voltammogram and integration yielding a large area. Theoretically, ferrocene alkanethiols are modeled as 6.6 Å spheres and a surface coverage of 7.71×10^{-10} is calculated. For a fully loaded close packed film, there is some agreement between the experimental and theoretical values. Differences are most likely due to different solvation spheres around the molecules in the thiol coating solution.

The FWHM values for Chidsey's ferrocene containing films were approximately 230 mV for the cathodic and anodic waves. These values were much greater than the theoretical value of 90/n mV, indicating that the ferrocenes were interacting with one

another. The high FWHM value is evident from the extremely broadened peak on the voltammogram shown in Figure 1.10. The broadened waves for fully loaded films therefore could not allow for a single rate constant to be determined. Hence, the film had to be diluted in order to determine k°.

Dimeric Ferrocene Alkanethiol Monolayers

Many self-assembled alkanethiol monolayers containing monomeric ferrocenes have been synthesized and studied electrochemically, [6,13,15,16] but alkanethiol monolayers containing dimeric ferrocenes have not been extensively reported. The effect of another electroactive substitiuent within the monolayer can have profound effects on the observed thermodynamic and kinetic properties.

The study of dimeric ferrocene alkanethiols on gold has concentrated on investigating the effect of another electroactive site within the monolayer. The ability of a system to contain mixed valence functionalities is attractive because the properties of the mixed valent state are often not the sum of those of the monovalent states. Monolayers containing two ferrocenes have been reported by Filler[17] and Kubo[18] et al. These studies will be the focus throughout this section.

Filler[17] et al. constructed a variety of diferrocenylethane tagged alkanethiol SAMs having different chain lengths of six, twelve, and sixteen methylene units between the electrode surface and the inner ferrocene. Voltammograms for the six-carbon derivative are shown in Figure 1.11. The voltammograms for monolayer films containing two ferrocenes are not drastically different than those containing one ferrocene. The most noticeable difference is that the voltammogram displays two waves in both the anodic and cathodic directions. The peaks are reasonably symmetric, with the first redox wave

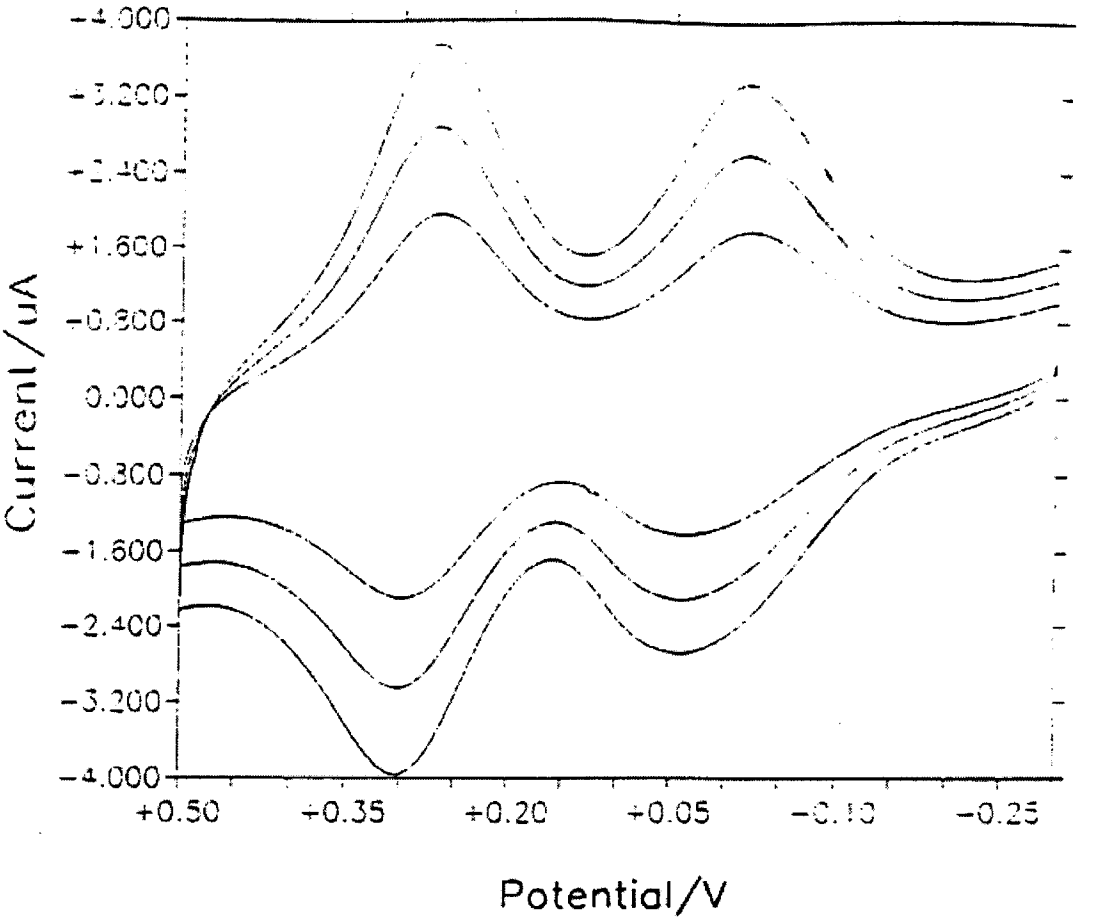


Figure 1.11: Cyclic voltammogram for 6-(1,2-diferrocenylethylcarbonyl)pentanethiol. Working electrode: Gold; Counter electrode: Silver wire; Reference electrode; Ag wire. Reprinted from reference 17.

diferrocenylethane group was modeled as a 12 Å sphere. The measured surface coverages indicated the formation of a closely packed monolayer on the surface.

The ordering of the monolayer was probed by examining FWHM values. The monolayer having a six-carbon chain between the inner ferrocene and the electrode produced a value of 150 mV for the first redox wave and 124 mV for the second redox wave. The twelve-carbon derivative demonstrated values of 105 mV for both redox waves. FWHM values for the fifteen-carbon chain could not be determined due to poorly resolved redox waves. While the FWHM values for the diferrocenylethane monolayers were larger than the theoretical value of 90/n mV, they were much smaller than those reported for monomeric ferrocenes, further indicating ordered films.

Kubo[18] et al. constructed alkanethiol SAMs containing biferrocene. Two symmetrical one electron transfers were observed, with the first wave centered at 197 mV and the second at 600 mV. The oxidation of the outer ferrocene occurred at lower potentials, as seen with Filler's compounds, due to the presence of an electron withdrawing carbonyl substituent on the inner ferrocene.

The major difference between the biferrocene films synthesized by Kubo and those containing 1,2-diferrocenylethane terminal groups, was that oxidation of the biferrocene group was found to be chemically irreversible. When the potential scan was limited to 500 mV, so that only the outer ferrocene was oxidized, the peak current ratios deviated from unity, indicating a chemically irreversible process. The results demonstrated that the homogeneous chemical reaction followed second order kinetics. When the potential was scanned to 900 mV, both redox waves were observed. The peak current ratios again

deviated from unity. However, when the larger potential limit was used, the reaction was found to obey first order kinetics.

Two rate constants for the biferrocene monolayer were obtained by the method of Laviron. The outer ferrocene produced a more rapid rate constant of 0.93(±0.02) s^{-1}, compared to a slower value of 0.64(±0.02) $s^{-1}$for the inner ferrocene. The electron transfer for the outer ferrocene occurred more rapidly, despite the fact it is farther from the electrode surface. Upon oxidation of the outer ferrocene, a counter ion from the electrolyte solution must supply a charge compensating anion to the ferricenium cation. A charge compensating anion must also be supplied when the inner ferrocene is oxidized. Kubo speculated that forcing an anion past the anion located at the outer ferrocene was limiting the rate of the electron transfer. This inversion of rate constants was not observed in the diferrocenylethane tagged monolayers studied by Filler.

Kubo et al. obtained a surface coverages of 4.6 x 10^{-10} mol/cm^2 which were similar to those obtained for monomeric ferrocenes. This indicated the formation of a closely packed monolayer.

The biferrocene films produced FWHM values of approximately 100 mV. The peaks were relatively narrow and the values were in close agreement with the theoretical value of 90/n mV. This provided evidence that the ferrocenes were non-interacting, allowing the extraction of a single rate constant.

Monolayer chemistry is widely studied to obtain fundamental thermodynamic and kinetic information concerning the rate of electron transfers. They have become increasingly attractive systems to model electron transfer because of the ability to tailor the interface on the molecular level. Various methods of tailoring include monolayers

containing two, rather than one ferrocene, altering the distance from the ferrocene to the electrode surface, or altering the distance between the two ferrocenes. The latter approach has not been reported in the literature, and is the focus of the research outlined in this thesis.

Research Proposal

The goal of this research endeavor is to increase the alkane chain length separating two ferrocenes to explore the extent of communication between them and the possible increase in order through the attachment of an alkane chain on the backside of inner ferrocene. Effects of the bridging alkane chain will be quantified through the determination of heterogeneous electron transfer rate constants, surface coverages, and FWHM values. Another area of interest is the possibility of a thermodynamic price for oxidation of the inner ferrocene due to ion migration into a non-polar alkane environment. The data obtained will be compared to the previous studies done by Chidsey, Filler and Kubo. Although, this is a novel area of self-assembled monolayer chemistry, the fundamental principles described previously are the same.

1,6-diferrocenylhexane will be synthesized, tagged with an alkanethiol, purified and adsorbed onto a polycrystalline gold electrode. The electrochemical properties of SAMs constructed from this molecule will be probed via the previously explained cyclic voltammetry method. The cyclic voltammograms should produce four peaks and provide thermodynamic and kinetic data for comparison with the literature.

X-ray crystallography will be used to provide pertinent structural information concerning the diferrocenylhexane head group and packing orientation on the gold surface. Single crystal X-ray diffraction data will be obtained for any of the compounds

synthesized during the pathway to the final alkanethiol product. The orientation of the ferrocenes with respect to each other, as well as the unit cell-packing scheme, will be the focus of such experiments.

Cyclic voltammetry provides a wide range of information concerning self-assembled monolayers. A single experiment can allow extraction of heterogeneous electron transfer rate constants, thermodynamic properties such as the formal potential of each ferrocene, and how well the monolayer covers the gold electrode surface. The structural characteristics of the monolayer are found indirectly by performing this simple electrochemical experiment. The research presented will provide information useful to future endeavors in interfacial chemistry.

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CHAPTER TWO

SYNTHESIS AND CHARACTERIZATION

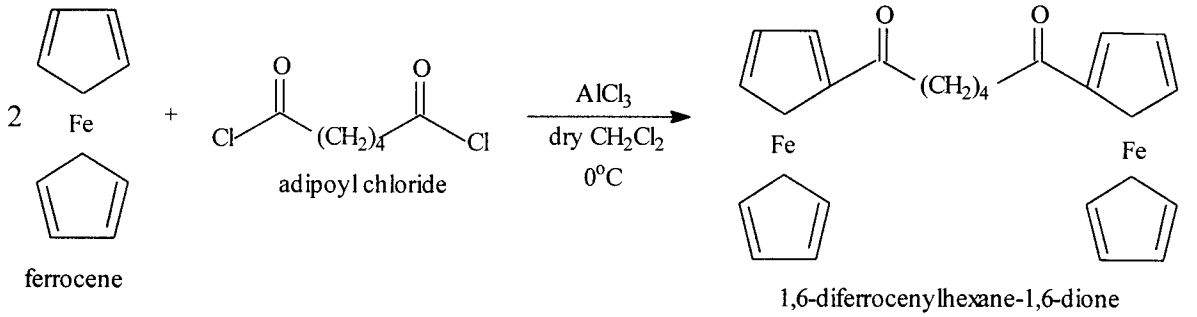
The production of a compound containing two ferrocene moieties bridged by a six-carbon chain is synthetically quite involved (see Figure 2.1). SAMs containing monomeric ferrocenes have been extensively studied [1-4], but little attention has been paid to monolayers containing oligomeric ferrocenes.

The initial step was a Friedel-Crafts acylation, in which adipoyl chloride, in the presence of $AlCl_3$ in dry methylene chloride, was used to link the two ferrocenes together. The two carbonyls in the bridge were reduced under Clemmensen reduction conditions, using a zinc-mercury amalgam and HCl in toluene. Upon reduction, another Friedel-Crafts acylation was performed with 6-bromohexanoyl chloride, under the same conditions as above. The final step in the reaction sequence was a nucleophilic displacement of bromide with thiolacetic acid, followed by displacement of acetic acid from the thioacetyl group using dilute NaOH.

Chemicals

Adipoyl chloride (Aldrich, 99%), aluminum chloride (Aldrich, 98%), argon (Praxair, 99.999%), 6-bromohexanoyl chloride (Aldrich, 97%), calcium hydride (Aldrich, 95%), deuterated chloroform (Aldrich, 99%), ethanol (Pharmco, absolute, 100%), ethyl acetate (Pharmco, 99.98%), ferrocene (Aldrich, 98%), hexane (Pharmco, 99.99%), hydrochloric acid (Fisher, certified ACS plus), magnesium sulfate (Fisher, certified ACS, 99%), mercuric chloride (Mallinckrodt, 98%), silica gel (Aldrich, 200-400 mesh, 60 Å), sodium

Step One: Friedel-Crafts Acylation



Step Two: Clemmensen Reduction

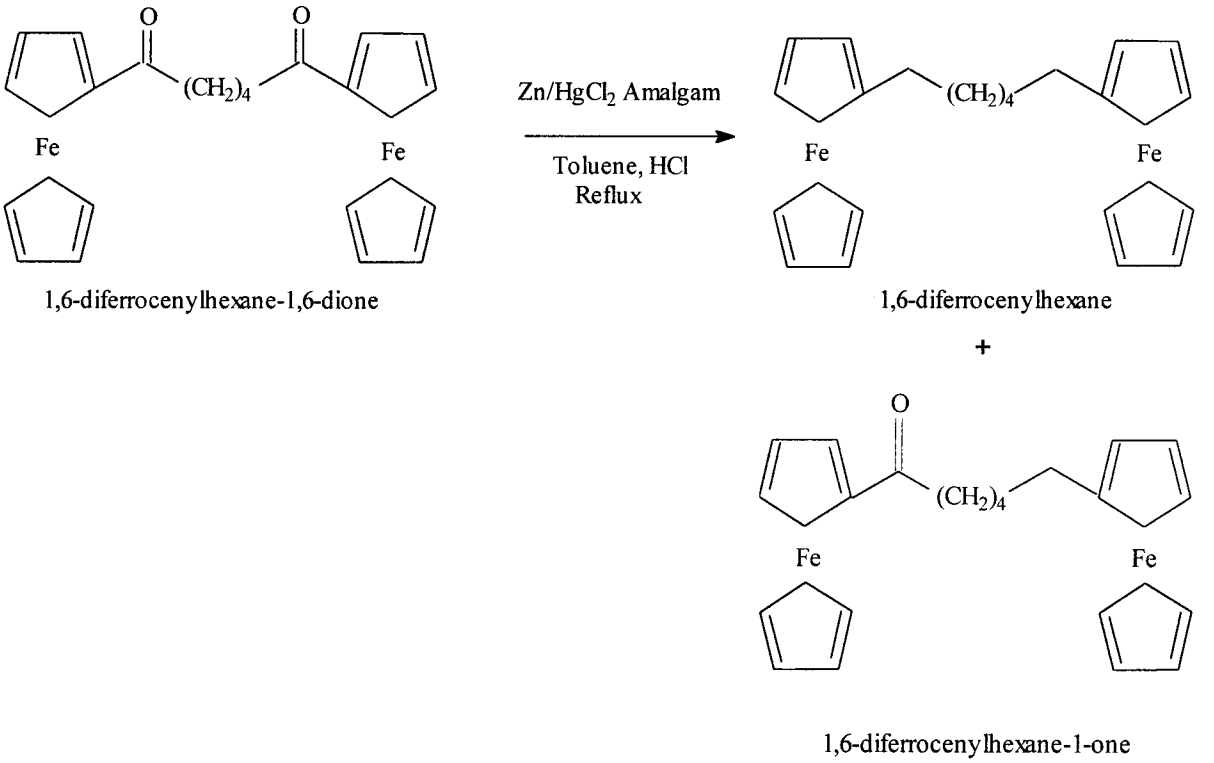
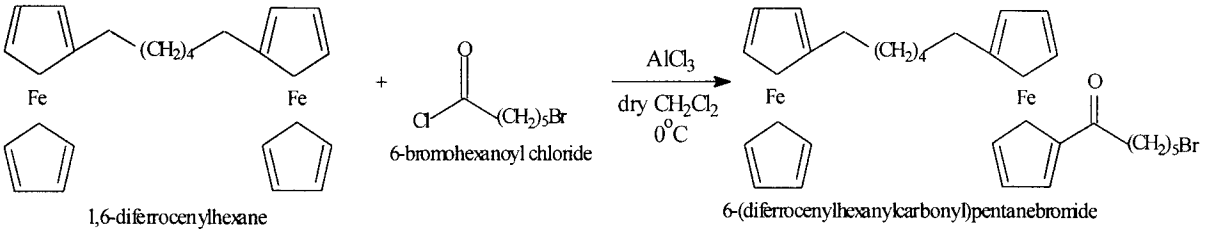
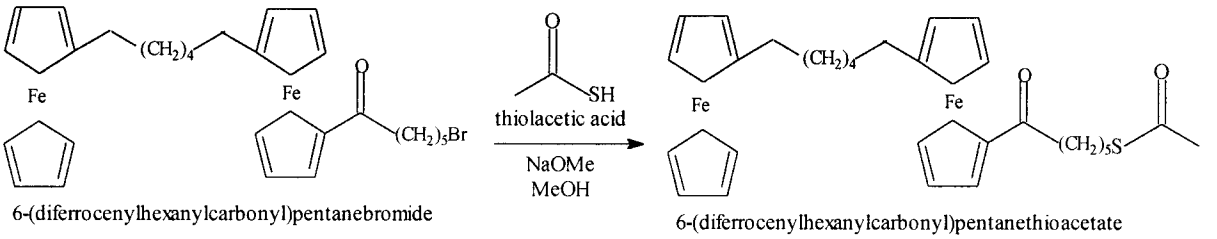


Figure 2.1: Schematic of Synthetic Pathway

Step Three: Friedel-Crafts Acylation



Step Four: Thiolation



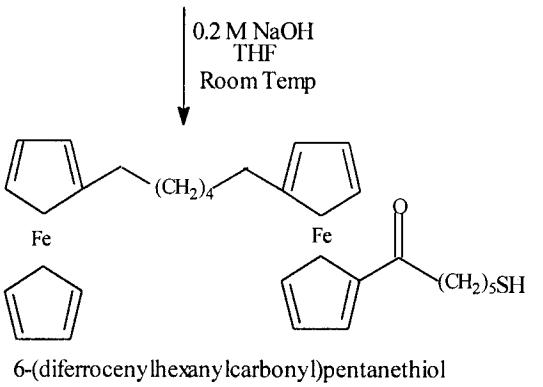


Figure 2.1, Continued: Schematic of Synthetic Pathway

chloride (Fisher, certified ACS, 99%), sodium hydroxide (Fisher, 97%), sodium sulfate (Fisher, certified ACS, 99%), tetrahydrofuran (Fisher, 99%), thiolacetic acid (Aldrich, 95%), toluene (Fisher, certified ACS, 99.9%) and zinc dust (Aldrich, 98%) were used as received.

Methylene chloride (Fisher, certified ACS, Fisher, 99.9%) was distilled over CaH_2 under nitrogen and used immediately. Methanol (Pharmco, 99.89%) was also distilled and used immediately. For reactions in which an inert atmosphere was required, pre-purified argon was delivered via a Schlenk line. Where appropriate, glassware was oven dried overnight at 110 °C and cooled under flowing argon. An overhead mechanical stirrer was used for reactions in which vigorous stirring was required.

Instrumentation

^{1}H and ^{13}C NMR spectra were obtained using a Varian-Gemini 2000 400 MHz NMR spectrometer using a deuterium lock, with chemical shifts reported as parts per million (ppm) downfield from TMS. IR spectra were obtained using an FT/IR 410 JASCO spectrometer, with the sample prepared as a KBr pellet and peak positions reported in wavenumbers. Direct probe mass spectrometry was performed using a Finnigan Model GCQ ion-trap spectrometer utilizing electron ionization to fragment the molecule.

Synthesis of 1,6-diferrocenylhexane-1,6-dione and 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

A modified version of the Friedel-Crafts acylation described by Chidsey[2], was used to prepare 1,6-diferrocenylhexane-1,6-dione and 1-ferrocenylcarbonyl-2-ferrocenyl-cyclopentene. Ferrocene (61.23 g, 0.329 mol) was dissolved in 700 mL of dry methylene chloride and cooled in an ice bath for fifteen minutes. Adipoyl chloride (24 mL, 0.165

mol) and anhydrous aluminum chloride (43.64 g, 0.327 mol) were added to the dissolved ferrocene. The reaction changed immediately from orange to deep purple. The ice bath was removed after fifteen minutes. After one and half-hours of stirring, 250 mL of deionized water was added dropwise via an addition funnel. The reaction began to slowly reflux and the color gradually turned back to orange. After an additional hour of stirring, the organic phase was extracted with deionized water until the aqueous layer was colorless, followed by three extractions with brine solution. The product was dried overnight over anhydrous sodium sulfate. The solvent was removed under reduced pressure and the crude product was purified via column chromatography using silica gel as the stationary phase and 75%/25% hexane/ethyl acetate as the eluent. Upon purification, two products were isolated. The first product (R_f = 0.7, 56% yield) was 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene, while the second (R_f = 0.5, 28% yield) was 1,6-diferrocenylhexane-1,6-dione.

Spectroscopic Data for 1,6-diferrocenylhexane-1,6-dione

^{1}H NMR (400 MHz, $CDCl_3$, ppm) 1.799 (broad m, 4H, peak E), 2.774 (t, 4H, peak D), 4.201 (s, 10H, peak A), 4.499 (t, 4H, peak B), 4.798 (t, 4H, peak C)

^{13}C NMR (400 MHz, $CDCl_3$, ppm) 25.715 (2C, peak G), 40.850 (2C, peak F), 70.492 (10C, peak A), 70.939 (4C, peak B), 73.352 (4C, peak C), 80.159 (2C, peak D), 205.191 (2C, peak E)

IR spectroscopy (ν_{max}/cm^{-1}) 3000-2950 (CH_2 stretching), 1658.48 (C=O stretching), 1453.10 (CH_2 bending), 1258.32 (C-C bending), 1069.33 (CH stretching), 827.31 (C=C stretching)

Mass spectrometry: parent ion peak at 482 m/z

Spectroscopic Data for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

^{1}H NMR (400 MHz, $CDCl_3$, ppm) 1.256 (m, 2H, peak E), 2.076 (q, 1H, peak F), 2.888 (t, 2H, peak D), 4.072 (s, 5H, peak I), 4.105 (s, 2H, peak H), 4.162 (s, 5H, peak A), 4.194 (s, 2H, peak G), 4.418 (s, 2H, peak B), 4.668 (s, 2H, peak C)

^{13}C NMR (400 MHz, $CDCl_3$, ppm) 24.349 (1C, peak I), 38.765 (1C, peaks H), 39.189 (1C, peak G), 69.567 (2C, peak L), 69.977 (2C, peak M), 70.250 (5C, peak N), 70.933 (5C, peak A), 71.570 (2C, peak B), 73.255 (2C, peak C), 80.181 (1C, peak D), 81.312 (1C, peak K), 136.984 (1C, peak J), 142.143 (1C, peak F), 203.248 (1C, peak E)

IR spectroscopy (ν_{max}/cm^{-1}) 3000-2950 (CH_2 stretching), 1631.48 (C=O stretching), 1444.42 (CH_2 bending), 1270.86 (C-C bending), 1103.08 (CH stretching), 823.46 (C=C stretching)

Mass spectrometry: parent ion peak at 464 m/z.

Synthesis of 1,6-diferrocenylhexane and 1,6-diferrocenylhexane-1-one

A Clemmensen reduction was carried out on the purified 1,6-diferrocenylhexane-1,6-dione to reduce the carbonyls into methylene groups according to the method of Creager[3]. The 1,6-diferrrocenylhexane-1,6-dione (8.49 g, 0.018 mol) was dissolved in 100 mL of toluene and transferred to a three neck round bottom flask. A zinc-mercury amalgam was prepared by dissolving mercuric chloride (1.20 g, 0.00442 mol) in 30 mL of deionized water, followed by addition of zinc dust (17.59 g, 0.269 mol). Deionized water (30 mL) and concentrated hydrochloric acid (12 M, 47 mL, 1.54 mol) were added to the solution and the mixture was heated to reflux under static argon for six hours. An overhead mechanical stirrer was used to ensure the biphasic mixture was in proper contact with the amalgam at all times throughout the reaction. After two and a half hours, an additional

portion of HCl (12 mL, 0.394 mol) was added, followed by a similar addition two and half hours later. The reaction was allowed to stir for another hour. Once the mixture had cooled to room temperature, the organic portion was extracted three times with deionized water, followed by three extractions with brine solution. The resulting crude product was then dried over anhydrous sodium sulfate overnight and the solvent was removed under reduced pressure. The product was purified using column chromatography with silica gel as the stationary phase and 75%/25% hexane/ethyl acetate as the mobile phase. Two products were isolated, those being the fully reduced product, 1,6-diferrocenylhexane (R_f = 0.6, 76 % yield), and the monoreduced product, 1,6-diferrocenylhexane-1-one (R_f = 0.4, yield 8.8%). Both products were isolated and fully characterized.

Spectroscopic Data for 1,6-diferrocenylhexane

^{1}H NMR (400 MHz, $CDCl_3$, ppm) 1.337 (broad m, 4H, peak F), 1.500 (broad m, 4H, peak E), 2.308 (t, 4H, peak D), 4.054 (m, 4H, peak C), 4.071 (m, 4H, peak B), 4.106 (m, 10H, peak A)

^{13}C NMR (400 MHz, $CDCl_3$, ppm) 22.799 (2C, peak G), 29.620 (4C, peak F), 31.175 (4C, peak E), 67.114 (4C, peak C), 68.169 (4C, peak B), 68.594 (10C, peak A), 89.617 (2C, peak D)

IR spectroscopy (ν_{max}/cm^{-1}) 2917.77 cm^{-1}-2847.38 cm^{-1} (CH_2 stretching), 1393.32 cm^{-1} (CH_2 bending), 1104.05 cm^{-1} (C-C bending), 1020.16 cm^{-1} (CH stretching), 815.74 cm^{-1} (C=C stretching)

Mass spectrometry: parent ion peak occurs at 454 m/z

Spectroscopic Data for 1,6-diferrocenylhexane-1-one

^{1}H NMR (400 MHz, $CDCl_3$, ppm) 1.408 (t, 2H, peak F), 1.555 (t, 2H, peak G), 1.725 (t, 2H, peak E), 2.347 (t, 2H, peak H), 2.695 (t, 2H, peak D), 4.050 (m, 1H, peak I), 4.073 (m, 2H, peak J), 4.102 (s, 5H, peak K), 4.192 (s, 5H, peak A), 4.487 (s, 2H, peak B), 4.777 (s, 2H, peak C)

^{13}C NMR (400 MHz, $CDCl_3$, ppm) 25.700 (1C, peak G), 30.722 (1C, peaks H and I), 32.361 (1C, peak J), 40.896 (1C, peak F), 68.278 (2C, peak L), 69.325 (2C, peak M), 69.711 (2C, peak N), 70.478 (2C, peak A), 70.895 (5C, peak B), 73.277 (5C, peak C), 80.280 (1C, peak D), 90.462 (1C, peak K), 205.403 (1C, peak E)

IR spectroscopy (ν_{max}/cm^{-1}) 2927.89 cm^{-1} (CH_2 stretching), 1675.84 cm^{-1} (C=O stretching), 1454.06 cm^{-1} (CH_2 bending), 1248.68 cm^{-1} (C-C bending), 1103.57 cm^{-1} (C-C stretching), 1025.46 cm^{-1} (CH stretching), 817.67 cm^{-1}(C=C stretching)

Mass spectrometry: parent ion peak at occurs at 468 m/z

Synthesis of 6-(diferrocenylhexanylcarbonyl)pentanebromide

Another Friedel Crafts acylation, as reported by Chidsey[2], was carried out on the purified 1,6-diferrocenylhexane. A 300 mL, oven-dried round bottom flask was cooled under flowing argon and 40 mL of dry methylene chloride was used to dissolve the 1,6-diferrocenylhexane (6.02 g, 0.0133 mol). The flask was stoppered and cooled in an ice bath for fifteen minutes. The 6-bromohexanoyl chloride (2.0 mL, 0.0131 mol) was added and the ice bath was removed. Anhydrous $AlCl_3$ (1.80g, 0.0135 mol) was then added to the mixture, which immediately turned from orange to deep purple. The mixture was stirred for one and half-hours under static argon and then quenched with 27 mL of deionized water, added via an additional funnel. The solution was then stirred for an

additional half-hour. The organic phase was extracted three times with deionized water until the aqueous layer was colorless, followed by three extractions with brine solution. The resulting organic phase was dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The crude product was purified using column chromatography with silica gel as the stationary phase and 80%/20% hexane/ethyl acetate as the eluent. Five products were isolated after running several columns. The second compound (R_f = 0.6, 0.5% yield) was the desired product, 6-(diferrocenylhexanyl-carbonyl)pentanebromide.

Spectroscopic Data for 6-(diferrocenylhexanylcarbonyl)pentanebromide

^{1}H NMR (400 MHz, $CDCl_3$, ppm) 1.254 (broad s, 2H, peak F), 1.352 (t, 4H, peak M), 1.540 (m, 4H, peak E), 1.731 (t, 2H, peak L), 1.928 (q, 2H, peak N), 2.300 (t, 4H, peak D), 2.786 (m, 2H, peak K), 3.445 (t, 2H, peak O), 4.029 (broad d, 2H, peak C), 4.047 (broad d, 2H, peak B), 4.086 (s, 5H, peak A), 4.111 (s, 4H, peaks G and H), 4.408 (q, 2H, peak I), 4.589 (q, 2H, peak J)

^{13}C NMR (400 MHz, $CDCl_3$, ppm) 24.676 (2C, peak G), 29.349 (1C, peak P), 30.669 (2C, peak F), 30.814 (2C, peak E), 32.331 (1C, peak Q), 34.000 (1C, peak O), 35.009 (1C, peak R), 41.215 (1C, peak N), 68.141 (2C, peak C), 69.218 (2C, peak B), 69.628 (5C, peak A), 70.758 (2C, peak H), 71.350 (2C, peak I), 71.722 (2C, peak J), 74.484 (2C, peak K), 76.949 (1C, peak L), 93.231 (2C, peak D), 206.260 (1C, peak M)

Mass spectrometry: The parent ion peak occurs at 631 m/z

Synthesis of 6-(diferrocenylhexanylcarbonyl)pentanethiol

The purified product was thiolated by dissolving sodium methoxide (0.03 g, 0.555 mmol) in 25 mL of distilled methanol according to the method of Hickman[5] et.al.

Thiolacetic acid (35 μL, 0.037 g, 0.388 mmol) was added to the methanol via a syringe. The 6-(diferrocenylhexanylcarbonyl)pentanebromide (0.15 g, 0.238 mmol) was dissolved in 25 mL of freshly distilled methanol and added to the reaction flask. The reaction was refluxed under static argon for eighteen hours. The methanol was removed under reduced pressure and the product was collected as an orange syrup. The crude product was purified via column chromatography with silica gel as the stationary phase and 60%/40% hexane/ethyl acetate as the mobile phase. The purified thioacetate salt (0.020 g, 0.0319 mmol) was dissolved in 10 mL of deoxygenated tertrahydrofuran. Two drops of deoxygenated 0.2 M NaOH (0.04 g in 50 mL deionized water) was added and the solution was stirred at room temperature overnight. The THF was removed under reduced pressure and the product was purified via column chromatography using a silica gel as the stationary phase and 60%/40% hexane/ethyl acetate as the eluent. The final product, 6-(diferrocenylhexanylcarbonyl)pentanethiol (R_f = 0.5, 75 % yield), was isolated and fully characterized.

Spectroscopic Data for 6-(diferrocenylhexanylcarbonyl)pentanethiol

^{1}H NMR (400 MHz, $CDCl_3$, ppm) 1.240 (s, 1H, peak P), 1.258 (m, 4H, peak F), 1.353 (t, 4H, peak M), 1.501 (m, 2H, peak N), 1.573 (m, 4H, peak E), 1.742 (t, 2H, peak L), 2.294 (t, 4H, peak D), 2.494 (m, 2H, peak O), 2.784 (m, 2H, peak K), 4.039 (m, 2H, peak C), 4.062 (m, 2H, peak B), 4.094 (broad m, 5H, peak A), 4.130 (s, 2H, peak G), 4.147 (s, 2H, peak H), 4.404 (q, 2H, peak I), 4.595 (q, 2H, peak J)

^{13}C NMR (400 MHz, $CDCl_3$, ppm) 25.108 (2C, peak G), 29.630 (1C, peak P), 30.434 (1C, peak Q), 30.677 (2C, peak F), 30.821 (2C, peak E), 31.595 (1C, peak O), 33.181 (1C, peak R), 41.306 (1C, peak N), 68.126 (2C, peak C), 69.203 (2C, peak B), 69.605

(5C, peak A), 70.743 (2C, peak H), 71.350 (2C, peak I), 71.783 (2C, peak J), 74.438 (2C, peak K), 76.995 (1C, peak L), 93.193 (2C, peak D), 206.420 (1C, peak M)

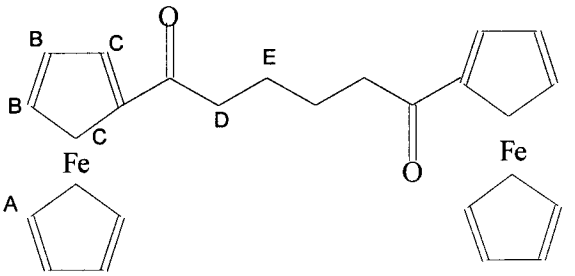
Mass spectrometry: The parent ion peak occurs at 585 m/z

RESULTS AND DISCUSSION

Characterization of 1,6-diferrocenylhexane-1,6-dione

The ^{1}H NMR of 1,6-diferrocenylhexane-1,6-dione in $CDCl_3$ is shown in Figure 2.2. The broad peak at 1.255 ppm is from the hexane used to purify the product. The inner methylene protons on the six-carbon chain joining the two ferrocenes show a broad signal at 1.799 ppm (peak E). The protons neighboring the carbonyl were shifted downfield to 2.774 ppm (peak D) due to the electron withdrawing carbonyl substituent. The protons on the bottom cyclopentadienyl (Cp) ring showed a strong singlet at 4.201 ppm (peak A). This peak will recur throughout the following ^{1}H NMR assignments and will be very distinguishable from other peaks. The two protons on the top Cp ring that are two bonds away from the carbonyl shows a triplet at 4.798 ppm (peak C) and the protons three bonds away from the carbonyl show a triplet at 4.499 ppm (peak B). Protons in this region are common for carbonyl substituted ferrocene compounds.

^{13}C NMR of 1,6-diferrocenylhexane-1,6-dione was also performed in $CDCl_3$ and is shown in Figure 2.3. The carbons in the methylene bridge that are the farthest from the oxygen should be shifted upfield with the adjacent carbons downfield. The methylene carbon two bonds away from the carbonyl is located at 25.715 ppm (peak G) while the carbon one away is at 40.850 ppm (peak F). The region in the ^{13}C spectra between 70 and 80 ppm had to be magnified to assign the remaining peaks, as shown in Figure 2.4. The bottom Cp ring carbons are at 70.492 ppm (peak A), which is a characteristic peak



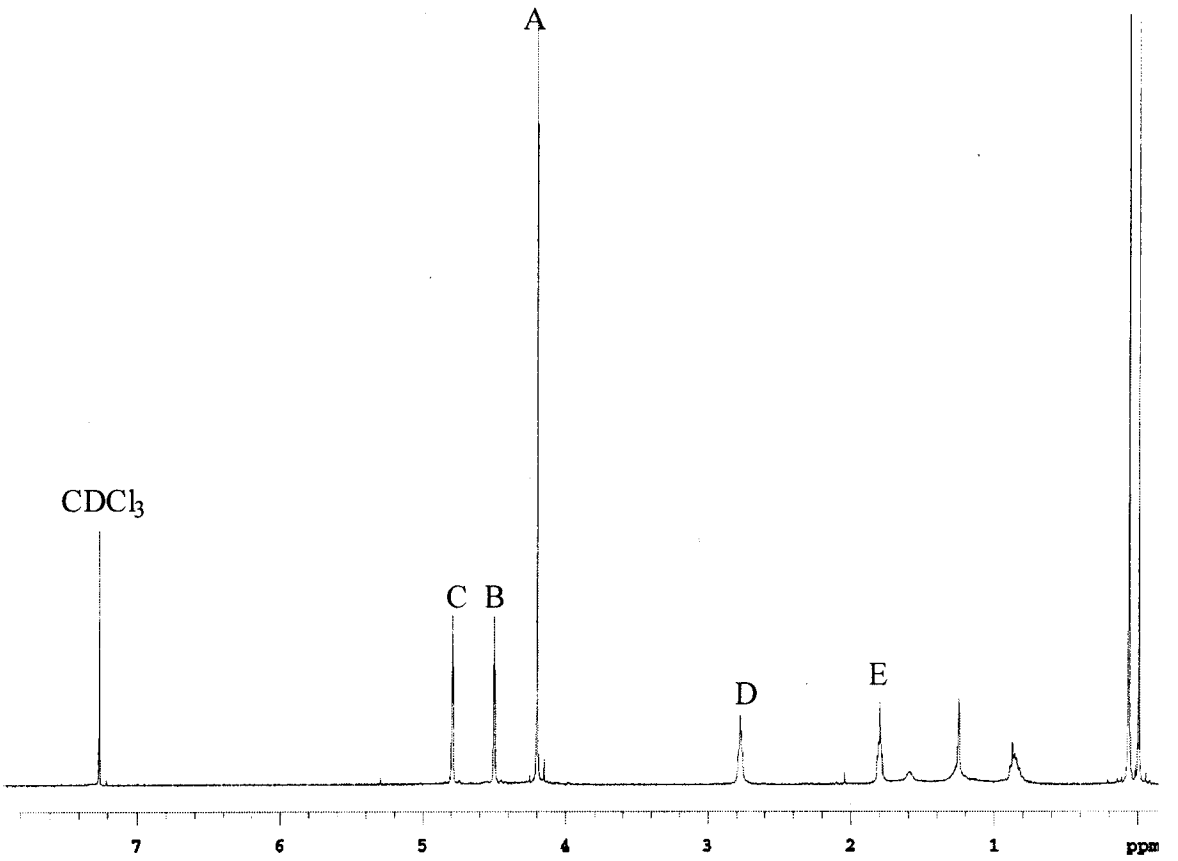
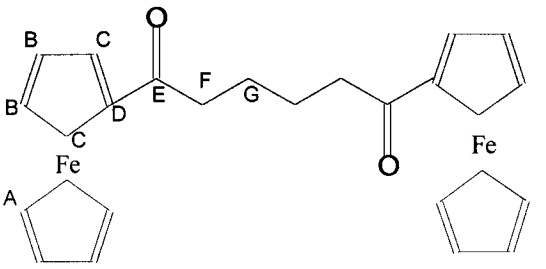


Figure 2.2: ^{1}H NMR spectrum of 1,6-diferrocenylhexane-1,6-dione



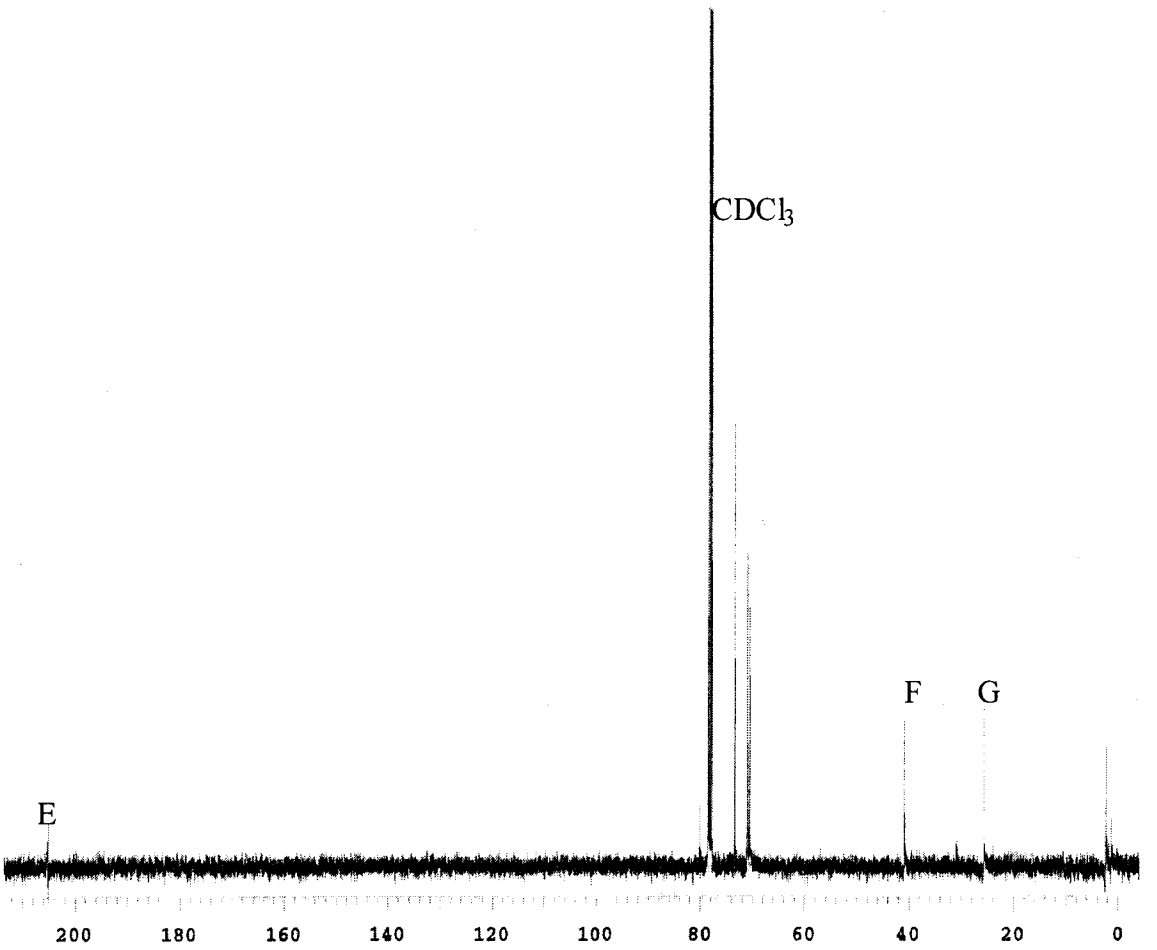


Figure 2.3: ^{13}C NMR spectrum of 1,6-diferrocenylhexane-1,6-dione

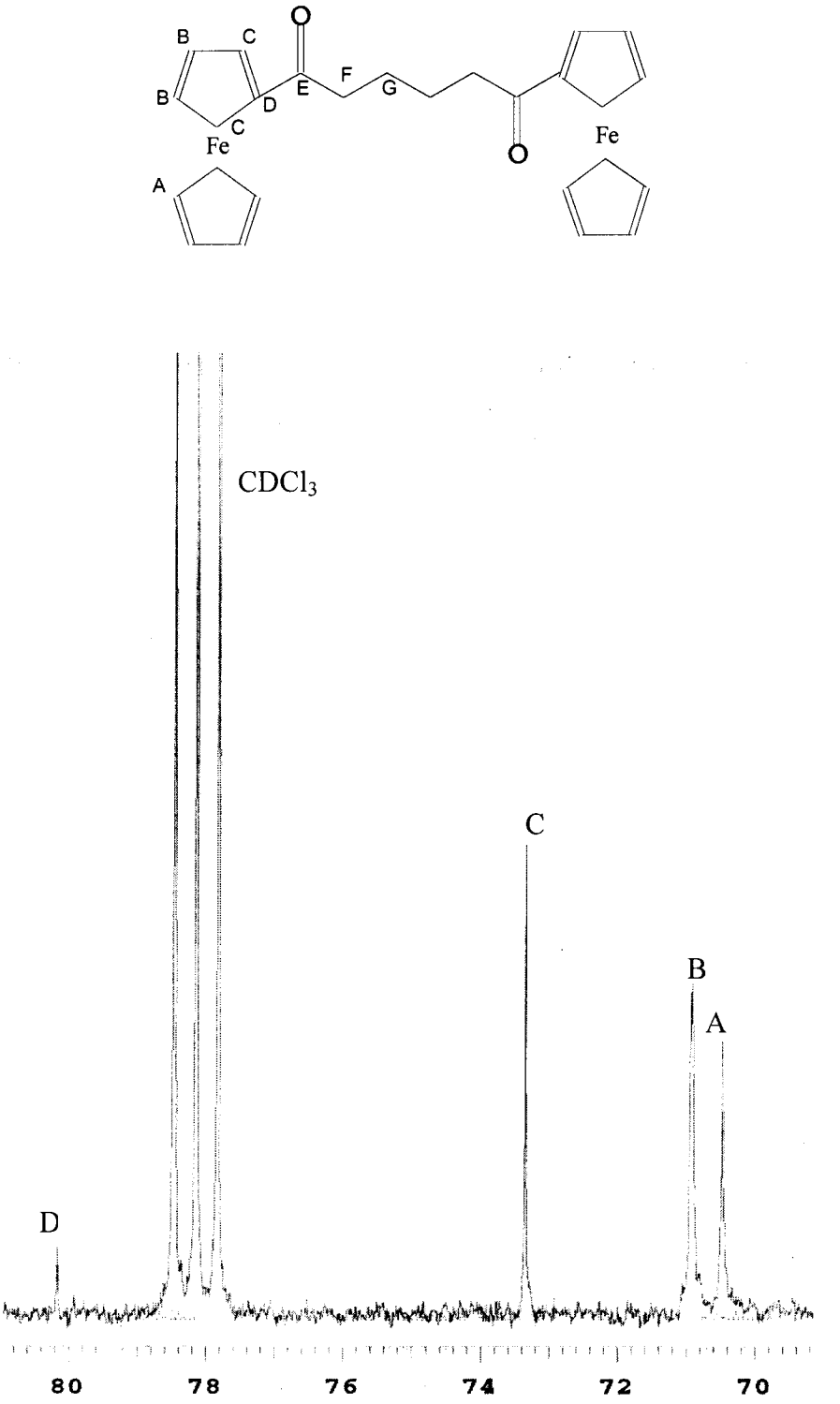


Figure 2.4: ^{13}C NMR spectrum close up from 70-85 ppm of 1,6-diferrocenylhexane-1,6-dione

in the ferrocene compounds. The carbons in the top Cp ring that are two and three bonds away from the carbonyl show chemical shifts at 73.352 ppm (peak C) and 70.939 ppm (peak B), respectively. The carbon in the Cp ring directly attached to the carbonyl, shows a low intensity peak at 80.159 ppm (peak D). The low intensity is due to the fact no protons are attached to that carbon. The carbonyl carbon was easily assigned at 205.191 ppm (peak E).

The IR spectrum, shown in Figure 2.5, was assigned with close attention to a strong absorbing carbonyl stretch at 1658.48 cm^{-1}. Stretching from the C=C bonds in the Cp rings occurs between 3000 and 2950 cm^{-1}, with CH_2 bending from the methylenes at 1453.10 cm^{-1}. Single carbon-carbon bonds in the methylene bridge occurred at 1258.32 cm^{-1} and 827.31 cm^{-1}. CH stretching at 1069.33 cm^{-1} was attributed to the Cp rings.

Direct probe mass spectrometry on 1,6-diferrocenylhexane-1,6-dione dissolved in CH_2Cl_2 was performed and the results are shown in Figure 2.6. The parent ion peak is easily assigned at 482 m/z. A common feature in fragmenting of ferrocene compounds, is the loss of a bottom Cp ring. This is evident from the peak at 417 m/z. Refer to Table 2.1 for the assignments of the remaining major fragments.

Characterization of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

The ^1H NMR spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene in $CDCl_3$ is shown in Figure 2.7. The protons the farthest upfield at 1.256 (peak E) are located at the apex of the cyclopentene ring. The protons adjacent to the apex are located at 2.706 ppm (peak F) and 2.888 ppm (peak D). Peak D is shifted downfield from the other protons due to the carbonyl substituent. The large singlet at 4.072 ppm (peak I) is assigned to the bottom Cp ring protons closest to the cyclopentene ring. The other unsubstituted Cp

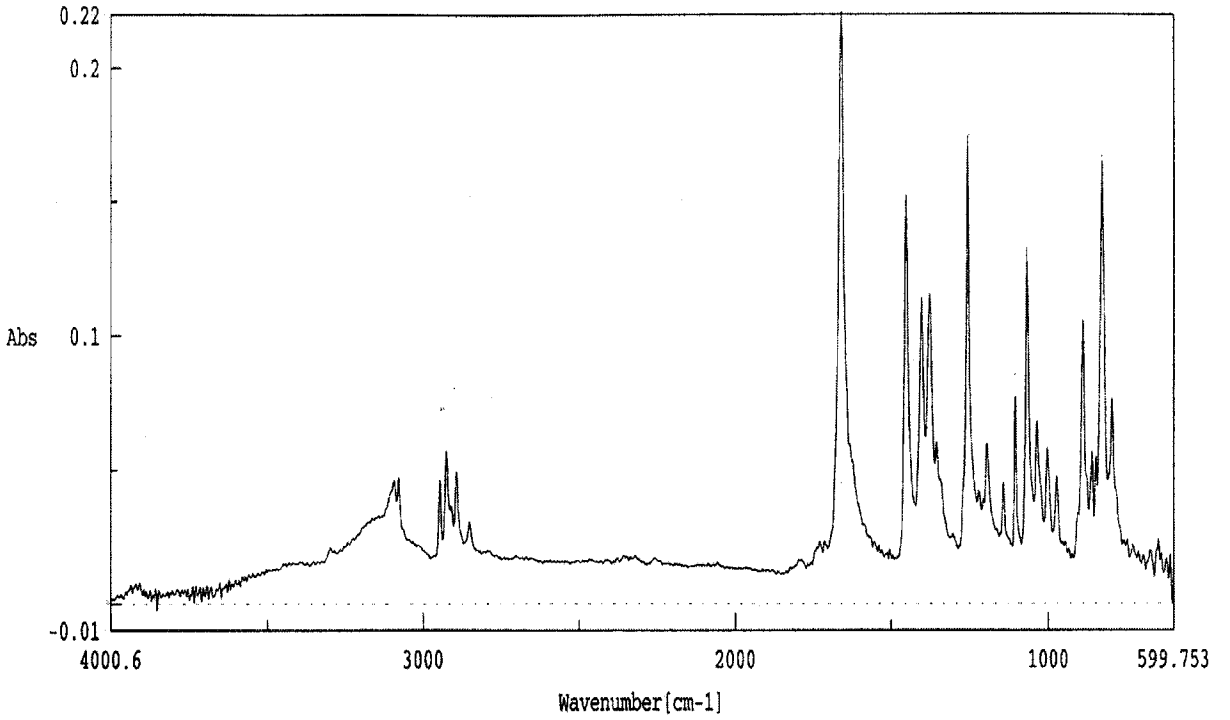


Figure 2.5: IR spectrum of 1,6-diferrocenylhexane-1,6-dione

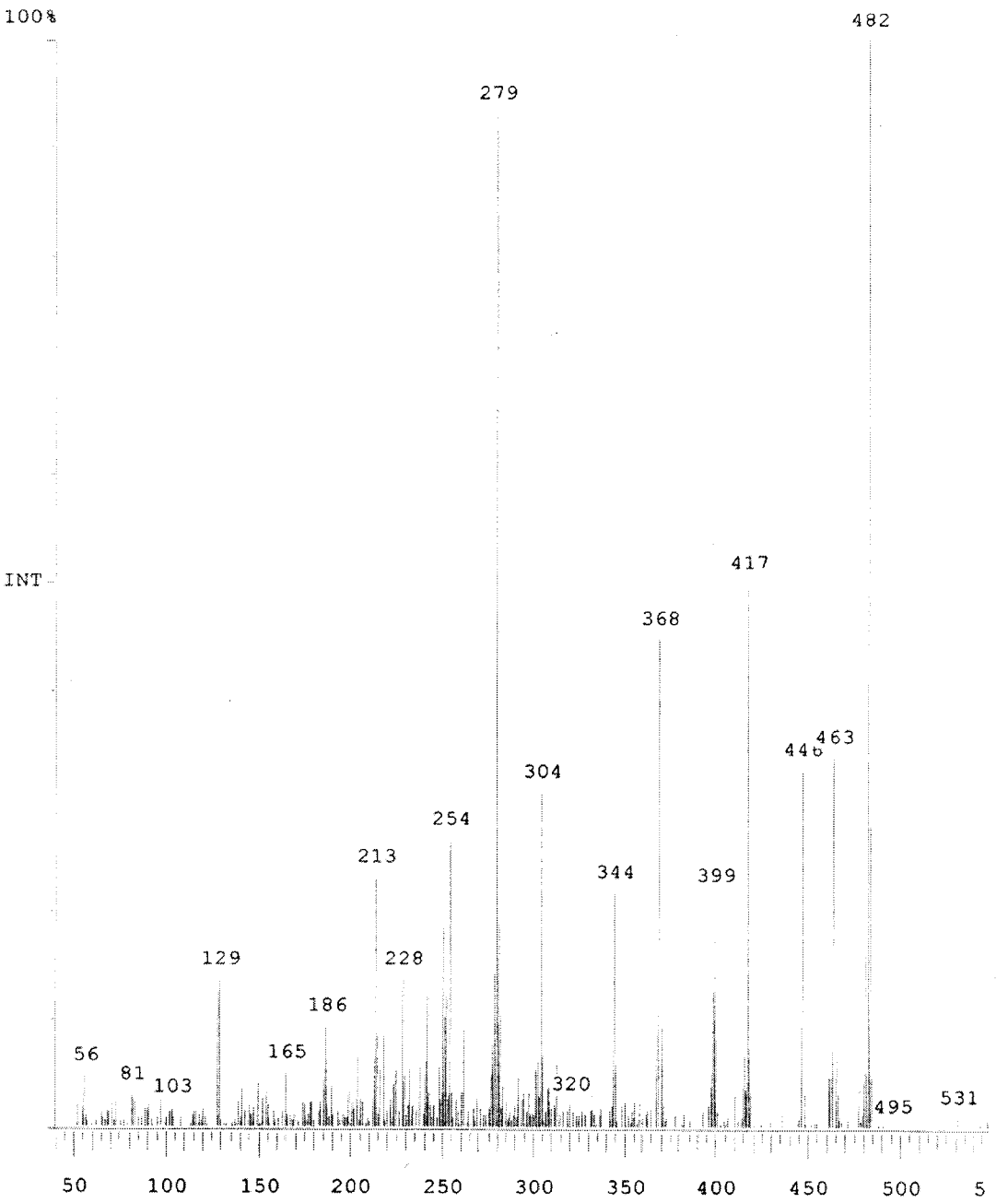
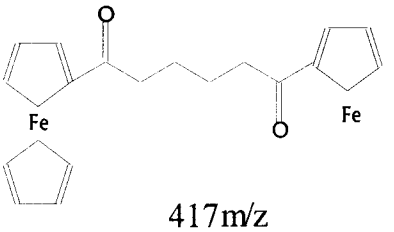


Figure 2.6: Mass spectrum of 1,6-diferrocenylhexane-1,6-dione

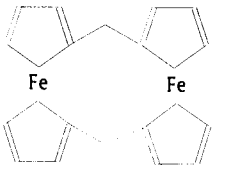
Table 2.1

Assigned Fragments from 1,6-diferrocenylhexane-1,6-dione Mass Spectrum

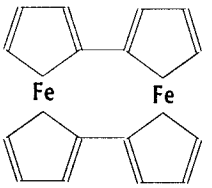
Fragments



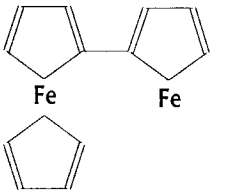
417m/z



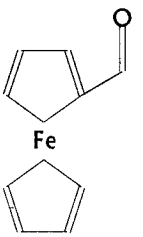
399 m/z



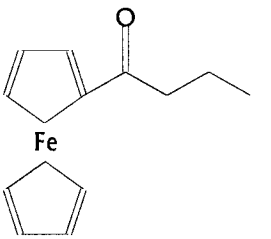
368 m/z



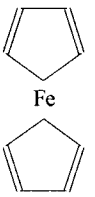
304 m/z



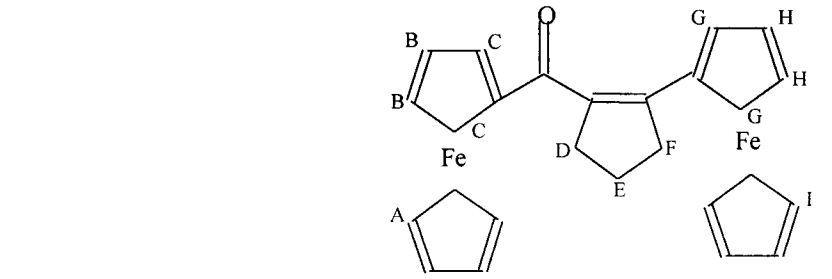
213 m/z



254 m/z



186 m/z



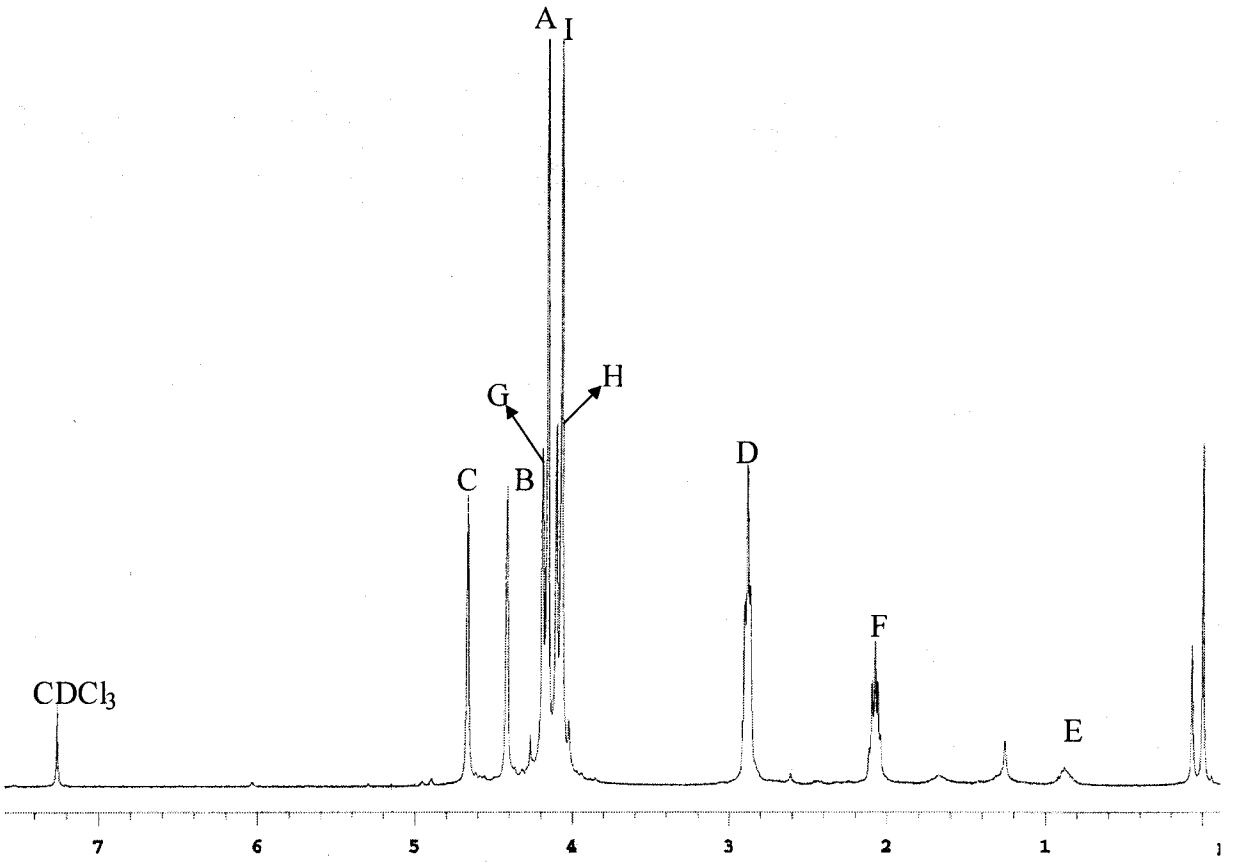
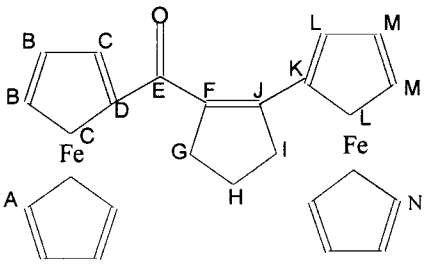


Figure 2.7: ^{1}H NMR spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

ring protons are a singlet at 4.162 ppm (peak A). The protons on the top Cp ring adjacent to the cyclopentene ring are shown in the same region at 4.105 ppm (peak H) and 4.194 ppm (peak G). However, the similar protons on the other Cp ring are shifted downfield due to the proximity of the electron withdrawing carbonyl substituent. The protons two and three bonds away from the carbonyl are shown at 4.668 ppm (peak C) and 4.418 ppm (peak B), respectively.

The ^{13}C NMR spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene in $CDCl_3$ is shown in Figure 2.8. The methylene carbon at the apex of the five-membered ring showed a peak at 38.765 ppm (peak H). The adjacent methylene carbons at 24.349 ppm (peak I) and 39.189 ppm (peak G) were extremely close to one another, but peak G was shifted downfield due to the proximity of the carbonyl substituent. The ^{13}C spectra in the region from 70 to 80 ppm was expanded and is shown in Figure 2.9. The carbons in the top Cp ring directly attached to the cyclopentene ring demonstrated chemical shifts at 69.567 ppm (peak L) and 69.977 ppm (peak M), which were one and two bonds away, respectively. The carbons on the lower Cp ring attached to the cyclopentene ring were found downfield slightly at 70.250 ppm (peak N). The characteristic peak at 70.933 ppm (peak A) was assigned to the bottom Cp ring carbons of the ferrocene attached to the carbonyl. The four carbons in the upper ring that were two and three bonds away from the carbonyl were downfield from peak A at 73.255 ppm (peak C) and 71.570 ppm (peak B), respectively. The carbon in the ferrocene ring to which the carbonyl is directly attached is located at 80.181 ppm (peak D) while the carbon in the other Cp ring attached to the cyclopentene is at 81.312 ppm (peak K). The sp^2 carbons in the five-membered ring to which the ferrocene and carbonyl are directly attached, are located at



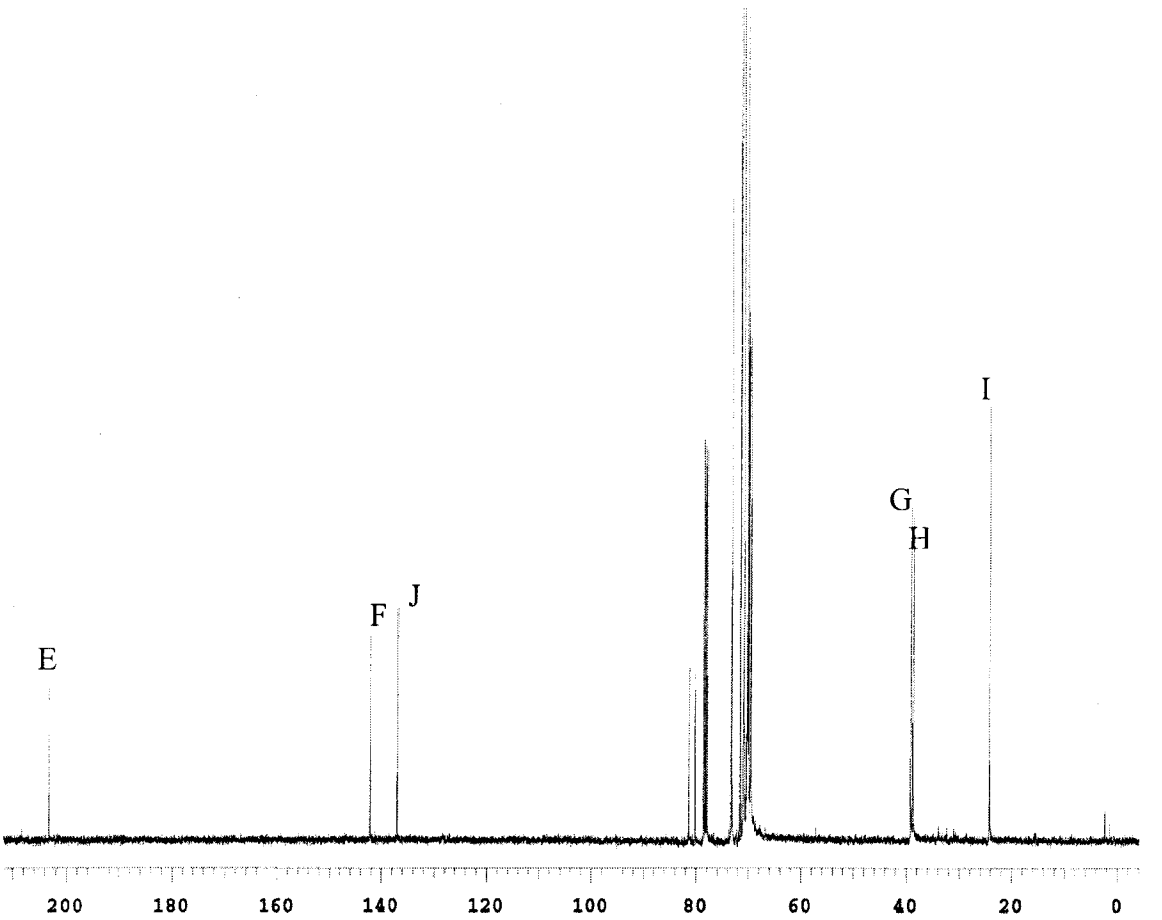
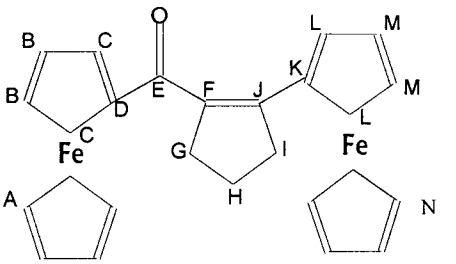


Figure 2.8: ^{13}C NMR spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene



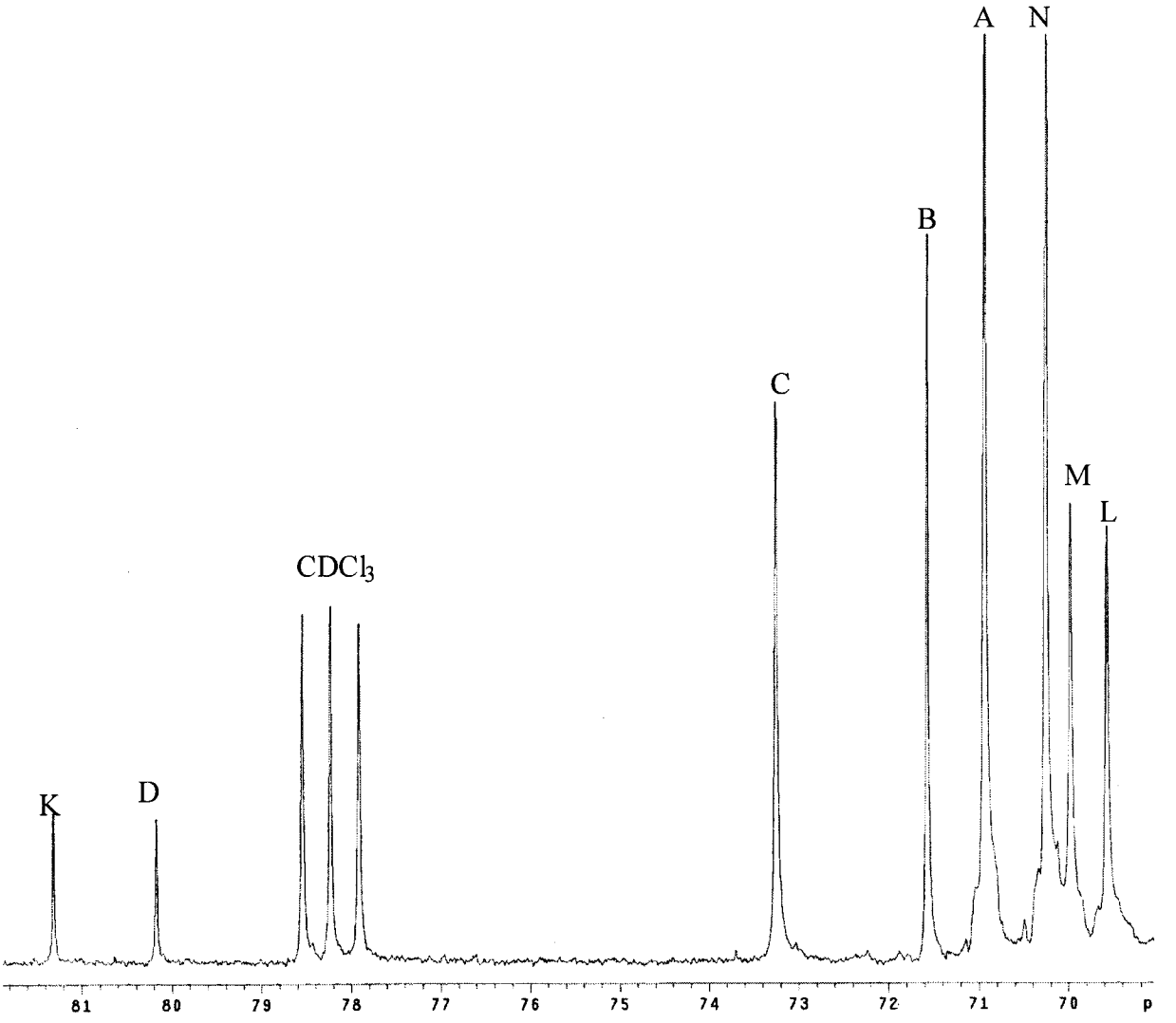


Figure 2.9: ^{13}C NMR spectrum close up from 69-82 ppm of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

136.984 ppm (peak J) and 142.143 ppm (peak F), respectively. Lastly, the carbonyl carbon displays the characteristic chemical shift at 203.248 ppm (peak E).

To aid the in the ^{13}C NMR assignments, due to the complexity of this molecule, an Attached Proton Test (APT) was performed. Spectra of this nature will distinguish between carbons that have even or odd numbered protons attached to it. Carbons with even number of protons attached, i.e. zero or two, will show chemical shifts that point up, while carbons with odd number of carbons attached, i.e. one or three, will display chemical shifts that point down. This spectrum confirmed the ^{13}C NMR assignments and is shown in Figure 2.10.

The IR spectrum is shown in Figure 2.11 and displays a strong carbonyl stretch at 1631.48 cm^{-1}. Methylene stretching and bending from the Cp rings appears at 3000-2950 cm^{-1} and 1444.42 cm^{-1}, respectively. Unsaturated carbon bending from the methylene bridge was evident from the peak at 1270.86 cm^{-1} and saturated carbons in the Cp rings displayed absorbances at 832.46 cm^{-1}. The C-H stretching from the Cp rings were assigned to the peak at 1103.08 cm^{-1}.

Direct probe mass spectrometry analysis indicated that the parent ion peak occurred at 464 m/z and is shown in Figure 2.12. The next major fragment, 399 m/z, was due to the loss of a bottom Cp ring. The assignment of the remaining fragments is shown in Table 2.2.

Characterization of 1,6-diferrocenylhexane

The ^{1}H NMR spectrum of 1,6-diferrocenylhexane in $CDCl_3$ is shown in Figure 2.13. The inner methylene protons in the carbon bridge were located upfield at 1.337 ppm (peak F). The next two methylene protons were shifted downfield to 1.500 ppm (peak E)

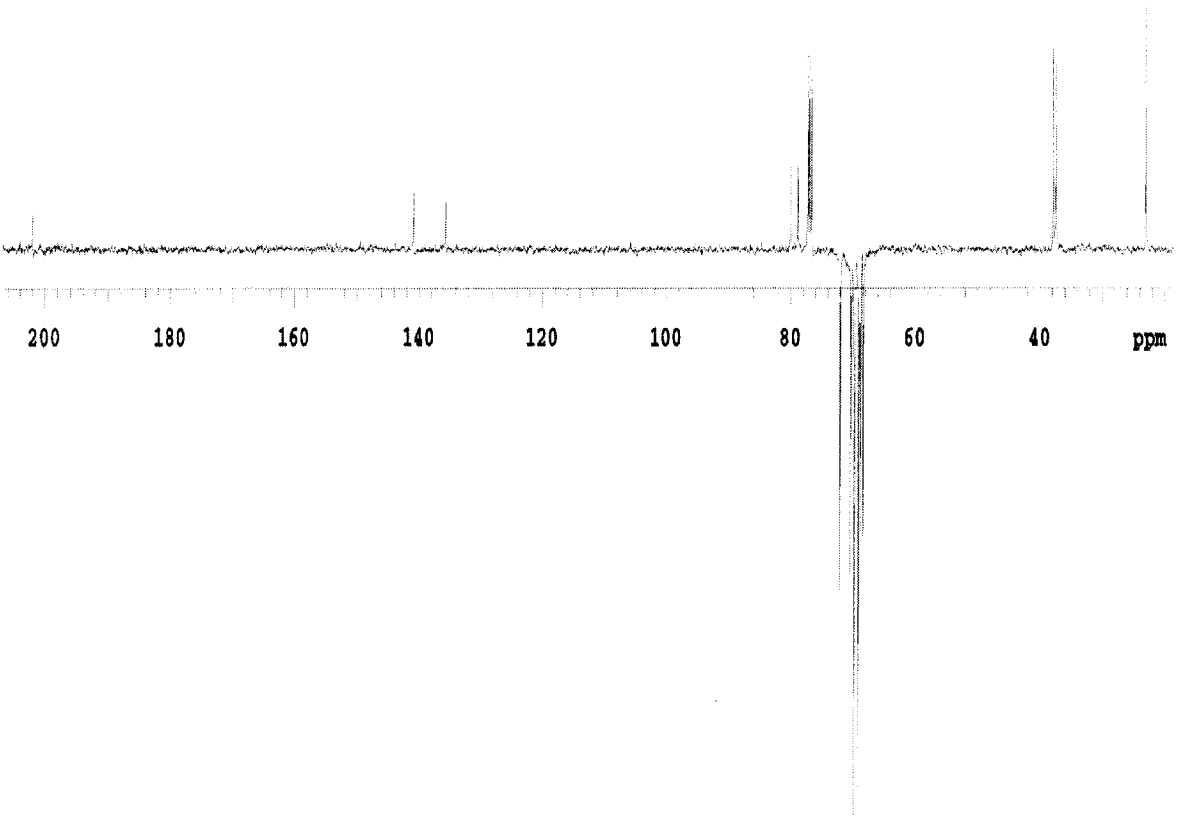


Figure 2.10: APT spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

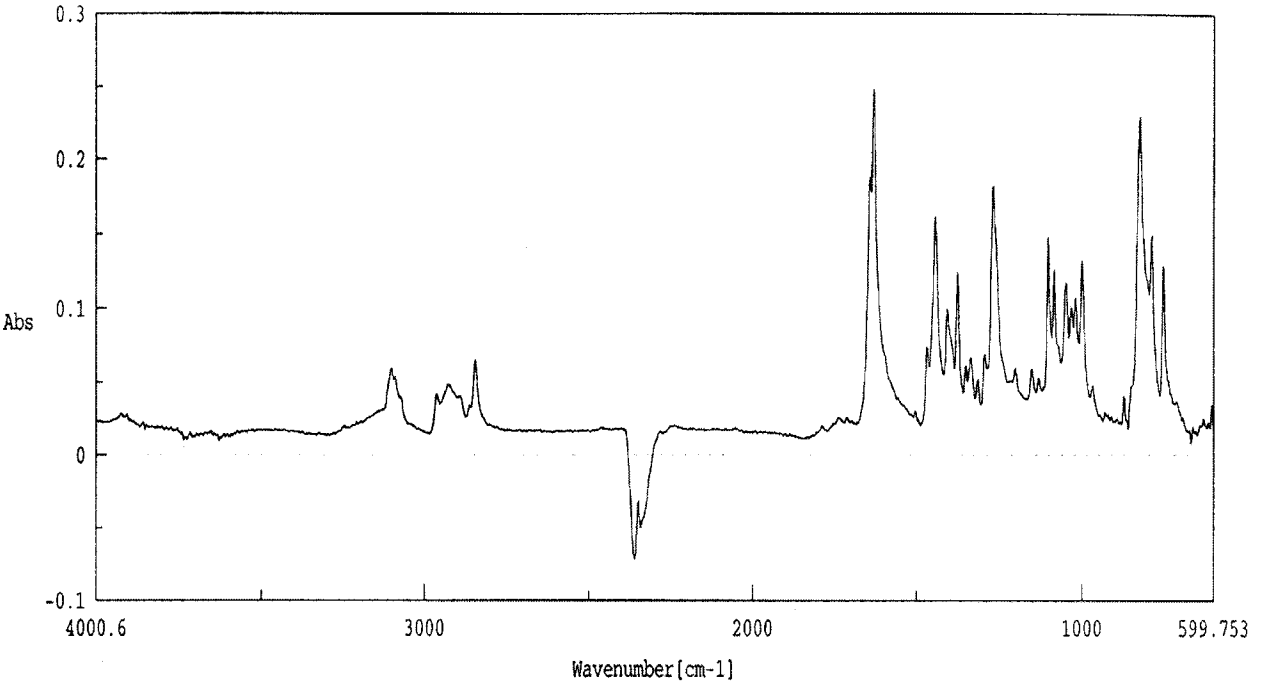


Figure 2.11: IR spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

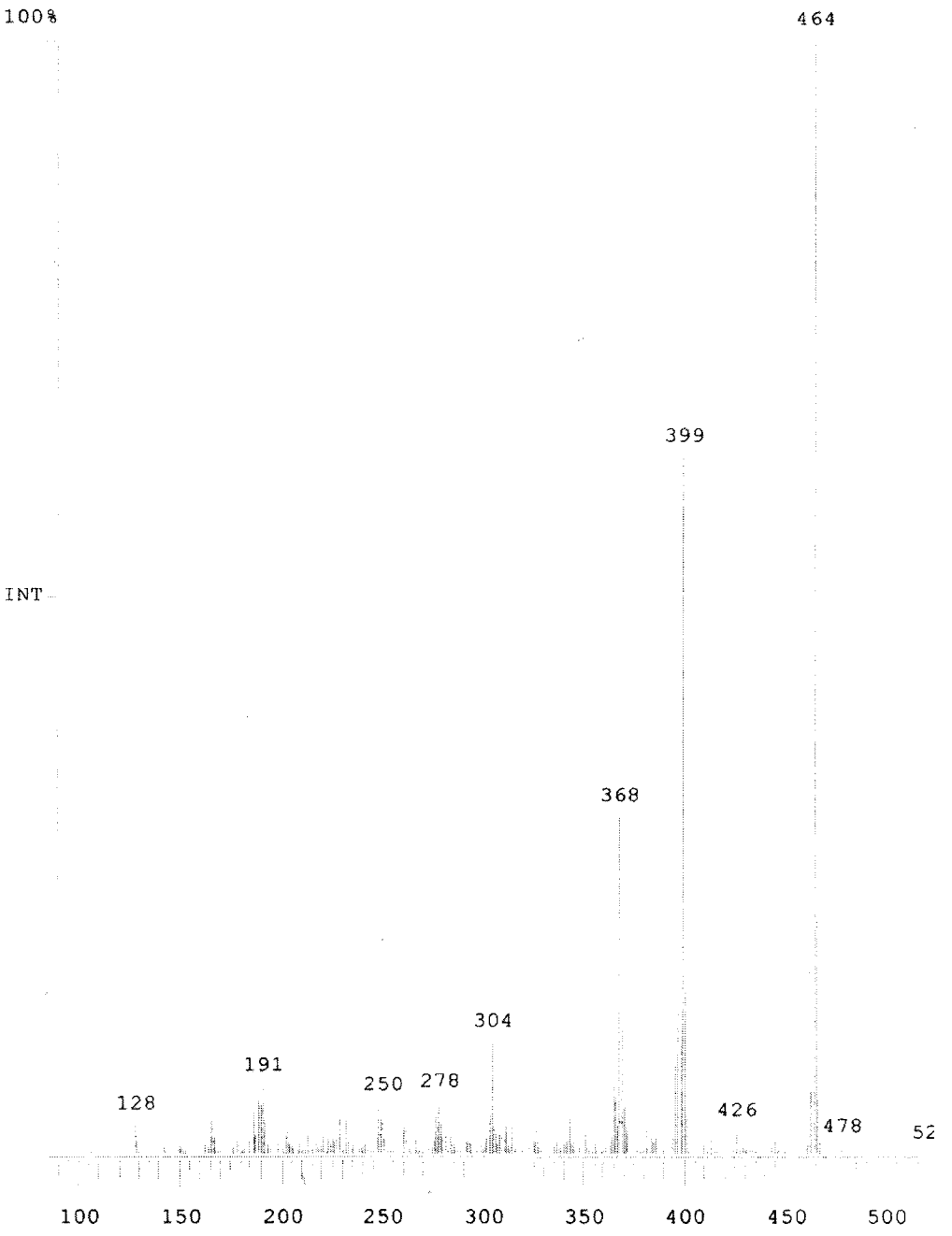
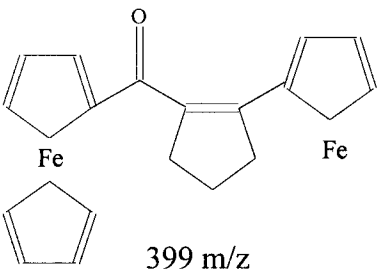


Figure 2.12: Mass spectrum of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Table 2.2

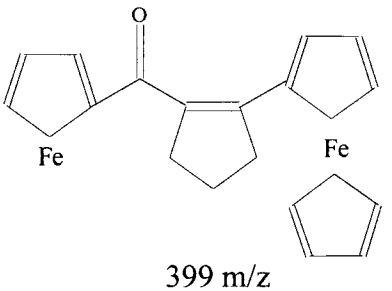
Assigned Fragments from 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene Mass Spectrum

Fragments

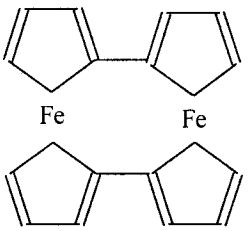


399 m/z

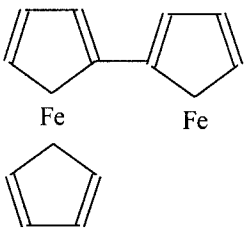
or



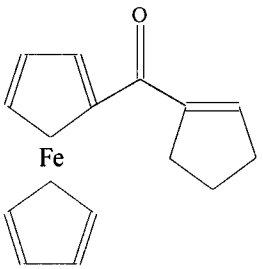
399 m/z



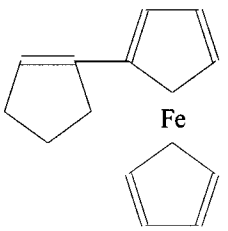
368 m/z



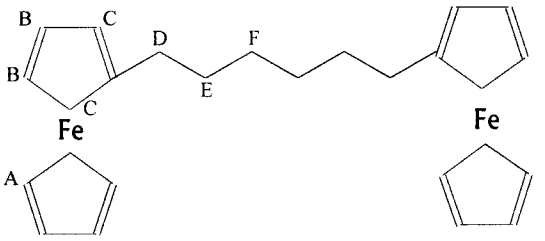
304 m/z



278 m/z



250 m/z



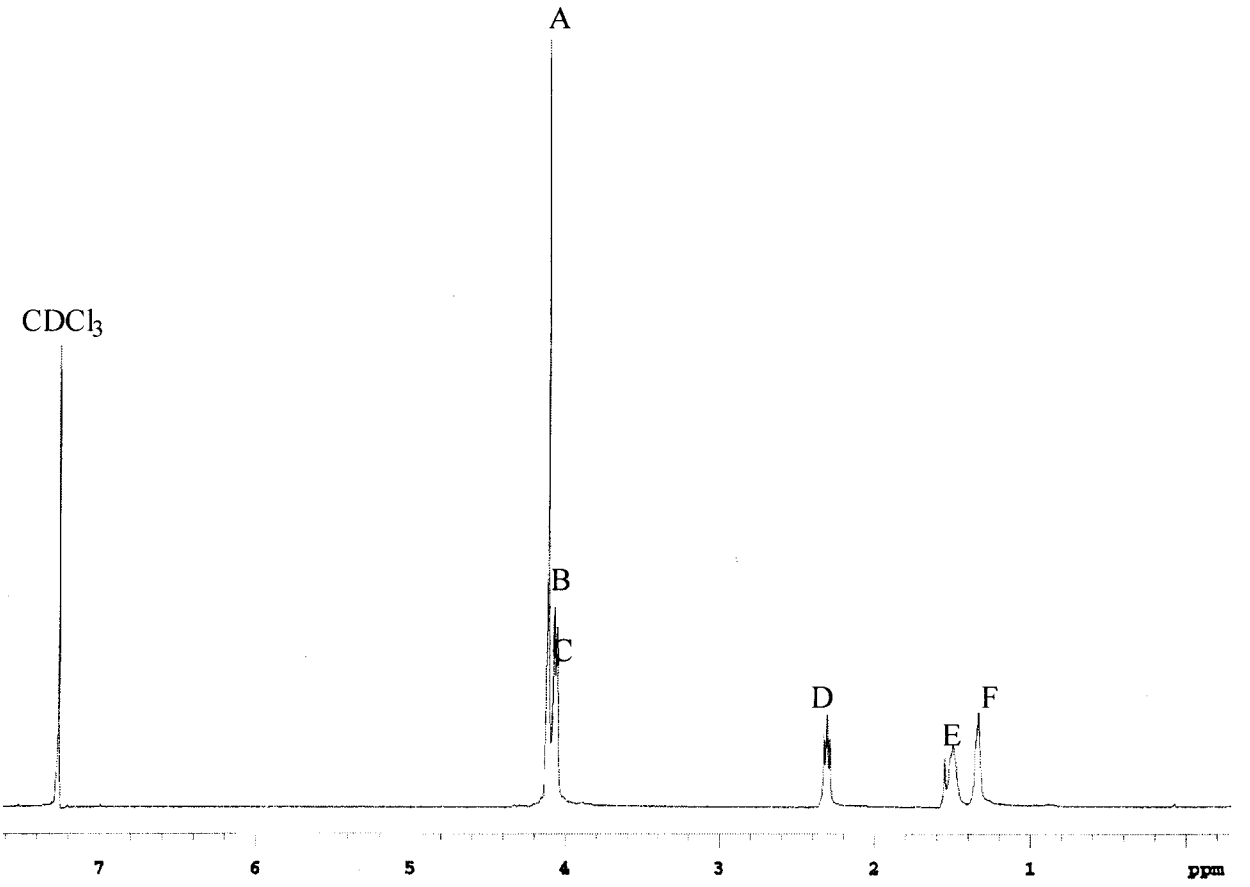


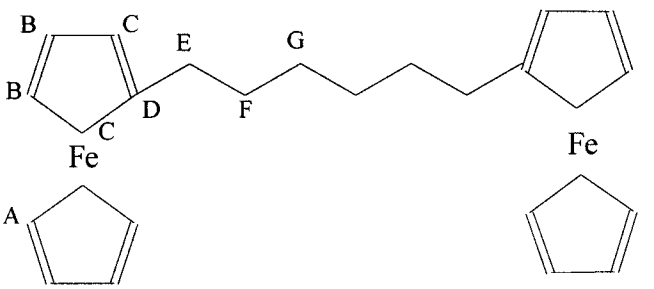
Figure 2.13: ^{1}H NMR spectrum of 1,6-diferrocenylhexane

and 2.303 ppm (peak D). The protons on the top Cp ring were shifted upfield by the electron donating alkyl substituent showing chemical shifts of 4.054 ppm (peak C) and 4.071 ppm (peak B). This was an indication that the reduction was successful. The Cp protons on the bottom ring gave a strong singlet at 4.106 ppm (peak A), as expected.

The ^{13}C NMR spectrum of 1,6-diferrocenylhexane was performed in $CDCl_3$ and is shown in Figure 2.14. The inner most methylene carbons in the bridge were shifted upfield to 22.799 ppm (peak G) as compared to 1,6-diferrocenylhexane-1,6-dione. The next two peaks were the carbons located one and two bonds away from the ferrocene at 31.175 ppm (peak E) and 29.620 ppm (peak F), respectively. The carbons in the top Cp ring one bond away from the electron donating bridge show a chemical shift value of 67.114 ppm (peak C) and the carbons two bonds away occur at 68.169 ppm (peak B). The five carbons in the bottom Cp ring were indicated by the intense peak at 68.594 ppm (peak A). The carbon in the top Cp ring to which the methylene bridge is bonded, shows a chemical shift of 89.617 ppm (peak D). The absence of the carbonyl peak around 200 ppm also indicated that the reduction was successful.

The IR spectrum is shown in Figure 2.15 and displays no carbonyl stretch at approximately 1600 cm^{-1}. The methylene stretching from the Cp rings showed peaks at 2917.77 cm^{-1} and 2847.38 cm^{-1}. Single carbon-carbon bond stretching from the methylene bridge occurred at 1104.05 cm^{-1}. The C-H stretching from the Cp rings was evident at 1020.16 cm^{-1}. Unsaturated carbon-carbon bond stretching from the Cp rings was assigned to the peak at 815.74 cm^{-1}.

Shown in Figure 2.16 is the mass spectrum of the fully reduced product and shows the parent ion peak at 454 m/z. The fragment assignments are shown in Table 2.3.



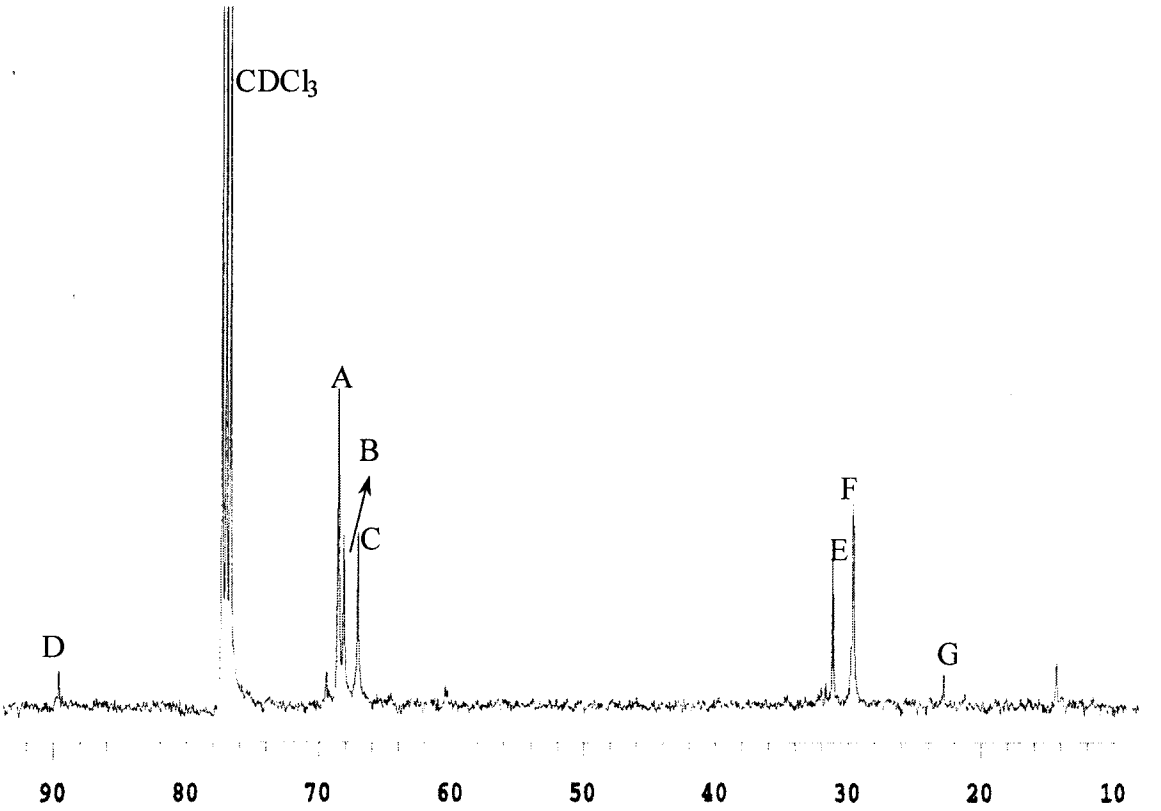


Figure 2.14: ^{13}C NMR spectrum of 1,6-diferrocenylhexane

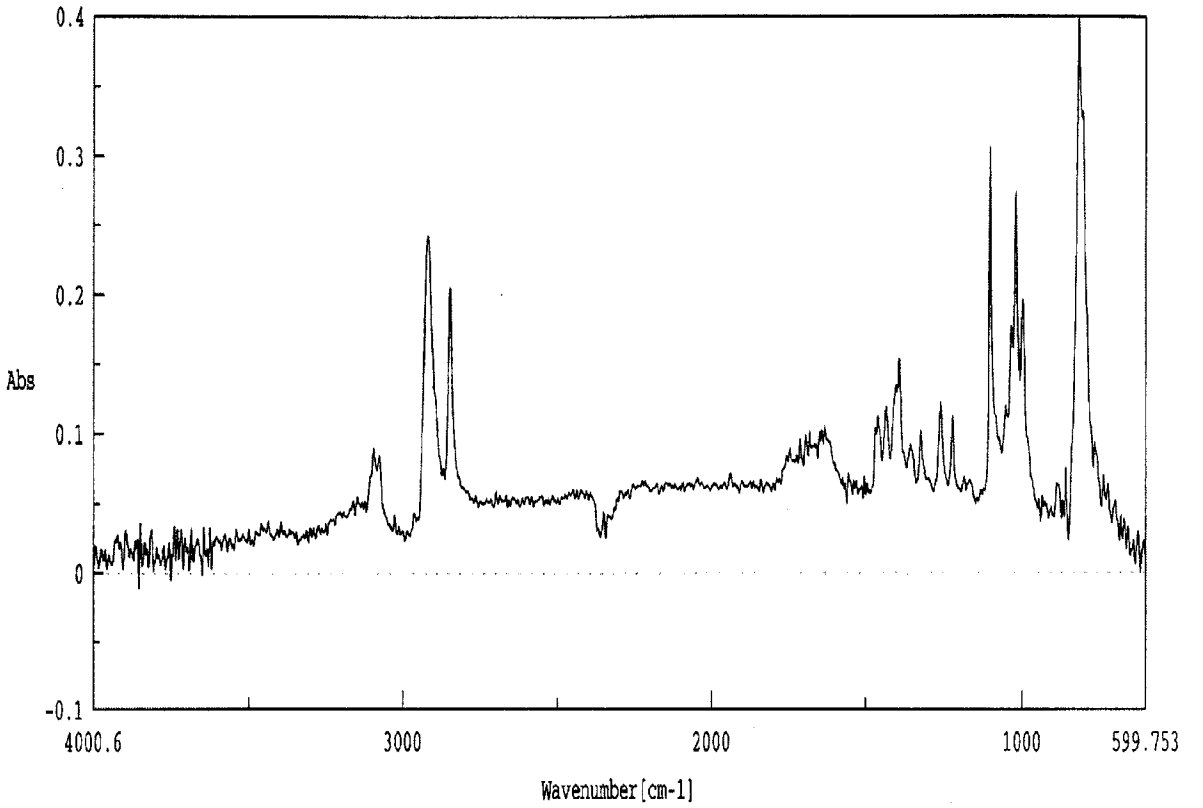


Figure 2.15: IR spectrum of 1,6-diferrocenylhexane

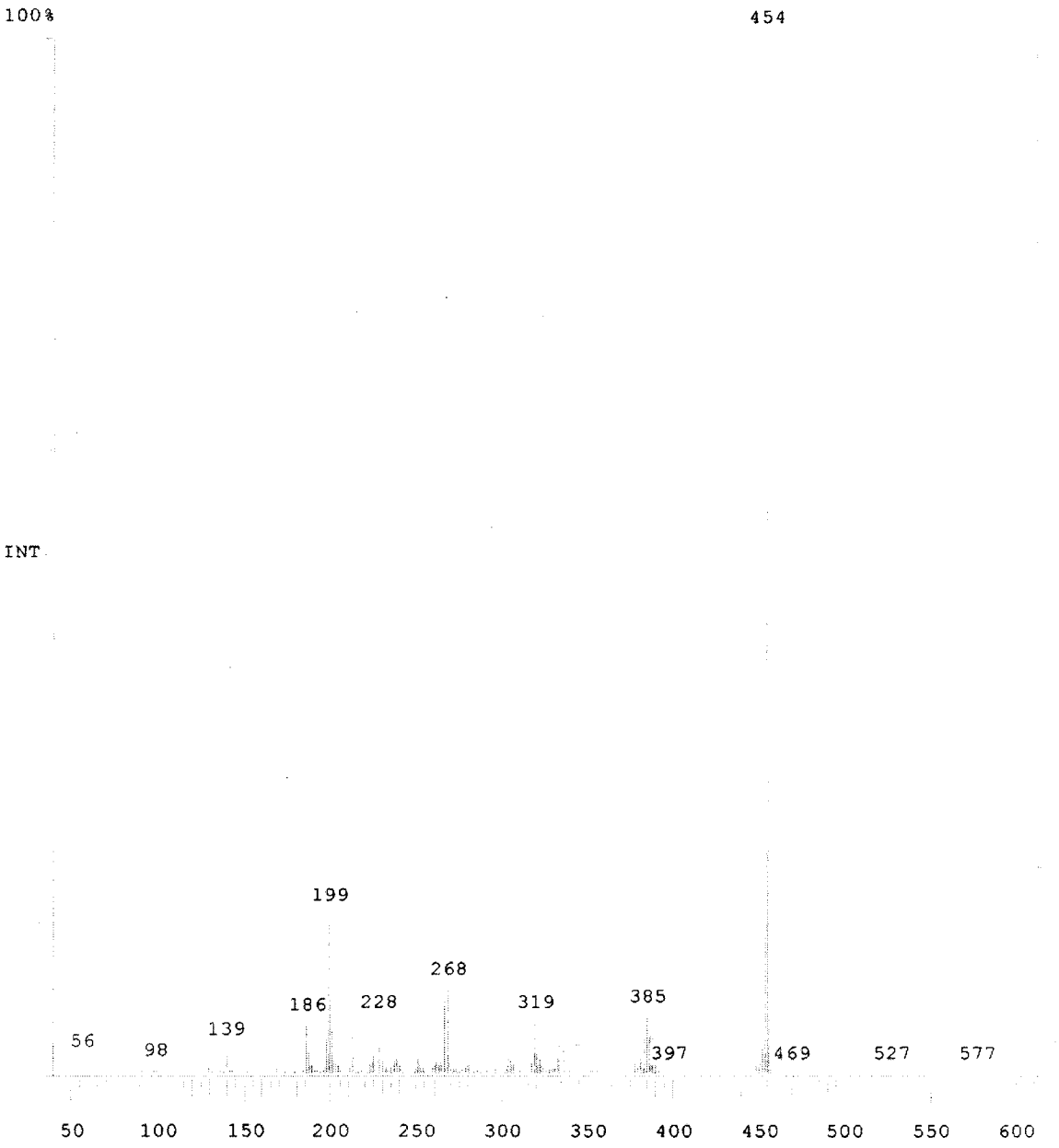
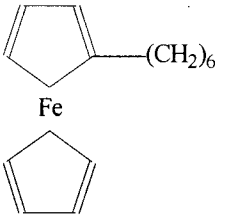


Figure 2.16: Mass spectrum of 1,6-diferrocenylhexane

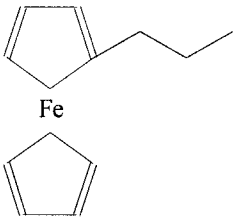
Table 2.3

Assigned Fragments from 1,6-diferrocenylhexane Mass Spectrum

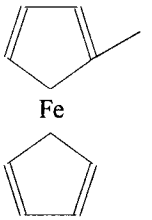
Fragments



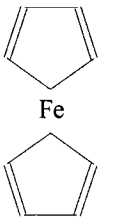
268 m/z



228 m/z



199 m/z

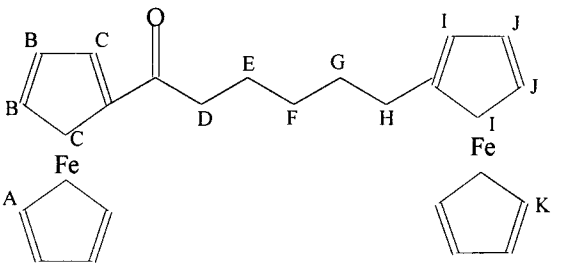


186 m/z

Characterization of 1,6-diferrocenylhexane-1-one

The ^{1}H NMR spectrum of 1,6-diferrocenylhexane is shown in Figure 2.17. The three peaks close to one another and the furthest upfield were assigned to the methylene protons on the three inner carbons in the bridge. The innermost protons showed a broad triplet at 1.408 ppm (peak F) while the adjacent protons were triplets at 1.555 ppm (peak G) and 1.725 ppm (peak E). Peak E was shifted downfield due to the carbonyl. The two protons adjacent to the top alkyl substituted Cp ring demonstrated a chemical shift of 2.347 ppm (peak H) while the peak at 2.695 ppm (peak D) was assigned to the protons closest to the carbonyl. The top Cp ring protons attached to the six carbon chain two and three bonds away, were evident in the spectrum at 4.073 ppm (peak J) and 4.050 ppm (peak I). The two intense singlets at 4.102 ppm (peak K) and 4.192 ppm (peak A) were attributed to the protons on the bottom Cp rings. Peak A was shifted downfield slightly because of the proximity to the carbonyl. The protons located on the top Cp ring that are two and three bonds away from the carbonyl display chemical shifts at 4.777 ppm (peak C) and 4.487 ppm (peak B), respectively.

The ^{13}C NMR spectrum of 1,6-diferrocenylhexane-1-one is shown in Figure 2.18. The methylene carbon two bonds away from the carbonyl was the peak furthest upfield at 25.700 ppm (peak G). The peak at 30.722 ppm (peaks H and I) was assigned to the next two carbons in the methylene bridge. The peaks were superimposed on one another due to the similar environment of each carbon. The next peak at 32.361 ppm (peak J) is due to the carbon one bond away from the ferrocene. The carbon adjacent to the carbonyl was shifted downfield the most, with respect to the other carbons in the bridge at 40.896 ppm (peak F). Figure 2.19 is an expanded view of the ^{13}C NMR spectrum from 65-95



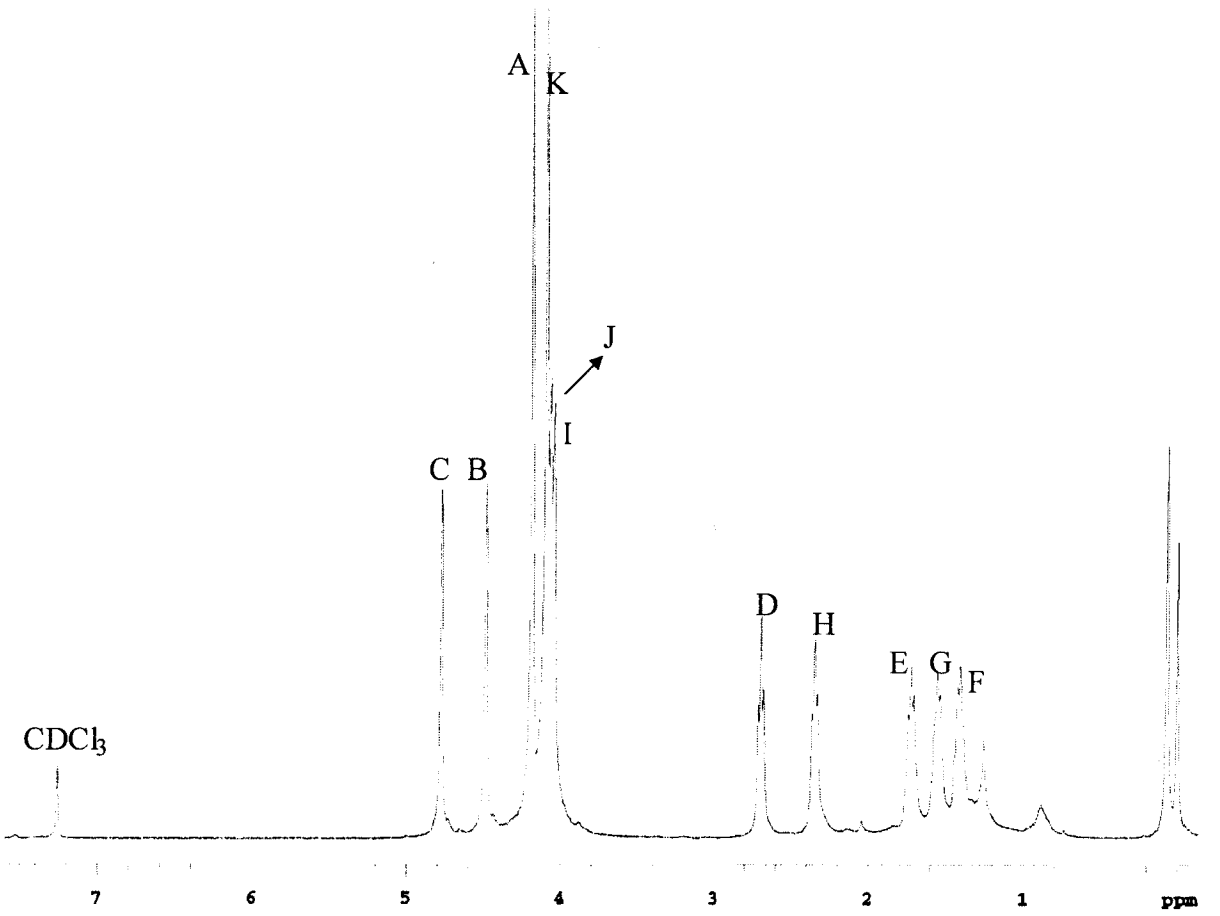
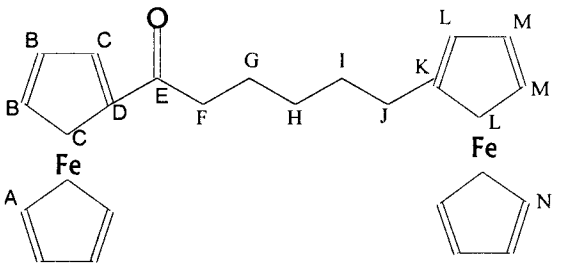


Figure 2.17: ^{1}H NMR spectrum of 1,6-diferrocenylhexane-1-one



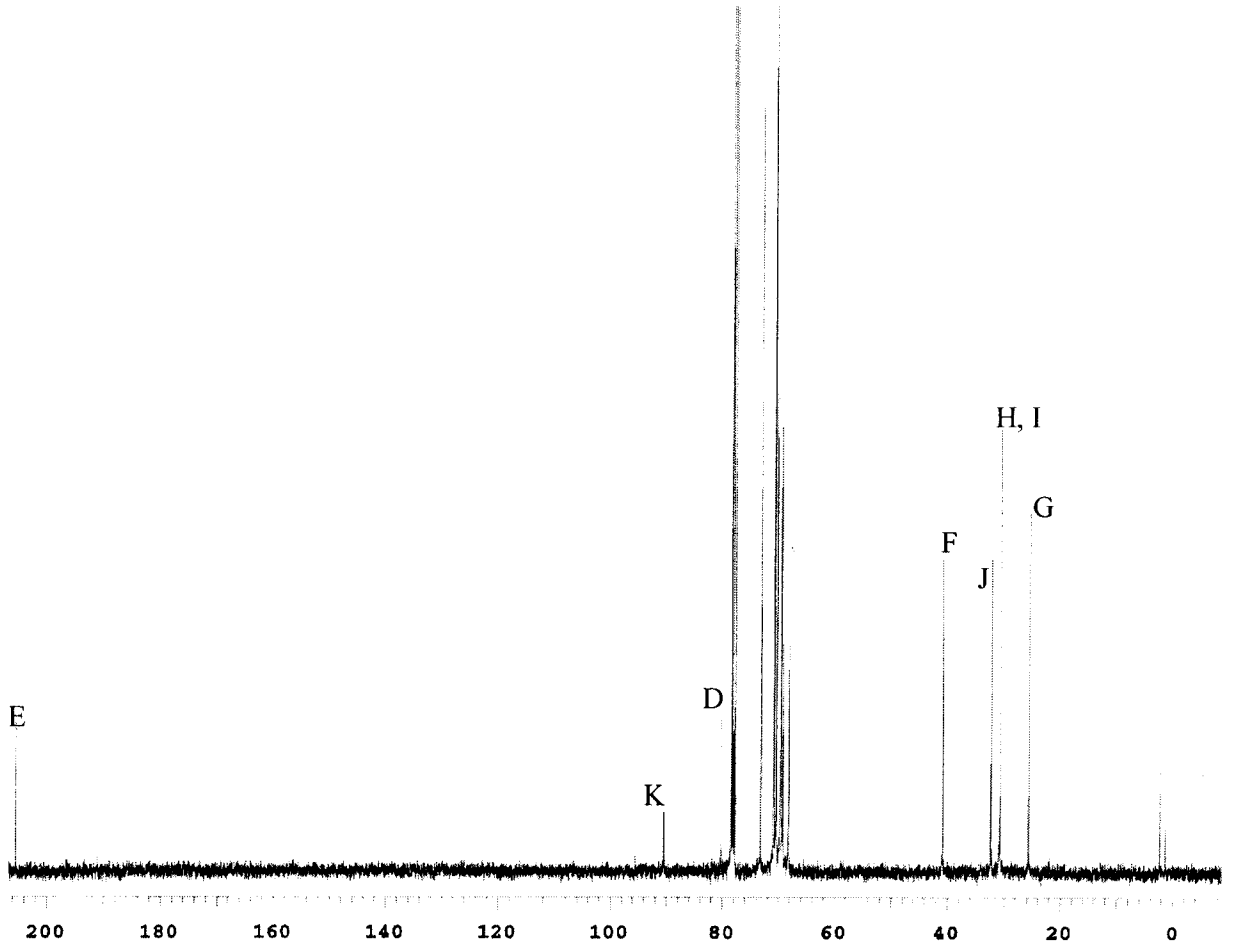


Figure 2.18: ^{13}C NMR spectrum of 1,6-diferrocenylhexane-1-one

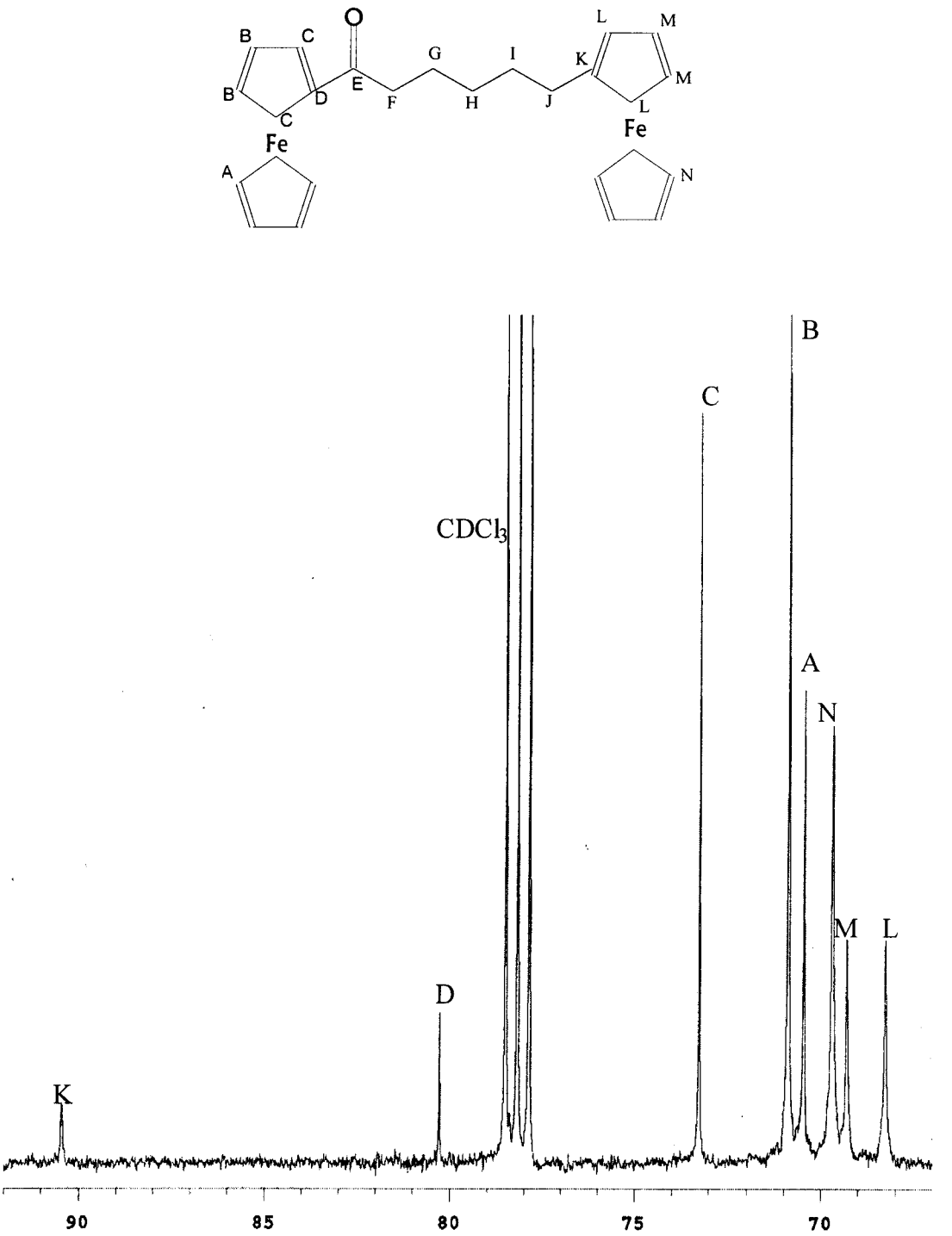


Figure 2.19: ^{13}C NMR spectrum close up from 65-95 ppm of 1,6-diferrocenylhexane-1-one

ppm. The top Cp carbons on the ferrocene attached to the methylene bridge are located at 68.278 ppm (peak L) and 69.325 ppm (peak M). The carbons closest to the electron donating methylene bridge are shifted upfield (peak L) more than the adjacent carbons in the ring (peak M). The carbons in the bottom alkyl substituted Cp ring appear at 69.711 ppm (peak N). The bottom Cp ring carbons attached to the carbonyl display a chemical shift of 70.478 ppm (peak A) downfield with respect to the other bottom Cp ring carbons. The top Cp ring carbons three bonds away from the carbonyl occur at 70.895 ppm (peak B) and two bonds away occur at 73.277 ppm (peak C). The carbon in the top Cp ring attached directly to the carbonyl carbon is located at 80.280 ppm (peak D). The other Cp ring carbon attached to the methylene bridge is downfield at 90.462 ppm (peak K). The carbonyl carbon is easily seen at 205.403 ppm (peak E).

The IR spectrum of 1,6-diferrocenylhexane-1-one is shown in Figure 2.20. The carbonyl stretching peak is easily assigned at 1675.84 cm^{-1}. Methylene stretching occurs at 2927.89 cm^{-1} from the six-carbon chain bridging the two ferrocenes and methylene bending is assigned at 1454.06 cm^{-1}. Single carbon-carbon bond bending and stretching in the methylene bridge, occurs at 1248.68 cm^{-1} and 1103.57 cm^{-1}, respectively. Stretching from the CH groups is assigned to the peak at 1025.46 cm^{-1}. Unsaturated carbon bond stretching from the Cp ring carbons is assigned to the 817.67 cm^{-1} peak.

The mass spectrum obtained from direct probe analysis displayed the parent ion peak at 468 m/z and is shown in Figure 2.21. The loss of a bottom Cp ring is evident from the peak at 403 m/z. The remaining fragments were assigned and can be seen in Table 2.4.

Characterization of 6-(diferrocenylhexanylcarbonyl)pentanebromide

The NMR assignments for 6-(diferrocenylhexanylcarbonyl)pentanebromide were

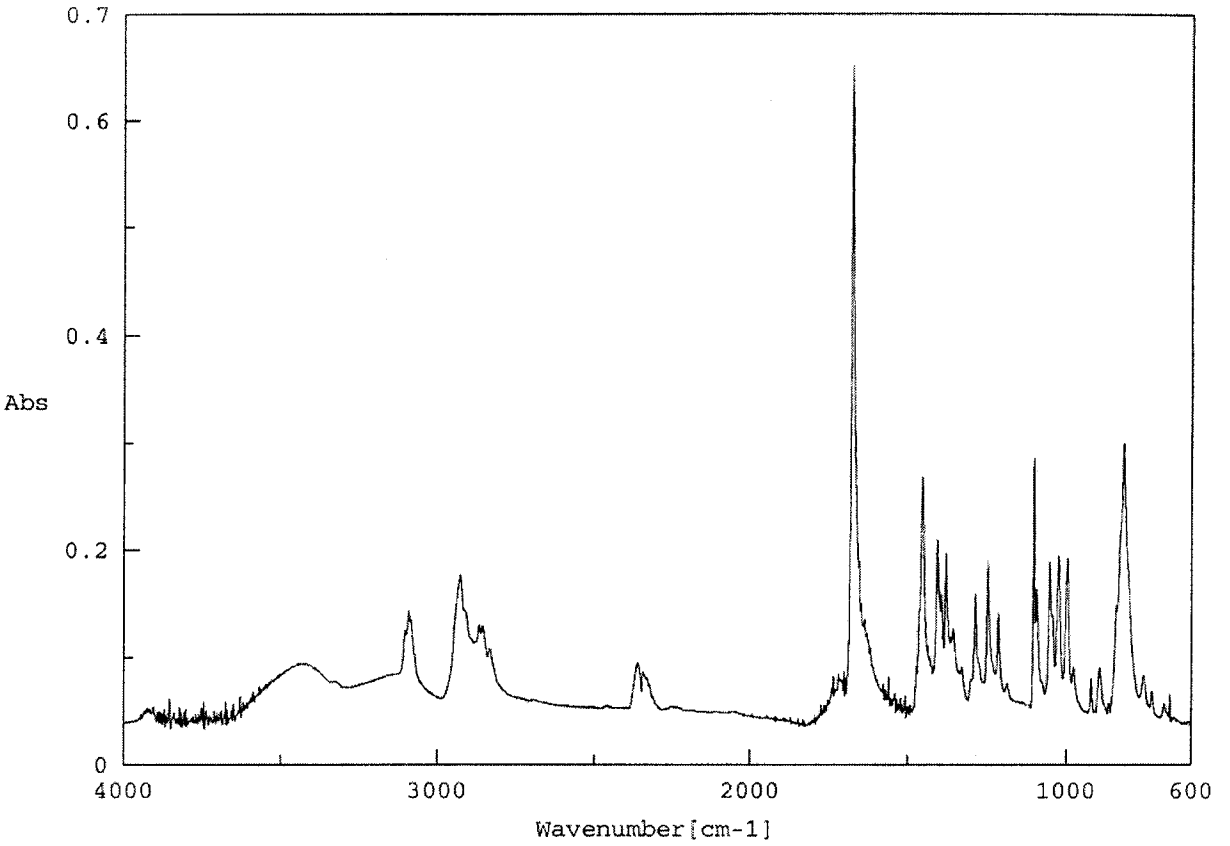


Figure 2.20: IR spectrum of 1,6-diferrocenylhexane-1-one

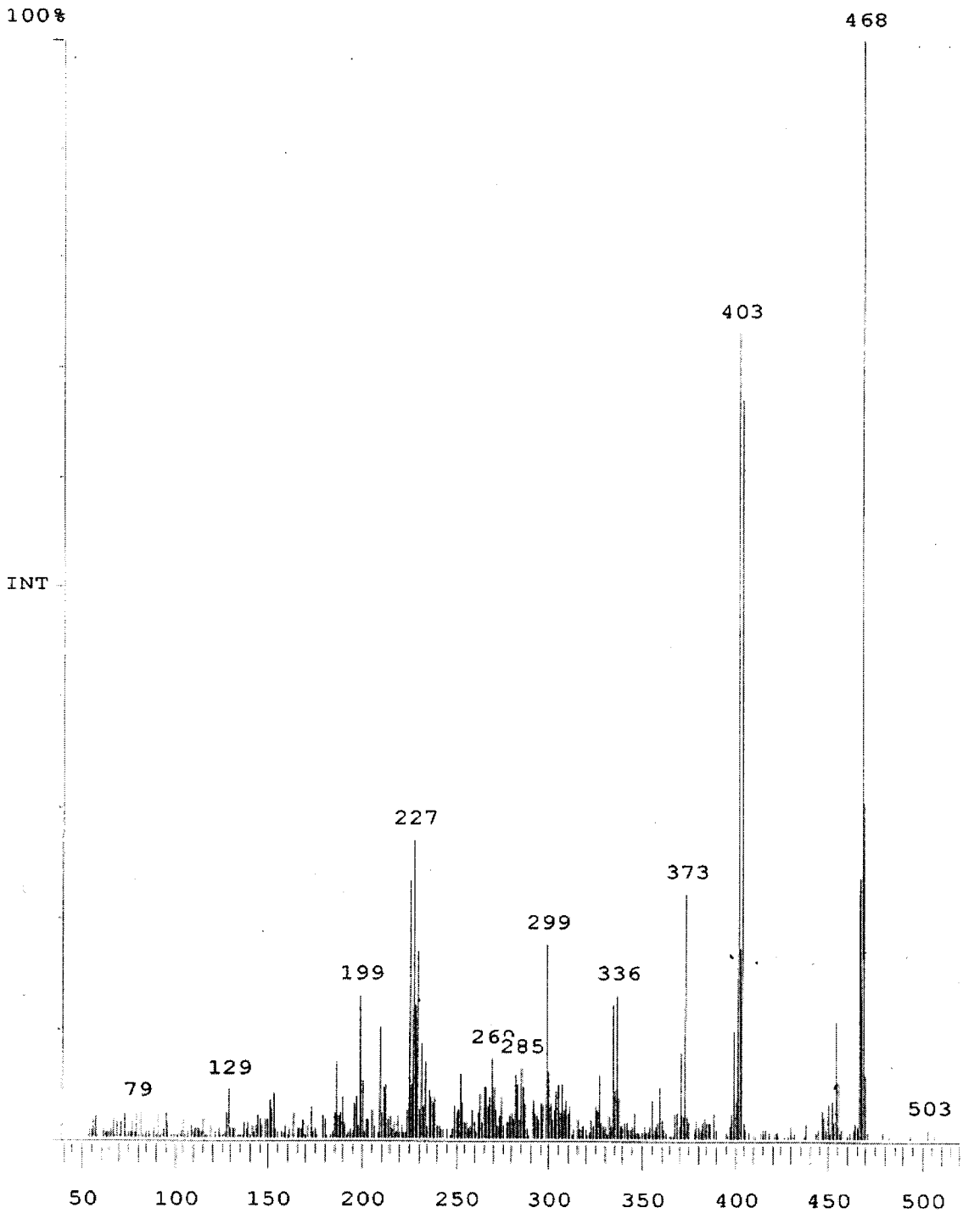
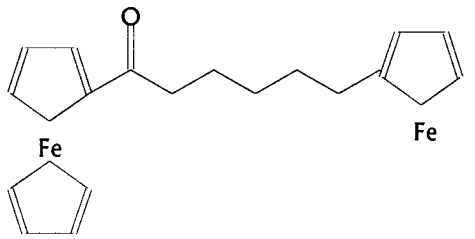


Figure 2.21: Mass spectrum of 1,6-diferrocenylhexane-1-one

Table 2.4

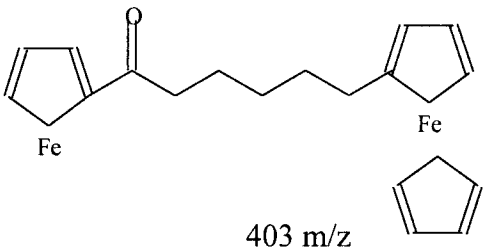
Assigned Fragments from 1,6-diferrocenylhexane-1-one Mass Spectrum

Fragments

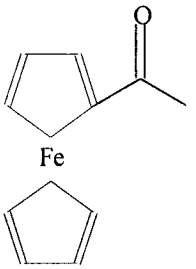


403

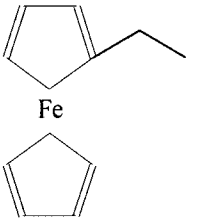
or



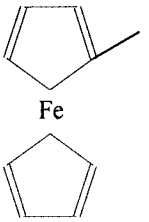
403 m/z



227 m/z



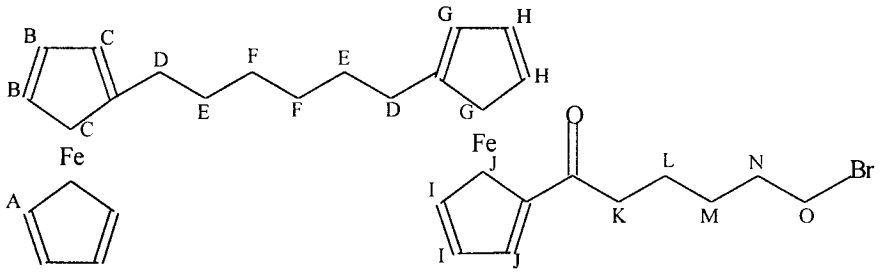
213 m/z



199 m/z

somewhat difficult due to the broad multiplets upfield. A portion of the ^{1}H NMR from 1.2 ppm to 2.0 ppm is shown in Figure 2.22. The four center methylene protons in the bridge joining the two ferrocenes show a chemical shift of 1.254 ppm (peak F). The broad triplet at 1.352 ppm (peak M) was assigned to the methylene protons three away from the bromine. The methylene protons two bonds away from the top Cp rings display a broad multiplet at 1.540 ppm (peak E). The multiplet downfield at 1.731 ppm (peak L) is associated with protons located two carbons away from the carbonyl on the bottom ring. The pentet at 1.928 ppm (peak N) are the protons two away from the bromine. Shown in Figure 2.23 is the ^{1}H NMR spectrum from 2.3 ppm to 3.5 ppm. The broad triplet at 2.300 ppm (peak D) are the protons adjacent to the top Cp rings. The protons neighboring the carbonyl show a chemical shift downfield at 2.786 ppm (peak K) due to the electron withdrawing nature of the oxygen. The protons adjacent to the bromine are shifted downfield at 3.445 ppm (peak O). The remaining ^{1}H NMR spectrum is shown in Figure 2.24. The protons that are on the top Cp ring of the ferrocene with no substitution on the bottom ring, show characteristic chemical shifts values of 4.029 ppm (peak C) and 4.047 ppm (peak B). The intense signal at 4.086 ppm (peak A) are the five protons on the bottom unsubstituted Cp ring. The other top Cp ring protons are shifted downfield slightly because of the carbonyl substituted on the lower ring at 4.111 ppm (peaks G and H). The protons on the bottom Cp ring attached to the carbonyl that are two and three bonds away are at 4.589 ppm (peak J) and 4.408 ppm (peak I), respectively. These chemical shift values are similar in nature to those reported for 1,6-diferrocenylhexane and 1,6-diferrocenylhexane-1-one.

A portion of the ^{13}C NMR spectrum of 6-(diferrocenylhexanylcarbonyl)pentane-



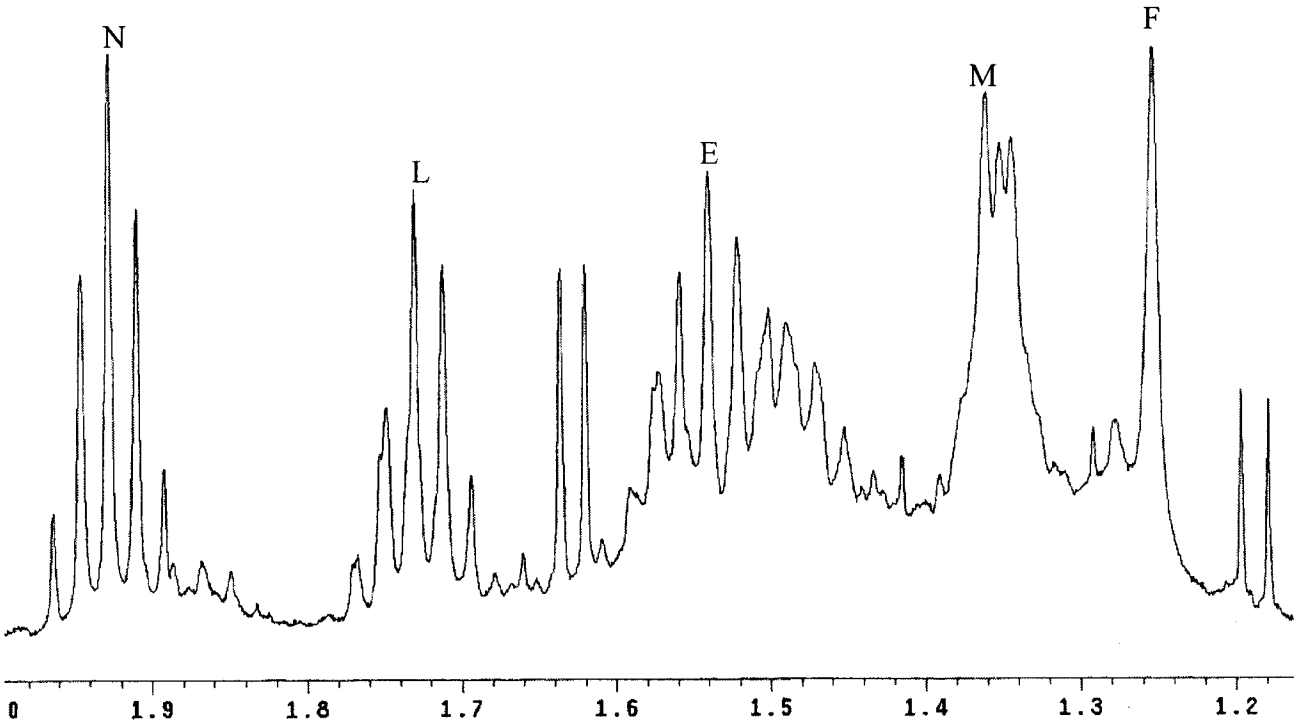
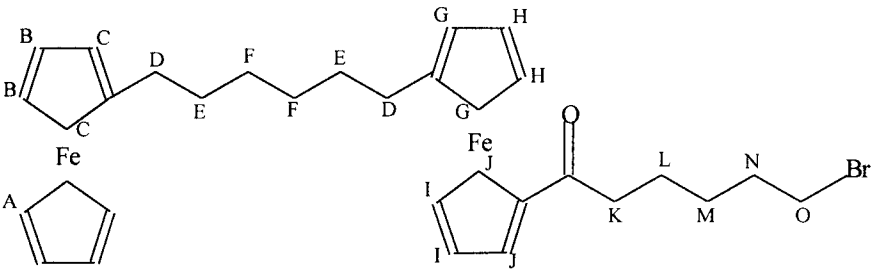


Figure 2.22: ^{1}H NMR spectrum close up from 1.2-2.0 ppm of 6-(diferrocenylhexanylcarbonyl)pentanebromide



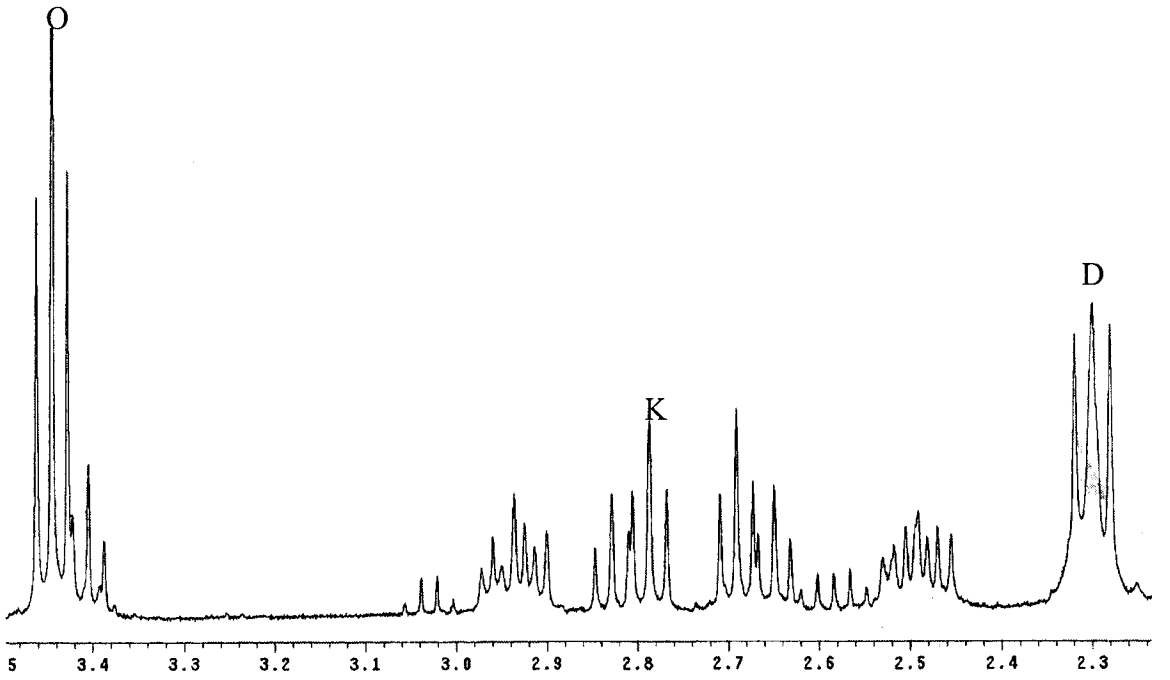
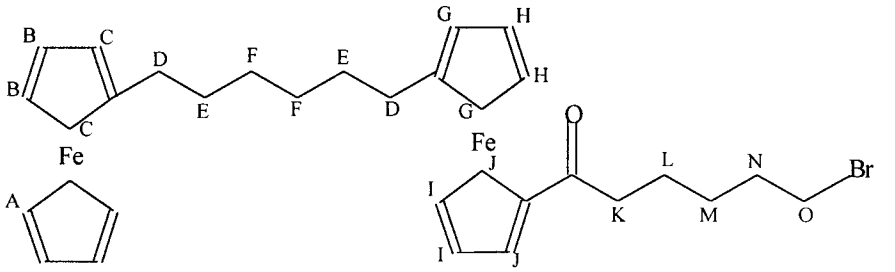


Figure 2.23: ^{1}H NMR spectrum close up from 2.3-3.5 ppm of 6-(diferrocenylhexanylcarbonyl)pentanebromide



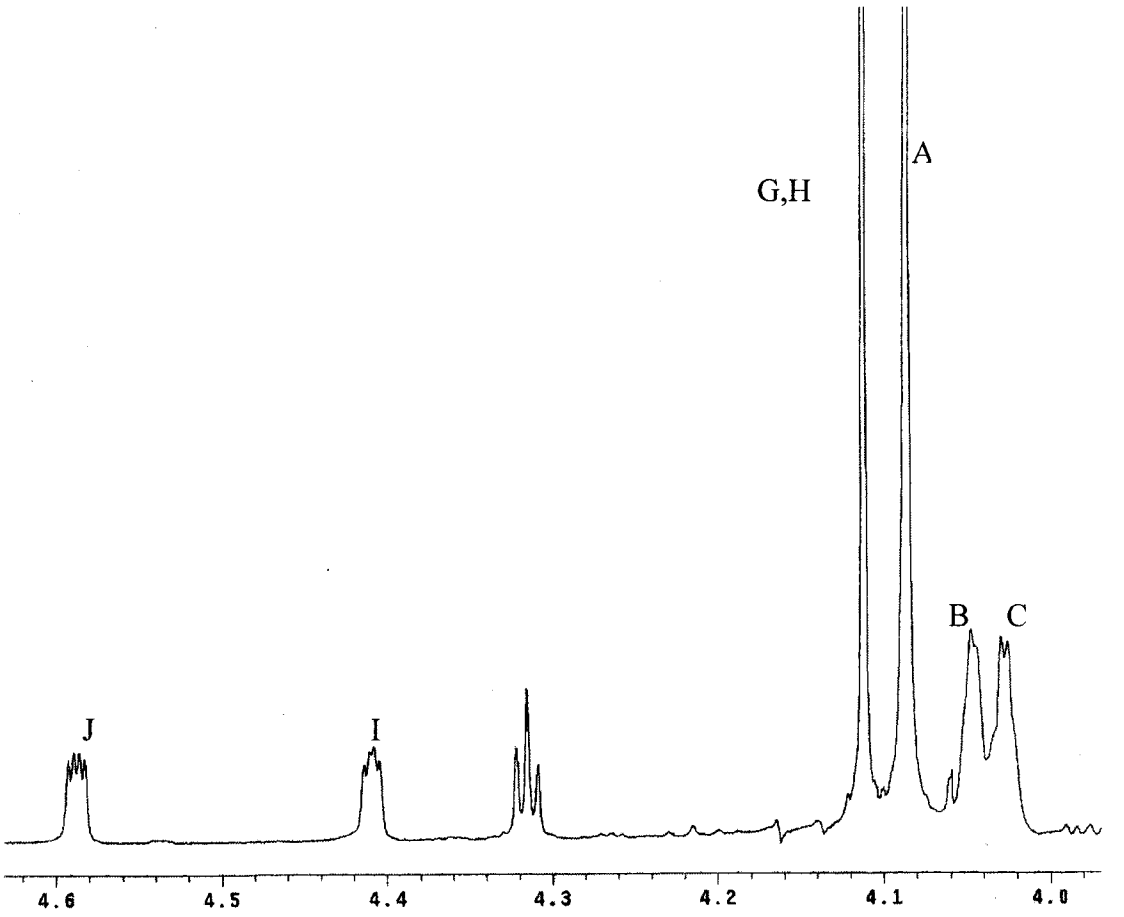
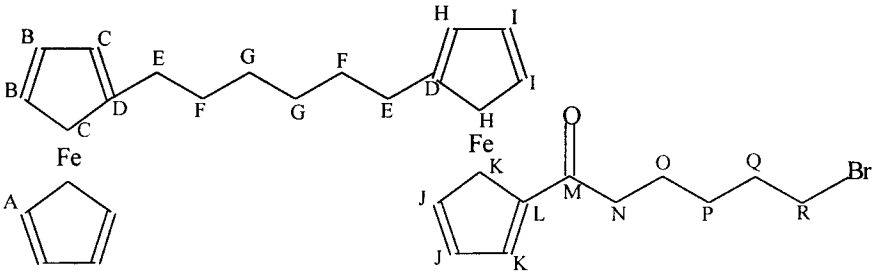


Figure 2.24: ^{1}H NMR spectrum close up from 4.0-4.6 ppm of 6-(diferrocenylhexanylcarbonyl)pentanebromide



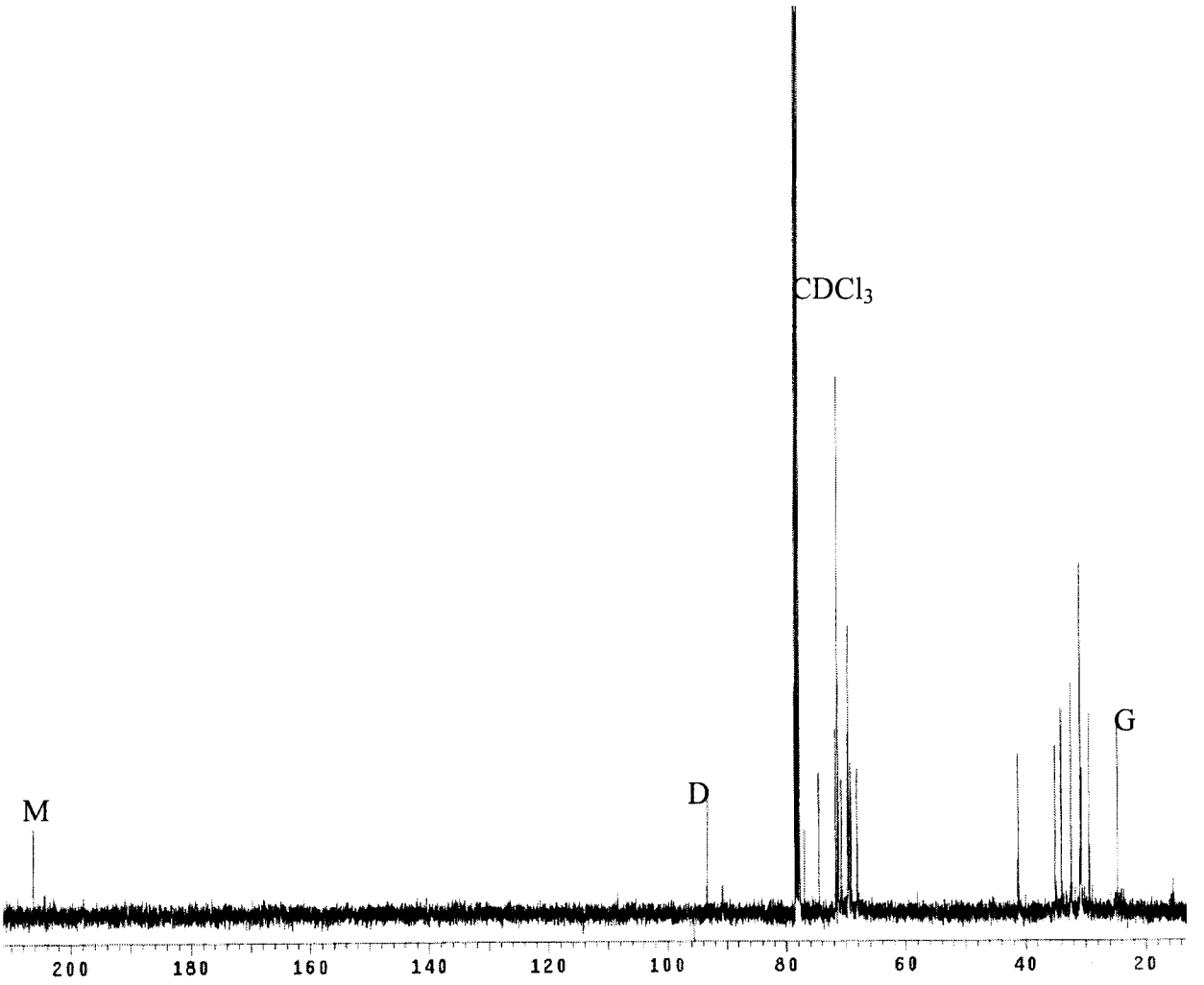


Figure 2.25: ^{13}C NMR spectrum of 6-(diferrocenylhexanylcarbonyl)pentanebromide

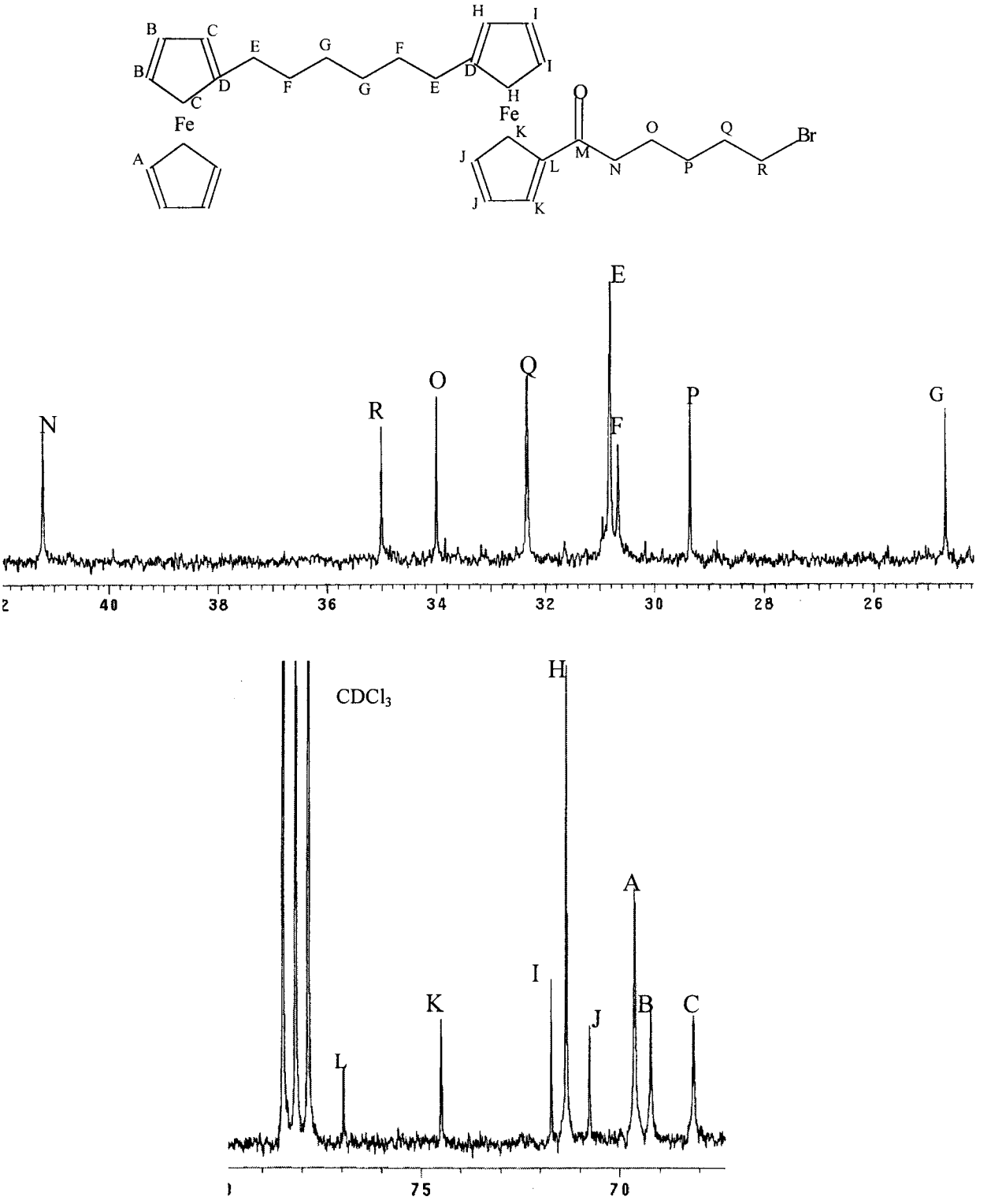


Figure 2.26: ^{13}C NMR spectrum close up from 25-42 ppm and 65-80 ppm 6-(diferrocenylhexanylcarbonyl)pentanebromide

chemical shift of 76.949 ppm (peak L). The remaining carbons are seen in Figure 2.25 of the full carbon spectrum. The carbons in the top Cp rings to which the methylene bridge is attached are located at 93.231 ppm (peak D). The carbonyl carbon is easily assigned at 206.260 ppm (peak M).

The mass spectrum of 6-(diferrocenylhexanylcarbonyl)pentanebromide is shown in Figure 2.27. The parent ion peak is located at 630 m/z with the next major peak at 550 m/z, indicating the loss of the bromine. The loss of the bottom Cp ring, common in these types of compounds, was assigned to 485 m/z. The loss of the entire six-carbon chain on the bottom Cp ring was evident from the peak at 453 m/z. The remaining fragments are assigned in Table 2.5.

Characterization of 6-(diferrocenylhexanylcarbonyl)pentanethiol

The ^{1}H NMR spectrum of 6-(diferrocenylhexanylcarbonyl)pentanethiol in $CDCl_3$ is located in Figure 2.28. The peak assignments were similar to those of the 6-(diferrocenylhexanylcarbonyl)pentanebromide. The proton attached to the thiol was difficult to assign because of the various overlapping multiplets located upfield. The peak at 1.240 ppm (peak P) was assigned to the proton attached to the sulfur. The four protons on the bridging inner methylene carbons were near peak P at 1.258 ppm (peak F). The broad triplet at 1.353 ppm (peak M) was assigned to the inner protons that are located three bonds away from the thiol. Protons that are two bonds away from the thiol, demonstrate a chemical shift of 1.501 ppm (peak N). The protons that are located on the carbons in the methylene bridge that are two bonds away from the top Cp rings are located at 1.573 ppm (peak E). The chemical shift located at 1.742 ppm (peak L) were assigned to the protons two bonds away from the carbonyl. The broad triplet at 2.294

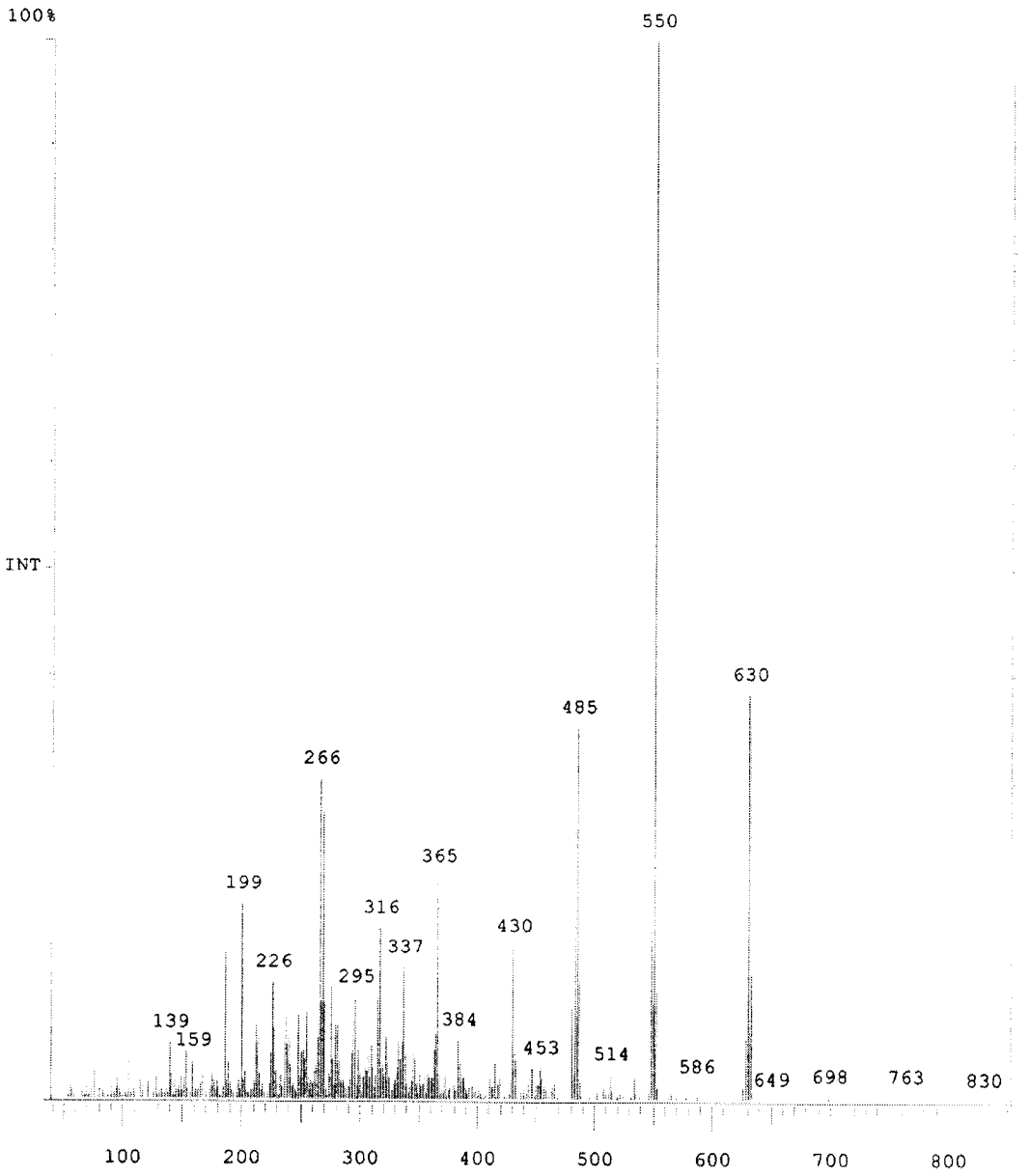
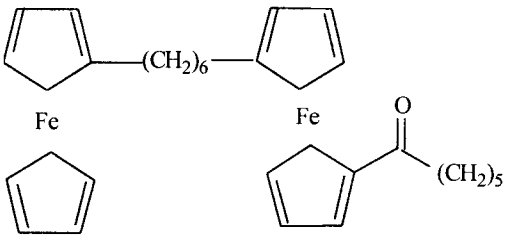


Figure 2.27: Mass spectrum of 6-(diferrocenylhexanylcarbonyl)pentanebromide

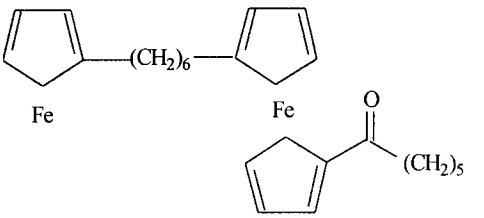
Table 2.5

Assigned Fragments from 6-(diferrocenylhexanylcarbonyl)pentanebromide Mass Spectrum

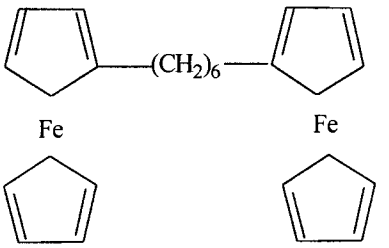
Fragments



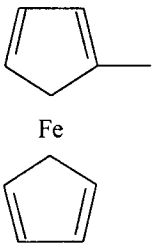
550 m/z



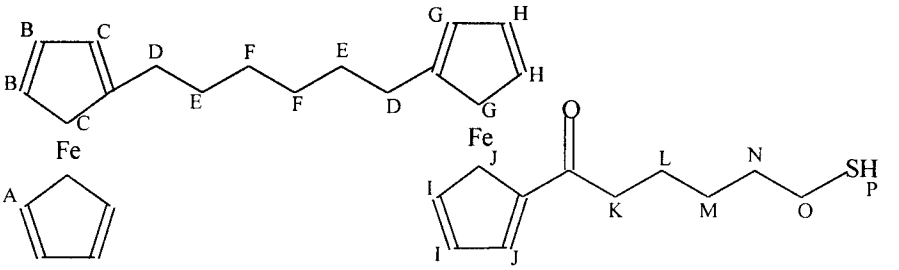
485 m/z



453 m/z



199 m/z



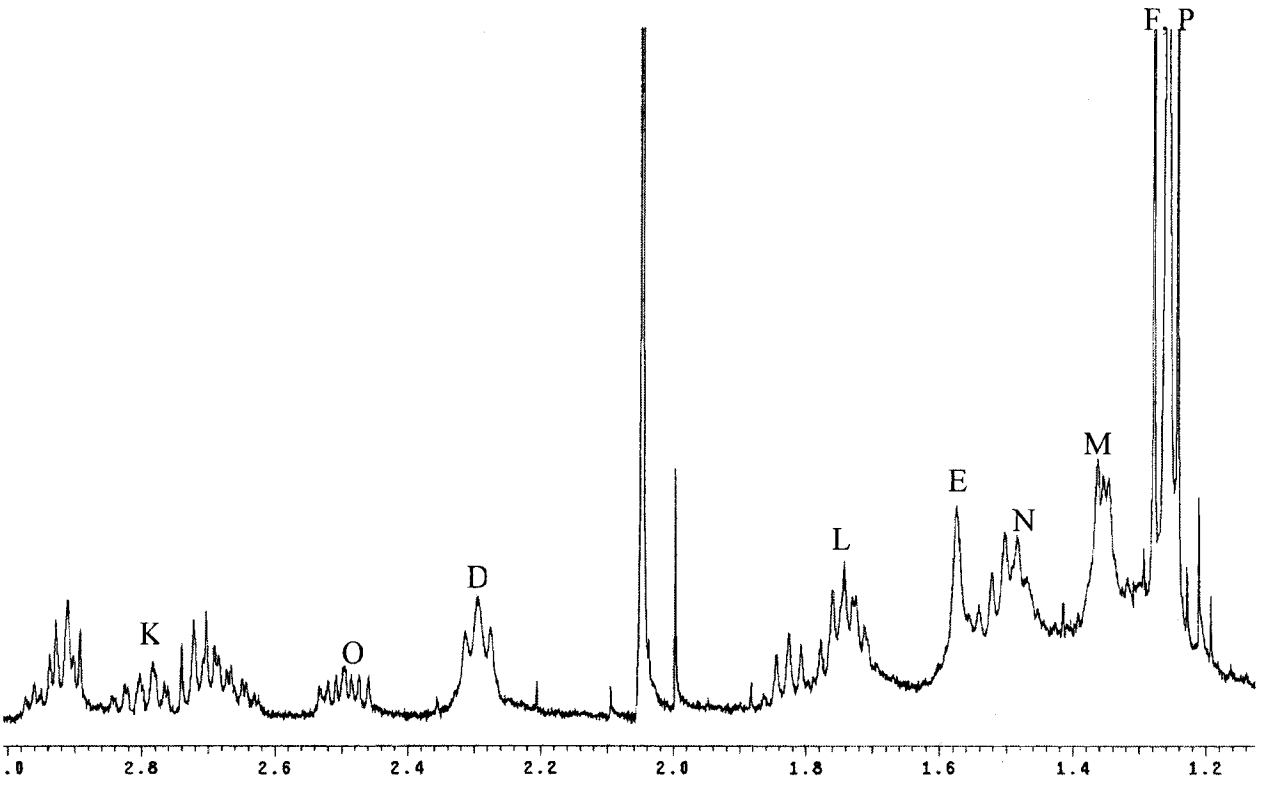
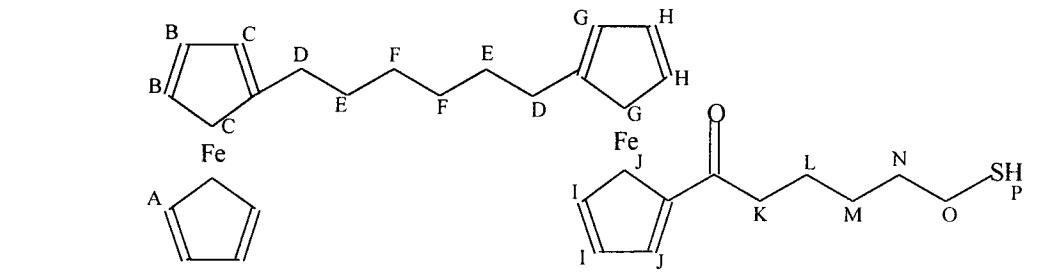


Figure 2.28: ^{1}H NMR spectrum close up from 1.2-3.0 ppm of 6-(diferrocenylhexanylcarbonyl)pentanethiol

ppm (peak D) were result of the protons in the methylene bridge adjacent to the top Cp rings. The multiplet at 2.494 ppm (peak O) were the protons on the carbon next to the sulfur. Another broad multiplet downfield at 2.784 ppm (peak K) is assigned to the protons adjacent to the carbonyl. Figure 2.29 is a close up from 1.2 ppm to 3.0 ppm to expand the various multiplets. The top Cp ring protons of the ferrocene without bottom ring substitution were characteristic at 4.039 ppm (peak C) and 4.062 ppm (peak B). The strong singlet at 4.094 ppm (peak A) were the five protons on the bottom Cp ring. The other top Cp ring protons were located at 4.130 ppm (peak G) and 4.147 ppm (peak H). Peak H was shifted downfield because of the proximity of the carbonyl. The remaining four protons on the bottom substituted Cp ring that are two and three bonds away from the carbonyl are located at 4.595 ppm (peak J) and 4.404 ppm (peak I), respectively.

The ^{13}C NMR spectrum in $CDCl_3$ of 6-(diferrocenylhexanylcarbonyl)pentanethiol is shown in Figure 2.30. The innermost carbons in the methylene bridge are located the farthest upfield at 25.108 ppm (peak G). The carbon three bonds away from the thiol are downfield at 29.630 ppm (peak P) while the carbon two bonds away from the thiol was assigned at 30.434 ppm (peak Q). The remaining carbons in the methylene bridge that are one and two bonds away from the top Cp rings are at 30.821 ppm (peak E) and 30.677 ppm (peak F), respectively. The carbon two bonds away from the carbonyl was shifted downfield to 31.595 ppm (peak O) relative to the previous chemical shifts due to the carbonyl. The carbon that is directly attached to the thiol displays a chemical shift of 33.181 ppm (peak R). The carbon adjacent to the carbonyl was significantly shifted downfield from the other peaks at 41.306 ppm (peak N). The carbons in the top Cp ring



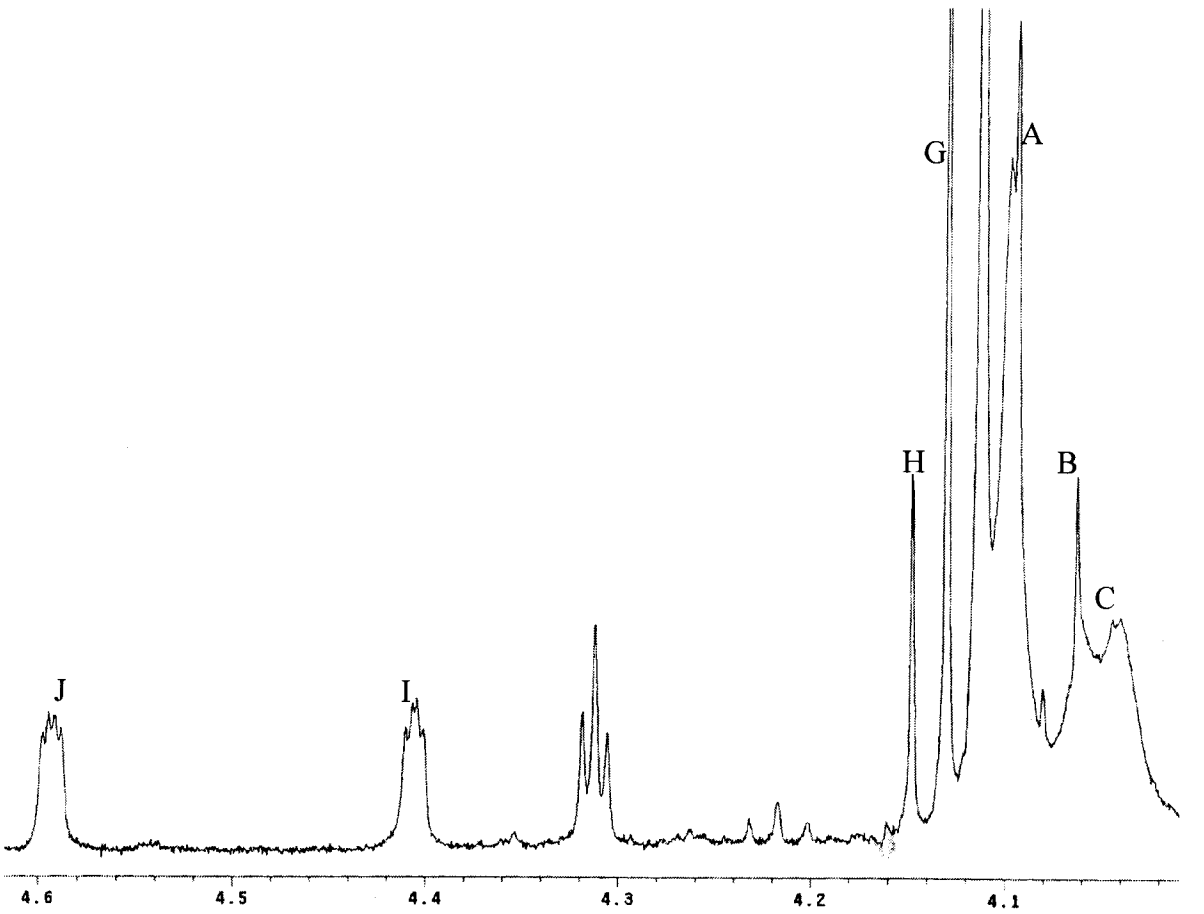


Figure 2.29: ^{1}H NMR spectrum close up from 4.0-4.6 ppm of 6-(diferrocenylhexanylcarbonyl)pentanethiol

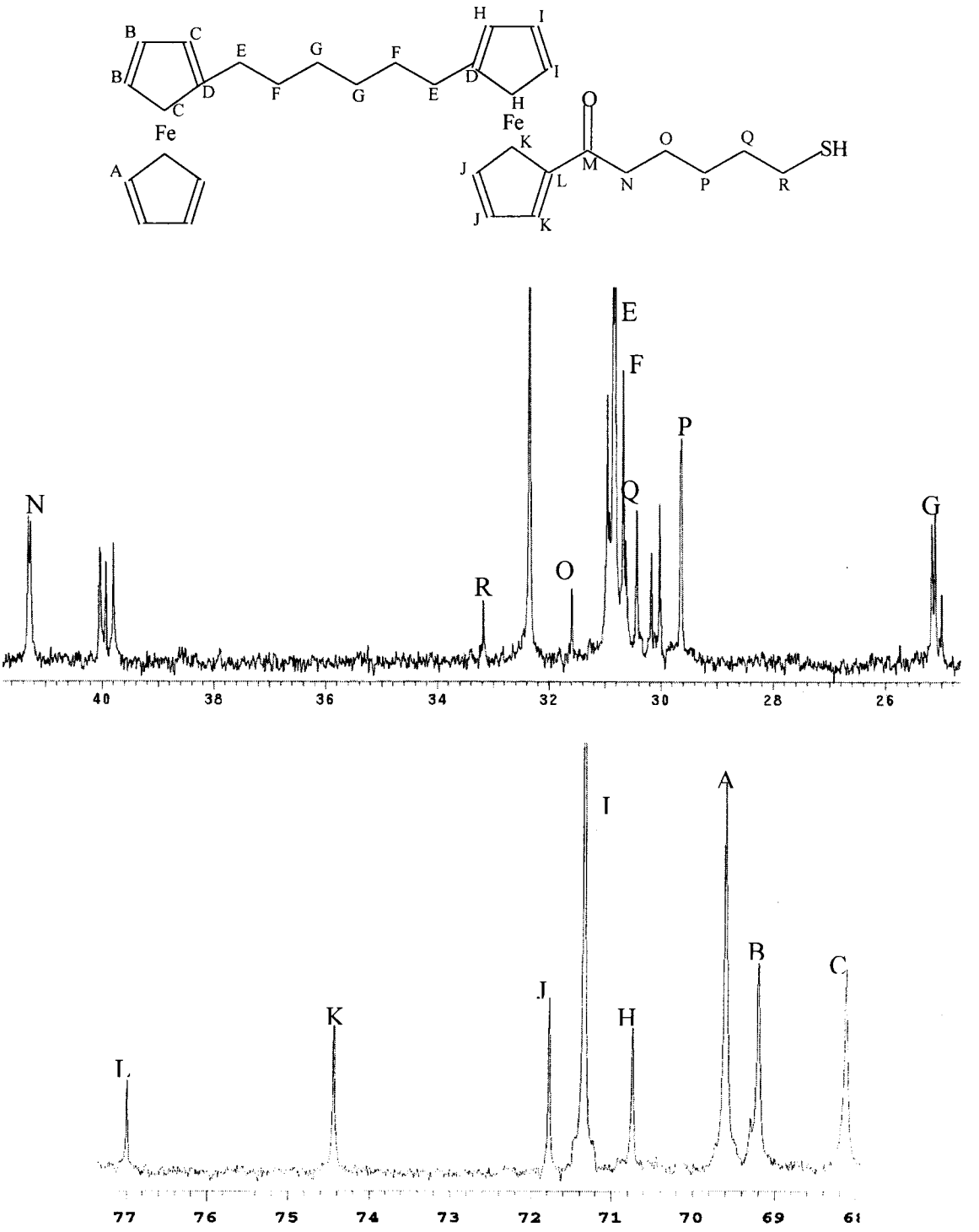


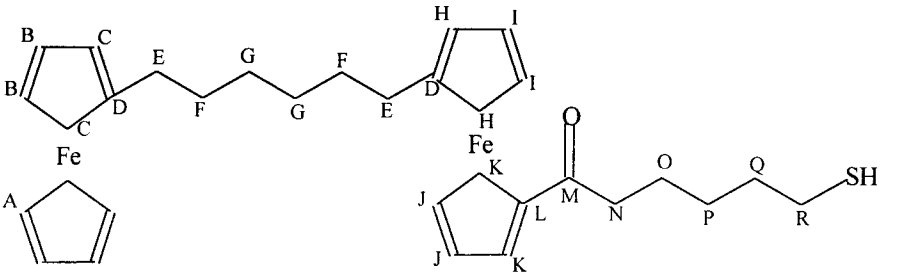
Figure 2.30: ^{13}C NMR spectrum close up from 25-45 ppm and 68-77 ppm of 6-(diferrocenylhexanylcarbonyl)pentanethiol

demonstrated characteristic chemical shifts at 68.126 ppm (peak C) and 69.203 ppm (peak B), which are two and three bonds away from the methylene bridge, respectively. The strong signal at 69.605 ppm (peak A) is assigned to the five carbons on the bottom unsubstituted Cp ring. The other top Cp ring carbons with bottom ring substitution are located at 70.743 ppm (peak H) and 71.350 ppm (peak I). The chemical shifts at 71.783 ppm (peak J) and 74.438 ppm (peak K) are due to the carbons in the bottom ring that are three and two bonds away from the carbonyl, respectively. The carbon in the Cp ring attached directly to the carbonyl is located at 76.995 ppm (peak L). Figure 2.31 displays the entire ^{13}C NMR spectrum in which the remaining two peaks were assigned. The low intensity signal at 93.193 ppm (peak D) was assigned to the carbons in the top Cp rings to which the methylene bridge is directly attached. The distinct peak at 206.420 ppm (peak M) was easily assigned to the carbonyl carbon.

The mass spectrum of 6-(diferrocenylhexanylcarbonyl)pentanethiol in CH_2Cl_2 is shown in Figure 2.32 and the parent ion peak is easily seen at 584 m/z. The other major fragment at 453 m/z results from the loss of the entire six-carbon thiol chain substituted on the lower Cp ring. The remaining fragments are assigned in Table 2.6.

Conclusion

The synthetic pathway as presented in Figure 2.1 was carried out to produce the final thiolated product, 6-(diferrocenylhexanylcarbonyl)pentanethiol. The intermediate products in all the reactions were purified via column chromatography and fully characterized using ^{1}H, ^{13}C NMR, IR, and mass spectrometry. The ^{1}H and ^{13}C NMR values were similar to those reported in the literature.[1-4] The reported spectroscopic data verifies that all the products were synthesized, as expected. For three of the compounds,



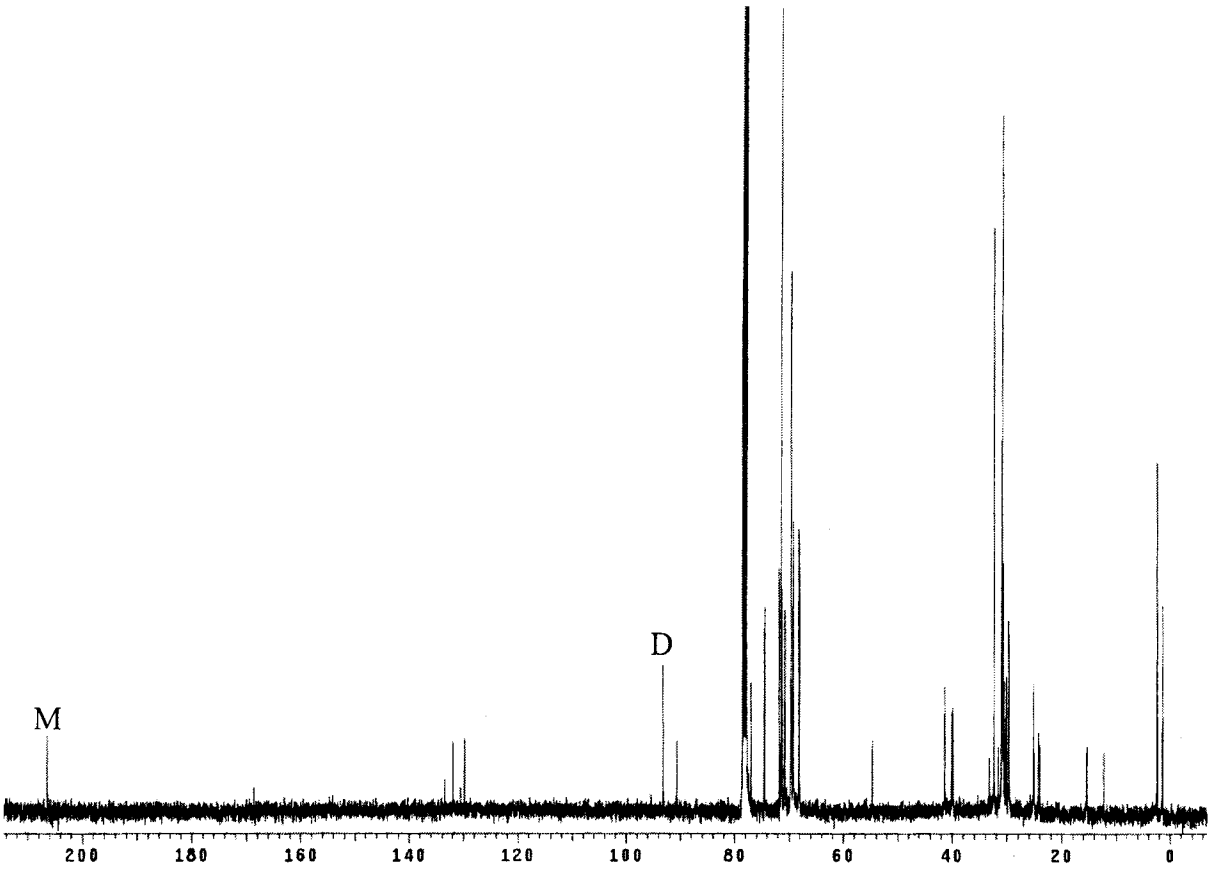


Figure 2.31: ^{13}C NMR spectrum of 6-(diferrocenylhexanylcarbonyl)pentanethiol

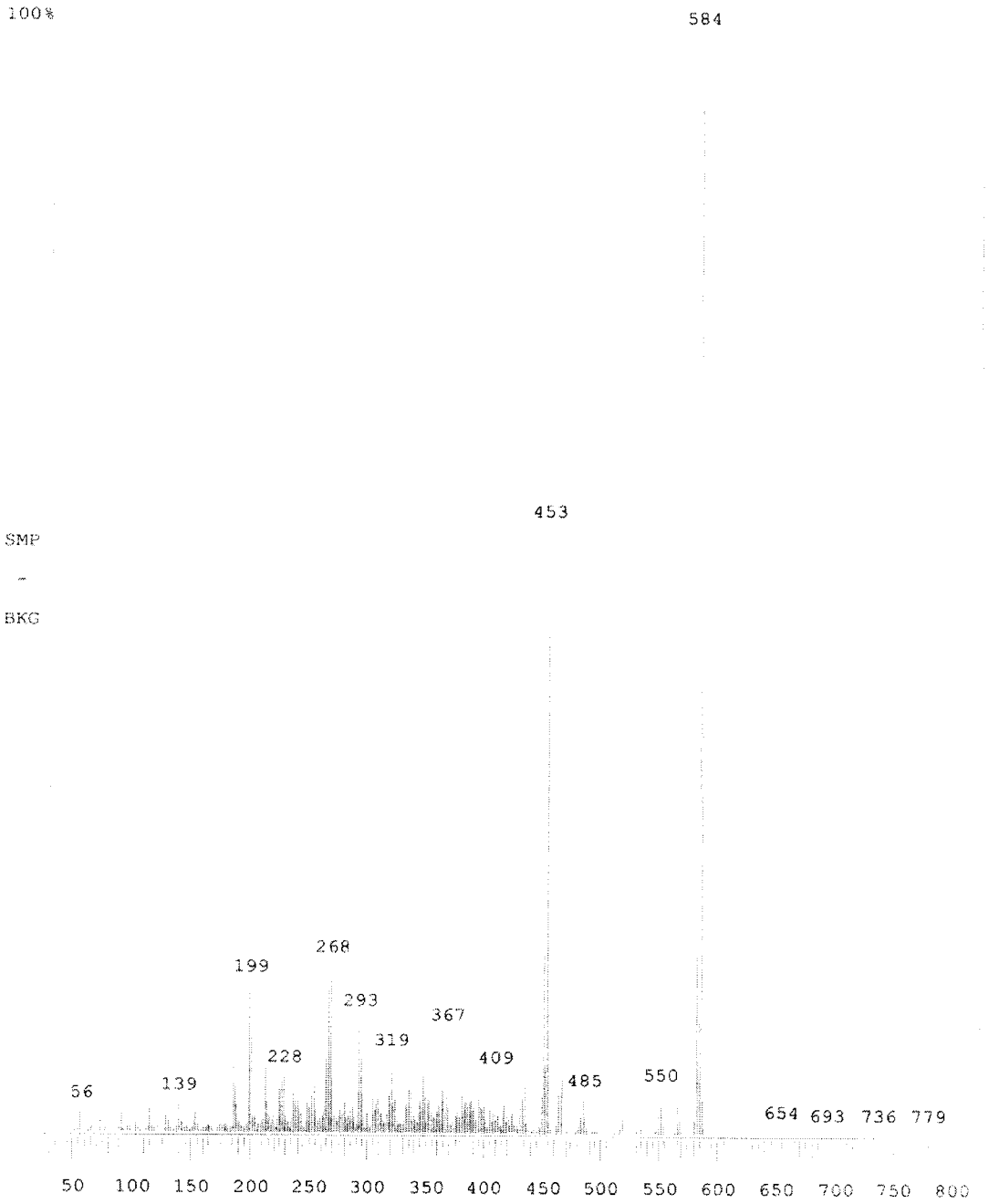
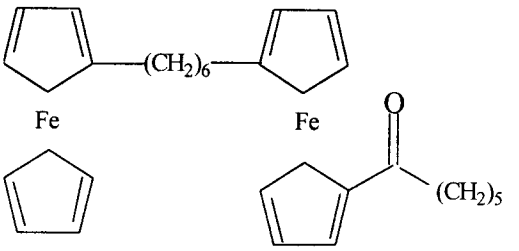


Figure 2.32: Mass spectrum of 6-(diferrocenylhexanylcarbonyl)pentanethiol

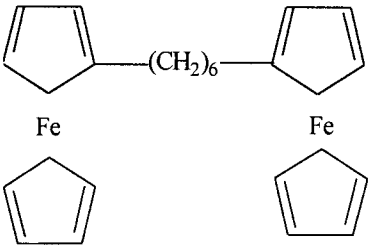
Table 2.6

Assigned Fragments from 6-(diferrocenylhexanylcarbonyl)pentanethiol Mass Spectrum

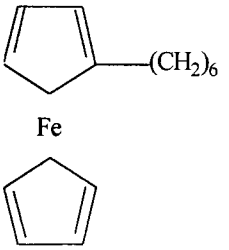
Fragments



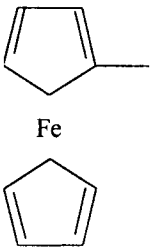
550 m/z



453 m/z



268 m/z



199 m/z

the spectroscopic data was further supported by single crystal X-ray diffraction analysis.

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CHAPTER THREE

X-RAY CRYSTALLOGRAPHY

Single crystals of 1,6-diferrocenylhexane-1,6-dione, 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene, and 1,6-diferrocenylhexane were obtained and X-ray crystallography was used to deduce their respective solid state structures. The crystal data for 1,6-diferrocenylhexane-1,6-dione and 1,6-diferrocenylhexane produced similar results, each belonging to the monoclinic crystal system and having space groups of P2(1)/n and P2(1)/c, respectively.

An unexpected chiral reaction product, 1-ferrocenylcarbonyl-2-ferrocenyl-cyclopentene, was the most interesting. Single crystal X-ray crystallographic analysis demonstrated that the molecule contained two chiral centers. The BASF parameter was approximately 50%, indicating a nearly racemic mixture. The X-ray data for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene indicates that the triclinic crystal has a space group of P1.

Experimental

All crystals were grown via kinetically controlled solvent evaporation. Both the 1,6-diferrocenylhexane-1,6-dione and 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene crystals precipitated out of a 75%/25% hexane/ethyl acetate solvent system, while the 1,6-diferrocenylhexane precipitated out of a an 80%/20% hexane/ethyl acetate solvent system. The crystals were examined under an optical microscope to observe their quality before mounting. The crystals that were chosen had clean edges with no observable cracks throughout. Crystals were mounted on the end of a glass capillary using epoxy.

Attempts were made to obtain X-ray quality single crystals of 1,6-diferrocenylhexane-1-one, but proved to be unsuccessful.

Instrumentation

The X-ray diffraction data for 1,6-diferrocenylhexane-1,6-dione was collected on a Siemens P4 Single Crystal Diffractometer equipped with a serial detector utilizing molybdenum radiation (MoKα, λ=0.71073 Å). A copper radiation source could not be utilized because the iron centers in ferrocene absorb the emitted radiation. XSCANS operating program from Bruker (Siemens) was used for data collection in which photo, hemisphere, fractional and thin shell searches were performed. Prior to theta:2theta data collection, Bravais lattice and Laue group symmetry routines determined crystal lattice symmetry and refined the unit cell parameters. Empirical psi scans corrected for absorption in the collected data. Structure refinement was done with Bruker SHELXTL-XP and SHELXTL-XL software packages, and tables of bond lengths, angles and structure factors were prepared using SHELXTL-XCIF.

Data collection for the remaining two crystals, 1-ferrocenylcarbonyl-2-ferrocenyl-cyclopentene and 1,6-diferrocenylhexane, was done on a Bruker SMART 1k CCD Single Crystal Diffractometer at Kent State University. Mo radiation (MoKα, λ=0.71073 Å) in a 2.4 kW fine focus sealed tube was used as the source of the X-rays. The crystals of these two compounds were much smaller in size, and data collection would have taken significantly more time with a serial detector than with a Bruker CCD detector. A complete sphere of data was collected in 1800 frames, with an exposure time of ten seconds per frame and a width of 0.30° with ω scans. Approximately 450 frames of data were used to determine the initial unit cell parameters. Bravais lattice and Laue

symmetry were determined in a program called SMART that refined the final cell. All of the generated data was integrated in SAINT and empirical absorption correction was performed using SADABS (written by George Sheldrick, University of Göttingen, 1996). Structure refinement and results for both structures were also done using the Bruker SHELXTL-XP, SHELXTL-XL, and SHELXTL-XCIF software package.

X-ray Diffraction Analysis of 1,6-diferrocenylhexane-1,6-dione

Single crystals of 1,6-diferrocenylhexane-1,6-dione were obtained following purification via column chromatography in which the crystals precipitated out of 75%/25% hexane/ethyl acetate. The crystal was centered in the X-ray beam and a twenty-minute rotation photo was obtained. The total number of reflections found was 6669, of which 3072 were unique. Upon completion of data collection, empirical psi-scans were performed to correct for absorption effects, including corrections for absorption by the glass capillary.

Direct Methods structure solution yielded the resulting structure in which all non-hydrogen atoms were assigned anisotropically. All hydrogen atoms were refined isotropically and convergence was achieved for all atomic positions with an R value of 0.1094 for all data. The high symmetry of the molecule produced a monoclinic crystal belonging to the P2(1)/n space group. Crystal structure data and refinement results are shown in Table 3.1. An ORTEP plot of 50% ellipsoids and the unit cell, generated in SHELXTL-XP, of 1,6-diferrocenylhexane-1,6-dione are shown in Figure 3.1 and Figure 3.2, respectively. The bond lengths, angles, and anisotropic and isotropic displacement coordinates as well as the hydrogen coordinates, are found in Tables 3.2 to 3.6.

Table 3.1

Crystal Data and Structure Refinement for 1,6-diferrocenylhexane-1,6-dione

Empirical formula	$C_{26}H_{26}Fe_2O_2$
Formula weight	482.17
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 5.7654(5) Å alpha = 90° b=22.7859(16)Å beta=101.778(6)° c = 8.2065(5) Å gamma = 90°
Volume	1055.39(13) A^3
Z, Calculated density	2, 1.517 Mg/m^3
Absorption coefficient	1.395 mm^{-1}
F(000)	500
Crystal size	0.05 x 0.42 x 0.18 mm
Theta range for data collection	1.79 to 29.99 deg.
Limiting indices	$-8 \le h \le 8, -32 \le k \le 32, -11 \le l \le 11$
Reflections collected / unique	6669 / 3072 [R(int) = 0.0765]
Completeness to theta = 29.99	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.5460 and 0.4435
Refinement method	Full-matrix least-squares on F^2
Hydrogen Atom Positions	Refined
Data / restraints / parameters	3072 / 0 / 189
Goodness-of-fit on F^2	0.958
Final R indices [I>2sigma(I)]	$R1(F)^a = 0.0521$, $wR2(F^2)^b = 0.1329$
R indices (all data)	$R1(F)^a = 0.1094$, $wR2(F^2)^b = 0.1779$
Extinction coefficient	0.011(3)
Largest diff. peak and hole	0.660 and -0.958 $e.A^{-3}$

$^a R_1(F) = \Sigma \big| |F_o| - |F_c| \big| / \Sigma |F_o|$ with $F_o > 4.0\sigma(F)$.

$^b wR_2(F^2) = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$ with $F_o > 4.0\sigma(F)$, and $w^{-1} = \sigma^2(F_o)^2 + (W \cdot P)^2 + T \cdot P$, where $P = (Max(F_o^2, 0) + 2F_c^2)/3$, W = 0.1000, and T = 0.00.

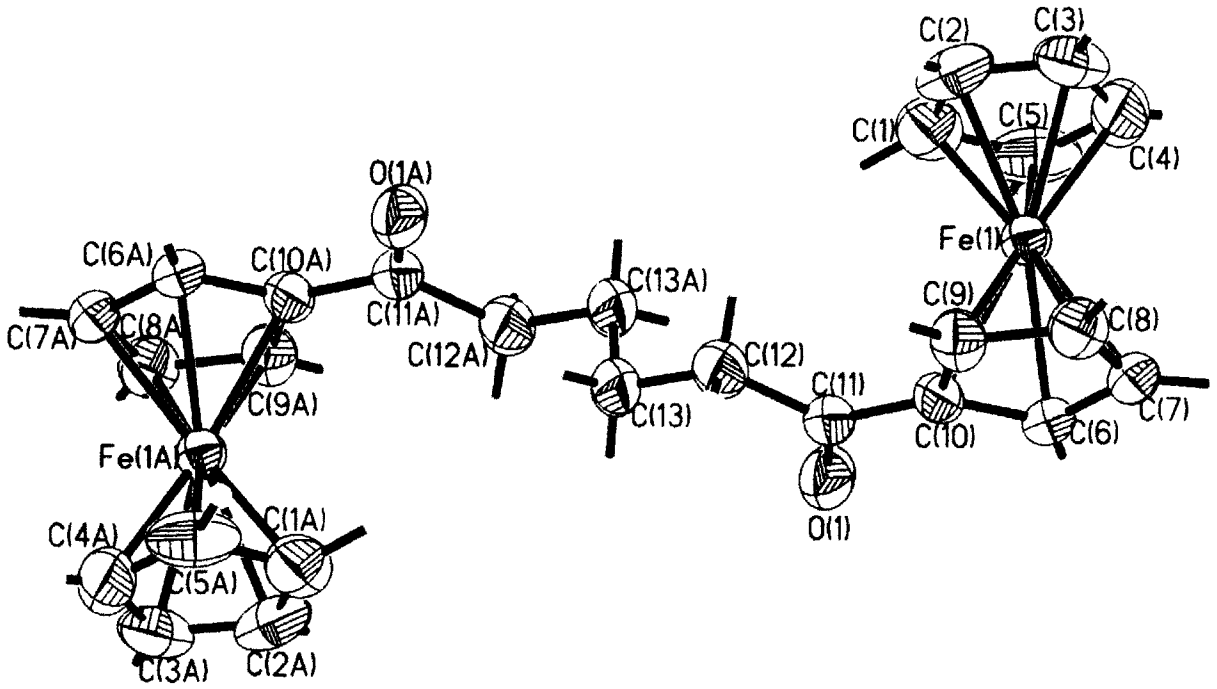

Figure 3.1: ORTEP plot of 1,6-diferrocenylhexane-1,6-dione (50% ellipsoids)

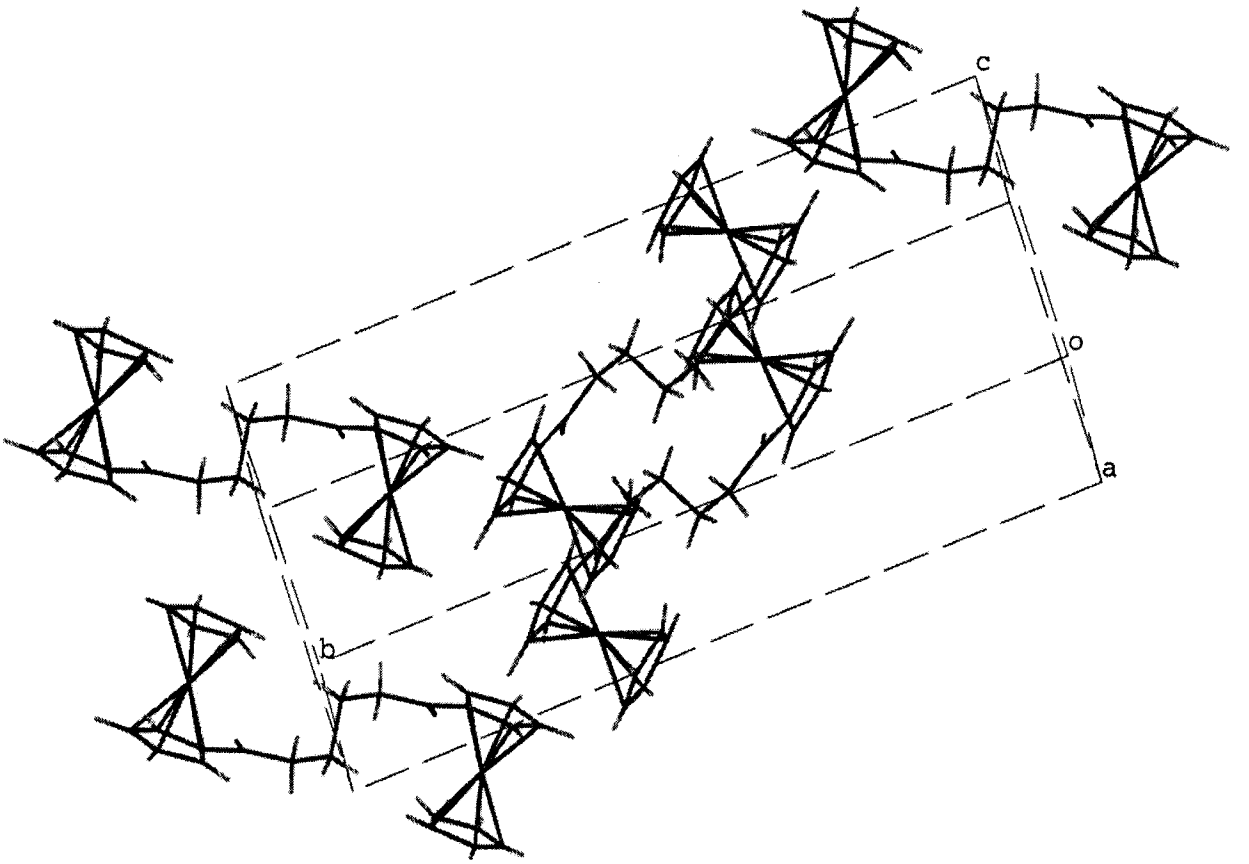

Figure 3.2: Unit cell of 1,6-diferrocenylhexane-1,6-dione

Table 3.2

Atomic Coordinates ($x10^4$) and Equivalent Isotropic Displacement Parameters ($A^2 x 10^3$) for 1,6-diferrocenylhexane-1,6-dione. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom Number	x	y	z	U(eq)
Fe(1)	7845(1)	1520(1)	4558(1)	36(1)
O(1)	3861(6)	1224(1)	356(4)	56(1)
C(1)	6619(12)	719(2)	5089(6)	66(2)
C(2)	8972(12)	770(2)	5830(7)	66(2)
C(3)	9281(11)	1239(2)	6910(6)	62(1)
C(4)	7070(15)	1485(3)	6848(7)	70(2)
C(5)	5361(10)	1170(3)	5724(7)	73(2)
C(6)	6129(8)	2080(2)	2753(4)	40(1)
C(7)	7918(9)	2389(2)	3873(5)	48(1)
C(8)	10128(9)	2119(2)	3870(5)	50(1)
C(9)	9755(8)	1639(2)	2740(5)	45(1)
C(10)	7233(7)	1609(2)	2040(4)	38(1)
C(11)	5974(8)	1163(2)	927(4)	40(1)
C(12)	7277(8)	622(2)	531(5)	46(1)
C(13)	5774(10)	167(2)	-484(5)	51(1)

Table 3.3

Anisotropic Displacement Parameters ($A^2 \times 10^3$) for 1,6-diferrocenylhexane-1,6-dione. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$

Atom Number	U11	U22	U33	U23	U13	U12
Fe(1)	39(1)	34(1)	34(1)	2(1)	6(1)	-2(1)
O(1)	61(2)	43(2)	57(2)	-6(1)	-6(2)	2(2)
C(1)	94(4)	50(3)	52(2)	9(2)	12(3)	-28(3)
C(2)	73(4)	53(3)	75(3)	30(3)	21(3)	18(3)
C(3)	66(3)	72(3)	41(2)	18(2)	-5(2)	-8(3)
C(4)	121(6)	50(3)	52(3)	3(2)	47(3)	5(3)
C(5)	52(3)	92(4)	73(3)	44(3)	11(3)	-7(3)
C(6)	50(2)	33(2)	37(2)	6(1)	5(2)	4(2)
C(7)	72(3)	31(2)	40(2)	3(2)	5(2)	-4(2)
C(8)	54(3)	44(2)	51(2)	3(2)	7(2)	-17(2)
C(9)	48(2)	46(2)	45(2)	-1(2)	19(2)	-6(2)
C(10)	45(2)	37(2)	31(2)	1(1)	6(2)	-4(2)
C(11)	50(2)	35(2)	35(2)	2(1)	6(2)	-1(2)
C(12)	51(3)	48(2)	41(2)	0(2)	15(2)	0(2)
C(13)	79(3)	41(2)	39(2)	-3(2)	21(2)	5(2)

Table 3.4

Bond lengths [Å] for 1,6-diferrocenylhexane-1,6-dione

Fe(1)-C(4)	2.021(5)
Fe(1)-C(5)	2.041(5)
Fe(1)-C(10)	2.034(3)
Fe(1)-C(1)	2.037(5)
Fe(1)-C(2)	2.038(5)
Fe(1)-C(9)	2.045(4)
Fe(1)-C(3)	2.042(4)
Fe(1)-C(6)	2.049(4)
Fe(1)-C(8)	2.052(4)
Fe(1)-C(7)	2.060(4)
C(12)-C(13)	1.491(6)
C(12)-C(11)	1.513(6)
C(12)-H(12B)	0.93(4)
C(12)-H(12A)	0.83(4)
O(1)-C(11)	1.221(5)
C(10)-C(9)	1.451(6)
C(9)-C(8)	1.421(6)
C(6)-C(7)	1.420(6)
C(6)-H(6)	1.01(5)
C(6)-C(10)	1.432(5)
C(8)-C(7)	1.416(7)
C(8)-H(8)	1.03(5)
C(7)-H(7)	1.00(5)
C(1)-C(2)	1.374(9)
C(1)-C(5)	1.417(9)
C(1)-H(1)	1.06(8)
C(3)-C(2)	1.376(8)
C(3)-C(4)	1.384(9)
C(3)-H(3)	0.95(9)
C(2)-H(2)	0.82(7)
C(4)-C(5)	1.402(9)
C(4)-H(4)	0.60(5)
C(5)-H(5)	1.19(5)
C(13)-C(13)#1	1.516(9)
C(13)-H(13A)	0.94(4)
C(13)-H(13B)	0.94(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z

Table 3.5

Bond Angles [degrees] for 1,6-diferrocenylhexane-1,6-dione

C(4)-Fe(1)-C(5)	40.4(3)	C(2)-Fe(1)-C(6)	161.5(2)
C(4)-Fe(1)-C(10)	157.4(3)	C(9)-Fe(1)-C(6)	69.07(18)
C(5)-Fe(1)-C(10)	121.5(2)	C(3)-Fe(1)-C(6)	157.1(2)
C(4)-Fe(1)-C(1)	67.2(2)	C(4)-Fe(1)-C(8)	123.9(2)
C(5)-Fe(1)-C(1)	40.7(3)	C(5)-Fe(1)-C(8)	160.0(3)
C(10)-Fe(1)-C(1)	108.11(18)	C(10)-Fe(1)-C(8)	69.06(17)
C(4)-Fe(1)-C(2)	66.3(3)	C(1)-Fe(1)-C(8)	157.6(3)
C(5)-Fe(1)-C(2)	67.2(3)	C(2)-Fe(1)-C(8)	122.8(2)
C(10)-Fe(1)-C(2)	125.1(2)	C(9)-Fe(1)-C(8)	40.58(17)
C(1)-Fe(1)-C(2)	39.4(2)	C(3)-Fe(1)-C(8)	108.0(2)
C(4)-Fe(1)-C(9)	159.8(3)	C(6)-Fe(1)-C(8)	68.30(19)
C(5)-Fe(1)-C(9)	158.1(2)	C(4)-Fe(1)-C(7)	108.2(2)
C(10)-Fe(1)-C(9)	41.69(17)	C(5)-Fe(1)-C(7)	124.0(2)
C(1)-Fe(1)-C(9)	122.5(2)	C(10)-Fe(1)-C(7)	68.67(15)
C(2)-Fe(1)-C(9)	108.8(2)	C(1)-Fe(1)-C(7)	161.2(3)
C(4)-Fe(1)-C(3)	39.8(3)	C(2)-Fe(1)-C(7)	157.4(2)
C(5)-Fe(1)-C(3)	67.8(2)	C(9)-Fe(1)-C(7)	68.27(19)
C(10)-Fe(1)-C(3)	160.8(2)	C(3)-Fe(1)-C(7)	122.2(2)
C(1)-Fe(1)-C(3)	66.9(2)	C(6)-Fe(1)-C(7)	40.44(16)
C(2)-Fe(1)-C(3)	39.4(2)	C(8)-Fe(1)-C(7)	40.3(2)
C(9)-Fe(1)-C(3)	123.8(2)	C(13)-C(12)-C(11)	115.4(4)
C(4)-Fe(1)-C(6)	122.1(2)	C(13)-C(12)-H(12B)	110(2)
C(5)-Fe(1)-C(6)	107.5(2)	C(11)-C(12)-H(12B)	106(2)
C(10)-Fe(1)-C(6)	41.05(15)	C(13)-C(12)-H(12A)	110(3)
C(1)-Fe(1)-C(6)	125.1(2)	C(11)-C(12)-H(12A)	106(3)
H(12B)-C(12)-H(12A)	109(4)	C(9)-C(10)-Fe(1)	69.6(2)
C(6)-C(10)-C(11)	124.9(4)	C(11)-C(10)-Fe(1)	121.8(3)
C(6)-C(10)-C(9)	107.2(3)	O(1)-C(11)-C(10)	119.4(4)
C(9)-C(10)-C(11)	127.7(4)	O(1)-C(11)-C(12)	120.7(4)
C(6)-C(10)-Fe(1)	70.1(2)	C(8)-C(9)-Fe(1)	70.0(2)
C(10)-C(11)-C(12)	119.8(4)	C(10)-C(6)-H(6)	126(3)
C(8)-C(9)-C(10)	107.5(4)	Fe(1)-C(6)-H(6)	125(2)
C(10)-C(9)-Fe(1)	68.7(2)	C(9)-C(8)-C(7)	108.6(4)
C(8)-C(9)-H(9)	128(3)	C(9)-C(8)-Fe(1)	69.4(2)
C(10)-C(9)-H(9)	124(3)	C(7)-C(8)-Fe(1)	70.2(3)
Fe(1)-C(9)-H(9)	132(3)	C(9)-C(8)-H(8)	121(3)
C(7)-C(6)-C(10)	108.1(4)	C(7)-C(8)-H(8)	131(3)
C(7)-C(6)-Fe(1)	70.2(2)	Fe(1)-C(8)-H(8)	130(2)
C(10)-C(6)-Fe(1)	68.9(2)	C(8)-C(7)-C(6)	108.6(4)
C(7)-C(6)-H(6)	126(2)	C(8)-C(7)-Fe(1)	69.6(2)

Table 3.5., Continued

C(6)-C(7)-Fe(1)	69.4(2)	C(1)-C(2)-H(2)	131(4)
C(8)-C(7)-H(7)	128(3)	Fe(1)-C(2)-H(2)	111(4)
C(6)-C(7)-H(7)	123(3)	C(3)-C(4)-C(5)	109.6(5)
Fe(1)-C(7)-H(7)	127(3)	C(3)-C(4)-Fe(1)	70.9(3)
C(2)-C(1)-C(5)	107.9(5)	C(5)-C(4)-Fe(1)	70.6(3)
C(2)-C(1)-Fe(1)	70.3(3)	C(3)-C(4)-H(4)	126(6)
C(5)-C(1)-Fe(1)	69.8(3)	C(5)-C(4)-H(4)	125(6)
C(2)-C(1)-H(1)	133(5)	Fe(1)-C(4)-H(4)	127(5)
C(5)-C(1)-H(1)	117(5)	H(5)-C(5)-C(4)	149(3)
Fe(1)-C(1)-H(1)	113(4)	H(5)-C(5)-C(1)	106(3)
C(2)-C(3)-C(4)	107.1(5)	C(4)-C(5)-C(1)	105.7(5)
C(2)-C(3)-Fe(1)	70.1(3)	H(5)-C(5)-Fe(1)	126(3)
C(4)-C(3)-Fe(1)	69.2(3)	C(4)-C(5)-Fe(1)	69.0(3)
C(2)-C(3)-H(3)	113(5)	C(1)-C(5)-Fe(1)	69.5(3)
C(4)-C(3)-H(3)	140(5)	C(12)-C(13)-C(13)#1	113.2(4)
Fe(1)-C(3)-H(3)	122(5)	C(12)-C(13)-H(13A)	113(3)
C(3)-C(2)-C(1)	109.7(6)	C(13)#1-C(13)-H(13A)	105(3)
C(3)-C(2)-Fe(1)	70.5(3)	C(12)-C(13)-H(13B)	106(3)
C(1)-C(2)-Fe(1)	70.3(3)	C(13)#1-C(13)-H(13B)	112(3)
C(3)-C(2)-H(2)	117(4)	H(13A)-C(13)-H(13B)	109(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z

Table 3.6

Hydrogen coordinates (x 10^4) and Isotropic Displacement Parameters (A^2 x 10^3) for 1,6-diferrocenylhexane-1,6-dione.

Atom Number	x	y	z	U(eq)
H(1)	5710(160)	490(30)	4020(100)	120(30)
H(2)	10170(120)	640(30)	5560(70)	72(18)
H(3)	10900(150)	1310(30)	7410(100)	120(30)
H(4)	6860(110)	1690(20)	7260(70)	46(17)
H(5)	3320(90)	1090(20)	5120(70)	620(30)
H(6)	4380(80)	2170(19)	2530(50)	45(12)
H(7)	7590(90)	2740(20)	4540(60)	65(15)
H(8)	11810(90)	2240(20)	4460(50)	51(12)
H(9)	10900(90)	1406(18)	2390(50)	44(12)
H(12A)	8300(70)	740(17)	30(50)	26(9)
H(12B)	8010(70)	462(16)	1550(50)	26(9)
H(13A)	4710(80)	325(19)	-1390(60)	42(11)
H(13B)	6830(90)	-80(20)	-880(60)	54(13)

X-ray Diffraction Analysis of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

The data set for this crystal was obtained with the help of Dr. Casey Raymond at Kent State University using the Bruker CCD system. The crystal was centered in the X-ray path and a one-minute rotation photo was taken. A full data set was collected, integrated, and corrected for absorption, as stated previously. A total of 9526 total reflections were collected, with 8551 of those being unique.

Prior to X-ray analysis, it was not known that this molecule was chiral. Structure refinement indicated that the molecule was chiral with the value of the BASF parameter being approximately 50%, indicating a nearly racemic mixture. The triclinic crystal is a part of the P1 space group due to the low symmetry of the molecule. Direct methods were used for structure refinement using SHELXTL software. The majority of non-hydrogen atoms were easily assigned anisotropically, but C16, C17, C36, and C37 were initially non-positive definite, meaning these atoms had negative mean square thermal displacement parameters. Since the structure has two molecules in the asymmetric unit, the non-positive definite atoms were constrained to have the same parameters as their symmetrical component in the other molecule using a command called EADP. This command allowed anisotropic refinement of these atoms, and refinement converged upon to an R value of 0.1335. The majority of hydrogen atoms were refined isotropically, while the remaining were assigned using the HFIX command. The constraint on the assigned hydrogens was removed, but refinement attempts proved unsuccessful. Therefore, the constraint was reinstated and the hydrogen atoms emerged as expected. Crystal data and refinement results are summarized in Table 3.7 and ORTEP plots of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene displaying 50% ellipsoids are shown in

Table 3.7

Crystal Data and Structure Refinement for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Empirical formula	$C_{26}H_2Fe_2O$
Formula weight	464.15
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P1
Unit cell dimensions	a = 8.4097(6)Å alpha = 93.7510(10)° b = 10.3097(8)Å beta=100.6130(10)° c=12.1100(9)Å gamma= 98.2110(10)°
Volume	1016.86(13) A^3
Z, Calculated density	2,1.516 Mg/m^3
Absorption coefficient	1.441 mm^{-1}
F(000)	480
Crystal size	0.02 x 0.05 x 0.10 mm
Theta range for data collection	1.72 to 28.29 deg.
Limiting indices	$-11 \le h \le 11$, $-13 \le k \le 13$, $-16 \le l \le 15$
Reflections collected / unique	9546 / 8551 [R(int) = 0.0277]
Completeness to theta = 28.29	97.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Hydrogen Atom Positions	Mixed Refinement and Constrained
Data / restraints / parameters	8551 / 3 / 500
Goodness-of-fit on F^2	1.008
Final R indices [I>2sigma(I)]	$R1(F)^a = 0.0651$, $wR2(F^2)^b = 0.1202$
R indices (all data)	$R1(F)^a = 0.1335$, $wR2(F^2)^b = 0.1460$
Absolute structure parameter	0.46(5)
Largest diff. peak and hole	0.514 and -0.357 $e.A^{-3}$

$^a R_1(F) = \Sigma \| |F_o| - |F_c| \| / \Sigma |F_o|$ with $F_o > 4.0\sigma(F)$.

$^b wR_2(F^2) = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$ with $F_o > 4.0\sigma(F)$, and $w^{-1} = \sigma^2(F_o)^2 + (W \cdot P)^2 + T \cdot P$, where $P = (Max(F_o^2, 0) + 2F_c^2)/3$, W = 0.0599, and T = 0.14.

Figures 3.3 and 3.4. Figure 3.5 displays the unit cell, followed by tables of bond lengths, angles, and anisotropic displacement parameters in Tables 3.8 to 3.12. Appendix B includes the structure factor tables generated in XCIF.

X-ray Diffraction Analysis of 1,6-diferrocenylhexane

Data collection for this crystal was also performed at Kent State University under the supervision of Dr. Casey Raymond. Data collection generated 1800 frames of data in which 9429 reflections were generated and 2594 were unique. Data integration and empirical absorption correction were performed in SAINT and SADABS, respectively.

Due to the high symmetry of the fully reduced product, the crystal belonged to the monoclinic crystal system, just as 1,6-diferrrocenylhexane-1,6-dione, with a space group of P2(1)/c. Direct methods were used for crystal structure refinement and all non-hydrogen atoms were assigned isotropically. However, only H6, HllA, and H11B could be refined. The remaining hydrogen positions were calculated using the HFIX constraint. The constraint was removed and refinement of the hydrogen positions was again attempted, but failed. Thus the HFIX constraint had to be reinstated to include all of the hydrogens in the structure. The final structure converged to a final R value of 0.0960 for all data. The crystal data and refinement results are shown in Table 3.13. An ORTEP plot of the fully reduced molecule displaying 50% ellipsoids is shown in Figure 3.6, followed by the orientation in the unit cell in Figure 3.7. Crystal data and refinement results, as well as bond lengths and angles can be found in Table 3.14 to Table 3.18.

RESULTS AND DISCUSSION

Characterization of 1,6-diferrocenylhexane-1,6-dione

The bond lengths for the structure were compared to those reported in the

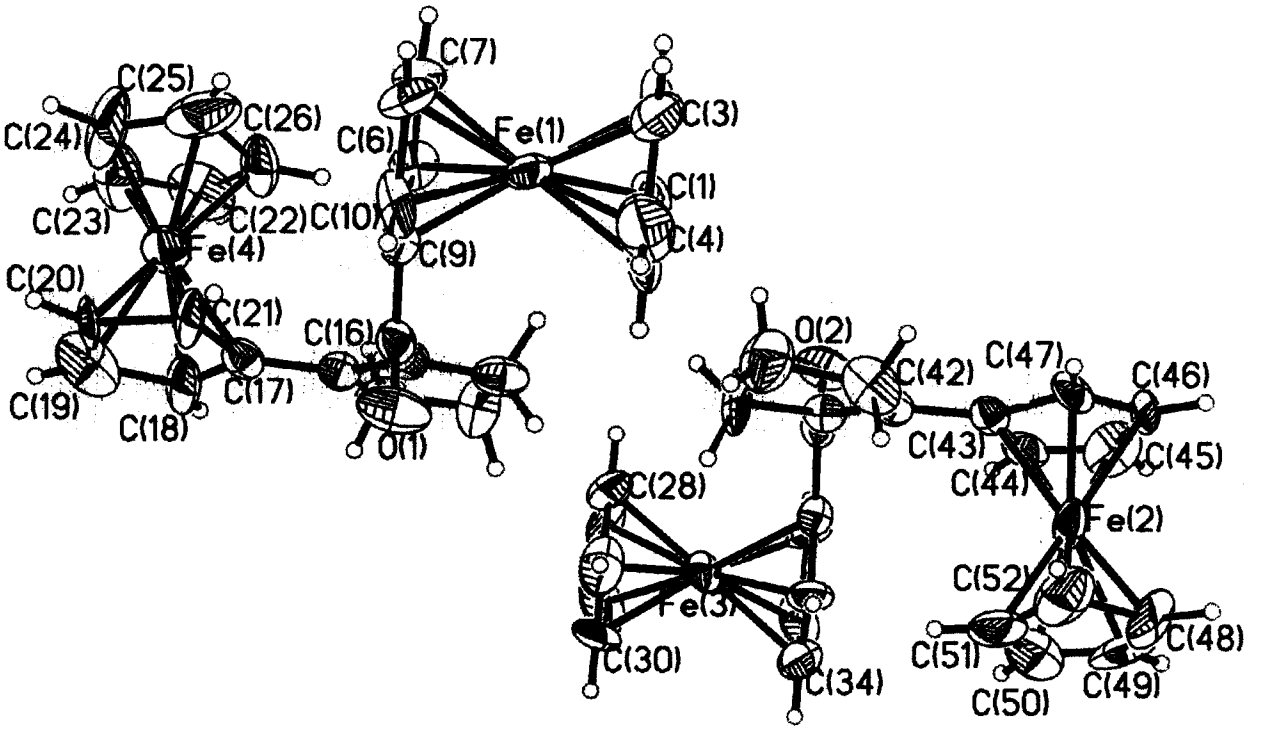

Figure 3.3: ORTEP plot of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene (50% ellipsoids)

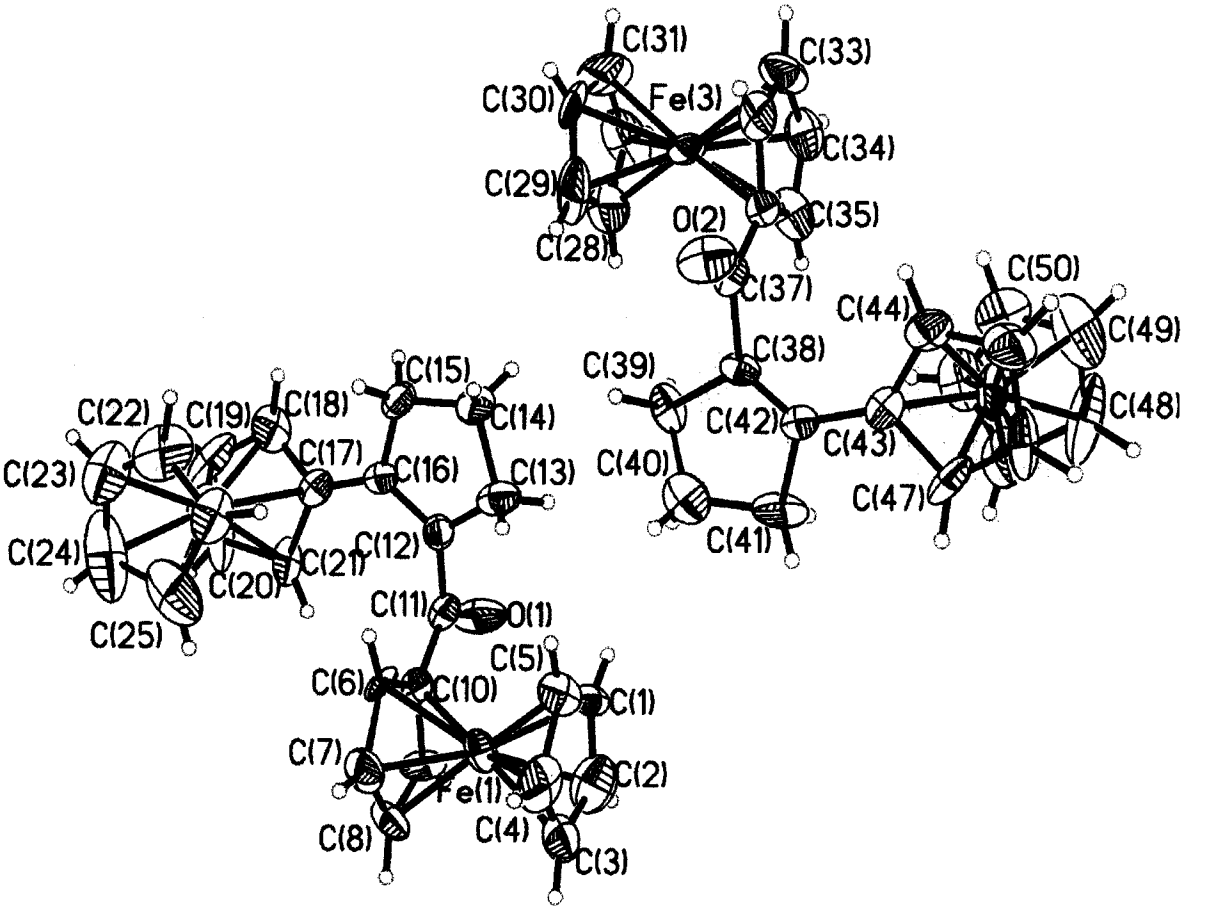

Figure 3.4: ORTEP plot of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene (50% ellipsoids)

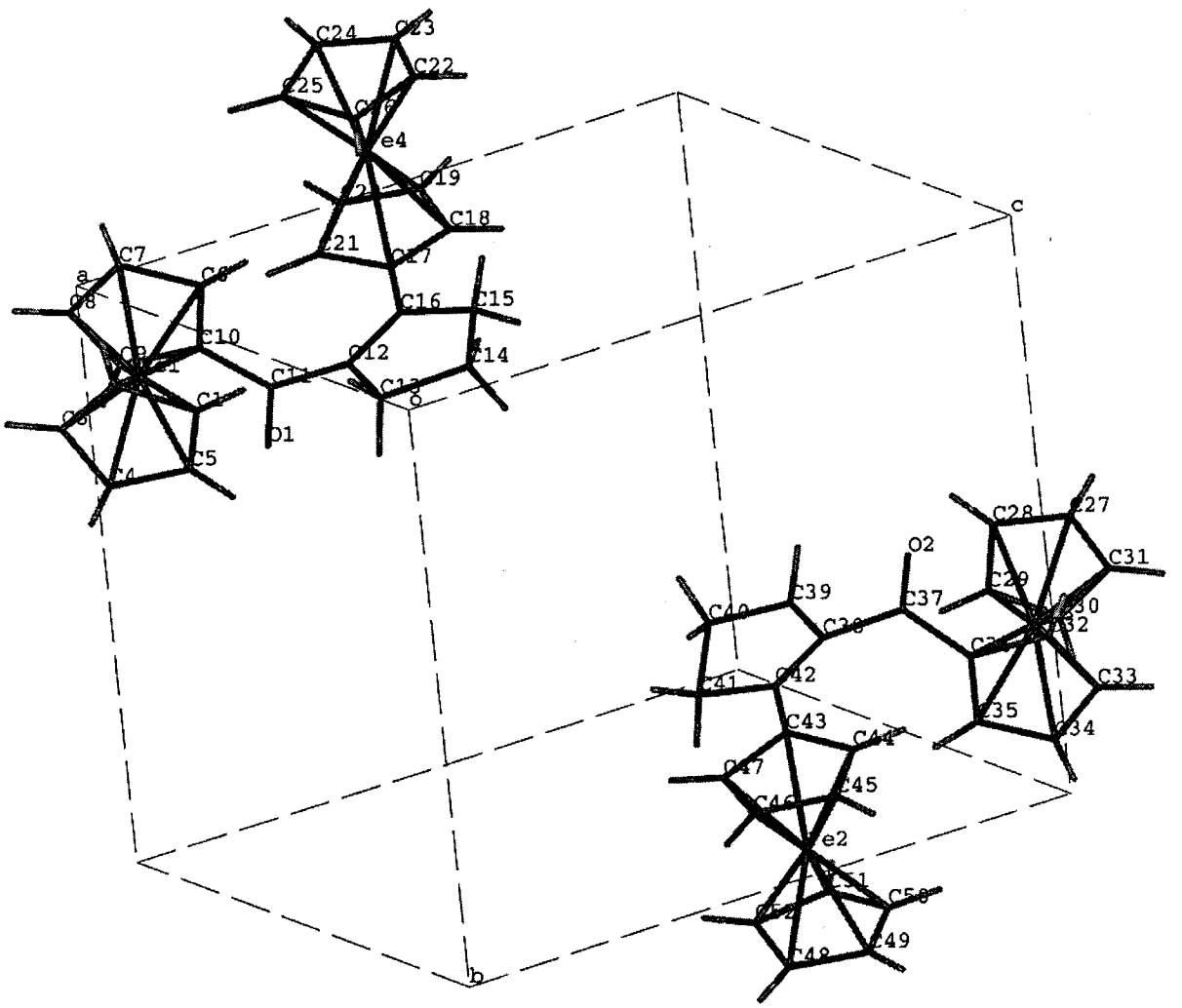

Figure 3.5: Unit cell of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Table 3.8

Atomic Coordinates ($x10^4$) and Equivalent Isotropic Displacement Parameters ($A^2 x 10^3$) for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom Number	x	y	z	U(eq)
Fe(1)	1921(2)	2590(1)	1845(1)	39(1)
Fe(2)	3650(2)	10946(2)	7547(1)	47(1)
Fe(3)	-1512(2)	6399(1)	8915(1)	39(1)
Fe(4)	-3243(2)	-1959(2)	3210(2)	52(1)
O(1)	-2537(14)	2717(13)	1505(10)	64(3)
O(2)	3053(14)	6330(12)	9344(9)	57(3)
C(1)	3022(16)	3900(15)	3272(13)	46(4)
C(2)	4220(20)	3494(16)	2620(15)	67(5)
C(3)	3940(20)	3833(14)	1551(16)	64(5)
C(4)	2440(20)	4478(18)	1449(18)	76(6)
C(5)	2026(17)	4462(13)	2555(11)	47(4)
C(6)	775(17)	965(12)	2399(11)	40(3)
C(7)	1940(20)	637(16)	1721(15)	52(4)
C(8)	1522(19)	1009(13)	629(12)	46(4)
C(9)	98(16)	1594(13)	622(9)	47(4)
C(10)	-363(18)	1558(13)	1682(11)	35(1)
C(11)	-1686(18)	2088(13)	2089(12)	36(1)
C(12)	-1854(16)	2045(13)	3281(12)	37(3)
C(13)	-1049(16)	3096(13)	4149(11)	47(4)
C(14)	-1780(20)	2766(15)	5240(11)	50(4)
C(15)	-2801(17)	1461(12)	4903(11)	49(4)
C(16)	-2854(16)	1087(13)	3689(12)	34(1)
C(17)	-3783(17)	-90(14)	3136(12)	36(1)
C(18)	-4915(19)	-848(14)	3566(12)	54(4)
C(19)	-5680(20)	-1982(17)	2759(16)	78(6)
C(20)	-4963(16)	-1894(12)	1823(13)	58(5)
C(21)	-3740(17)	-676(12)	2015(10)	43(3)
C(22)	-2120(20)	-2510(20)	4677(14)	76(6)
C(23)	-2900(20)	-3534(17)	4042(16)	78(5)
C(24)	-2270(30)	-3622(17)	3087(19)	113(10)
C(25)	-960(30)	-2440(20)	3126(17)	94(7)
C(26)	-1040(20)	-1712(15)	4212(13)	57(4)
C(27)	-2110(20)	4544(14)	9369(16)	65(5)
C(28)	-1490(20)	4500(13)	8422(16)	74(5)
C(29)	-2670(20)	5143(17)	7640(16)	73(5)

Table 3.8, Continued

C(30)	-3790(18)	5537(17)	8169(18)	73(6)
C(31)	-3360(20)	5160(20)	9286(18)	84(6)
C(32)	367(16)	7391(11)	10094(12)	47(4)
C(33)	-1050(20)	7968(16)	10088(15)	66(5)
C(34)	-1560(20)	8403(16)	9028(15)	54(5)
C(35)	-489(17)	8096(14)	8361(13)	50(4)
C(36)	746(18)	7451(13)	8995(12)	35(1)
C(37)	2059(17)	6822(13)	8656(12)	36(1)
C(38)	2302(16)	6951(13)	7467(10)	31(3)
C(39)	1380(20)	5856(13)	6533(12)	62(5)
C(40)	2260(30)	6085(18)	5639(15)	76(5)
C(41)	3138(18)	7554(15)	5808(9)	55(4)
C(42)	3186(16)	7840(13)	7079(11)	34(1)
C(43)	4249(17)	9081(14)	7720(12)	36(1)
C(44)	4288(16)	9735(15)	8778(12)	46(3)
C(45)	5360(20)	10847(16)	8983(11)	63(5)
C(46)	6138(16)	11010(12)	8033(14)	58(5)
C(47)	5481(16)	9983(14)	7265(13)	50(4)
C(48)	3240(30)	12650(17)	6850(20)	106(9)
C(49)	2570(30)	12569(18)	7811(18)	91(7)
C(50)	1430(20)	11490(20)	7607(16)	68(5)
C(51)	1330(20)	10864(17)	6627(17)	68(5)
C(52)	2510(30)	11454(17)	6009(16)	76(6)

Table 3.9

Bond lengths [Å] for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Fe(1)-C(7)	2.012(16)	O(2)-C(37)	1.253(18)
Fe(1)-C(9)	2.028(11)	C(1)-C(5)	1.32(2)
Fe(1)-C(10)	2.027(14)	C(1)-C(2)	1.48(2)
Fe(1)-C(6)	2.027(11)	C(1)-H(1)	0.9300
Fe(1)-C(5)	2.044(12)	C(2)-C(3)	1.35(2)
Fe(1)-C(4)	2.040(18)	C(2)-H(2)	0.9300
Fe(1)-C(2)	2.050(15)	C(3)-C(4)	1.50(3)
Fe(1)-C(3)	2.074(16)	C(3)-H(3)	0.9300
Fe(1)-C(8)	2.070(14)	C(4)-C(5)	1.44(2)
Fe(1)-C(1)	2.101(13)	C(4)-H(4)	0.9300
Fe(2)-C(47)	2.015(14)	C(5)-H(5)	0.9300
Fe(2)-C(51)	2.046(17)	C(6)-C(7)	1.45(2)
Fe(2)-C(50)	2.035(18)	C(6)-C(10)	1.405(19)
Fe(2)-C(49)	2.049(15)	C(6)-H(6)	0.9300
Fe(2)-C(52)	2.068(17)	C(7)-C(8)	1.40(2)
Fe(2)-C(48)	2.043(14)	C(7)-H(7)	0.9300
Fe(2)-C(44)	2.052(15)	C(8)-C(9)	1.41(2)
Fe(2)-C(45)	2.059(15)	C(8)-H(8)	0.9300
Fe(2)-C(43)	2.070(14)	C(9)-C(10)	1.409(17)
Fe(2)-C(46)	2.057(13)	C(9)-H(9)	0.9300
Fe(3)-C(29)	1.957(17)	C(10)-C(11)	1.46(2)
Fe(3)-C(31)	2.002(15)	C(11)-C(12)	1.479(19)
Fe(3)-C(30)	2.011(16)	C(12)-C(16)	1.381(18)
Fe(3)-C(33)	2.026(16)	C(12)-C(13)	1.455(19)
Fe(3)-C(28)	2.011(14)	C(13)-C(14)	1.594(19)
Fe(3)-C(32)	2.024(14)	C(13)-H(13A)	0.9700
Fe(3)-C(35)	2.046(15)	C(13)-H(13B)	0.9700
Fe(3)-C(36)	2.030(14)	C(14)-C(15)	1.478(19)
Fe(3)-C(27)	2.045(13)	C(14)-H(14A)	0.9700
Fe(3)-C(34)	2.069(16)	C(14)-H(14B)	0.9700
Fe(4)-C(23)	1.995(16)	C(15)-C(16)	1.486(19)
Fe(4)-C(26)	1.995(15)	C(15)-H(15A)	0.9700
Fe(4)-C(19)	2.020(17)	C(15)-H(15B)	0.9700
Fe(4)-C(24)	2.011(19)	C(16)-C(17)	1.40(2)
Fe(4)-C(18)	2.024(16)	C(17)-C(18)	1.35(2)
Fe(4)-C(20)	2.016(12)	C(17)-C(21)	1.459(19)
Fe(4)-C(22)	2.009(13)	C(18)-C(19)	1.46(2)
Fe(4)-C(21)	2.050(13)	C(18)-H(18)	0.9300
Fe(4)-C(17)	2.046(14)	C(19)-C(20)	1.38(2)
Fe(4)-C(25)	2.06(2)	C(19)-H(19)	0.9300
O(1)-C(11)	1.200(18)	C(20)-C(21)	1.482(16)

Table 3.9, Continued

C(20)-H(20)	0.9300	C(37)-C(38)	1.503(18)
C(21)-H(21)	0.9300	C(38)-C(42)	1.266(18)
C(22)-C(23)	1.28(3)	C(38)-C(39)	1.555(16)
C(22)-C(26)	1.36(2)	C(39)-C(40)	1.43(2)
C(22)-H(22)	0.9300	C(39)-H(39A)	0.9700
C(23)-C(24)	1.36(3)	C(39)-H(39B)	0.9700
C(23)-H(23)	0.9300	C(40)-C(41)	1.57(2)
C(24)-C(25)	1.51(3)	C(40)-H(40A)	0.9700
C(24)-H(24)	0.9300	C(40)-H(40B)	0.9700
C(25)-C(26)	1.49(2)	C(41)-C(42)	1.540(17)
C(25)-H(25)	0.9300	C(41)-H(41A)	0.9700
C(26)-H(26)	0.9300	C(41)-H(41B)	0.9700
C(27)-C(31)	1.29(3)	C(42)-C(43)	1.53(2)
C(27)-C(28)	1.34(2)	C(43)-C(44)	1.40(2)
C(27)-H(27)	0.9300	C(43)-C(47)	1.498(18)
C(28)-C(29)	1.49(3)	C(44)-C(45)	1.331(19)
C(28)-H(28)	0.9300	C(44)-H(44)	0.9300
C(29)-C(30)	1.33(3)	C(45)-C(46)	1.43(2)
C(29)-H(29)	0.9300	C(45)-H(45)	0.9300
C(30)-C(31)	1.43(3)	C(46)-C(47)	1.34(2)
C(30)-H(30)	0.9300	C(46)-H(46)	0.9300
C(31)-H(31)	0.9300	C(47)-H(47)	0.9300
C(32)-C(33)	1.40(2)	C(48)-C(49)	1.38(3)
C(32)-C(36)	1.428(19)	C(48)-C(52)	1.53(3)
C(32)-H(32)	0.9300	C(48)-H(48)	0.9300
C(33)-C(34)	1.40(2)	C(49)-C(50)	1.34(3)
C(33)-H(33)	0.9300	C(49)-H(49)	0.9300
C(34)-C(35)	1.37(2)	C(50)-C(51)	1.30(2)
C(34)-H(34)	0.9300	C(50)-H(50)	0.9300
C(35)-C(36)	1.443(19)	C(51)-C(52)	1.44(3)
C(35)-H(35)	0.9300	C(51)-H(51)	0.9300
C(36)-C(37)	1.46(2)	C(52)-H(52)	0.9300

Table 3.10

Bond Angles [degrees] for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

C(7)-Fe(1)-C(9)	67.2(6)	C(5)-Fe(1)-C(1)	37.0(6)
C(7)-Fe(1)-C(10)	68.4(6)	C(4)-Fe(1)-C(1)	67.7(7)
C(9)-Fe(1)-C(10)	40.7(5)	C(2)-Fe(1)-C(1)	41.8(6)
C(7)-Fe(1)-C(6)	42.1(6)	C(3)-Fe(1)-C(1)	68.5(7)
C(9)-Fe(1)-C(6)	68.5(5)	C(8)-Fe(1)-C(1)	160.6(6)
C(10)-Fe(1)-C(6)	40.6(5)	C(47)-Fe(2)-C(51)	130.4(7)
C(7)-Fe(1)-C(5)	159.9(6)	C(47)-Fe(2)-C(50)	165.0(7)
C(9)-Fe(1)-C(5)	126.1(6)	C(51)-Fe(2)-C(50)	37.0(7)
C(10)-Fe(1)-C(5)	110.6(6)	C(47)-Fe(2)-C(49)	155.5(8)
C(6)-Fe(1)-C(5)	123.8(5)	C(51)-Fe(2)-C(49)	64.9(7)
C(7)-Fe(1)-C(4)	156.0(7)	C(50)-Fe(2)-C(49)	38.2(8)
C(9)-Fe(1)-C(4)	108.6(7)	C(47)-Fe(2)-C(52)	107.5(7)
C(10)-Fe(1)-C(4)	125.0(7)	C(51)-Fe(2)-C(52)	40.9(7)
C(6)-Fe(1)-C(4)	160.7(7)	C(50)-Fe(2)-C(52)	67.6(8)
C(5)-Fe(1)-C(4)	41.4(7)	C(49)-Fe(2)-C(52)	70.9(8)
C(7)-Fe(1)-C(2)	107.6(7)	C(47)-Fe(2)-C(48)	122.7(9)
C(9)-Fe(1)-C(2)	159.0(6)	C(51)-Fe(2)-C(48)	66.0(8)
C(10)-Fe(1)-C(2)	158.6(6)	C(50)-Fe(2)-C(48)	64.3(8)
C(6)-Fe(1)-C(2)	122.3(7)	C(49)-Fe(2)-C(48)	39.5(8)
C(5)-Fe(1)-C(2)	65.5(7)	C(52)-Fe(2)-C(48)	43.6(8)
C(4)-Fe(1)-C(2)	67.3(8)	C(47)-Fe(2)-C(44)	67.4(5)
C(7)-Fe(1)-C(3)	118.6(6)	C(51)-Fe(2)-C(44)	124.5(7)
C(9)-Fe(1)-C(3)	124.7(6)	C(50)-Fe(2)-C(44)	111.2(6)
C(10)-Fe(1)-C(3)	162.5(7)	C(49)-Fe(2)-C(44)	123.3(7)
C(6)-Fe(1)-C(3)	154.8(6)	C(52)-Fe(2)-C(44)	157.2(7)
C(5)-Fe(1)-C(3)	68.6(6)	C(48)-Fe(2)-C(44)	158.2(8)
C(4)-Fe(1)-C(3)	42.7(7)	C(47)-Fe(2)-C(45)	66.5(6)
C(2)-Fe(1)-C(3)	38.2(7)	C(51)-Fe(2)-C(45)	155.0(8)
C(7)-Fe(1)-C(8)	40.0(6)	C(50)-Fe(2)-C(45)	122.3(7)
C(9)-Fe(1)-C(8)	40.4(6)	C(49)-Fe(2)-C(45)	107.4(7)
C(10)-Fe(1)-C(8)	68.8(6)	C(52)-Fe(2)-C(45)	162.5(8)
C(6)-Fe(1)-C(8)	69.7(6)	C(48)-Fe(2)-C(45)	124.4(8)
C(5)-Fe(1)-C(8)	159.9(6)	C(44)-Fe(2)-C(45)	37.8(5)
C(4)-Fe(1)-C(8)	121.3(7)	C(47)-Fe(2)-C(43)	43.0(5)
C(2)-Fe(1)-C(8)	122.5(7)	C(51)-Fe(2)-C(43)	111.3(7)
C(3)-Fe(1)-C(8)	105.6(7)	C(50)-Fe(2)-C(43)	126.2(7)
C(7)-Fe(1)-C(1)	125.2(7)	C(49)-Fe(2)-C(43)	158.8(8)
C(9)-Fe(1)-C(1)	157.8(6)	C(52)-Fe(2)-C(43)	121.1(6)
C(10)-Fe(1)-C(1)	122.1(6)	C(48)-Fe(2)-C(43)	160.6(9)
C(6)-Fe(1)-C(1)	107.3(6)	C(44)-Fe(2)-C(43)	39.7(6)

Table 3.10, Continued

C(45)-Fe(2)-C(43)	66.7(6)	C(32)-Fe(3)-C(27)	109.0(7)
C(47)-Fe(2)-C(46)	38.5(6)	C(35)-Fe(3)-C(27)	167.6(7)
C(51)-Fe(2)-C(46)	164.0(8)	C(36)-Fe(3)-C(27)	128.7(7)
C(50)-Fe(2)-C(46)	155.9(7)	C(29)-Fe(3)-C(34)	125.2(8)
C(49)-Fe(2)-C(46)	121.2(7)	C(31)-Fe(3)-C(34)	120.0(9)
C(52)-Fe(2)-C(46)	124.4(8)	C(30)-Fe(3)-C(34)	106.0(7)
C(48)-Fe(2)-C(46)	108.4(8)	C(33)-Fe(3)-C(34)	40.0(7)
C(44)-Fe(2)-C(46)	66.3(6)	C(28)-Fe(3)-C(34)	166.7(8)
C(45)-Fe(2)-C(46)	40.8(7)	C(32)-Fe(3)-C(34)	68.3(6)
C(43)-Fe(2)-C(46)	68.5(5)	C(35)-Fe(3)-C(34)	39.0(6)
C(29)-Fe(3)-C(31)	66.6(8)	C(36)-Fe(3)-C(34)	68.4(6)
C(29)-Fe(3)-C(30)	39.1(8)	C(27)-Fe(3)-C(34)	152.6(7)
C(31)-Fe(3)-C(30)	41.7(8)	C(23)-Fe(4)-C(26)	68.2(7)
C(29)-Fe(3)-C(33)	159.9(8)	C(23)-Fe(4)-C(19)	107.8(7)
C(31)-Fe(3)-C(33)	106.7(7)	C(26)-Fe(4)-C(19)	158.1(8)
C(30)-Fe(3)-C(33)	123.2(7)	C(23)-Fe(4)-C(24)	39.7(9)
C(29)-Fe(3)-C(28)	44.2(8)	C(26)-Fe(4)-C(24)	70.6(6)
C(31)-Fe(3)-C(28)	66.3(8)	C(19)-Fe(4)-C(24)	121.0(8)
C(30)-Fe(3)-C(28)	70.4(6)	C(23)-Fe(4)-C(18)	119.7(8)
C(33)-Fe(3)-C(28)	152.6(8)	C(26)-Fe(4)-C(18)	119.4(6)
C(29)-Fe(3)-C(32)	159.1(7)	C(19)-Fe(4)-C(18)	42.4(7)
C(31)-Fe(3)-C(32)	123.4(7)	C(24)-Fe(4)-C(18)	155.4(10)
C(30)-Fe(3)-C(32)	160.3(6)	C(23)-Fe(4)-C(20)	126.4(6)
C(33)-Fe(3)-C(32)	40.5(6)	C(26)-Fe(4)-C(20)	158.9(7)
C(28)-Fe(3)-C(32)	119.4(6)	C(19)-Fe(4)-C(20)	40.0(7)
C(29)-Fe(3)-C(35)	110.8(7)	C(24)-Fe(4)-C(20)	110.0(6)
C(31)-Fe(3)-C(35)	154.5(8)	C(18)-Fe(4)-C(20)	69.3(6)
C(30)-Fe(3)-C(35)	119.7(7)	C(23)-Fe(4)-C(22)	37.4(8)
C(33)-Fe(3)-C(35)	66.5(7)	C(26)-Fe(4)-C(22)	39.8(7)
C(28)-Fe(3)-C(35)	130.9(7)	C(19)-Fe(4)-C(22)	124.6(7)
C(32)-Fe(3)-C(35)	68.5(5)	C(24)-Fe(4)-C(22)	64.7(8)
C(29)-Fe(3)-C(36)	124.0(7)	C(18)-Fe(4)-C(22)	107.3(7)
C(31)-Fe(3)-C(36)	161.5(8)	C(20)-Fe(4)-C(22)	160.5(8)
C(30)-Fe(3)-C(36)	156.1(7)	C(23)-Fe(4)-C(21)	165.9(6)
C(33)-Fe(3)-C(36)	68.3(6)	C(26)-Fe(4)-C(21)	119.7(6)
C(28)-Fe(3)-C(36)	109.5(6)	C(19)-Fe(4)-C(21)	69.4(6)
C(32)-Fe(3)-C(36)	41.3(5)	C(24)-Fe(4)-C(21)	129.0(9)
C(35)-Fe(3)-C(36)	41.5(5)	C(18)-Fe(4)-C(21)	68.2(6)
C(29)-Fe(3)-C(27)	66.9(8)	C(20)-Fe(4)-C(21)	42.7(5)
C(31)-Fe(3)-C(27)	37.1(8)	C(22)-Fe(4)-C(21)	155.4(7)
C(30)-Fe(3)-C(27)	66.9(8)	C(23)-Fe(4)-C(17)	151.5(8)
C(33)-Fe(3)-C(27)	120.1(7)	C(26)-Fe(4)-C(17)	103.8(6)
C(28)-Fe(3)-C(27)	38.7(7)	C(19)-Fe(4)-C(17)	68.9(6)

Table 3.10, Continued

C(24)-Fe(4)-C(17)	165.9(10)	Fe(1)-C(5)-H(5)	125.2
C(18)-Fe(4)-C(17)	38.6(6)	C(7)-C(6)-C(10)	105.3(11)
C(20)-Fe(4)-C(17)	70.4(5)	C(7)-C(6)-Fe(1)	68.4(8)
C(22)-Fe(4)-C(17)	119.7(7)	C(10)-C(6)-Fe(1)	69.7(7)
C(21)-Fe(4)-C(17)	41.7(5)	C(7)-C(6)-H(6)	127.3
C(23)-Fe(4)-C(25)	70.2(8)	C(10)-C(6)-H(6)	127.4
C(26)-Fe(4)-C(25)	42.9(7)	Fe(1)-C(6)-H(6)	126.1
C(19)-Fe(4)-C(25)	158.0(9)	C(8)-C(7)-C(6)	110.7(13)
C(24)-Fe(4)-C(25)	43.6(9)	C(8)-C(7)-Fe(1)	72.3(9)
C(18)-Fe(4)-C(25)	158.0(7)	C(6)-C(7)-Fe(1)	69.5(7)
C(20)-Fe(4)-C(25)	122.6(7)	C(8)-C(7)-H(7)	124.6
C(22)-Fe(4)-C(25)	67.7(8)	C(6)-C(7)-H(7)	124.6
C(21)-Fe(4)-C(25)	106.9(7)	Fe(1)-C(7)-H(7)	125.2
C(17)-Fe(4)-C(25)	123.6(8)	C(7)-C(8)-C(9)	105.3(13)
C(5)-C(1)-C(2)	104.6(14)	C(7)-C(8)-Fe(1)	67.8(9)
C(5)-C(1)-Fe(1)	69.1(7)	C(9)-C(8)-Fe(1)	68.2(7)
C(2)-C(1)-Fe(1)	67.2(8)	C(7)-C(8)-H(8)	127.4
C(5)-C(1)-H(1)	127.7	C(9)-C(8)-H(8)	127.4
C(2)-C(1)-H(1)	127.7	Fe(1)-C(8)-H(8)	128.2
Fe(1)-C(1)-H(1)	127.4	C(10)-C(9)-C(8)	110.2(12)
C(3)-C(2)-C(1)	112.1(16)	C(10)-C(9)-Fe(1)	69.6(7)
C(3)-C(2)-Fe(1)	71.8(10)	C(8)-C(9)-Fe(1)	71.4(8)
C(1)-C(2)-Fe(1)	71.0(8)	C(10)-C(9)-H(9)	124.9
C(3)-C(2)-H(2)	124.0	C(8)-C(9)-H(9)	124.9
C(1)-C(2)-H(2)	123.9	Fe(1)-C(9)-H(9)	125.6
Fe(1)-C(2)-H(2)	124.9	C(9)-C(10)-C(6)	108.5(13)
C(2)-C(3)-C(4)	105.5(16)	C(9)-C(10)-C(11)	130.1(13)
C(2)-C(3)-Fe(1)	69.9(9)	C(6)-C(10)-C(11)	121.3(12)
C(4)-C(3)-Fe(1)	67.5(9)	C(9)-C(10)-Fe(1)	69.7(7)
C(2)-C(3)-H(3)	127.2	C(6)-C(10)-Fe(1)	69.7(8)
C(4)-C(3)-H(3)	127.3	C(11)-C(10)-Fe(1)	123.1(10)
Fe(1)-C(3)-H(3)	126.8	O(1)-C(11)-C(12)	117.9(13)
C(5)-C(4)-C(3)	104.3(16)	O(1)-C(11)-C(10)	120.4(13)
C(5)-C(4)-Fe(1)	69.4(9)	C(12)-C(11)-C(10)	121.0(12)
C(3)-C(4)-Fe(1)	69.9(9)	C(16)-C(12)-C(13)	112.3(12)
C(5)-C(4)-H(4)	127.9	C(16)-C(12)-C(11)	125.4(12)
C(3)-C(4)-H(4)	127.9	C(13)-C(12)-C(11)	122.2(11)
Fe(1)-C(4)-H(4)	124.6	C(12)-C(13)-C(14)	105.4(11)
C(1)-C(5)-C(4)	113.5(14)	C(12)-C(13)-H(13A)	110.7
C(1)-C(5)-Fe(1)	73.9(9)	C(14)-C(13)-H(13A)	110.7
C(4)-C(5)-Fe(1)	69.2(8)	C(12)-C(13)-H(13B)	110.7
C(1)-C(5)-H(5)	123.2	C(14)-C(13)-H(13B)	110.7
C(4)-C(5)-H(5)	123.2	H(13A)-C(13)-H(13B)	108.8

Table 3.10, Continued

C(15)-C(14)-C(13)	103.6(12)	C(20)-C(21)-H(21)	127.2
C(15)-C(14)-H(14A)	111.0	Fe(4)-C(21)-H(21)	127.9
C(13)-C(14)-H(14A)	111.0	C(23)-C(22)-C(26)	115.4(18)
C(15)-C(14)-H(14B)	111.0	C(23)-C(22)-Fe(4)	70.7(10)
C(13)-C(14)-H(14B)	111.0	C(26)-C(22)-Fe(4)	69.5(9)
H(14A)-C(14)-H(14B)	109.0	C(23)-C(22)-H(22)	122.2
C(14)-C(15)-C(16)	109.3(11)	C(26)-C(22)-H(22)	122.4
C(14)-C(15)-H(15A)	109.8	Fe(4)-C(22)-H(22)	129.6
C(16)-C(15)-H(15A)	109.8	C(22)-C(23)-C(24)	108.9(19)
C(14)-C(15)-H(15B)	109.8	C(22)-C(23)-Fe(4)	71.9(10)
C(16)-C(15)-H(15B)	109.8	C(24)-C(23)-Fe(4)	70.8(10)
H(15A)-C(15)-H(15B)	108.3	C(22)-C(23)-H(23)	125.7
C(17)-C(16)-C(12)	129.6(13)	C(24)-C(23)-H(23)	125.4
C(17)-C(16)-C(15)	121.5(12)	Fe(4)-C(23)-H(23)	123.3
C(12)-C(16)-C(15)	109.0(12)	C(23)-C(24)-C(25)	108.7(15)
C(16)-C(17)-C(18)	124.1(14)	C(23)-C(24)-Fe(4)	69.5(12)
C(16)-C(17)-C(21)	127.0(13)	C(25)-C(24)-Fe(4)	70.1(10)
C(18)-C(17)-C(21)	109.0(13)	C(23)-C(24)-H(24)	125.7
C(16)-C(17)-Fe(4)	128.4(10)	C(25)-C(24)-H(24)	125.6
C(18)-C(17)-Fe(4)	69.8(9)	Fe(4)-C(24)-H(24)	126.3
C(21)-C(17)-Fe(4)	69.3(8)	C(26)-C(25)-C(24)	100.9(19)
C(17)-C(18)-C(19)	109.9(13)	C(26)-C(25)-Fe(4)	66.0(9)
C(17)-C(18)-Fe(4)	71.6(10)	C(24)-C(25)-Fe(4)	66.3(12)
C(19)-C(18)-Fe(4)	68.7(9)	C(26)-C(25)-H(25)	129.5
C(17)-C(18)-H(18)	125.1	C(24)-C(25)-H(25)	129.6
C(19)-C(18)-H(18)	125.0	Fe(4)-C(25)-H(25)	129.4
Fe(4)-C(18)-H(18)	126.2	C(22)-C(26)-C(25)	105.7(16)
C(20)-C(19)-C(18)	107.7(12)	C(22)-C(26)-Fe(4)	70.6(9)
C(20)-C(19)-Fe(4)	69.8(9)	C(25)-C(26)-Fe(4)	71.1(9)
C(18)-C(19)-Fe(4)	68.9(9)	C(22)-C(26)-H(26)	127.2
C(20)-C(19)-H(19)	126.2	C(25)-C(26)-H(26)	127.1
C(18)-C(19)-H(19)	126.2	Fe(4)-C(26)-H(26)	122.8
Fe(4)-C(19)-H(19)	126.7	C(31)-C(27)-C(28)	112.9(19)
C(19)-C(20)-C(21)	108.0(13)	C(31)-C(27)-Fe(3)	69.6(10)
C(19)-C(20)-Fe(4)	70.1(9)	C(28)-C(27)-Fe(3)	69.3(8)
C(21)-C(20)-Fe(4)	69.9(6)	C(31)-C(27)-H(27)	123.5
C(19)-C(20)-H(20)	126.0	C(28)-C(27)-H(27)	123.6
C(21)-C(20)-H(20)	126.0	Fe(3)-C(27)-H(27)	129.4
Fe(4)-C(20)-H(20)	125.6	C(27)-C(28)-C(29)	102.0(16)
C(17)-C(21)-C(20)	105.5(13)	C(27)-C(28)-Fe(3)	72.0(9)
C(17)-C(21)-Fe(4)	69.0(7)	C(29)-C(28)-Fe(3)	66.0(8)
C(20)-C(21)-Fe(4)	67.4(7)	C(27)-C(28)-H(28)	129.0
C(17)-C(21)-H(21)	127.3	C(29)-C(28)-H(28)	129.0

Table 3.10, Continued

Fe(3)-C(28)-H(28)	124.7	C(35)-C(36)-C(32)	105.8(12)
C(30)-C(29)-C(28)	110.3(17)	C(35)-C(36)-C(37)	131.6(13)
C(30)-C(29)-Fe(3)	72.7(11)	C(32)-C(36)-C(37)	122.3(12)
C(28)-C(29)-Fe(3)	69.8(9)	C(35)-C(36)-Fe(3)	69.9(9)
C(30)-C(29)-H(29)	124.9	C(32)-C(36)-Fe(3)	69.1(8)
C(28)-C(29)-H(29)	124.9	C(37)-C(36)-Fe(3)	120.6(10)
Fe(3)-C(29)-H(29)	124.2	O(2)-C(37)-C(36)	122.4(13)
C(29)-C(30)-C(31)	104.1(16)	O(2)-C(37)-C(38)	120.7(13)
C(29)-C(30)-Fe(3)	68.2(10)	C(36)-C(37)-C(38)	116.4(12)
C(31)-C(30)-Fe(3)	68.8(10)	C(42)-C(38)-C(37)	129.7(12)
C(29)-C(30)-H(30)	128.0	C(42)-C(38)-C(39)	112.0(12)
C(31)-C(30)-H(30)	127.9	C(37)-C(38)-C(39)	118.3(12)
Fe(3)-C(30)-H(30)	126.5	C(40)-C(39)-C(38)	102.1(12)
C(27)-C(31)-C(30)	110.6(16)	C(40)-C(39)-H(39A)	111.3
C(27)-C(31)-Fe(3)	73.2(9)	C(38)-C(39)-H(39A)	111.3
C(30)-C(31)-Fe(3)	69.5(10)	C(40)-C(39)-H(39B)	111.4
C(27)-C(31)-H(31)	124.7	C(38)-C(39)-H(39B)	111.4
C(30)-C(31)-H(31)	124.7	H(39A)-C(39)-H(39B)	109.2
Fe(3)-C(31)-H(31)	124.1	C(39)-C(40)-C(41)	108.6(14)
C(33)-C(32)-C(36)	107.1(13)	C(39)-C(40)-H(40A)	110.0
C(33)-C(32)-Fe(3)	69.8(9)	C(41)-C(40)-H(40A)	109.9
C(36)-C(32)-Fe(3)	69.6(8)	C(39)-C(40)-H(40B)	110.0
C(33)-C(32)-H(32)	126.5	C(41)-C(40)-H(40B)	110.0
C(36)-C(32)-H(32)	126.4	H(40A)-C(40)-H(40B)	108.3
Fe(3)-C(32)-H(32)	125.7	C(42)-C(41)-C(40)	99.2(12)
C(32)-C(33)-C(34)	110.1(15)	C(42)-C(41)-H(41A)	111.9
C(32)-C(33)-Fe(3)	69.7(9)	C(40)-C(41)-H(41A)	111.9
C(34)-C(33)-Fe(3)	71.6(9)	C(42)-C(41)-H(41B)	111.9
C(32)-C(33)-H(33)	124.9	C(40)-C(41)-H(41B)	111.9
C(34)-C(33)-H(33)	124.9	H(41A)-C(41)-H(41B)	109.6
Fe(3)-C(33)-H(33)	125.3	C(38)-C(42)-C(41)	112.6(12)
C(35)-C(34)-C(33)	107.2(14)	C(38)-C(42)-C(43)	127.7(13)
C(35)-C(34)-Fe(3)	69.6(9)	C(41)-C(42)-C(43)	119.6(11)
C(33)-C(34)-Fe(3)	68.3(9)	C(44)-C(43)-C(47)	102.2(13)
C(35)-C(34)-H(34)	126.4	C(44)-C(43)-C(42)	132.3(13)
C(33)-C(34)-H(34)	126.4	C(47)-C(43)-C(42)	125.3(13)
Fe(3)-C(34)-H(34)	127.2	C(44)-C(43)-Fe(2)	69.4(9)
C(34)-C(35)-C(36)	109.7(14)	C(47)-C(43)-Fe(2)	66.6(8)
C(34)-C(35)-Fe(3)	71.4(9)	C(42)-C(43)-Fe(2)	123.0(10)
C(36)-C(35)-Fe(3)	68.7(8)	C(45)-C(44)-C(43)	112.3(13)
C(34)-C(35)-H(35)	125.2	C(45)-C(44)-Fe(2)	71.4(9)
C(36)-C(35)-H(35)	125.1	C(43)-C(44)-Fe(2)	70.8(8)
Fe(3)-C(35)-H(35)	126.4	C(45)-C(44)-H(44)	123.9

Table 3.10, Continued

C(43)-C(44)-H(44)	123.9	Fe(2)-C(48)-H(48)	127.2
Fe(2)-C(44)-H(44)	125.5	C(48)-C(49)-C(50)	105.8(18)
C(44)-C(45)-C(46)	108.8(13)	C(48)-C(49)-Fe(2)	70.0(9)
C(44)-C(45)-Fe(2)	70.8(9)	C(50)-C(49)-Fe(2)	70.3(11)
C(46)-C(45)-Fe(2)	69.5(8)	C(48)-C(49)-H(49)	127.0
C(44)-C(45)-H(45)	125.6	C(50)-C(49)-H(49)	127.1
C(46)-C(45)-H(45)	125.6	Fe(2)-C(49)-H(49)	124.2
Fe(2)-C(45)-H(45)	125.6	C(51)-C(50)-C(49)	113.1(19)
C(47)-C(46)-C(45)	107.1(12)	C(51)-C(50)-Fe(2)	72.0(11)
C(47)-C(46)-Fe(2)	69.1(8)	C(49)-C(50)-Fe(2)	71.5(10)
C(45)-C(46)-Fe(2)	69.7(9)	C(51)-C(50)-H(50)	123.5
C(47)-C(46)-H(46)	126.4	C(49)-C(50)-H(50)	123.4
C(45)-C(46)-H(46)	126.5	Fe(2)-C(50)-H(50)	124.7
Fe(2)-C(46)-H(46)	126.3	C(50)-C(51)-C(52)	113.1(18)
C(46)-C(47)-C(43)	109.6(14)	C(50)-C(51)-Fe(2)	71.0(11)
C(46)-C(47)-Fe(2)	72.4(9)	C(52)-C(51)-Fe(2)	70.3(10)
C(43)-C(47)-Fe(2)	70.4(8)	C(50)-C(51)-H(51)	123.5
C(46)-C(47)-H(47)	125.3	C(52)-C(51)-H(51)	123.4
C(43)-C(47)-H(47)	125.2	Fe(2)-C(51)-H(51)	127.0
Fe(2)-C(47)-H(47)	123.6	C(48)-C(52)-Fe(2)	67.3(9)
C(49)-C(48)-C(52)	110.4(18)	C(51)-C(52)-H(52)	131.3
C(49)-C(48)-Fe(2)	70.5(9)	C(48)-C(52)-H(52)	131.4
C(52)-C(48)-Fe(2)	69.1(8)	Fe(2)-C(52)-H(52)	124.4
C(49)-C(48)-H(48)	124.9	C(51)-C(52)-C(48)	97.3(17)
C(52)-C(48)-H(48)	124.7	C(51)-C(52)-Fe(2)	68.7(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z

Table 3.11

Anisotropic Displacement Parameters ($A^2 \times 10^3$) for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$

Atom Number	U11	U22	U33	U23	U13	U12
Fe(1)	38(1)	32(1)	49(1)	4(1)	2(1)	19(1)
Fe(2)	54(1)	28(1)	46(1)	-1(1)	-14(1)	-7(1)
Fe(3)	31(1)	45(1)	44(1)	1(1)	23(1)	-5(1)
Fe(4)	47(2)	49(1)	56(2)	16(1)	-4(1)	12(1)
O(1)	52(7)	102(9)	54(6)	27(6)	25(5)	35(6)
O(2)	47(6)	87(8)	42(6)	23(5)	3(4)	23(5)
C(1)	29(7)	56(8)	44(7)	-17(6)	-2(5)	-6(6)
C(2)	51(10)	61(10)	71(12)	-9(9)	-3(8)	-29(7)
C(3)	64(10)	38(7)	96(13)	1(8)	32(9)	12(7)
C(4)	65(12)	72(11)	86(13)	17(10)	4(9)	-1(9)
C(5)	42(7)	47(7)	46(7)	-26(5)	24(5)	-19(6)
C(6)	56(8)	35(6)	39(7)	28(5)	25(6)	7(5)
C(7)	42(10)	45(9)	72(12)	3(8)	15(8)	20(7)
C(8)	59(9)	43(7)	41(8)	-2(6)	12(6)	29(6)
C(9)	46(8)	71(9)	11(5)	-21(5)	5(5)	-24(6)
C(10)	40(2)	32(2)	32(3)	2(2)	9(2)	2(2)
C(11)	31(2)	33(2)	41(2)	8(2)	9(2)	-1(2)
C(12)	32(8)	30(7)	52(9)	2(6)	17(6)	4(6)
C(13)	45(7)	60(8)	46(8)	20(6)	21(6)	23(6)
C(14)	80(10)	46(7)	15(5)	3(5)	4(6)	-6(7)
C(15)	52(8)	36(7)	74(10)	24(6)	39(7)	18(6)
C(16)	32(2)	38(2)	32(2)	6(2)	10(2)	7(2)
C(17)	31(2)	40(2)	36(3)	12(2)	1(2)	5(2)
C(18)	61(9)	49(7)	35(7)	-12(6)	-13(6)	-9(6)
C(19)	55(11)	87(12)	95(14)	59(11)	17(9)	-5(9)
C(20)	39(8)	23(6)	85(11)	-5(7)	-43(7)	-8(5)
C(21)	63(8)	27(6)	23(6)	-3(5)	-22(5)	-8(5)
C(22)	73(12)	114(15)	36(8)	33(10)	-22(8)	31(11)
C(23)	84(13)	72(11)	59(10)	19(8)	-21(9)	-8(9)
C(24)	150(20)	52(10)	91(15)	-23(9)	-86(14)	14(11)
C(25)	103(16)	100(14)	86(15)	3(11)	-8(11)	73(13)
C(26)	60(9)	52(7)	42(8)	3(6)	-17(6)	-12(6)
C(27)	82(13)	25(7)	98(13)	17(7)	55(10)	-10(7)

Table 3.11, Continued

C(28)	62(9)	29(7)	135(15)	20(8)	19(9)	17(6)
C(29)	83(12)	55(10)	76(11)	-9(8)	27(9)	-8(8)
C(30)	25(8)	75(11)	117(16)	-24(10)	8(9)	21(7)
C(31)	58(10)	101(13)	92(14)	-10(11)	52(10)	-31(9)
C(32)	48(8)	30(6)	75(9)	17(6)	22(6)	29(6)
C(33)	48(9)	76(10)	69(11)	-31(8)	32(8)	-16(7)
C(34)	56(11)	41(8)	64(12)	1(8)	1(9)	16(7)
C(35)	40(7)	49(8)	58(9)	-3(6)	-10(6)	24(6)
C(36)	40(2)	32(2)	32(3)	2(2)	9(2)	2(2)
C(37)	31(2)	33(2)	41(2)	8(2)	9(2)	-1(2)
C(38)	36(8)	43(8)	14(6)	2(5)	0(5)	10(6)
C(39)	80(10)	43(8)	42(8)	-32(6)	3(7)	-28(7)
C(40)	93(13)	64(10)	67(11)	-11(8)	22(10)	3(9)
C(41)	57(9)	94(11)	10(5)	-6(6)	1(5)	6(7)
C(42)	32(2)	38(2)	32(2)	6(2)	10(2)	7(2)
C(43)	31(2)	40(2)	36(3)	12(2)	1(2)	5(2)
C(44)	31(6)	56(8)	57(9)	12(7)	19(6)	13(6)
C(45)	91(12)	68(11)	32(7)	8(7)	11(7)	20(9)
C(46)	26(7)	29(6)	97(12)	-9(7)	-25(7)	-8(5)
C(47)	26(6)	51(8)	79(10)	37(7)	21(6)	4(6)
C(48)	90(15)	33(8)	180(20)	62(12)	-23(15)	8(8)
C(49)	104(15)	61(11)	109(15)	2(10)	-13(11)	63(11)
C(50)	51(10)	90(13)	64(12)	18(10)	7(8)	13(9)
C(51)	54(9)	64(9)	84(12)	13(9)	-11(8)	35(7)
C(52)	100(15)	55(10)	74(12)	25(9)	6(10)	23(9)

Table 3.12

Hydrogen Coordinates ($x10^4$) and Isotropic Displacement Parameters ($A^2 \times 10^3$) for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Atom Number	x	y	z	U(eq)
H(1)	2981	3783	4022	56
H(2)	5080	3057	2912	81
H(3)	4539	3695	996	76
H(4)	1892	4812	817	92
H(5)	1142	4815	2741	57
H(6)	780	815	3148	48
H(7)	2844	234	1978	62
H(8)	2064	895	34	55
H(9)	-453	1952	6	56
H(13A)	-1282	3943	3917	56
H(13B)	128	3115	4298	56
H(14A)	-915	2733	5883	59
H(14B)	-2440	3417	5429	59
H(15A)	-3902	1489	5029	58
H(15B)	-2343	811	5355	58
H(18)	-5171	-676	4271	65
H(19)	-6507	-2642	2859	94
H(20)	-5204	-2495	1186	70
H(21)	-3083	-353	1523	52
H(22)	-2290	-2318	5405	91
H(23)	-3747	-4122	4208	93
H(24)	-2589	-4297	2507	135
H(25)	-297	-2220	2610	113
H(26)	-461	-889	4513	69
H(27)	-1689	4170	10015	77
H(28)	-575	4159	8288	88
H(29)	-2619	5252	6890	87
H(30)	-4658	5961	7880	88
H(31)	-3894	5331	9871	101
H(32)	947	7035	10700	56
H(33)	-1563	8051	10699	79
H(34)	-2467	8821	8816	65
H(35)	-549	8278	7613	60
H(39A)	1443	4986	6783	74
H(39B)	240	5953	6303	74
H(40A)	1515	5916	4915	91

Table 3.12, Continued

H(40B)	3070	5498	5652	91
H(41A)	4228	7638	5637	66
H(41B)	2501	8117	5360	66
H(44)	3641	9427	9281	55
H(45)	5564	11423	9634	75
H(46)	6947	11698	7961	69
H(47)	5751	9851	6559	59
H(48)	4018	13336	6738	127
H(49)	2852	13147	8463	110
H(50)	779	11215	8116	82
H(51)	577	10110	6351	81
H(52)	2751	11191	5317	91

Table 3.13

Crystal Data and Structure Refinement for 1,6-diferrocenylhexane

Empirical formula	$C_{26}H_{30}Fe_2$
Formula weight	454.20
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.8908(11) Å alpha = 90° b = 8.3936(7)Å beta = 98.572(2)° c = 10.0431(9) Å gamma = 90°
Volume	1074.53(16) A^3
Z, Calculated density	2, 1.404 Mg/m^3
Absorption coefficient	1.358 mm^{-1}
F(000)	476
Crystal size	0.06 x 0.10 x 0.04 mm
Theta range for data collection	1.60 to 28.28 deg.
Limiting indices	$-17 \leq h \leq 17, -10 \leq k \leq 10, -13 \leq l \leq 13$
Reflections collected / unique	9429 / 2594 [R(int) = 0.0494]
Completeness to theta = 28.28	97.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Hydrogen Atom Positions	Constrained
Data / restraints / parameters	2594 / 0 / 127
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	$R1(F)^a = 0.0637$, $wR2(F^2)^b = 0.1420$
R indices (all data)	$R1(F)^a = 0.0960$, $wR2(F^2)^b = 0.1552$
Largest diff. peak and hole	0.426 and -0.424 $e.A^{-3}$

$^a R_1(F) = \Sigma \| |F_o| - |F_c| \| / \Sigma |F_o|$ with $F_o > 4.0\sigma(F)$.

$^b wR_2(F^2) = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$ with $F_o > 4.0\sigma(F)$, and $w^{-1} = \sigma^2(F_o)^2 + (W \cdot P)^2 + T \cdot P$, where $P = (Max(F_o^2, 0) + 2F_c^2)/3$, W = 0.0600, and T = 1.18.

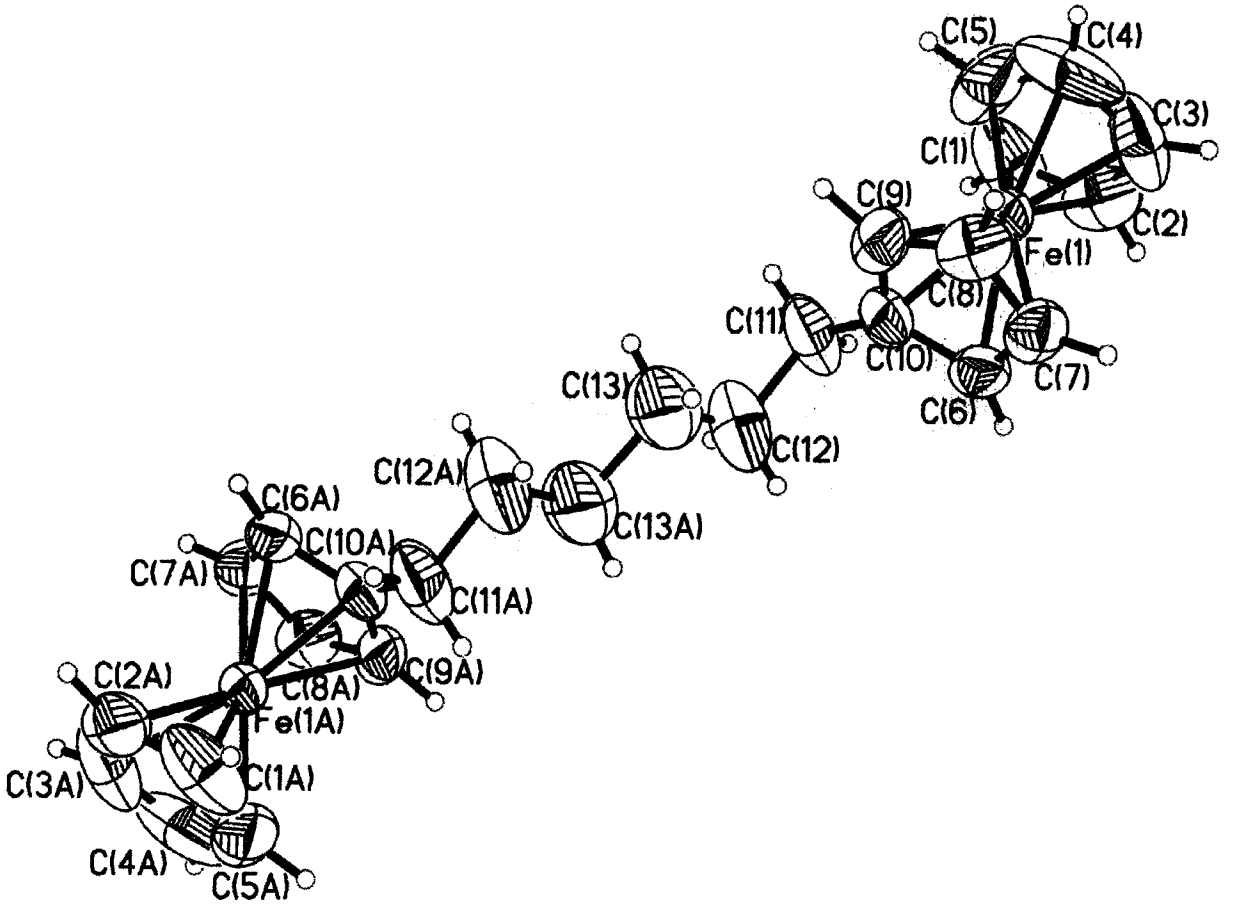

Figure 3.6: ORTEP plot of 1,6-diferrocenylhexane (50% ellipsoids)

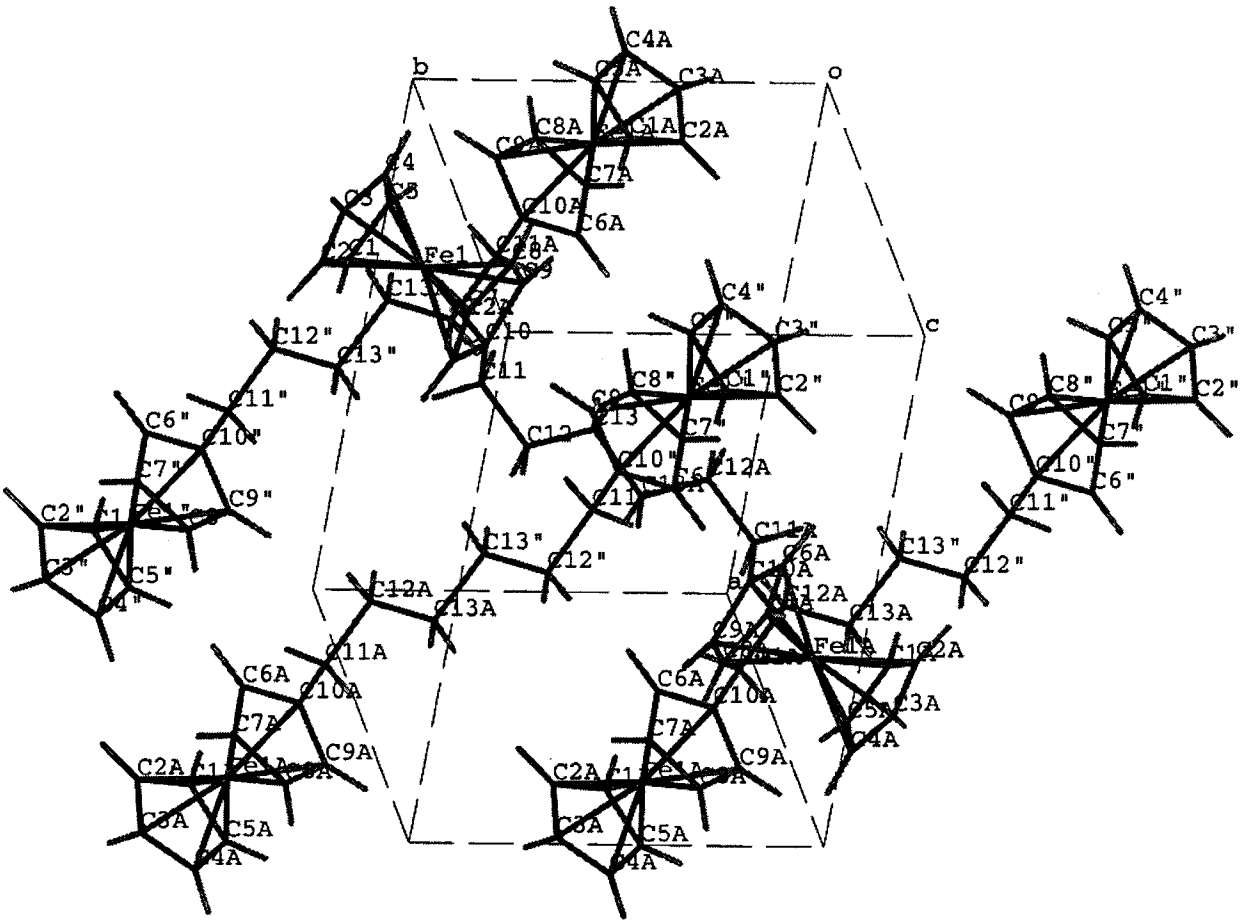

Figure 3.7: Unit cell of 1,6-diferrocenylhexane

Table 3.14

Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (A^2 x 10^3) for 1,6-diferrocenylhexane. U(eq) is defined as one third of the trace of the orthogonalizedUij tensor.

Atom Number	x	y	z	U(eq)
Fe(1)	1894(1)	10132(1)	3653(1)	50(1)
C(1)	2444(5)	11477(10)	2270(9)	110(3)
C(2)	2071(7)	12438(6)	3194(6)	95(2)
C(3)	1050(7)	12117(9)	3138(8)	109(3)
C(4)	781(6)	10979(13)	2237(11)	138(4)
C(5)	1622(12)	10561(9)	1684(6)	138(4)
C(6)	2833(4)	9588(5)	5394(4)	64(1)
C(7)	1782(4)	9501(6)	5573(4)	67(1)
C(8)	1293(4)	8363(6)	4679(4)	71(1)
C(9)	2043(4)	7749(5)	3929(4)	69(1)
C(10)	3020(4)	8518(5)	4369(4)	64(1)
C(11)	4036(4)	8259(7)	3847(6)	100(2)
C(12)	4835(5)	7164(9)	4722(8)	128(3)
C(13)	4548(7)	5590(8)	4590(9)	137(3)

Table 3.15

Bond Lengths [Å] for 1,6-diferrocenylhexane

C(1)-C(5)	1.369(11)
C(1)-C(2)	1.370(9)
C(1)-Fe(1)	1.999(5)
C(1)-H(1)	0.9800
C(2)-C(3)	1.335(9)
C(2)-Fe(1)	2.010(5)
C(2)-H(2)	0.9800
C(3)-C(4)	1.326(11)
C(3)-Fe(1)	2.015(5)
C(3)-H(3)	0.9800
C(4)-C(5)	1.337(11)
C(4)-Fe(1)	1.995(6)
C(4)-H(4)	0.9800
C(5)-Fe(1)	1.990(6)
C(5)-H(5)	0.9800
C(6)-C(7)	1.395(7)
C(6)-C(10)	1.414(6)
C(6)-Fe(1)	2.025(4)
C(6)-H(6)	0.9800
C(7)-C(8)	1.396(6)
C(7)-Fe(1)	2.026(4)
C(7)-H(7)	0.9800
C(8)-C(9)	1.408(6)
C(8)-Fe(1)	2.026(4)
C(8)-H(8)	0.9800
C(9)-C(10)	1.426(6)
C(9)-Fe(1)	2.024(4)
C(9)-H(9)	0.9800
C(10)-C(11)	1.497(7)
C(10)-Fe(1)	2.036(4)
C(11)-C(12)	1.552(8)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.373(10)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(13)#1	1.654(14)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

Table 3.16

Bond Angles [degrees] for 1,6-diferrocenylhexane

C(5)-C(1)-C(2)	107.1(6)	Fe(1)-C(7)-H(7)	126.1
C(5)-C(1)-Fe(1)	69.5(4)	C(7)-C(8)-C(9)	108.3(4)
C(2)-C(1)-Fe(1)	70.4(3)	C(7)-C(8)-Fe(1)	69.8(2)
C(5)-C(1)-H(1)	126.4	C(9)-C(8)-Fe(1)	69.6(2)
C(2)-C(1)-H(1)	126.4	C(7)-C(8)-H(8)	125.8
Fe(1)-C(1)-H(1)	126.4	C(9)-C(8)-H(8)	125.8
C(3)-C(2)-C(1)	107.2(6)	Fe(1)-C(8)-H(8)	125.8
C(3)-C(2)-Fe(1)	70.8(3)	C(8)-C(9)-C(10)	108.3(4)
C(1)-C(2)-Fe(1)	69.6(3)	C(8)-C(9)-Fe(1)	69.7(2)
C(3)-C(2)-H(2)	126.4	C(10)-C(9)-Fe(1)	69.9(2)
C(1)-C(2)-H(2)	126.4	C(8)-C(9)-H(9)	125.8
Fe(1)-C(2)-H(2)	126.4	C(10)-C(9)-H(9)	125.8
C(4)-C(3)-C(2)	109.3(7)	Fe(1)-C(9)-H(9)	125.8
C(4)-C(3)-Fe(1)	69.9(4)	C(6)-C(10)-C(9)	105.9(4)
C(2)-C(3)-Fe(1)	70.4(3)	C(6)-C(10)-C(11)	126.9(5)
C(4)-C(3)-H(3)	125.4	C(9)-C(10)-C(11)	127.2(5)
C(2)-C(3)-H(3)	125.4	C(6)-C(10)-Fe(1)	69.2(2)
Fe(1)-C(3)-H(3)	125.4	C(9)-C(10)-Fe(1)	69.0(2)
C(3)-C(4)-C(5)	109.1(8)	C(11)-C(10)-Fe(1)	126.0(3)
C(3)-C(4)-Fe(1)	71.5(4)	C(10)-C(11)-C(12)	115.5(5)
C(5)-C(4)-Fe(1)	70.2(4)	C(10)-C(11)-H(11A)	108.4
C(3)-C(4)-H(4)	125.5	C(12)-C(11)-H(11A)	108.4
C(5)-C(4)-H(4)	125.5	C(10)-C(11)-H(11B)	108.4
Fe(1)-C(4)-H(4)	125.5	C(12)-C(11)-H(11B)	108.4
C(4)-C(5)-C(1)	107.3(7)	H(11A)-C(11)-H(11B)	107.5
C(4)-C(5)-Fe(1)	70.6(4)	C(13)-C(12)-C(11)	111.6(7)
C(1)-C(5)-Fe(1)	70.3(4)	C(13)-C(12)-H(12A)	109.3
C(4)-C(5)-H(5)	126.3	C(11)-C(12)-H(12A)	109.3
C(1)-C(5)-H(5)	126.3	C(13)-C(12)-H(12B)	109.3
Fe(1)-C(5)-H(5)	126.3	C(11)-C(12)-H(12B)	109.3
C(7)-C(6)-C(10)	109.6(4)	H(12A)-C(12)-H(12B)	108.0
C(7)-C(6)-Fe(1)	69.9(3)	C(12)-C(13)-C(13)#1	111.6(9)
C(10)-C(6)-Fe(1)	70.1(2)	C(12)-C(13)-H(13A)	109.3
C(7)-C(6)-H(6)	125.2	C(13)#1-C(13)-H(13A)	109.3
C(10)-C(6)-H(6)	125.2	C(12)-C(13)-H(13B)	109.3
Fe(1)-C(6)-H(6)	125.2	C(13)#1-C(13)-H(13B)	109.3
C(6)-C(7)-C(8)	107.9(4)	H(13A)-C(13)-H(13B)	108.0
C(6)-C(7)-Fe(1)	69.8(2)	C(5)-Fe(1)-C(4)	39.2(3)
C(8)-C(7)-Fe(1)	69.9(2)	C(5)-Fe(1)-C(1)	40.2(3)
C(6)-C(7)-H(7)	126.1	C(4)-Fe(1)-C(1)	66.1(3)
C(8)-C(7)-H(7)	126.1	C(5)-Fe(1)-C(2)	66.9(3)

Table 3.16, Continued

C(4)-Fe(1)-C(2)	65.6(3)	C(3)-Fe(1)-C(7)	110.4(2)
C(1)-Fe(1)-C(2)	40.0(3)	C(9)-Fe(1)-C(7)	68.29(19)
C(5)-Fe(1)-C(3)	65.6(3)	C(6)-Fe(1)-C(7)	40.30(19)
C(4)-Fe(1)-C(3)	38.6(3)	C(5)-Fe(1)-C(8)	127.9(4)
C(1)-Fe(1)-C(3)	65.7(3)	C(4)-Fe(1)-C(8)	109.5(3)
C(2)-Fe(1)-C(3)	38.7(3)	C(1)-Fe(1)-C(8)	165.7(3)
C(5)-Fe(1)-C(9)	108.3(2)	C(2)-Fe(1)-C(8)	152.5(3)
C(4)-Fe(1)-C(9)	119.5(3)	C(3)-Fe(1)-C(8)	120.3(3)
C(1)-Fe(1)-C(9)	128.1(3)	C(9)-Fe(1)-C(8)	40.68(18)
C(2)-Fe(1)-C(9)	166.2(3)	C(6)-Fe(1)-C(8)	67.7(2)
C(3)-Fe(1)-C(9)	152.7(3)	C(7)-Fe(1)-C(8)	40.31(18)
C(5)-Fe(1)-C(6)	153.3(5)	C(5)-Fe(1)-C(10)	118.8(3)
C(4)-Fe(1)-C(6)	165.9(4)	C(3)-Fe(1)-C(10)	165.9(4)
C(1)-Fe(1)-C(6)	119.9(3)	C(9)-Fe(1)-C(10)	41.11(18)
C(2)-Fe(1)-C(6)	110.0(2)	C(6)-Fe(1)-C(10)	40.75(17)
C(3)-Fe(1)-C(6)	129.7(3)	C(7)-Fe(1)-C(10)	68.81(19)
C(9)-Fe(1)-C(6)	68.09(18)	C(2)-Fe(1)-C(10)	128.5(3)
C(5)-Fe(1)-C(7)	165.2(4)	C(4)-Fe(1)-C(10)	152.6(4)
C(4)-Fe(1)-C(7)	128.8(4)	C(1)-Fe(1)-C(10)	108.2(2)
C(1)-Fe(1)-C(7)	153.1(3)	C(8)-Fe(1)-C(10)	68.9(2)
C(2)-Fe(1)-C(7)	119.8(2)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z

Table 3.17

Anisotropic Displacement Parameters ($A^2 \times 10^3$) for 1,6-diferrocenylhexane. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$

Atom Number	U11	U22	U33	U23	U13	U12
Fe(1)	60(1)	42(1)	47(1)	4(1)	8(1)	4(1)
C(1)	100(5)	126(6)	117(5)	77(5)	62(4)	38(4)
C(2)	148(6)	53(3)	76(4)	19(3)	-13(4)	-21(3)
C(3)	127(6)	88(5)	127(6)	49(4)	64(5)	59(4)
C(4)	100(5)	128(8)	163(9)	81(7)	-58(6)	-17(5)
C(5)	287(14)	74(4)	45(3)	5(3)	1(5)	33(7)
C(6)	82(3)	52(2)	53(2)	4(2)	-9(2)	2(2)
C(7)	90(3)	66(3)	47(2)	5(2)	16(2)	3(2)
C(8)	84(3)	66(3)	61(3)	12(2)	10(2)	-21(2)
C(9)	110(4)	41(2)	55(3)	4(2)	9(3)	1(2)
C(10)	76(3)	50(2)	64(3)	11(2)	5(2)	17(2)
C(11)	94(4)	90(4)	120(5)	24(3)	27(4)	50(3)
C(12)	122(6)	98(5)	164(7)	4(5)	24(5)	45(4)
C(13)	183(8)	76(4)	139(6)	12(4)	-15(6)	13(5)

Table 3.18

Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters (A^2 x 10^3) for 1,6-diferrocenylhexane

Atom Number	x	y	z	U(eq)
H(1)	3160	11467	2053	132
H(2)	2472	13238	3767	114
H(3)	577	12633	3685	131
H(4)	75	10533	2000	166
H(5)	1639	9778	963	165
H(6)	3357	10302	5887	77
H(7)	1447	10125	6217	80
H(8)	553	8052	4582	85
H(9)	1914	6938	3223	83
H(11A)	4364	9287	3763	120
H(11B)	3885	7803	2952	120
H(12A)	5523	7299	4455	153
H(12B)	4883	7475	5660	153
H(13A)	4437	5305	3643	164
H(13B)	3891	5437	4934	164

International Tables of Crystallography and are in agreement.[1] Sp^2 hybridized carbon bond lengths were approximately 1.4 Å with the carbon-hydrogen bonds in agreement with the typical 1.0 Å. Sp^3 hybridized carbon-carbon bond lengths were consistent with the theoretical values of 1.5 Å. The iron bond lengths to the carbons in the cyclopentene rings were in agreement with one another, displaying lengths of 2.0 Å, which are typical of ferrocene derivatives. The bond angles between the iron and carbons in the ring above and below also demonstrated agreement with literature values.[2,3] The carbon-carbon bond angles in the Cp rings were also in agreement with literature values.[2,3]

The planarity of the top and bottom Cp rings was calculated in XSHELL. The equation of the mean plane and atomic deviations from the planes are given in Table A-1 and A-2 of Appendix A. The plane defined by C1 to C5 had a maximum deviation of 0.0020 Å, attributed to C1. The top Cp ring, containing C6 to C10, had a maximum deviation of 0.0042 Å at C9.

The planarity of the Cp ring with respect to the carbonyl was also investigated. The plane that included O1 and C6 to C10 showed a maximum deviation of 0.0046 Å from the plane due to C8. It is interesting to note that the carbonyl lies in the plane of the Cp ring to maximize electronic interactions between the Cp ring and the carbonyl group.

Due to the symmetry of 1,6-diferrocenylhexane1,6-dione, half of the structure was in the asymmetric unit and the grow command was used to generate the other half. Utilizing this command put the ferrocenes 180 °C out of phase with respect to one another. The planarity calculations for the Cp rings produced the same results as previously stated. In addition, the top and bottom Cp rings of the ferrocenes, were eclipsed with respect to one another.

Characterization of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

The sp^2 carbon-carbon bonds in the Cp rings demonstrated the appropriate bond lengths, 2.0 Å from the iron centers, as well as with respect to each other, 1.4 Å . The carbon-carbon sp^2 and sp^3 bond lengths in the cyclopentene ring were consistent with literature values at 1.3 Å and 1.5 Å, respectively. The bond between C12 and C16 was longer than expected for a double bond, suggesting the presence of a single bond. However, the results from the mass spectrometry and ^{13}C NMR experiments clearly demonstrate the presence of a C=C double bond. In addition the bond angles associated with C12, C16, C38, and C42 are in accordance with sp^2 hybridized carbons, further indicating the presence of a carbon-carbon double bond. Thus, it was concluded that the cyclopentene ring contained a double bond.

The coplanarity of the Cp rings within the ferrocene with respect to the carbonyl group was calculated. The maximum deviation in the plane defined by C6 to C11 containing O1, occurred at O1 with a value of 0.0567 Å, while the plane defined by O2 and C32 to C37 was 0.0462 Å at C37. The carbonyl, as in 1,6-diferrocenylhexane-1,6-dione, is coplanar with the adjacent Cp ring to maximize electronic interactions. The equations for the plane, as well as the atom deviations from the plane, are shown in Tables B-1 and B-2 in Appendix B. Figure 3.8 displays an ORTEP plot illustrating the coplanarity of the carbonyl with the adjacent Cp ring.

The planarity of the cyclopentene ring with respect to the adjacent Cp ring was also calculated in XSHELL. The maximum deviation from the plane was 0.1195 Å at C12 in the plane defined by C12 to C21. Thus, the cyclopentene group and the neighboring Cp ring are nearly coplanar with respect to one another. The plane that included C38 to C47

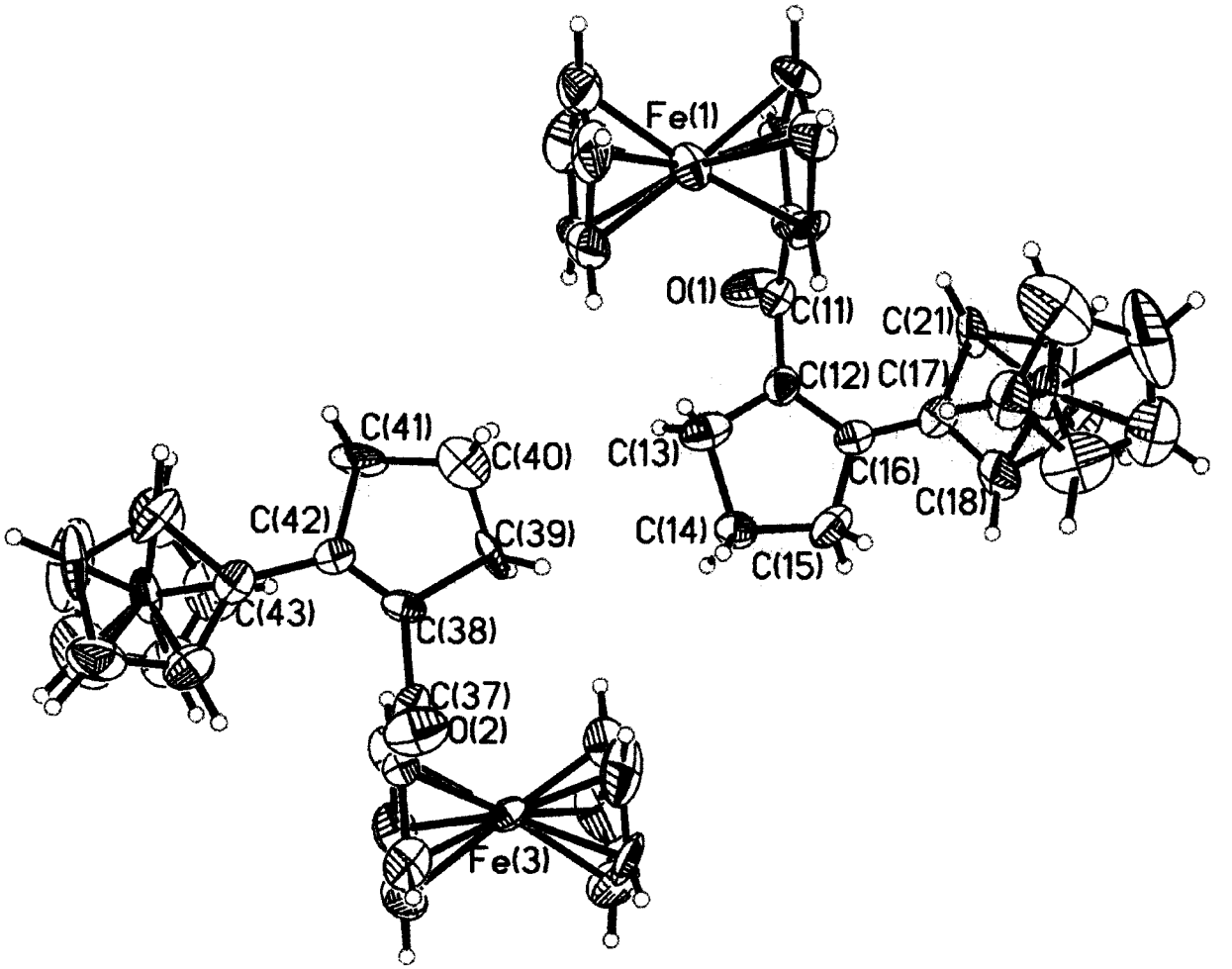

Figure 3.8: ORTEP plot of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene (50% ellipsoids) demonstrating coplanarity of carbonyl with adjacent Cp ring.

demonstrated a maximum deviation of 0.2523 Å at C41 also demonstrating the near coplanarity between the cyclopentene and Cp rings. An ORTEP plot shown in Figure 3.9 shows the coplanarity between the cyclopentene ring and the adjacent Cp ring. The equation of the planes for the five-membered ring, as well as atomic deviations from the plane can be found in Tables B-3 and B-4 in Appendix B.

The planarity of the Cp rings was calculated for the four ferrocenes 1-ferrocenyl-carbonyl-2-ferrocenylcylcopentene was also calculated. The equations of the mean planes and atomic deviations are located in Tables B-5 to B-12 for all eight Cp rings. The greatest deviation from planarity between all of the Cp rings occurred at C14 with a deviation of 0.0501 Å. Eclipsing of the top and bottom Cp rings was evident in all of the ferrocene groups.

The planarity of the cyclopentene rings were also determined and the deviations from the calculated plane are shown in Table B-13 and Table B-14 in Appendix B. The plane defined by C12 to C16 had a maximum deviation of 0.0501 Å at C14. The cyclopentene ring containing C38 to C42, deviated by 0.1300 Å from the plane at C40. Figure 3.9 gives an edge on view of the five membered ring and the maximum deviation at C40 is easily seen in this ORTEP plot.

Figure 3.9 also illustrates that the orientation of the carbonyl is out of the plane relative to the cyclopentene ring. This is attributed to steric interactions between the carbonyl group and the adjacent five-membered ring.

Characterization of 1,6-diferrocenylhexane

Bond lengths between the sp^2 carbon atoms in the Cp rings produced values of approximately 1.4 Å, which are typical of sp^2 hybridized carbons. The carbon-iron bond

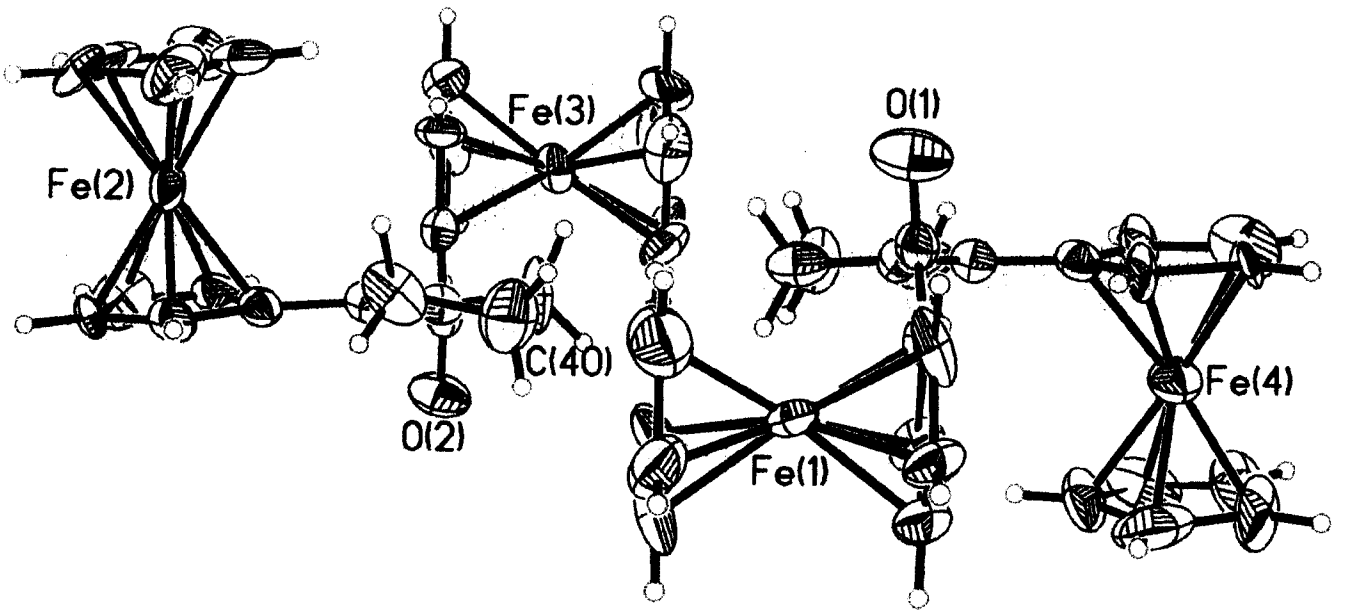

Figure 3.9: ORTEP plot of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene (50% ellipsoids) demonstrating coplanarity of cyclopentene ring with adjacent Cp ring.

bond lengths centers were also in agreement with theoretical values of 2.0 Å. The sp^3 hybridized carbon-carbon bonds in the six-carbon bridge were approximately 1.5 Å. The carbon-hydrogen bonds throughout the molecule produced typical 1.0 Å bond lengths. The bond angles were also investigated and were in agreement with those found in literature.[2,3]

The maximum deviation from planarity for the bottom Cp ring was 0.0060 Å from the plane that included C1 to C5 and was due to C2. The planarity of the top ring only showed a 0.0040 Å deviation from the mean plane defined by C6 to C10 that was attributed to C6. Table C-1 and C-2 in Appendix C shown the equations of the mean plane and the atomic deviations for both the bottom and top rings. In addition, the top and bottom Cp rings were slightly staggered relative to one another, but not to an appreciable degree.

The grow command was also used to generate the remaining half of 1,6-diferrocenyl-hexane, not shown in the asymmetric unit. The ferrocenes were therefore 180° out of phase with respect to one another.

Conclusions

The crystal structures for the compounds, 1,6-diferrocenylhexane-1,6-dione, 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene, and 1,6-diferrocenylhexane are presented. The structures of the fully oxidized and fully reduced compounds produced results that were consistent with literature values and refinement was straightforward. Since the structure of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentane was not known prior to structure refinement, the results were surprising, i.e.chirality.

All three crystals produced bond lengths and angles that were similar with respect to one another, and were also in agreement with those reported in the literature.[1-3] The sp^2 carbon bond lengths were approximately 1.3 Å to 1.4 Å and sp^3-sp^2 carbon bond lengths were 1.5 Å. The carbon bonds to the iron centers were all consistent at 2.0 Å and the carbon-hydrogen bonds were approximately 1.0 Å.

The top and bottom Cp rings were coplanar in all three crystal structures. The carbonyl moieties in both the 1,6-diferrocenylhexane-1,6-dione and 1-ferrocenyl-carbonyl-2-ferrocenylcyclopentene were found to be coplanar with the adjacent Cp rings, allowing for maximization of electronic interactions between the two. The deviation from planarity of the oxygen in the 1,6-diferrocenylhexane-1,6-dione was compared to both oxygen's in 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene. The plane defined by O1 and O2 in the chiral crystal, was 0.0552 Å and 0.0006 Å, respectively, different than the plane containing O1 in 1,6-diferrocenylhexane-1,6-dione.

The 1,6-diferrocenylhexane-1,6-dione and 1,6-diferrocenylhexane products both crystallized in the monoclinic crystal system. The space groups were different, with 1,6-diferrocenylhexane-1,6-dione belonged to the P2(1)/n and 1,6-diferrocenylhexane to the P2(1)/c space group. For these structures, it was observed that adjacent ferrocene groups in the molecule were rotated 180° out of phase relative to one another. The 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene was observed to be in the triclinic crystal system with a space group of P1, the lowest symmetry possible.

In all three crystals the relative eclipsing of the Cp rings within the ferrocenes were investigated using XSHELL. The top and bottom Cp rings in the fully oxidized and chiral crystals were eclipsed with respect to one another. The Cp rings in 1,6-

diferrocenylhexane were somewhat staggered, but to a negligible degree.

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CHAPTER FOUR

ELECTROCHEMISTRY

Cyclic voltammetry was the principle electrochemical technique used to study the synthesized diferrocenes. A four-part synthesis was carried out, as stated in Chapter Two, to prepare 6-(diferrocenylhexanylcarbonyl)pentanethiol. Solution CV was performed on four of the synthesized precursors, 1,6-diferrocenylhexane-1,6-dione, 1-ferrocenyl-carbonyl-2-ferrocenylcyclopentene, 1,6-diferrocenylhexane and 1,6-diferrocenylhexane-1-one. The redox potentials of the diferrocenes in solution were used to compare and assign the waves observed in the monolayer electrochemistry. Chemical and electrochemical reversibility, formal potentials, and ΔE_p values were investigated and compared to previous work performed on dimeric ferrocene complexes in solution.[1,2] To demonstrate that solution voltammetry was a diffusion controlled process, graphs of peak current versus the square root of the scan rate (i_p v. $\nu^{1/2}$) were created.

The electrochemical investigation of monolayers constructed from 6-(diferrocenyl-hexanylcarbonyl)pentanethiol was the ultimate goal of this project. The data presented is a preliminary study in diferrocene tagged alkanethiol monolayers. Rate constants, surface coverages and full width at half maximum (FWHM) values are reported for the monolayers. The values obtained for each are compared to previously reported work on 1,2-diferrocenylethane containing monolayers and the various monomeric ferrocene alkanethiol monolayers produced by Chidsey[3,4].

Chemicals

Acetonitrile (Fisher, HPLC grade, 99.9%), aluminiun oxide (LECO Corp., 1.0 μm

powder), methylene chloride (Fisher, certified ACS, 99.9%), and perchloric acid (Fisher, certified ACS, 74%), were used as received.

Tetra-*n*-butylammonium perchlorate (Fluka, 98%) was recrystallized three times from ethanol.

Instrumentation

A Bio-Analytical Systems (BAS) 100B Potentiostat was used to perform the cyclic voltammetry experiments. The software used in data analysis was included in the potentiostat package. Platinum and gold disc (1.6 mm diameter) working electrodes, platinum wire counter electrodes, and aqueous Ag/AgCl and non-aqueous $Ag/AgNO_3$ electrodes were purchased from Bio-Analytical Systems.

Electrode Preparation

Solution voltammetry experiments were performed at a platinum disc working electrode. Before each use, the electrode was hand polished for fifteen minutes on a flocked twill polishing cloth with an aqueous suspension of 1.0 micron Al_2O_3, until a mirror finish was obtained. The electrode was sonicated for fifteen minutes in deionized water to remove residual aluminum oxide, rinsed with water and electrolyte before transferring it to the cell.

The polycrystalline gold electrodes used for monolayer electrochemistry were polished by hand on a flocked twill polishing cloth for one and a half hours using an aqueous suspension of 1.0 micron Al_2O_3. The electrode was sonicated for fifteen minutes in deionized water to ensure all of the Al_2O_3 was removed, followed by rinsing with water and electrolyte solution. Prior to soaking the electrode in the thiol coating solution, the gold electrode surface was electrochemically reduced in a 1.0 M $HClO_{4(aq)}$ solution

by performing 50 cyclic voltammetric sweeps between –1500 mV and 1500 mV, ending at –1500 mV. The electrode was rinsed with deionized water and methylene chloride before immersing it in the monolayer coating solution.

Solution Voltammetry

Cyclic voltammetry was performed on four of the synthesized precursors; 1,6-diferrocenylhexane-1,6-dione, 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene, 1,6-diferrocenylhexane, and 1,6-diferrocenylhexane-1-one. Solutions were prepared as 1.0 mM in the ferrocene compounds and 0.1 M in recrystallized tertra-*n*-butylammonium perchlorate (TBAP) in HPLC grade acetonitrile.

Data analysis was performed by constructing a spreadsheet in Microsoft Excel in which ΔE_p, $i_{p,a}/i_{p,c}$, and $E^{\circ'}$ values were calculated as a function of scan rate. These values are shown in Tables D-1 to D-4 in Appendix D. The data were then examined for chemical and electrochemical reversibility. Graphs of $i_{p,a}$ versus $\nu^{1/2}$ were constructed for all four solutions to demonstrate that electron transfer was diffusion controlled.

Monolayer Preparation

Monolayers were produced by preparing a 1.0 mM coating solution of 6-(diferrocenylhexanylcarbonyl)pentanethiol (0.01 g, 0.017 mol) dissolved in methylene chloride. The electrodes were prepared as stated previously and soaked in the thiol solution overnight with gentle stirring.

Data analysis consisted of calculating ΔE_p, $i_{p,a}/i_{p,c}$, and $E^{\circ'}$ as a function of scan rate. The peak areas, used for surface coverage determinations, as well as FWHM values for each wave were determined using the BAS software. A spreadsheet was constructed in Microsoft Excel and the data is tabulated in Tables D-5 to D-7 of Appendix D. The data

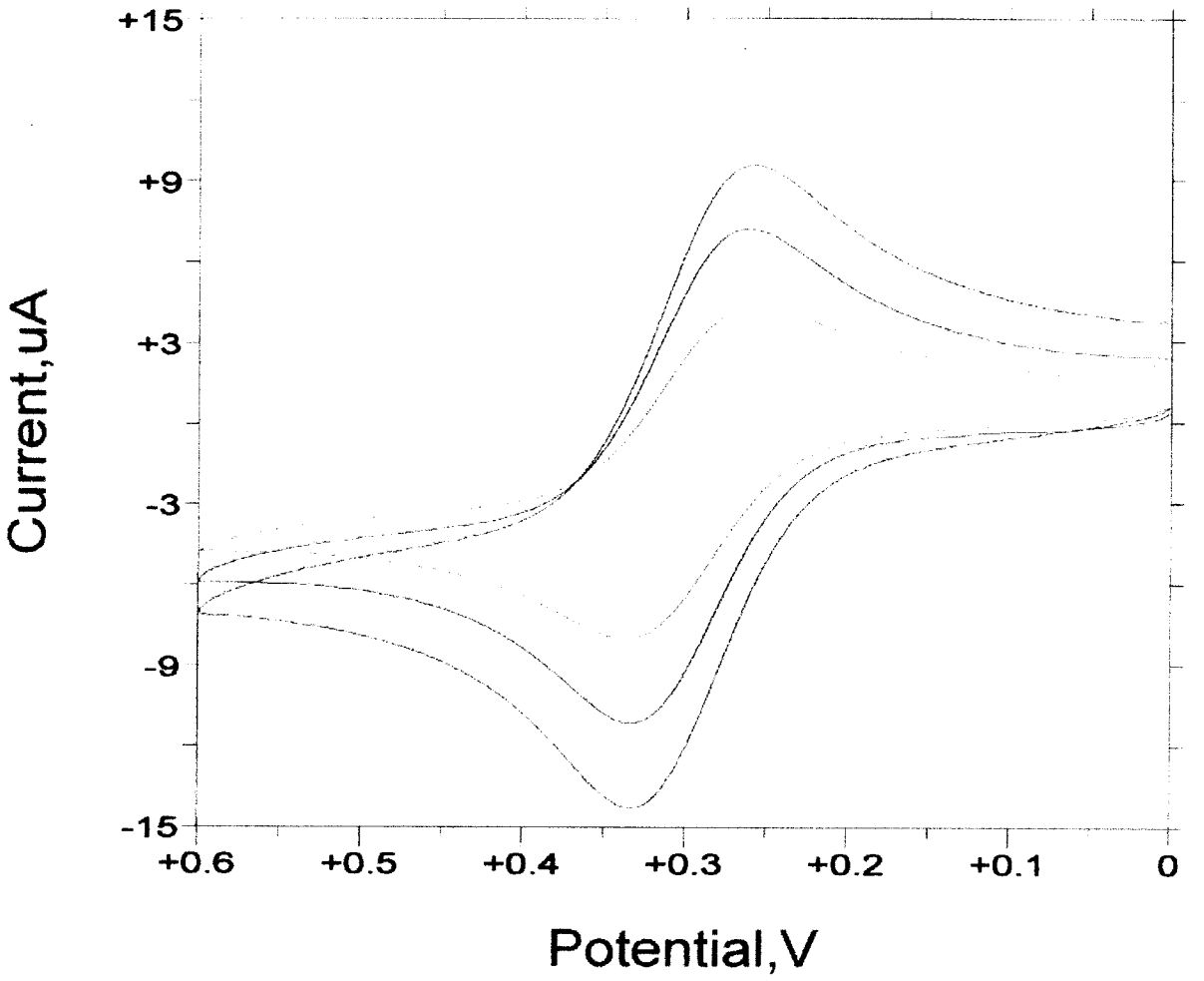
were examined for chemical and electrochemical reversibility, formal potentials and electrochemical accessibility. To illustrate that the thiol was a surface confined species, a plot of $i_{p,a}$ versus scan rate was constructed.

Solution Voltammetry of 1,6-diferrocenylhexane-1,6-dione

A scan rate study was performed on the solution from 25 mV/sec to 500 mV/sec at 25 mV/sec intervals and from 500 mV/sec to 1000 mV/sec at 50 mV/sec intervals. The data is tabulated in Appendix D in Table D-1. Shown in Figure 4.1, is a series of voltammograms at 150 mV/sec, 100 mV/sec, and 50 mV/sec scan rates. The voltammograms displayed a single, two-electron oxidation centered at an $E^{\circ\prime}$ of 271.5 mV. The cathodic and anodic waves were symmetrical with respect to each other, with minimal peak tailing and broadening. The ratio of $i_{p,a}/i_{p,c}$ was approximately one. ΔE_p was approximately 94.5 mV and independent of scan rate.

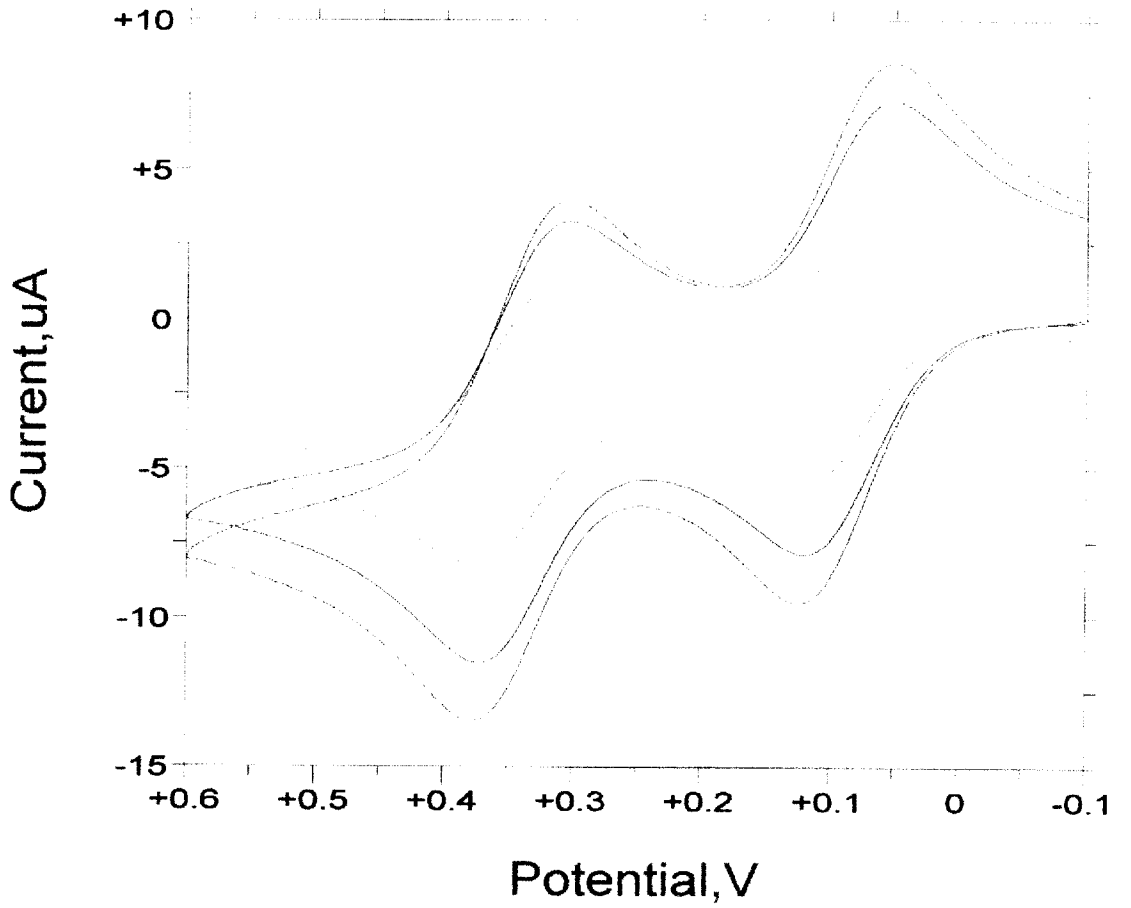
Solution Voltammetry of 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

A full scan rate study was performed on the 1-ferrocenylcarbonyl-2-ferrocenyl-cyclopentene and tabulated data is found in Table D-2 of Appendix D. Voltammograms at scan rates of 150 mV/sec, 100 mV/sec, and 50 mV/sec are shown in Figure 4.2. The voltammograms displayed two distinct one electron transfer waves, with $E^{\circ\prime}$'s centered at 87 mV for the first wave and 344 mV for the second wave. The waves were well defined and symmetrical in both the anodic and cathodic directions. The peak current ratios for both redox waves were approximately one at all scan rates. ΔE_p was approximately 80 mV for both redox waves and was independent of scan rate.



Line Color	Scan Rate
Blue	150 mV/sec
Red	100 mV/sec
Green	50 mV/sec

Figure 4.1: Cyclic voltammogram of 1.0 mM 1,6-diferrocenylhexane-1,6-dione with 0.1 M TBAP in CH_3CN. Working electrode: Platinum disc; Counter electrode: Platinum wire; Reference electrode: non-aqueous $Ag/AgNO_3$; Temperature: 25°C



Line Color	Scan Rate
Blue	150 mV/sec
Red	100 mV/sec
Green	50 mV/sec

Figure 4.2: Cyclic voltammogram of 1.0 mM 1-ferrocenylcarbonyl-2-ferrocenyl-cyclopentene with 0.1 M TBAP in CH_3CN. Working electrode; Platinum disc; Counter electrode; Platinum wire; Reference electrode: non-aqueous $Ag/AgNO_3$; Temperature: 25°C

Solution Voltammetry of 1,6-diferrocenylhexane

A full scan rate study was also performed on the fully reduced product, 1,6-diferrocenylhexane. The voltammograms for the 150 mV/sec, 100 mV/sec, and 50 mV/sec scan rates are shown in Figure 4.3. The remaining data is tabulated in Table D-3 of Appendix D. A single, two electron transfer wave was observed with $E^{\circ\prime}$ centered at -10.5 mV. The ratio of peak currents was approximately one and ΔE_p was 81.5 mV, both of which were independent of scan rate.

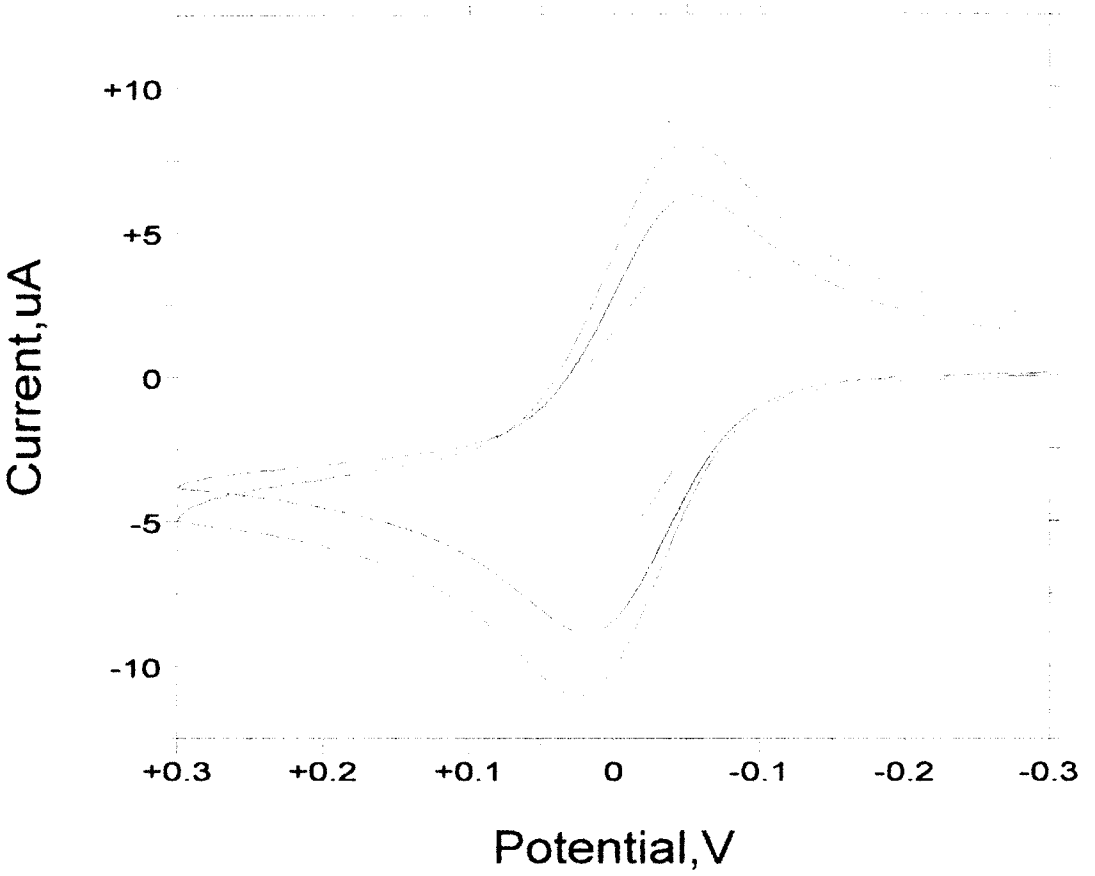
Solution Voltammetry of 1,6-diferrocenylhexane-1-one

A series of voltammograms for 150 mV/sec, 100 mV/sec, and 50 mV/sec scan rates are shown in Figure 4.4. The data for the remaining scan rates is located in Table D-4 of Appendix D. A full scan rate study displayed two, single electron transfer waves centered at 7 mV and 305 mV, respectively. The symmetrical waves produced peak current ratios equal to one at all scan rates. ΔE_p was 75 mV and 84 mV for the first and second redox waves, respectively, and was also independent of scan rate.

Monolayer Voltammetry of 6-(diferrocenylhexanylcarbonyl)pentanethiol

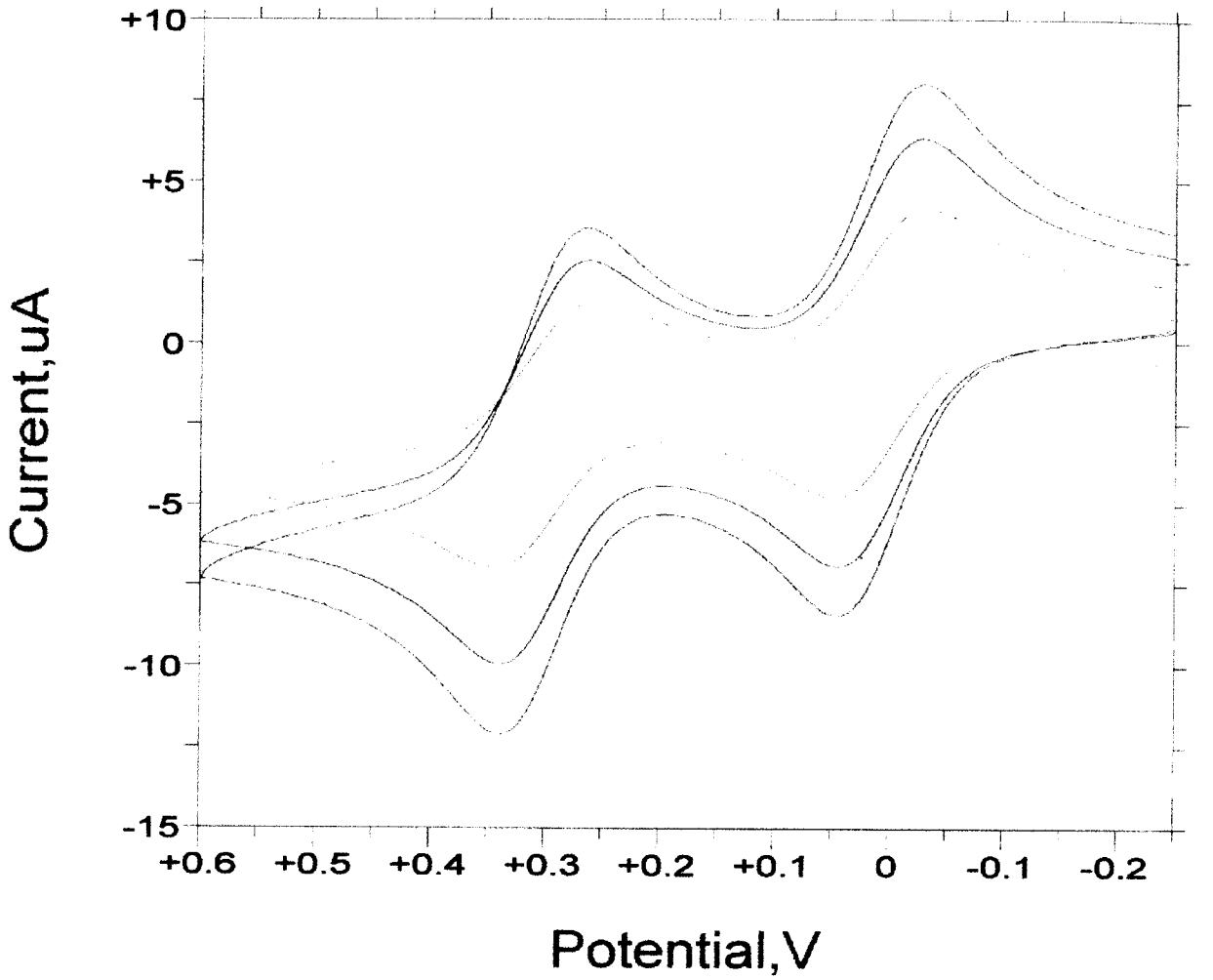
Scan rate studies from 25 mV/sec to 500 mV/sec were obtained between 0 mV and 800 mV. As a final step, the electrodes were cycled through the aforementioned potentials, for 100 sweeps. This was to determine if the monolayer was stable to extended cycling in perchloric acid. Three electrodes were prepared for the following monolayer study.

The first electrode did not produce well-defined peaks in the anodic direction but did produce well-defined peaks in the cathodic direction. Voltammograms at 150 mV/sec, 100 mV/sec and 50 mV/sec are shown in Figure 4.5, and illustrates the formation of a



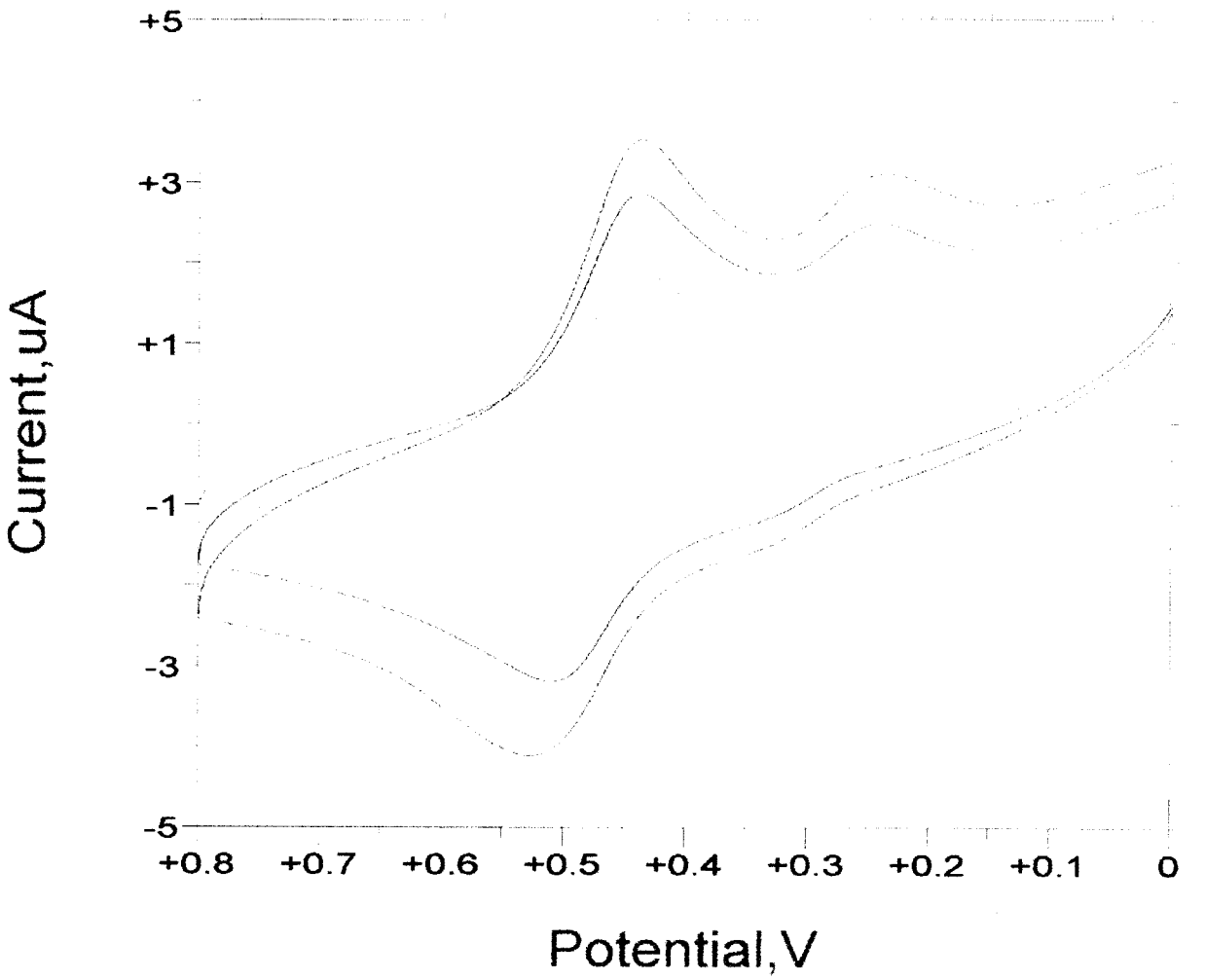
Line Color	Scan Rate
Blue	150 mV/sec
Red	100 mV/sec
Green	50 mV/sec

Figure 4.3: Cyclic voltammogram of 1.0 mM 1,6-diferrocenylhexane with 0.1 M TBAP in CH_3CN. Working electrode: Platinum disc; Counter electrode: Platinum wire; Reference electrode: non-aqueous $Ag/AgNO_3$; Temperature: 25°C



Line Color	Scan Rate
Blue	150 mV/sec
Red	100 mV/sec
Green	50 mV/sec

Figure 4.4: Cyclic voltammogram of 1.0 mM 1,6-diferrocenylhexane-1-one with 0.1 M TBAP in CH_3CN. Working electrode: Platinum disc; Counter electrode: Platinum wire; Reference electrode: non-aqueous $Ag/AgNO_3$; Temperature: 25°C



Line Color	Scan Rate
Blue	150 mV/sec
Red	100 mV/sec
Green	50 mV/sec

Figure 4.5: Poor cyclic voltammogram of 1.0 mM 6-(diferrocenylhexanylcarbonyl)-pentanethiol self-assembled monolayer. Working electrode: Gold disc; Counter electrode: Platinum wire; Reference electrode: aqueous Ag/AgCl; Temperature: 25°C

poor monolayer on the electrode surface. Because the first anodic peak was not well defined, the determination of the peak potentials and currents was difficult. The cathodic sweep produced peaks that were broadened and tailed, therefore the data was not included in any of the reported values. Table D-5 contains the data obtained, as well as the relevant calculations.

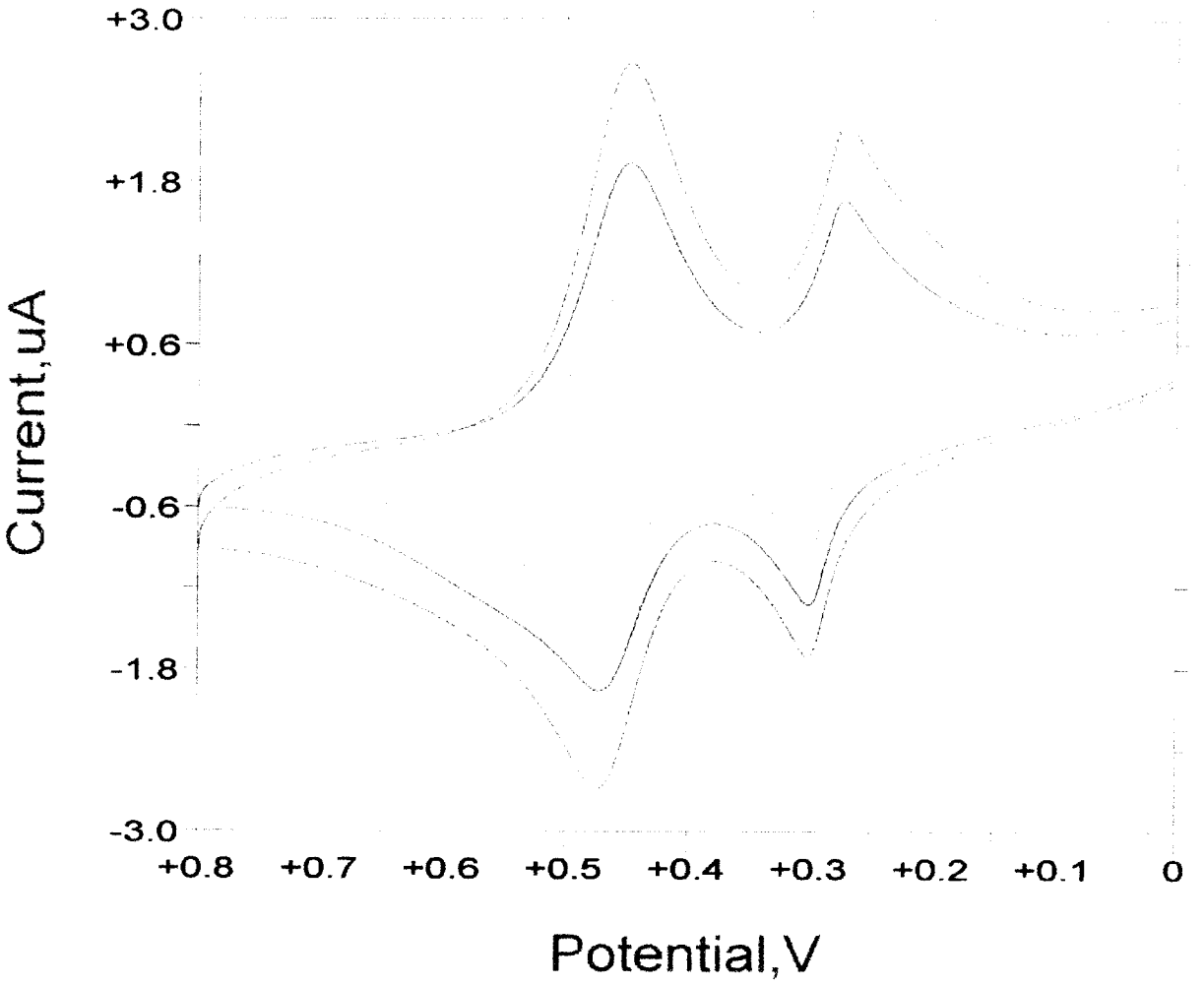
The second and third electrodes produced voltammograms, which displayed four well-defined peaks. The data produced from both electrodes were similar in nature, but the focus of analysis will be on the data obtained from the second electrode. The full data sets for both electrodes are located in Tables D-6 and D-7 of Appendix D.

Figure 4.6 displays a series of voltammograms at a variety of scan rates for the second electrode. Two, single electron transfer waves were observed in the cyclic voltammetry experiment. The first redox wave was centered at 285.5 mV, and the second wave was centered at 462.5 mV. Peak broadening and tailing did occur in the second anodic and first cathodic wave, but not to the degree seen with the first electrode. Peak current ratios were approximately one for both redox waves and are tabulated in Table D-6 in Appendix D. ΔE_p for the first redox wave was found to increase with increasing scan rate. The second redox wave produced ΔE_p values of approximately 27.5 mV that were independent of scan rate.

Surface coverages were calculated by integrating the area under the voltammetric waves. The formula used to calculate surface coverage was:

$$\Gamma = (\text{Area of peak})/(0.0402\ \text{cm}^2 nF\nu)$$

where 0.0402 cm^2 is the electrode surface area corrected for surface roughness.[5] The



Line Color	Scan Rate
Blue	150 mV/sec
Red	100 mV/sec
Green	50 mV/sec

Figure 4.6: Cyclic voltammogram of 1.0 mM of 6-(diferrocenylhexanylcarbonyl)-pentanethiol self-assembled monolayer. Working electrode: Gold disc; Counter electrode: Platinum wire; Reference electrode: aqueous Ag/AgCl; Temperature: 25°C

values obtained for each wave were tabulated and can be found in Table D-6 of Appendix D. The median surface coverages calculated from the anodic and cathodic peaks for the oxidation centered at 285.5 mV were 2.11 x 10^{-11} mol/cm^2 and 2.81 x 10^{-11} mol/cm^2, respectively. The redox wave centered at 462.5 mV displayed median surface coverages of 5.16 x 10^{-11} mol/cm^2 for the anodic wave and 7.29 x 10^{-11} mol/cm^2 for the cathodic wave. The surface coverage was also calculated for a CV taken after extended cycling. The surface coverage for the first anodic wave was determined to be 1.78 x 10^{-11} mol/cm^2.

FWHM values were obtained for all four waves displayed on the voltammogram. The peak centered at 285.5 mV displayed FWHM values of 44.9 mV and 85 mV for the anodic and cathodic waves, respectively. The peak centered at more anodic potentials displayed FWHM values of 80.2 mV and 86.8 mV for the anodic and cathodic waves, respectively. These values were obtained from the voltammogram at a scan rate of 200 mV/sec.

RESULTS AND DISCUSSION

Analysis of the Solution Voltammetry

The cyclic voltammograms for the symmetrically substituted compounds, 1,6-diferrocenylhexane-1,6-dione and 1,6-diferrocenylhexane, display single, two electron oxidations. While those that are asymmetrically substituted, 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene and 1,6-diferrocenylhexane-1-one, display two, single electron oxidations. The formal potentials obtained from the solution voltammetry of the compounds containing carbonyl substituted ferrocenes were determined to be

approximately 300 mV, while those containing alkyl or alkene substituents were determined to be approximately 50 mV. These potentials are characteristic of ferrocene containing compounds. It is well documented that formal potentials for carbonyl substituted ferrocenes are shifted to more anodic potentials with respect to ferrocene, due to the electron withdrawing nature of the substituent. Electron donating alkyl groups, shift the formal potentials cathodically with respect to ferrocene. The formal potentials obtained in this study were shifted cathodically by approximately 200 mV relative to literature values obtained in methylene chloride. The shift in $E^{\circ\prime}$ is attributed to the different solvent, acetonitrile, used in the current study.

The symmetrically substituted ferrocene compounds, 1,6-diferrocenylhexane-1,6-dione and 1,6-diferrocenylhexane, were investigated to determine if the ferrocenes were electronically communicating with one another. A study done by Ferguson[6] et al., demonstrated that symmetrical dimeric ferrocenes can produce two one-electron transfers, indicating that the ferrocenes are electronically "talking" to one another. The study found that a single, two-electron transfer wave for symmetrical ferrocene dimers indicated that the ferrocenes were not communicating with one another. Compounds displaying this type of behavior were given a Robin-Day classification of I-II. In the case of 1,6-diferrocenylhexane-1,6-dione and 1,6-diferrocenylhexane, a single two-electron transfer wave was displayed for each compound. Since the ΔE_p values were observed to be larger than the theoretical value of 59/n mV, the effects of solution iR made it difficult to unambiguously assign a Robin-Day classification. The symmetric ferrocenes were thus given a Robin-Day classification of I-II.

The ratio of the peak currents was calculated for all four compounds and are reported

in Tables D-1 to D-4 in Appendix D. The ratios for the four compounds were approximately one at all scan rates, indicating that each oxidation was chemically reversible.

The difference in peak potentials for each wave was also calculated for all four sets of voltammograms. The cyclic voltammetry experiments for each solution produced ΔE_p values that were approximately 90 mV, and were independent of scan rate. The theoretical value of ΔE_p at all scan rates for an electrochemically reversible system in solution is 57/n mV. The ΔE_p values were larger than 57/n mV due to solution iR effects. Electrochemical reversibility was therefore demonstrated for all four solutions. The peak potentials for each individual scan rate for all four compounds are tabulated in Tables D-1 to D-4 located in Appendix D.

To demonstrate that the electron transfers were diffusion controlled, graphs of the anodic peak current versus the square root of the scan rate were constructed and are presented in Figures 4.7 to 4.10. The resulting linear plots indicate that the electron transfers were diffusion controlled. The best-fit line was calculated and the resulting correlation coefficients are shown in the figures.

Analysis of 6-(diferrocenylhexanylcarbonyl)pentanethiol Self-Assembled Monolayer Voltammetry

The cyclic voltammograms for monolayers containing 6-(diferrocenylhexanyl-carbonyl)pentanethiol display two, single electron transfer waves centered at 263 mV and 463 mV. Based on substituent effects, the wave centered at 263 mV was assigned to the outer ferrocene and the wave at 463 mV was assigned to the carbonyl substituted (inner)

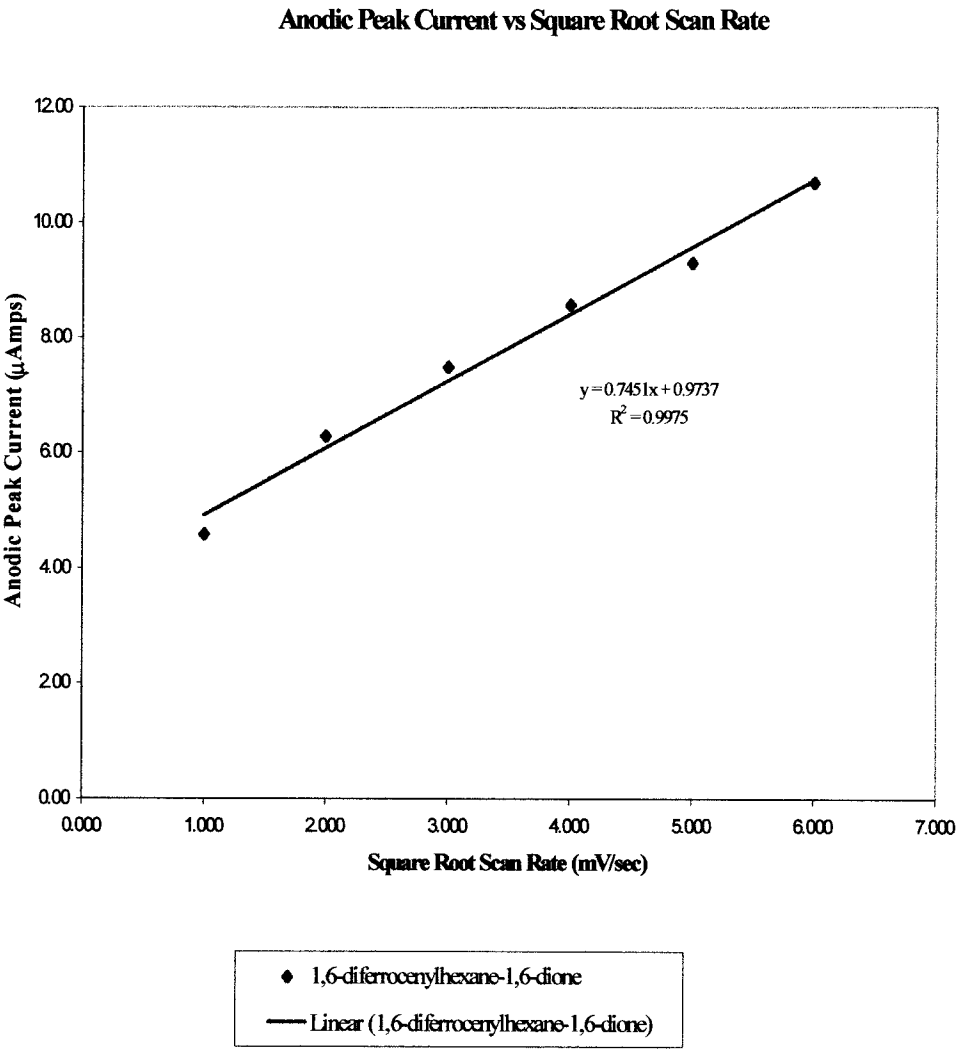


Figure 4.7: Plot of $i_{p,a}$ versus $\nu^{1/2}$ for 1,6-diferrocenylhexane-1,6-dione for the 25 mV/sec to 200 mV/sec scan rates.

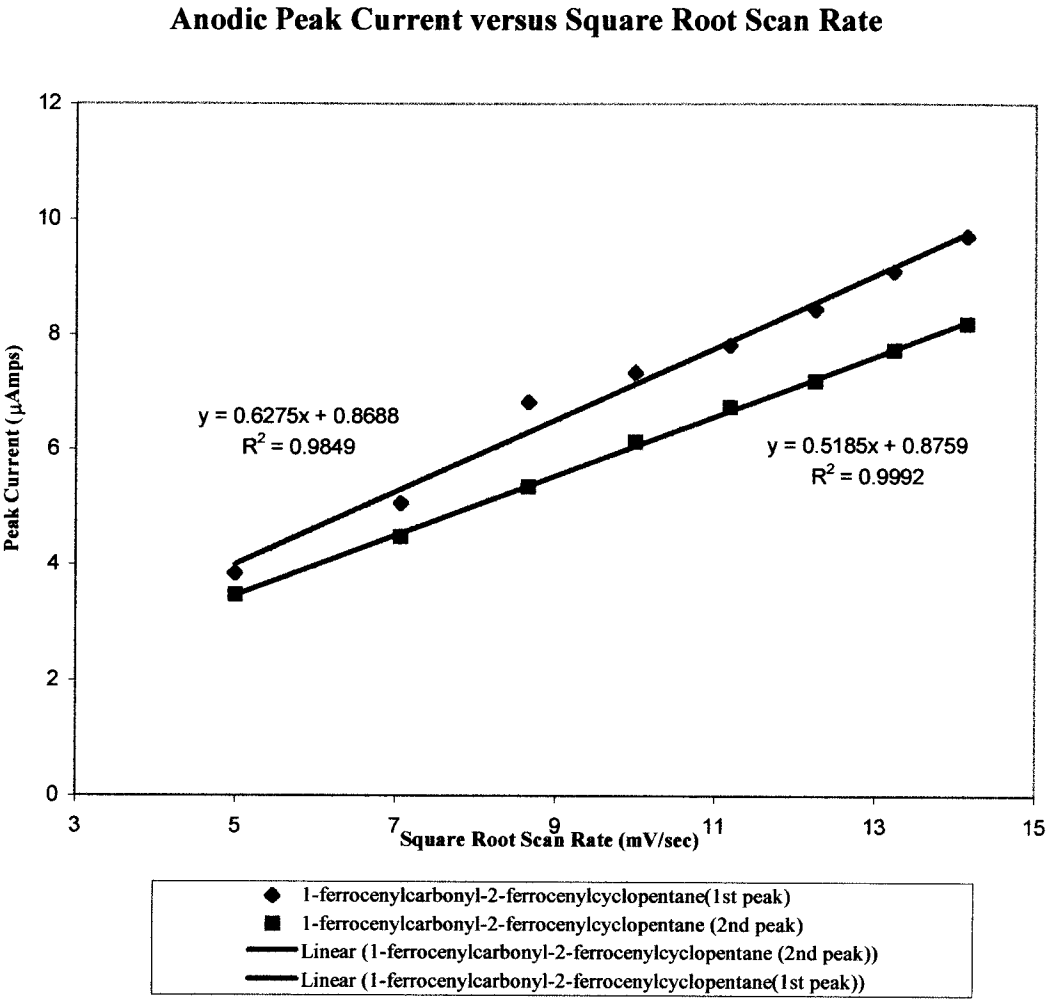


Figure 4.8: Plot $i_{p,a}$ versus $\nu^{1/2}$ for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene for the 25 mV/sec to 200 mV/sec scan

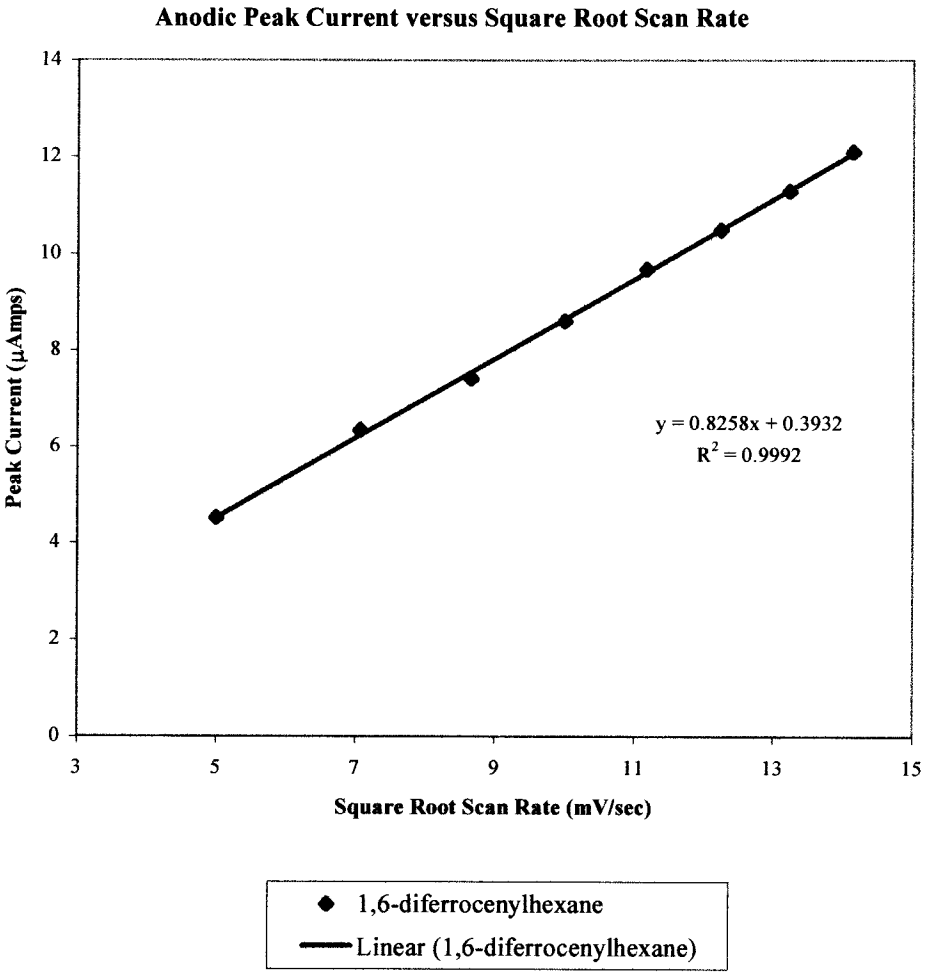


Figure 4.9: Plot $i_{p,a}$ versus $\nu^{1/2}$ for 1,6-diferrocenylhexane for the 25 mV/sec to 200 mV/sec scan rates

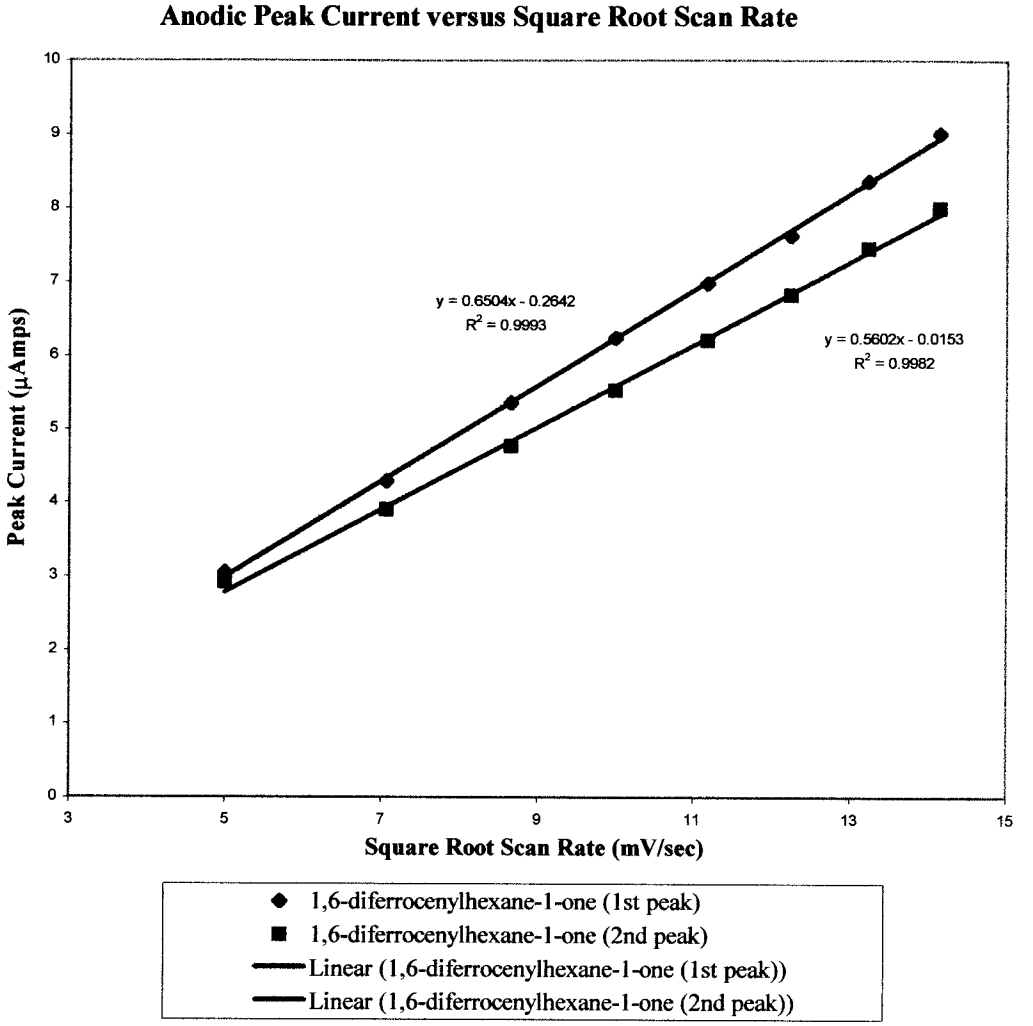


Figure 4.10: Plot $i_{p,a}$ versus $v^{1/2}$ for 1,6-diferrocenylhexane-1-one for the 25 mV/sec to 200 mV/sec scan rates.

ferrocene. The formal potentials are in good agreement with those reported by Kubo[2], but are significantly different than those reported by Filler because a different reference electrode was used. The redox waves were reasonably symmetric, but the waves associated with oxidation of the inner ferrocene and reduction of the outer ferrocene displayed significant tailing.

The peak current ratios were approximately one at all scan rates, indicating monolayers produced from 6-(diferrocenylhexanylcarbonyl)pentanethiol were chemically reversible. The values for the ratios were similar to those obtained by Filler, but different than those seen by Kubo, because the monolayers containing biferrocene were found to be chemically irreversible. These values are tabulated in Table D-6 in Appendix D.

The value of ΔE_p for oxidation of the inner ferrocene was approximately 27.5 mV and did not increase with increasing scan rate, indicating an electrochemically reversible process. A rate constant could not be calculated for the inner ferrocene because electron transfer was rapid on the voltammetric time scale. The outer ferrocene, however, demonstrated increasing ΔE_p values as the scan rate was increased from 25 mV/sec to 500 mV/sec. A plot of ΔE_p versus scan rate is shown in Figure 4.11. A heterogeneous electron transfer rate constant of 11.9 s^{-1}($\pm$0.2) was obtained via the method of Laviron, indicating that the monolayer was ordered.

To determine if the the redox active species was surface confined, a plot of $i_{p,a}$ versus scan rate was constructed. The plot demonstrated a linear relationship, indicating that the electron transfer was for a covalently bonded species. The plot is shown in Figure 4.12.

The surface coverages were calculated for all four waves of the 6-(diferrocenyl-hexanylcarbonyl)pentanethiol monolayer by integrating the charge under the

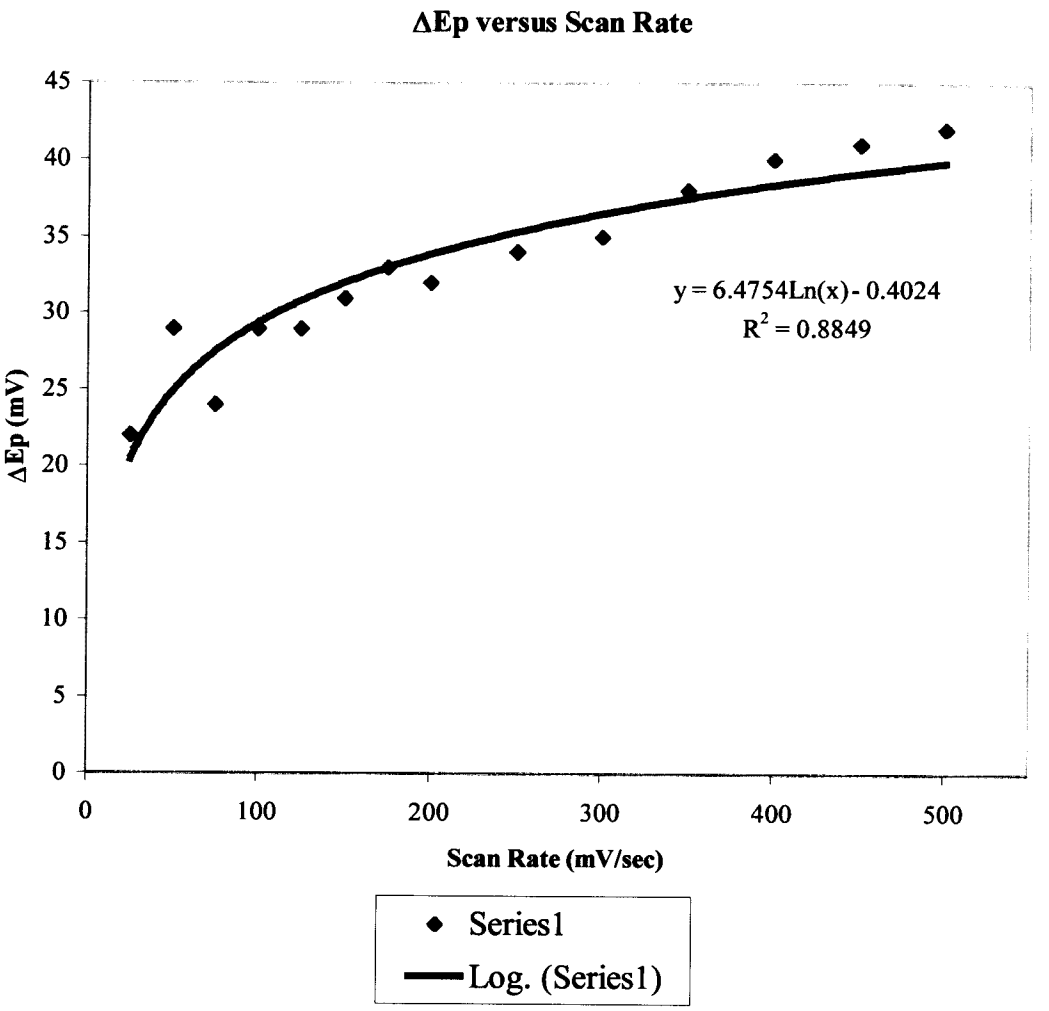


Figure 4.11: Plot of ΔE_p versus ν for 6-(diferrocenylhexanylcarbonyl)pentanethiol

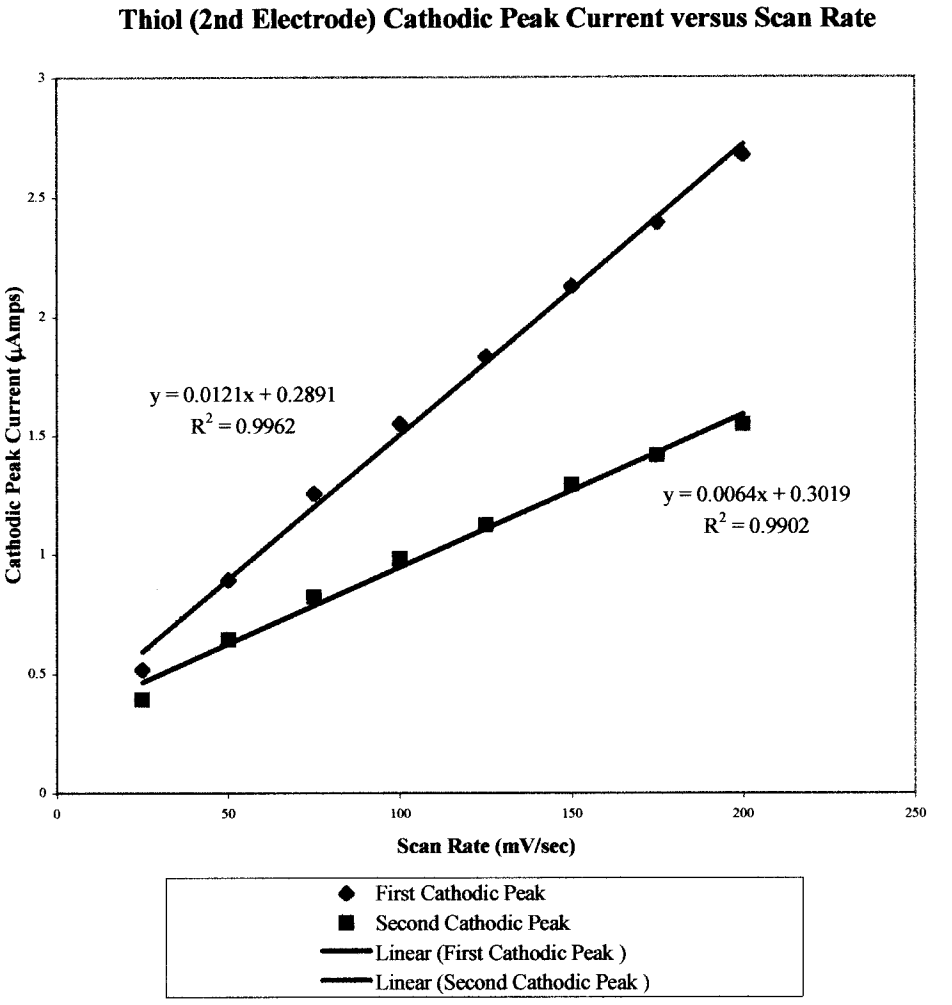


Figure 4.12: Plot of $i_{p,a}$ versus ν for 6-(diferrocenylhexanylcarbonyl)pentanethiol for the 25 mV/sec to 200 mV/sec scan rates

voltammetric waves and are corrected for surface roughness.[5] The inner ferrocene produced surface coverages of 7.29 x 10^{-11} mol/cm^2 and 5.16 x 10^{-11} mol/cm^2, for the anodic and cathodic waves, respectively. The difference in the surface coverages were attributed to tailing of the anodic wave. The outer ferrocene waves yielded surface coverages of 2.11 x 10^{-11} mol/cm^2 for the anodic wave and 2.81 x 10^{-11} mol/cm^2 for the cathodic wave. These values are lower than those reported by Chidsey and Filler for monomeric and dimeric ferrocene alkanethiol monolayers. This is attributed to the fact that the 6-(diferrocenylhexanylcarbonyl)pentanethiol head group occupies a much larger volume than either ferrocene and diferrocenylethane. The surface coverages from the inner ferrocene group indicates a densely packed monolayer.

The surface coverages measured for the outer ferrocene are approximately 40% of that for the inner ferrocene. This indicates that 60% of the outer ferrocene groups are not electrochemically accessible. This behavior is very different than that observed by Filler[1] and Mirkin[7]. The surface coverage of the outer ferrocene groups in diferrocenylethane tagged alkanethiol monolayers was found to be the same as that of the inner ferrocenes, indicating that both of the redox active molecules were electrochemically accessible. Mirkin et.al constructed monolayer films containing an inner azobenzene moiety separated from an outer ferrocene group via a butane chain. The results demonstrated that the *outer* ferrocene groups were electrochemically accessible, but the inner azobenzenes were not. This was attributed to the dense packing in the monolayer, which did not allow charge-compensating cations to enter the film upon reduction. Monolayer films tagged with diferrocenylhexane groups display the opposite behavior with respect to the films reported by Mirkin.

A possible explanation for this unusual behavior is that the majority of the outer ferrocenes prefer to fold over into the non-polar hexane region of the film, rather than fully extending into the aqueous solution. In such a situation, oxidation of the majority of the outer ferrocene groups would be difficult because the resulting cations do not like the hydrophobic chain environment. This issue will be addressed by performing voltammetry in less polar solvents, such as acetonitrile or methylene chloride. Solvents such as these could prevent the outer ferrocene groups from folding over into the hydrophobic alkane region, resulting in greater electrochemical accessibility.

Surface coverages were also obtained for the monolayer at 100 mV/sec after extended cycling in perchloric acid and are displayed in Table D-6 of Appendix D. The coverage from the anodic wave for the outer ferrocene decreased by approximately 27% when compared with the 100 mV/sec scan. In addition, the voltammetric waves were considerablely less well-defined after extended cycling, as shown in Figure 4.13. This data indicates that the monolayer was not stable with respect to extended cycling in perchloric acid.

The FWHM values were calculated by subtracting the potentials at half peak height. The FWHM values obtained for the second anodic wave and both cathodic waves were approximately 90/n mV. This was a strong indication that the ferrocene redox sites are isolated and not interacting with one another. The FWHM of 44.9 mV for the first anodic wave was not typical for a surface confined species. The wave was much sharper when compared to the other three, as seen in Figure 4.6. A structural rearrangement upon oxidation of the outer ferrocene could be an explanation for the narrow peaks, as observed in films containing polyvinyl ferrocene.[8]

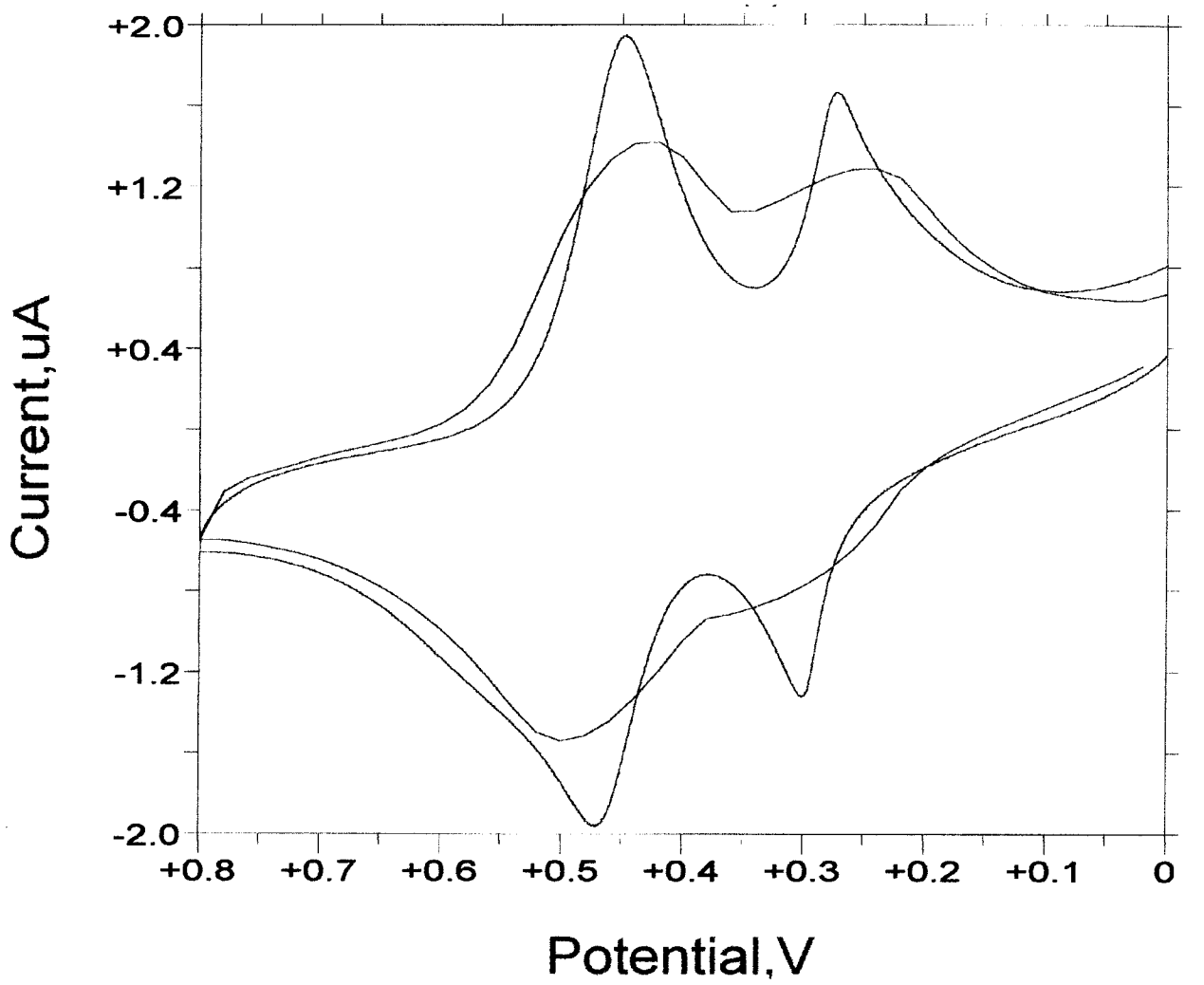


Figure 4.13: Cyclic voltammogram of 6-(diferrocenylhexanylcarbonyl)pentanethiol monolayer at 100 mV/sec (blue) and 100 sweeps (red) at 100 mV/sec.
Blue: Before extended cycling; Red: After extended cycling.

Conclusion

The ultimate goal of this research endeavor was to determine the effects of including a long alkane chain between two ferrocene moieties on monolayer voltammetry. The results from solution voltammetry experiments demonstrated that all four of the compounds that were synthesized, displayed oxidations at the appropriate potentials and that they were chemically and electrochemically reversible. The fully oxidized and fully reduced symmetrical compounds were assigned a Robin-Day classification of I-II. This indicated that the ferrocenes were not electronically communicating.

The monolayer study provided preliminary data concerning rate constants, surface coverages, and FWHM values for diferrocene alkanethiol monolayers with a six-carbon chain separating the ferrocenes. Both ferrocene oxidations were determined to be chemically reversible. The oxidation of the inner ferrocene was found to be electrochemically reversible, whereas the outer ferrocene was electrochemically irreversible. A rate constant of 11.9 s^{-1} was calculated based on Laviron's method.

The calculated surface coverages concluded that approximately 40% of the outer ferrocenes were electrochemically accessible. This unexpected result could be due to the outer ferrocene groups folding over into the hydrophobic alkane bridge. Further experiments in which less polar solvents will be employed, should address this issue.

FWHM values agreed with the theoretical value of 90/n mV for a surface confined species. This indicated that the ferrocene sites in the monolayer were ordered and non-interacting, a criterion for the extraction of a single rate constant. However, the first anodic wave produced a sharp, narrow peak and thus a small value of FWHM. This could possibly be due to a structural rearrangement upon oxidation of the outer ferrocene.

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APPENDIX A

Crystallography Data for 1,6-diferrocenylhexane-1,6-dione

Equations of Mean Plane for 1,6-diferrocenylhexane-1,6-dione

Table A-1

0.1396 * XO + 0.6041 * YO + 0.7846 * ZO = -1.1562
0.7877 * x + 13.7660 * y – 6.2742 * z = -1.1562

Deviation	Weight	Name
0.0020	1.00	C1
-0.0015	1.00	C2
0.0003	1.00	C3
0.0009	1.00	C4
-0.0017	1.00	C5

Table A-2

0.1297 * XO + 0.6044 * YO + 0.7861 * ZO = 2.1022
0.7318 * x + 13.7720 * y – 6.2982 * z = 2.1022

Deviation	Weight	Name
0.0016	1.00	C6
0.0010	1.00	C7
-0.0033	1.00	C8
0.0042	1.00	C9
-0.0035	1.00	C10

Table A-3

0.1287 * XO + 0.6037 * YO + 0.7867* ZO = 2.0932
0.7262 * x + 13.7566 * y – 6.3049 * z = 2.0932

Deviation	Weight	Name
0.0029	1.00	C6
0.0004	1.00	C7
-0.0046	1.00	C8
0.0044	1.00	C9
-0.0016	1.00	C10
-0.0015	1.00	O1

Table A-4
Observed and Calculated Structure Factors for 1,6-diferrocenylhexane-1,6-dione

h	k	l	10Fo	10Fc	10s
2	0	0	520	581	8
4	0	0	259	276	7
6	0	0	111	102	7
1	1	0	249	310	3
2	1	0	170	185	13
3	1	0	33	17	11
4	1	0	211	225	4
5	1	0	156	157	6
6	1	0	131	142	7
7	1	0	70	49	11
0	2	0	134	437	134
1	2	0	1936	1659	5
2	2	0	231	234	4
3	2	0	353	395	11
4	2	0	168	167	4
5	2	0	244	226	13
6	2	0	0	10	1
7	2	0	0	5	1
1	3	0	313	306	3
2	3	0	146	149	10
3	3	0	79	89	6
4	3	0	0	5	1
5	3	0	291	290	4
6	3	0	20	12	20
7	3	0	100	104	10
0	4	0	1681	1624	10
1	4	0	421	412	10
2	4	0	336	362	9
3	4	0	345	343	4
4	4	0	130	133	7
5	4	0	84	82	6
6	4	0	49	72	17
7	4	0	29	5	28
1	5	0	188	194	2
2	5	0	351	342	6
3	5	0	40	40	11
4	5	0	222	217	4
5	5	0	75	77	7
6	5	0	161	155	11
7	5	0	29	11	28
0	6	0	584	537	13
1	6	0	161	147	5
2	6	0	424	433	6
3	6	0	192	207	3
4	6	0	290	292	3
5	6	0	149	142	9
6	6	0	29	37	28
7	6	0	0	32	1
1	7	0	91	87	4
2	7	0	108	112	5
3	7	0	276	283	5
4	7	0	31	46	20
5	7	0	194	194	7
6	7	0	40	61	21
7	7	0	82	99	12
0	8	0	430	457	6
1	8	0	796	811	7
2	8	0	49	53	7
3	8	0	506	514	12
4	8	0	33	31	13
5	8	0	181	174	4
6	8	0	22	34	22
7	8	0	17	13	16
1	9	0	420	409	20
2	9	0	276	273	6
3	9	0	121	126	5
4	9	0	232	225	16
5	9	0	40	18	13
6	9	0	109	113	9
7	9	0	37	47	20
0	10	0	798	795	17
1	10	0	309	298	4
2	10	0	851	838	17
3	10	0	133	124	15
4	10	0	344	338	7
5	10	0	19	5	19
6	10	0	10	33	9
7	10	0	5	5	5
1	11	0	29	35	19
2	11	0	270	270	10
3	11	0	113	113	5
4	11	0	72	68	19
5	11	0	126	127	9
6	11	0	149	117	7
7	11	0	45	47	16
0	12	0	119	125	4
1	12	0	756	764	17
-1	16	1	167	160	5
0	16	1	65	64	5
1	16	1	95	92	6
2	12	0	453	427	6
3	12	0	465	456	8
4	12	0	183	183	4
5	12	0	75	78	24
6	12	0	0	6	1
7	12	0	0	5	1
1	13	0	344	341	4
2	13	0	14	18	14
3	13	0	192	186	5
4	13	0	21	7	21
5	13	0	114	123	8
6	13	0	17	2	17
7	13	0	54	74	17
0	14	0	591	585	8
1	14	0	501	490	6
2	14	0	324	316	4
3	14	0	206	198	4
4	14	0	116	108	5
5	14	0	60	81	14
6	14	0	24	9	24
7	14	0	34	2	19
1	15	0	91	90	5
2	15	0	43	48	11
3	15	0	85	81	7
4	15	0	170	162	7
5	15	0	35	43	14
6	15	0	138	123	8
7	15	0	7	9	7
0	16	0	305	315	7
1	16	0	213	205	4
2	16	0	283	281	4
3	16	0	18	30	17
4	16	0	211	210	5
5	16	0	0	27	1
6	16	0	0	5	1
1	17	0	142	140	4
2	17	0	36	29	15
3	17	0	121	117	6
4	17	0	51	59	14
5	17	0	135	121	8
6	17	0	43	64	43
0	18	0	100	102	6
1	18	0	308	313	4
2	18	0	34	39	23
3	18	0	232	231	4
4	18	0	53	53	13
5	18	0	32	41	31
6	18	0	10	0	10
1	19	0	50	58	12
2	19	0	79	82	19
3	19	0	33	16	17
4	19	0	118	120	17
5	19	0	114	109	8
6	19	0	71	78	14
0	20	0	179	181	9
1	20	0	174	165	8
2	20	0	300	307	14
3	20	0	0	19	1
4	20	0	160	164	15
5	20	0	36	49	29
6	20	0	0	19	1
1	21	0	76	74	7
2	21	0	36	22	13
3	21	0	149	155	7
4	21	0	159	140	7
5	21	0	9	15	9
0	22	0	397	391	27
1	22	0	272	258	4
2	22	0	113	108	6
3	22	0	181	183	6
4	22	0	65	56	12
5	22	0	31	47	30
1	23	0	10	5	9
2	23	0	0	12	1
3	23	0	115	123	9
4	23	0	33	22	27
5	23	0	79	84	12
0	24	0	17	38	16
1	24	0	281	257	5
2	24	0	181	178	6
3	24	0	113	114	10
4	24	0	51	66	25
5	24	0	59	43	12
1	25	0	11	9	10
2	25	0	52	64	14
3	25	0	15	14	15
4	25	0	83	79	29
-1	23	1	64	71	11
0	23	1	216	217	6
1	23	1	18	4	17
0	26	0	197	193	18
1	26	0	19	34	19
2	26	0	153	157	8
3	26	0	32	31	32
4	26	0	33	45	32
1	27	0	39	23	18
2	27	0	40	66	21
3	27	0	54	65	17
4	27	0	36	46	35
0	28	0	40	39	15
1	28	0	100	112	11
2	28	0	0	7	1
3	28	0	21	54	20
1	29	0	18	8	18
2	29	0	17	5	17
3	29	0	47	48	15
0	30	0	145	131	8
1	30	0	0	15	1
2	30	0	48	53	13
1	31	0	26	15	26
2	31	0	16	42	16
0	32	0	43	53	19
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-5	0	1	239	249	3
-3	0	1	638	668	13
-1	0	1	806	1217	805
1	0	1	357	359	5
3	0	1	116	132	11
5	0	1	156	141	4
7	0	1	123	111	10
-8	1	1	43	7	17
-7	1	1	34	5	24
-6	1	1	33	58	27
-5	1	1	74	76	7
-4	1	1	108	109	9
-3	1	1	331	341	4
-2	1	1	193	286	89
-1	1	1	378	902	377
0	1	1	465	561	4
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2	1	1	195	208	4
3	1	1	181	202	8
4	1	1	230	242	3
5	1	1	236	240	4
6	1	1	30	21	29
7	1	1	0	5	1
-8	2	1	139	105	9
-7	2	1	32	36	32
-6	2	1	198	188	5
-5	2	1	166	167	8
-4	2	1	374	389	14
-3	2	1	101	103	4
-2	2	1	338	384	17
-1	2	1	66	339	65
0	2	1	458	444	6
1	2	1	259	262	10
2	2	1	32	9	9
3	2	1	109	113	12
4	2	1	162	164	4
5	2	1	119	126	5
6	2	1	167	147	13
7	2	1	0	14	1
-8	3	1	8	12	8
-7	3	1	21	13	20
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-5	3	1	0	8	1
-4	3	1	246	261	3
-3	3	1	144	139	4
-2	3	1	516	548	9
-1	3	1	206	336	206
0	3	1	1318	1257	15
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2	3	1	398	461	7
3	3	1	90	88	14
4	3	1	397	419	6
5	3	1	15	17	14
6	3	1	93	88	8
7	3	1	25	17	24
-7	4	1	102	94	10
-6	4	1	134	118	6
-5	4	1	121	124	5
-4	4	1	291	306	17
-3	4	1	468	496	6
-2	4	1	17	12	17
-1	4	1	45	31	6
0	4	1	725	702	11
1	4	1	126	134	3
2	1	2	89	88	4
3	1	2	25	16	20
4	1	2	82	85	8
2	4	1	221	220	5
3	4	1	171	187	9
4	4	1	154	156	4
5	4	1	52	43	19
6	4	1	101	94	11
7	4	1	96	85	21
-7	5	1	26	6	25
-6	5	1	0	12	1
-5	5	1	78	87	6
-4	5	1	36	36	13
-3	5	1	334	361	4
-2	5	1	74	68	6
-1	5	1	683	694	13
0	5	1	70	26	5
1	5	1	872	867	5
2	5	1	126	123	3
3	5	1	348	374	4
4	5	1	34	28	12
5	5	1	204	210	12
6	5	1	0	20	1
7	5	1	0	12	1
-7	6	1	73	83	13
-6	6	1	107	92	8
-5	6	1	263	260	8
-4	6	1	169	164	4
-3	6	1	243	270	9
-2	6	1	207	193	11
-1	6	1	288	289	5
0	6	1	332	342	6
1	6	1	51	58	7
2	6	1	92	95	5
3	6	1	152	167	13
4	6	1	143	135	4
5	6	1	123	124	5
6	6	1	90	69	15
7	6	1	53	84	18
-7	7	1	35	7	25
-6	7	1	24	10	23
-5	7	1	33	24	23
-4	7	1	279	282	4
-3	7	1	267	257	3
-2	7	1	468	470	12
-1	7	1	235	227	3
0	7	1	198	193	2
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3	7	1	151	157	4
4	7	1	332	339	4
5	7	1	0	8	1
6	7	1	47	63	17
7	7	1	6	12	5
-8	8	1	19	26	19
-6	8	1	176	180	9
-5	8	1	48	47	24
-4	8	1	368	372	6
-3	8	1	326	311	4
-2	8	1	448	441	6
-1	8	1	152	153	9
0	8	1	74	76	4
1	8	1	305	302	4
2	8	1	117	130	11
3	8	1	105	123	5
4	8	1	101	98	5
5	8	1	27	5	17
6	8	1	147	138	7
7	8	1	16	21	16
-7	9	1	30	29	30
-6	9	1	38	36	18
-5	9	1	57	55	10
-4	9	1	0	16	1
-3	9	1	235	231	3
-2	9	1	176	182	4
-1	9	1	405	409	16
0	9	1	547	530	6
1	9	1	659	635	6
2	9	1	407	409	6
3	9	1	429	424	10
4	9	1	38	42	12
5	9	1	133	131	5
6	9	1	47	53	17
7	9	1	0	11	1
-7	10	1	92	90	28
-6	10	1	33	27	33
-5	10	1	339	319	5
-4	10	1	104	111	13
-3	10	1	424	434	6
-2	10	1	28	29	21
-5	7	2	337	337	4
-4	7	2	67	78	7
-3	7	2	456	474	6
-1	10	1	259	251	9
0	10	1	40	35	7
1	10	1	184	170	5
2	10	1	65	71	6
3	10	1	112	111	7
4	10	1	72	76	8
5	10	1	141	131	17
6	10	1	28	11	27
7	10	1	125	115	29
-7	11	1	19	10	18
-6	11	1	20	33	20
-5	11	1	69	70	13
-4	11	1	64	65	8
-3	11	1	126	130	5
-2	11	1	183	180	4
-1	11	1	356	376	8
0	11	1	293	277	3
1	11	1	728	717	6
2	11	1	221	225	3
3	11	1	315	313	4
4	11	1	202	206	5
5	11	1	64	65	12
6	11	1	12	19	12
7	11	1	0	17	1
-7	12	1	21	28	20
-6	12	1	159	149	10
-5	12	1	211	194	4
-4	12	1	343	328	6
-3	12	1	172	152	4
-2	12	1	245	239	7
-1	12	1	48	47	10
0	12	1	213	220	2
1	12	1	170	157	4
2	12	1	37	39	13
3	12	1	0	11	1
4	12	1	113	111	5
5	12	1	46	34	14
6	12	1	140	124	16
7	12	1	87	73	11
-7	13	1	10	1	10
-6	13	1	29	0	28
-5	13	1	39	71	23
-4	13	1	55	48	19
-3	13	1	74	54	7
-2	13	1	311	313	8
-1	13	1	201	206	3
0	13	1	751	772	5
1	13	1	28	14	21
2	13	1	536	518	6
3	13	1	59	67	8
4	13	1	92	96	7
5	13	1	21	31	20
6	13	1	72	74	39
7	13	1	0	6	1
-7	14	1	51	68	20
-6	14	1	96	93	10
-5	14	1	143	140	7
-4	14	1	247	230	10
-3	14	1	108	102	5
-2	14	1	321	310	7
-1	14	1	111	121	4
0	14	1	156	148	3
1	14	1	55	53	8
2	14	1	153	157	4
3	14	1	0	11	1
4	14	1	21	13	21
5	14	1	131	126	8
6	14	1	86	95	19
-7	15	1	0	2	1
-6	15	1	20	16	20
-5	15	1	28	8	28
-4	15	1	101	95	6
-3	15	1	264	263	4
-2	15	1	2	32	2
-1	15	1	329	316	4
0	15	1	104	106	3
1	15	1	512	500	19
2	15	1	198	199	6
3	15	1	273	277	4
4	15	1	22	20	22
5	15	1	113	99	8
6	15	1	20	26	19
-6	16	1	41	38	16
-5	16	1	229	213	8
-4	16	1	37	23	16
-3	16	1	113	109	5
-2	16	1	48	44	10
-7	13	2	69	81	16
-6	13	2	0	33	1
-5	13	2	224	210	6

Table A-4, Continued
Observed and Calculated Structure Factors for 1,6-diferrocenylhexane-1,6-dione

h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ
2	16	1	58	62	11	2	23	1	251	254	6	5	1	2	139	132	4	-2	7	2	206	195	3	-4	13	2	37	31	16
3	16	1	59	61	10	3	23	1	95	96	14	6	1	2	107	93	15	-1	7	2	0	35	1	-3	13	2	307	323	11
4	16	1	44	34	21	4	23	1	116	108	10	7	1	2	45	49	19	0	7	2	385	378	6	-2	13	2	95	102	6
5	16	1	151	134	7	5	23	1	0	22	1	-8	2	2	31	29	30	1	7	2	587	561	6	-1	13	2	394	408	6
6	16	1	31	38	30	-5	24	1	37	60	24	-7	2	2	55	67	16	2	7	2	223	231	3	0	13	2	62	58	4
-6	17	1	30	15	30	-4	24	1	122	103	9	-6	2	2	48	52	14	3	7	2	138	137	10	1	13	2	58	49	8
-5	17	1	26	48	26	-3	24	1	74	84	22	-5	2	2	83	92	8	4	7	2	115	113	5	2	13	2	146	139	4
-4	17	1	38	26	17	-2	24	1	137	121	20	-4	2	2	24	20	24	5	7	2	186	185	5	3	13	2	125	115	6
-3	17	1	163	157	5	-1	24	1	0	7	1	-3	2	2	158	192	62	6	7	2	36	29	16	4	13	2	56	57	8
-2	17	1	257	253	5	0	24	1	97	90	6	-2	2	2	11	13	10	7	7	2	108	86	17	5	13	2	39	41	20
-1	17	1	41	41	17	1	24	1	0	3	1	-1	2	2	115	102	8	-7	8	2	28	42	28	6	13	2	29	2	29
0	17	1	464	454	4	2	24	1	22	4	22	0	2	2	500	505	4	-6	8	2	37	11	14	-7	14	2	23	13	22
1	17	1	190	181	4	3	24	1	54	40	11	1	2	2	743	731	5	-5	8	2	55	46	10	-6	14	2	49	50	14
2	17	1	224	233	15	4	24	1	37	50	21	2	2	2	306	318	3	-4	8	2	55	32	9	-5	14	2	106	94	9
3	17	1	96	87	6	5	24	1	44	41	16	3	2	2	494	523	6	-3	8	2	0	18	1	-4	14	2	46	5	10
4	17	1	123	123	13	-5	25	1	29	26	28	4	2	2	149	166	15	-2	8	2	150	154	3	-3	14	2	103	100	9
5	17	1	65	79	13	-4	25	1	14	21	14	5	2	2	235	223	3	-1	8	2	438	453	6	-2	14	2	274	264	9
6	17	1	55	62	15	-3	25	1	36	48	36	6	2	2	41	30	13	0	8	2	233	218	2	-1	14	2	299	309	4
-6	18	1	82	93	17	-2	25	1	82	81	12	7	2	2	40	48	21	1	8	2	350	374	4	0	14	2	284	287	4
-5	18	1	20	13	19	-1	25	1	180	173	6	-8	3	2	34	5	26	2	8	2	18	42	17	1	14	2	229	226	3
-4	18	1	216	206	7	0	25	1	77	88	7	-7	3	2	139	134	7	3	8	2	388	396	6	2	14	2	234	228	8
-3	18	1	11	8	10	1	25	1	189	189	7	-6	3	2	0	4	1	4	8	2	0	6	1	3	14	2	113	109	5
-2	18	1	91	92	7	2	25	1	53	38	12	-5	3	2	239	252	3	5	8	2	127	134	7	4	14	2	223	213	5
-1	18	1	93	88	5	3	25	1	162	160	8	-4	3	2	101	107	5	6	8	2	10	29	10	5	14	2	122	113	7
0	18	1	188	186	3	4	25	1	64	59	14	-3	3	2	360	719	360	7	8	2	62	72	15	6	14	2	0	46	1
1	18	1	61	41	6	-4	26	1	20	6	20	-2	3	2	79	75	8	-7	9	2	59	68	14	-7	15	2	53	27	12
2	18	1	109	107	5	-3	26	1	144	127	11	-1	3	2	196	192	2	-6	9	2	152	138	6	-6	15	2	140	134	9
3	18	1	7	18	7	-2	26	1	12	6	11	0	3	2	911	901	11	-5	9	2	151	140	6	-5	15	2	73	78	15
4	18	1	128	127	8	-1	26	1	53	59	13	1	3	2	221	224	3	-4	9	2	336	326	4	-4	15	2	250	245	4
5	18	1	31	28	17	0	26	1	40	56	10	2	3	2	111	115	4	-3	9	2	171	180	8	-3	15	2	134	139	5
6	18	1	57	67	17	1	26	1	0	4	1	3	3	2	114	124	10	-2	9	2	388	408	7	-2	15	2	173	173	5
-6	19	1	14	7	14	2	26	1	0	32	1	4	3	2	49	42	8	-1	9	2	185	203	3	-1	15	2	90	93	5
-5	19	1	0	39	1	3	26	1	45	51	19	5	3	2	192	182	6	0	9	2	225	229	2	0	15	2	366	371	5
-4	19	1	107	102	10	4	26	1	0	16	1	6	3	2	21	30	21	1	9	2	160	145	4	1	15	2	106	96	13
-3	19	1	76	63	11	-4	27	1	0	11	1	7	3	2	98	92	21	2	9	2	113	109	4	2	15	2	96	93	5
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0	19	1	226	221	3	-1	27	1	104	108	9	-6	4	2	39	59	24	5	9	2	0	12	1	5	15	2	18	14	18
1	19	1	229	232	4	0	27	1	161	150	4	-5	4	2	86	82	17	6	9	2	56	75	14	6	15	2	101	82	10
2	19	1	109	100	5	1	27	1	89	95	10	-4	4	2	47	46	8	7	9	2	69	76	15	-7	16	2	31	17	31
3	19	1	208	213	4	2	27	1	110	109	13	-3	4	2	61	195	60	-7	10	2	19	7	19	-6	16	2	0	29	1
4	19	1	96	98	11	3	27	1	86	68	11	-2	4	2	39	143	38	-6	10	2	66	75	12	-5	16	2	49	40	19
5	19	1	58	71	18	4	27	1	48	53	15	-1	4	2	543	504	5	-5	10	2	76	67	12	-4	16	2	40	12	16
6	19	1	27	27	27	-3	28	1	41	56	19	0	4	2	473	489	3	-4	10	2	40	39	16	-3	16	2	60	59	9
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-4	20	1	3	34	2	0	28	1	0	18	1	3	4	2	255	274	5	-1	10	2	388	391	7	0	16	2	63	58	6
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0	20	1	159	156	3	-3	29	1	27	31	26	7	4	2	36	26	19	3	10	2	0	3	1	4	16	2	187	175	6
1	20	1	112	112	5	-2	29	1	42	62	21	-8	5	2	76	79	14	4	10	2	249	252	3	5	16	2	68	81	15
2	20	1	55	47	7	-1	29	1	86	82	11	-7	5	2	0	23	1	5	10	2	24	13	23	6	16	2	52	59	14
3	20	1	89	94	9	0	29	1	34	33	11	-6	5	2	174	179	15	6	10	2	135	127	21	-6	17	2	0	46	1
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5	20	1	146	123	9	2	29	1	109	102	20	-4	5	2	475	488	10	-7	11	2	44	36	18	-4	17	2	148	136	12
6	20	1	13	8	13	3	29	1	56	60	17	-3	5	2	0	3	1	-6	11	2	188	161	6	-3	17	2	223	221	6
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2	21	1	184	188	4	1	31	1	69	76	15	6	5	2	121	118	16	3	11	2	30	3	17	6	17	2	42	49	17
3	21	1	193	186	11	-8	0	2	74	63	13	7	5	2	0	1	1	4	11	2	94	93	5	-6	18	2	0	10	1
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5	21	1	58	61	15	-4	0	2	149	138	8	-6	6	2	25	27	25	6	11	2	123	96	9	-4	18	2	33	32	32
-5	22	1	41	53	22	-2	0	2	466	498	6	-5	6	2	43	41	17	7	11	2	0	22	1	-3	18	2	128	128	12
-4	22	1	139	124	8	0	0	2	1069	1099	10	-4	6	2	0	15	1	-7	12	2	49	51	15	-2	18	2	30	32	29
-3	22	1	73	80	17	2	0	2	565	621	5	-3	6	2	0	7	1	-6	12	2	39	22	18	-1	18	2	109	105	5
-2	22	1	204	197	6	4	0	2	318	350	4	-2	6	2	166	162	3	-5	12	2	101	103	6	0	18	2	38	35	10
-1	22	1	172	169	5	6	0	2	178	164	7	-1	6	2	157	153	5	-4	12	2	109	101	5	1	18	2	218	211	5
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1	22	1	10	10	10	-7	1	2	39	51	23	1	6	2	297	275	4	-2	12	2	91	95	6	3	18	2	171	165	8
2	22	1	24	52	23	-6	1	2	53	62	13	2	6	2	360	385	5	-1	12	2	340	346	4	4	18	2	45	53	17
3	22	1	32	37	27	-5	1	2	138	139	4	3	6	2	304	295	4	0	12	2	148	152	2	5	18	2	129	112	9
4	22	1	70	82	13	-4	1	2	486	491	10	4	6	2	200	203	4	1	12	2	480	482	6	6	18	2	24	9	24
5	22	1	30	19	29	-3	1	2	216	316	216	5	6	2	26	29	25	2	12	2	238	234	3	-6	19	2	110	102	20
-5	23	1	0	33	1	-2	1	2	583	594	5	6	6	2	92	88	11	3	12	2	358	353	6	-5	19	2	54	60	17
-4	23	1	22	42	22	-1	1	2	380	462	52	7	6	2	0	25	1	4	12	2	86	82	6	-4	19	2	103	85	9
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-2	23	1	174	177	7	1	1	2	331	328	5	-6	7	2	92	91	24	6	12	2	56	67	16	-2	19	2	219	211	11
-1	19	2	148	143	4	1	27	2	0	15	1	-1	4	3	320	333	4	-2	10	3	100	111	5	2	16	3	22	26	22
0	19	2	203	197	3	2	27	2	35	40	23	0	4	3	256	261	5	-1	10	3	624	640	14	3	16	3	0	4	1
1	19	2	19	35	19	3	27	2	0	23	1	1	4	3	309	312	4	0	10	3	192	190	3	4	16	3	89	91	17
2	19	2	9	14	8	-3	28	2	0	10	1	2	4	3	0	17	1	1	10	3	432	426	10	5	16	3	59	43	12
3	19	2	109	115	9	-2	28	2	28	2	28	3	4	3	41	53	11	2	10	3	18	26	18	6	16	3	46	55	17
4	19	2	24	33	23	-1	28	2	75	89	14	4	4	3	27	13	22	3	10	3	83	67	6	-6	17	3	0	17	1

Table A-4, Continued
Observed and Calculated Structure Factors for 1,6-diferrocenylhexane-1,6-dione

h	k	l	10Fo	10Fc	10σ
5	19	2	34	39	34
-6	20	2	16	24	15
-5	20	2	36	1	15
-4	20	2	35	57	22
-3	20	2	74	75	10
-2	20	2	92	86	19
-1	20	2	0	11	1
0	20	2	96	103	4
1	20	2	120	116	5
2	20	2	246	247	10
3	20	2	38	25	16
4	20	2	194	189	8
5	20	2	35	34	21
-6	21	2	62	67	19
-5	21	2	51	62	17
-4	21	2	154	140	13
-3	21	2	73	70	12
-2	21	2	136	123	5
-1	21	2	200	196	4
0	21	2	135	143	3
1	21	2	0	20	1
2	21	2	0	26	1
3	21	2	13	1	13
4	21	2	62	68	13
5	21	2	29	4	28
-5	22	2	0	7	1
-4	22	2	28	16	27
-3	22	2	35	28	18
-2	22	2	88	76	7
-1	22	2	209	205	6
0	22	2	143	140	3
1	22	2	203	205	6
2	22	2	108	118	8
3	22	2	149	158	22
4	22	2	55	61	17
5	22	2	65	80	15
-5	23	2	80	97	16
-4	23	2	24	34	24
-3	23	2	167	156	7
-2	23	2	22	32	21
-1	23	2	127	139	12
0	23	2	49	62	10
1	23	2	63	79	16
2	23	2	23	38	22
3	23	2	27	15	27
4	23	2	0	25	1
5	23	2	23	38	23
-5	24	2	24	18	23
-4	24	2	0	22	1
-3	24	2	0	6	1
-2	24	2	25	27	24
-1	24	2	78	91	12
0	24	2	171	168	4
1	24	2	183	176	8
2	24	2	124	132	9
3	24	2	136	128	8
4	24	2	39	75	38
-5	25	2	35	26	23
-4	25	2	99	91	22
-3	25	2	96	108	10
-2	25	2	139	126	8
-1	25	2	0	15	1
0	25	2	33	36	12
1	25	2	49	41	14
2	25	2	55	62	15
3	25	2	26	26	26
4	25	2	0	21	1
-4	26	2	32	15	32
-3	26	2	0	4	1
-2	26	2	37	32	17
-1	26	2	64	92	29
0	26	2	156	158	6
1	26	2	102	90	8
2	26	2	127	140	9
3	26	2	35	8	22
4	26	2	12	41	11
-4	27	2	69	85	19
-3	27	2	57	81	18
-2	27	2	122	96	9
-1	27	2	35	55	22
0	27	2	0	10	1
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-2	24	3	116	108	10
-1	24	3	184	182	11
0	24	3	121	120	8
1	24	3	110	98	8
2	24	3	108	99	8
3	24	3	14	18	14
4	24	3	0	10	1
-4	25	3	0	29	1
0	28	2	16	5	16
1	28	2	136	121	10
2	28	2	0	4	1
3	28	2	34	61	33
-3	29	2	64	63	15
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0	29	2	29	24	14
1	29	2	40	50	19
2	29	2	22	10	22
-2	30	2	20	23	20
-1	30	2	0	18	1
0	30	2	103	112	7
1	30	2	20	22	19
2	30	2	43	56	17
-1	31	2	48	47	17
0	31	2	20	24	19
1	31	2	35	13	18
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-5	0	3	148	180	15
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1	0	3	426	438	6
3	0	3	180	185	4
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7	0	3	41	41	14
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-5	1	3	54	138	53
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3	1	3	342	340	6
4	1	3	185	185	4
5	1	3	200	201	10
6	1	3	48	58	15
7	1	3	62	66	17
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-7	2	3	21	14	21
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-2	2	3	304	534	303
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2	2	3	471	488	5
3	2	3	14	18	14
4	2	3	107	101	6
5	2	3	25	5	25
6	2	3	57	39	11
7	2	3	19	15	18
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-4	3	3	74	72	6
-3	3	3	110	97	5
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-1	3	3	502	502	5
0	3	3	187	200	2
1	3	3	22	8	22
2	3	3	582	618	6
3	3	3	0	19	1
4	3	3	360	360	9
5	3	3	34	40	15
6	3	3	138	124	7
7	3	3	20	24	20
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-7	4	3	61	78	15
-6	4	3	60	49	11
-5	4	3	82	192	81
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-2	4	3	169	346	169
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6	4	3	25	35	25
7	4	3	29	16	28
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3	5	3	425	428	12
4	5	3	0	21	1
5	5	3	218	215	5
6	5	3	0	2	1
7	5	3	110	98	32
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7	6	3	27	39	26
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-2	7	3	106	103	4
-1	7	3	121	108	4
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1	7	3	218	218	3
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3	7	3	281	288	7
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6	7	3	134	129	8
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3	8	3	57	68	9
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6	8	3	24	40	23
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2	9	4	145	147	4
3	9	4	174	172	4
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4	10	3	59	56	7
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6	13	3	121	111	10
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2	14	3	113	98	5
3	14	3	92	85	7
4	14	3	13	44	13
5	14	3	35	4	15
6	14	3	25	32	24
-7	15	3	60	63	14
-6	15	3	17	2	16
-5	15	3	45	15	14
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-3	18	3	28	31	28
-2	18	3	303	294	7
-1	18	3	54	44	22
0	18	3	161	152	5
1	18	3	17	13	17
2	18	3	28	46	28
3	18	3	42	58	16
4	18	3	0	14	1
5	18	3	0	14	1
-6	19	3	0	6	1
-5	19	3	0	11	1
-4	19	3	0	7	1
-3	19	3	8	48	8
-2	19	3	111	111	5
-1	19	3	0	5	1
0	19	3	173	172	3
1	19	3	127	128	5
2	19	3	202	197	5
3	19	3	143	151	12
4	19	3	116	119	10
5	19	3	50	66	24
-6	20	3	0	16	1
-5	20	3	133	121	17
-4	20	3	25	21	25
-3	20	3	218	219	10
-2	20	3	74	58	7
-1	20	3	269	265	3
0	20	3	0	3	1
1	20	3	167	163	5
2	20	3	18	6	18
3	20	3	0	16	1
4	20	3	26	2	25
5	20	3	33	36	32
-6	21	3	0	28	1
-5	21	3	42	4	14
-4	21	3	17	24	17
-3	21	3	20	26	19
-2	21	3	64	71	12
-1	21	3	72	64	8
0	21	3	58	59	6
1	21	3	186	191	6
2	21	3	0	5	1
3	21	3	193	169	8
4	21	3	23	34	23
5	21	3	85	80	13
-5	22	3	19	21	19
-4	22	3	138	123	8
-3	22	3	151	137	7
-2	22	3	282	278	9
-1	22	3	64	61	9
0	22	3	181	184	4
1	22	3	20	43	20
2	22	3	62	61	11
3	22	3	33	37	24
4	22	3	0	19	1
-5	23	3	0	14	1
-4	23	3	46	25	13
-3	23	3	19	12	18
-2	23	3	36	23	18
-1	23	3	93	90	19
0	23	3	141	148	5
1	23	3	40	25	14
2	23	3	123	125	18
3	23	3	48	4	10
4	23	3	107	102	11
-5	24	3	67	78	14
-4	24	3	53	63	19
-3	23	4	0	16	1
-2	23	4	141	130	8
-2	23	4	48	47	15
-1	23	4	197	198	6
0	23	4	66	79	7
1	23	4	125	129	10
2	23	4	24	36	24
3	23	4	68	78	15
4	23	4	36	57	35

Table A-4, Continued
Observed and Calculated Structure Factors for 1,6-diferrocenylhexane-1,6-dione

h	k	l	10Fo	10Fc	10s
-3	25	3	0	10	1
-2	25	3	35	44	28
-1	25	3	123	123	9
0	25	3	21	41	20
1	25	3	64	86	15
2	25	3	53	59	11
3	25	3	85	81	10
4	25	3	61	71	15
-4	26	3	54	56	26
-3	26	3	77	68	13
-2	26	3	49	51	14
-1	26	3	102	113	9
0	26	3	40	58	11
1	26	3	95	104	10
2	26	3	0	22	1
3	26	3	42	8	16
-4	27	3	44	26	15
-3	27	3	35	6	35
-2	27	3	63	53	13
-1	27	3	117	105	25
0	27	3	121	120	6
1	27	3	0	47	1
2	27	3	35	24	13
3	27	3	54	68	15
-3	28	3	14	2	14
-2	28	3	69	79	15
-1	28	3	0	3	1
0	28	3	83	96	9
1	28	3	0	14	1
2	28	3	0	35	1
-3	29	3	48	14	12
-2	29	3	43	47	18
-1	29	3	4	15	3
0	29	3	52	58	11
1	29	3	29	41	29
2	29	3	91	81	11
-2	30	3	0	13	1
-1	30	3	75	91	15
0	30	3	37	30	14
1	30	3	23	42	22
-8	0	4	74	69	11
-6	0	4	22	127	22
-4	0	4	174	170	7
-2	0	4	133	125	3
0	0	4	455	449	5
2	0	4	345	364	4
4	0	4	178	175	4
6	0	4	135	134	8
-8	1	4	0	10	1
-7	1	4	36	27	23
-6	1	4	103	108	16
-5	1	4	121	118	11
-4	1	4	258	255	3
-3	1	4	156	153	4
-2	1	4	590	622	5
-1	1	4	336	349	13
0	1	4	384	421	4
1	1	4	345	351	4
2	1	4	374	384	6
3	1	4	136	137	4
4	1	4	179	180	4
5	1	4	0	5	1
6	1	4	32	21	23
-8	2	4	21	21	21
-7	2	4	132	119	8
-6	2	4	15	16	15
-5	2	4	60	64	8
-4	2	4	49	30	13
-3	2	4	44	17	13
-2	2	4	126	127	6
-1	2	4	56	43	7
0	2	4	16	20	15
1	2	4	523	530	5
2	2	4	139	143	4
3	2	4	369	372	6
4	2	4	0	10	1
5	2	4	153	133	11
6	2	4	39	32	17
-6	3	5	145	151	6
-5	3	5	70	58	10
-4	3	5	225	235	12
-3	3	5	15	37	15
-2	3	5	150	149	3
-1	3	5	96	85	4
0	3	5	119	119	2
1	3	5	178	177	3
2	3	5	159	150	3
3	3	5	18	13	17
4	3	5	124	123	6
5	3	5	54	49	13
2	3	4	32	6	12
3	3	4	281	285	3
4	3	4	21	16	21
5	3	4	0	6	1
6	3	4	0	3	1
-7	4	4	8	39	7
-6	4	4	152	141	10
-5	4	4	27	29	26
-4	4	4	87	82	7
-3	4	4	108	96	10
-2	4	4	49	39	20
-1	4	4	70	65	4
0	4	4	359	377	7
1	4	4	239	235	3
2	4	4	319	322	4
3	4	4	120	122	4
4	4	4	146	155	8
5	4	4	74	81	16
6	4	4	93	88	11
-7	5	4	12	5	12
-6	5	4	140	157	7
-5	5	4	56	58	9
-4	5	4	353	344	4
-3	5	4	65	62	10
-2	5	4	963	954	5
-1	5	4	0	7	1
0	5	4	624	643	4
1	5	4	155	154	3
2	5	4	277	282	3
3	5	4	0	13	1
4	5	4	103	101	5
5	5	4	0	24	1
6	5	4	0	5	1
-7	6	4	49	67	14
-6	6	4	17	31	17
-5	6	4	0	7	1
-4	6	4	47	32	9
-3	6	4	75	155	74
-2	6	4	98	90	4
-1	6	4	297	290	4
0	6	4	378	379	6
1	6	4	229	227	3
2	6	4	178	180	4
3	6	4	247	245	3
4	6	4	225	217	12
5	6	4	19	39	19
6	6	4	72	70	11
-7	7	4	59	63	16
-6	7	4	24	94	24
-5	7	4	230	222	17
-4	7	4	92	86	7
-3	7	4	356	357	4
-2	7	4	107	110	5
-1	7	4	1087	1071	5
0	7	4	357	357	3
1	7	4	453	445	6
2	7	4	152	151	5
3	7	4	121	121	4
4	7	4	20	22	19
5	7	4	0	4	1
6	7	4	0	17	1
-7	8	4	68	83	15
-6	8	4	15	37	7
-5	8	4	14	57	13
-4	8	4	10	15	9
-3	8	4	43	32	11
-2	8	4	111	93	7
-1	8	4	398	387	6
0	8	4	103	95	3
1	8	4	160	173	4
2	8	4	25	4	25
3	8	4	278	277	3
4	8	4	21	15	20
5	8	4	177	169	6
6	8	4	50	38	14
-7	9	4	45	17	13
-6	9	4	70	72	16
-5	9	4	94	135	93
-3	9	5	127	123	5
-2	9	5	0	20	1
-1	9	5	96	87	4
0	9	5	75	77	4
1	9	5	132	123	4
2	9	5	43	39	10
3	9	5	72	68	6
4	9	5	168	164	6
5	9	5	93	83	11
6	9	5	11	23	11
-7	10	5	2	5	2
-6	10	5	0	13	1
5	9	4	0	3	1
6	9	4	11	28	11
-7	10	4	26	21	25
-6	10	4	116	116	10
-5	10	4	31	19	27
-4	10	4	62	65	8
-3	10	4	0	3	1
-2	10	4	31	9	17
-1	10	4	431	420	6
0	10	4	237	245	4
1	10	4	0	24	1
2	10	4	187	199	4
3	10	4	0	21	1
4	10	4	265	253	5
5	10	4	27	50	27
6	10	4	81	95	24
-7	11	4	30	20	30
-6	11	4	65	82	13
-5	11	4	30	36	29
-4	11	4	171	161	4
-3	11	4	119	118	5
-2	11	4	364	365	5
-1	11	4	247	248	4
0	11	4	415	416	6
1	11	4	211	197	3
2	11	4	334	322	4
3	11	4	51	35	9
4	11	4	35	42	21
5	11	4	33	20	21
6	11	4	14	2	14
-7	12	4	53	74	26
-6	12	4	33	45	33
-5	12	4	102	120	8
-4	12	4	33	5	32
-3	12	4	57	54	8
-2	12	4	48	37	9
-1	12	4	133	139	4
0	12	4	151	138	4
1	12	4	187	189	4
2	12	4	0	26	1
3	12	4	213	209	4
4	12	4	207	185	6
5	12	4	134	130	8
6	12	4	0	9	1
-7	13	4	39	29	17
-6	13	4	0	10	1
-5	13	4	179	172	6
-4	13	4	40	32	16
-3	13	4	308	308	4
-2	13	4	0	18	1
-1	13	4	386	388	6
0	13	4	53	57	6
1	13	4	332	329	7
2	13	4	48	51	26
3	13	4	201	192	10
4	13	4	20	30	19
5	13	4	36	28	18
6	13	4	18	29	17
-7	14	4	0	30	1
-6	14	4	37	43	36
-5	14	4	62	63	13
-4	14	4	153	146	4
-3	14	4	56	70	13
-2	14	4	94	105	6
-1	14	4	290	286	4
0	14	4	186	192	2
1	14	4	0	21	1
2	14	4	198	195	4
3	14	4	115	101	5
4	14	4	96	100	10
5	14	4	109	110	10
6	14	4	68	68	14
-7	15	4	0	14	1
-6	15	4	131	119	9
-5	15	4	22	27	22
-4	15	4	275	261	5
-3	15	4	117	102	10
-2	15	4	236	230	4
-5	16	5	83	87	14
-4	16	5	52	50	15
-3	16	5	200	186	6
-2	16	5	125	115	4
-1	16	5	233	228	4
0	16	5	77	77	6
1	16	5	295	273	5
2	16	5	131	137	7
3	16	5	42	42	15
4	16	5	32	34	25
5	16	5	18	3	18
-6	17	5	100	95	11
-4	16	4	26	50	25
-3	16	4	62	55	7
-2	16	4	48	47	9
-1	16	4	181	183	4
0	16	4	138	137	3
1	16	4	91	89	6
2	16	4	187	174	4
3	16	4	59	44	11
4	16	4	147	145	8
5	16	4	38	59	30
-6	17	4	37	46	22
-5	17	4	157	162	8
-4	17	4	118	106	8
-3	17	4	305	298	4
-2	17	4	267	253	7
-1	17	4	239	224	4
0	17	4	176	160	4
1	17	4	292	274	3
2	17	4	139	127	4
3	17	4	64	83	12
4	17	4	0	27	1
5	17	4	0	6	1
-6	18	4	0	14	1
-5	18	4	42	30	15
-4	18	4	69	80	12
-3	18	4	34	46	33
-2	18	4	0	1	1
-1	18	4	145	141	4
0	18	4	18	29	17
1	18	4	211	197	4
2	18	4	3	32	3
3	18	4	123	116	8
4	18	4	0	12	1
5	18	4	112	96	11
-6	19	4	12	45	12
-5	19	4	94	74	40
-4	19	4	163	136	7
-3	19	4	255	244	5
-2	19	4	161	156	4
-1	19	4	194	187	4
0	19	4	242	239	5
1	19	4	154	138	8
2	19	4	138	141	7
3	19	4	56	72	15
4	19	4	30	12	20
5	19	4	27	5	27
-6	20	4	25	42	25
-5	20	4	17	28	17
-4	20	4	48	42	14
-3	20	4	14	11	14
-2	20	4	45	39	13
-1	20	4	84	82	6
0	20	4	82	79	5
1	20	4	124	136	7
2	20	4	152	153	8
3	20	4	29	54	28
4	20	4	119	115	9
-5	21	4	26	22	25
-4	21	4	135	115	8
-3	21	4	77	69	13
-2	21	4	180	185	6
-1	21	4	125	126	7
0	21	4	199	196	4
1	21	4	50	64	20
2	21	4	124	127	8
3	21	4	0	6	1
4	21	4	27	33	26
-5	22	4	72	69	14
-4	22	4	0	15	1
-3	22	4	37	55	24
-2	22	4	29	33	28
-1	22	4	67	66	17
0	22	4	102	108	6
1	22	4	33	34	21
2	22	4	80	91	10
3	22	4	81	76	21
4	22	4	28	47	28
-5	23	4	61	62	35
0	24	5	128	126	6
1	24	5	87	80	19
2	24	5	108	96	10
3	24	5	40	67	24
-4	25	5	0	33	1
-3	25	5	17	27	16
-2	25	5	47	52	15
-1	25	5	0	3	1
0	25	5	16	11	16
1	25	5	45	50	17
2	25	5	0	17	1
-3	26	5	60	62	21
-5	24	4	48	25	14
-4	24	4	0	28	1
-3	24	4	0	6	1
-2	24	4	0	3	1
-1	24	4	0	4	1
0	24	4	12	28	12
1	24	4	84	86	14
2	24	4	41	46	13
3	24	4	81	86	13
-4	25	4	85	85	17
-3	25	4	63	55	14
-2	25	4	146	151	7
-1	25	4	67	71	14
0	25	4	120	117	8
1	25	4	62	59	12
2	25	4	89	85	10
3	25	4	104	84	10
-4	26	4	0	12	1
-3	26	4	21	15	20
-2	26	4	0	2	1
-1	26	4	9	34	8
0	26	4	39	38	11
1	26	4	42	33	14
2	26	4	81	80	16
3	26	4	38	24	38
-3	27	4	112	123	18
-2	27	4	143	122	8
-1	27	4	88	92	13
0	27	4	54	77	11
1	27	4	20	44	20
2	27	4	51	55	15
-3	28	4	0	26	1
-2	28	4	0	6	1
-1	28	4	0	7	1
0	28	4	32	20	10
1	28	4	36	61	35
2	28	4	0	29	1
-2	29	4	42	49	41
-1	29	4	138	130	18
0	29	4	42	42	10
1	29	4	64	73	16
-1	30	4	0	18	1
-7	0	5	34	38	34
-5	0	5	195	192	7
-3	0	5	318	342	11
-1	0	5	407	421	8
1	0	5	481	478	5
3	0	5	330	340	4
5	0	5	46	52	15
-7	1	5	89	77	11
-6	1	5	123	90	17
-5	1	5	189	180	4
-4	1	5	69	49	8
-3	1	5	82	196	82
-2	1	5	135	138	3
-1	1	5	86	86	4
0	1	5	126	124	2
1	1	5	123	121	4
2	1	5	180	178	3
3	1	5	23	16	22
4	1	5	52	38	14
5	1	5	149	129	6
6	1	5	63	63	16
-7	2	5	40	12	13
-6	2	5	159	141	6
-5	2	5	38	44	19
-4	2	5	175	182	4
-3	2	5	0	7	1
-2	2	5	337	347	7
-1	2	5	171	171	3
0	2	5	623	643	4
1	2	5	195	194	4
2	2	5	415	404	10
3	2	5	13	29	13
4	2	5	105	96	8
5	2	5	9	17	8
6	2	5	22	18	22
-7	3	5	27	15	27
-4	5	6	179	168	4
-3	5	6	21	13	20
-2	5	6	349	343	12
-1	5	6	6	4	6
0	5	6	346	351	4
1	5	6	60	62	8
2	5	6	221	216	3
3	5	6	62	72	10
4	5	6	178	171	6
5	5	6	29	32	29
-7	6	6	3	24	3
-6	6	6	134	110	8

Table A-4, Continued
Observed and Calculated Structure Factors for 1,6-diferrocenylhexane-1,6-dione

h	k	l	10Fo	10Fc	10σ
6	3	5	143	115	8
-7	4	5	0	11	1
-6	4	5	92	64	20
-5	4	5	199	185	4
-4	4	5	88	89	5
-3	4	5	125	239	124
-2	4	5	249	256	3
-1	4	5	519	537	7
0	4	5	381	394	4
1	4	5	219	215	3
2	4	5	86	76	5
3	4	5	202	202	4
4	4	5	25	28	24
5	4	5	0	23	1
6	4	5	21	14	21
-7	5	5	113	103	9
-6	5	5	30	26	22
-5	5	5	219	213	7
-4	5	5	35	23	13
-3	5	5	175	190	11
-2	5	5	0	27	1
-1	5	5	32	20	12
0	5	5	71	60	3
1	5	5	271	258	3
2	5	5	38	38	15
3	5	5	120	117	9
4	5	5	12	15	11
5	5	5	192	170	11
6	5	5	0	17	1
-7	6	5	8	10	8
-6	6	5	51	40	39
-5	6	5	144	134	5
-4	6	5	87	77	7
-3	6	5	299	307	9
-2	6	5	198	203	3
-1	6	5	555	561	5
0	6	5	326	342	4
1	6	5	229	223	7
2	6	5	105	102	9
3	6	5	120	110	13
4	6	5	0	21	1
5	6	5	26	12	25
6	6	5	28	6	28
-7	7	5	61	59	15
-6	7	5	144	136	7
-5	7	5	0	25	1
-4	7	5	93	97	10
-3	7	5	22	23	21
-2	7	5	304	298	4
-1	7	5	67	66	6
0	7	5	134	139	3
1	7	5	84	86	5
2	7	5	219	216	3
3	7	5	133	134	5
4	7	5	175	164	11
5	7	5	37	38	14
6	7	5	56	76	16
-7	8	5	28	11	28
-6	8	5	33	34	26
-5	8	5	13	43	12
-4	8	5	124	275	123
-3	8	5	75	74	6
-2	8	5	500	495	10
-1	8	5	78	78	6
0	8	5	450	448	6
1	8	5	109	112	5
2	8	5	167	159	5
3	8	5	65	71	12
4	8	5	149	138	6
5	8	5	30	11	24
6	8	5	23	7	22
-7	9	5	50	62	35
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3	12	5	104	94	8
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3	10	7	139	131	11
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-6	8	6	0	10	1
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3	9	6	133	116	6
4	9	6	129	124	7
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0	10	6	21	35	21
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3	10	6	17	1	16
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2	18	7	78	101	12
3	18	7	23	31	22
-5	19	7	58	74	16
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1	19	7	32	33	21
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Table A-4, Continued
Observed and Calculated Structure Factors for 1,6-diferrocenylhexane-1,6-dione

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0	6	8	170	166	4
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2	6	8	89	81	8
3	6	8	24	2	24
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3	7	8	85	87	10
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-4	9	8	0	10	1
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0	9	8	163	157	4
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2	9	8	59	72	18
3	9	8	135	117	8
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3	9	9	24	20	23
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-1	5	11	103	97	35
0	5	11	21	23	21
-3	6	11	0	15	1
-2	6	11	0	10	1
-1	6	11	29	29	29
-4	12	9	34	39	17
-3	12	9	12	3	12
-2	12	9	0	28	1
-1	12	9	32	38	23
0	12	9	105	94	6
1	12	9	33	26	24
2	12	9	109	78	9
-5	13	9	12	10	12
-4	13	9	104	94	9
-3	13	9	25	14	25
-2	13	9	144	144	8
-1	13	9	0	4	1
0	13	9	56	69	9
1	13	9	0	17	1
2	13	9	74	69	11
-4	14	9	14	6	13
-3	14	9	39	35	19
-2	14	9	32	39	31
-1	14	9	39	29	13
0	14	9	0	18	1
1	14	9	89	88	11
2	14	9	44	57	18
-4	15	9	0	27	1
-3	15	9	186	171	8
-2	15	9	25	32	24
-1	15	9	117	116	8
0	15	9	17	36	16
1	15	9	78	60	9
2	15	9	30	15	29
-4	16	9	24	2	23
-3	16	9	16	8	15
-2	16	9	35	43	20
-1	16	9	69	66	10
0	16	9	25	40	22
1	16	9	58	53	13
-3	17	9	62	54	14
-2	17	9	133	121	9
-1	17	9	62	74	13
0	17	9	73	70	7
1	17	9	54	54	14
-3	18	9	0	11	1
-2	18	9	29	29	29
-1	18	9	0	5	1
0	18	9	42	46	9
-2	19	9	77	79	11
-1	19	9	50	50	14
0	19	9	44	63	12
-1	20	9	53	53	13
-4	0	10	81	92	13
-2	0	10	106	101	10
0	0	10	72	79	11
2	0	10	64	81	15
-5	1	10	28	31	27
-4	1	10	28	36	23
-3	1	10	52	62	16
-2	1	10	28	42	28
-1	1	10	34	55	22
0	1	10	108	106	6
1	1	10	47	43	14
2	1	10	40	53	20
-5	2	10	67	69	15
-4	2	10	17	12	16
-3	2	10	114	108	12
-2	2	10	36	21	12
-1	2	10	96	103	27
0	2	10	14	12	14
1	2	10	25	43	25
2	2	10	13	24	12
-5	3	10	61	53	11
0	6	11	11	5	10
-3	7	11	38	21	16
-2	7	11	69	75	12
-1	7	11	14	31	13
0	7	11	70	77	8
-2	8	11	16	53	15
-2	5	10	42	58	16
-1	5	10	0	28	1
0	5	10	31	45	12
1	5	10	19	7	18
2	5	10	55	70	17
-5	6	10	0	10	1
-4	6	10	0	24	1
-3	6	10	99	90	10
-2	6	10	52	61	14
-1	6	10	36	33	15
0	6	10	101	106	7
1	6	10	31	15	22
2	6	10	30	45	29
-5	7	10	72	71	14
-4	7	10	26	36	26
-3	7	10	32	41	31
-2	7	10	0	2	1
-1	7	10	0	16	1
0	7	10	15	15	14
1	7	10	47	49	15
2	7	10	23	15	22
-4	8	10	24	10	24
-3	8	10	43	53	42
-2	8	10	0	4	1
-1	8	10	133	129	7
0	8	10	0	3	1
1	8	10	97	80	28
2	8	10	4	18	4
-4	9	10	27	35	26
-3	9	10	6	1	6
-2	9	10	33	17	25
-1	9	10	29	31	23
0	9	10	10	29	10
1	9	10	47	38	13
-4	10	10	56	52	15
-3	10	10	0	9	1
-2	10	10	120	119	16
-1	10	10	26	41	25
0	10	10	93	86	16
1	10	10	0	5	1
-4	11	10	21	18	20
-3	11	10	18	11	17
-2	11	10	0	6	1
-1	11	10	0	25	1
0	11	10	15	20	15
1	11	10	35	40	15
-4	12	10	0	17	1
-3	12	10	103	87	16
-2	12	10	34	45	20
-1	12	10	78	93	12
0	12	10	39	38	11
1	12	10	22	51	21
-3	13	10	0	13	1
-2	13	10	45	25	13
-1	13	10	0	16	1
0	13	10	11	12	11
-3	14	10	0	8	1
-2	14	10	48	71	17
-1	14	10	86	71	15
0	14	10	48	61	12
-2	15	10	0	8	1
-1	15	10	17	2	16
-3	0	11	30	41	29
-1	0	11	0	2	1
-3	1	11	19	32	18
-2	1	11	23	39	23
-1	1	11	63	86	14
0	1	11	28	31	16
-3	2	11	0	20	1
-1	8	11	9	9	9
-2	9	11	10	32	9
-1	9	11	0	41	1

APPENDIX B

Crystallography Data for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Equations of Mean Plane for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

Table B-1

0.5973 * XO + 0.7897 * YO – 0.1399 * ZO = 5.0788
4.8754 * x + 7.3446 * y + 3.1518 * z = 5.0788

Deviation	Weight	Name
0.0567	1.00	O1
0.0025	1.00	C6
0.0408	1.00	C7
0.0033	1.00	C8
-0.0227	1.00	C9
-0.0517	1.00	C10
-0.0289	1.00	C11

Table B-2

0.5888 * XO + 0.7985 * YO – 0.1250 * ZO = 7.6427
4.8062 * x + 7.4463 * y + 2.9649 * z = 7.6427

Deviation	Weight	Name
0.0021	1.00	O2
0.0300	1.00	C32
-0.0337	1.00	C33
-0.0129	1.00	C34
0.0150	1.00	C35
0.0456	1.00	C36
-0.0462	1.00	C37

Table B-3

0.7418 * XO –0.6288 * YO – 0.2332 * ZO = 4.9937
6.0543 * x + -7.4372* y + 3.5489 * z = 4.9937

Deviation	Weight	Name
-0.1195	1.00	C12
-0.0103	1.00	C13
0.0247	1.00	C14
0.1110	1.00	C15
-0.0200	1.00	C16
0.0076	1.00	C17
-0.0795	1.00	C18
-0.1635	1.00	C19
0.0592	1.00	C20
0.1022	1.00	C21

Table B-4

0.7408 * XO –0.6273 * YO – 0.2402 * ZO = -1.0226
6.0465 * x + -7.4204 * y + 3.6331 * z = -1.0226

Deviation	Weight	Name
0.0919	1.00	C38
-0.0045	1.00	C39
0.1238	1.00	C40
-0.2523	1.00	C41
-0.0274	1.00	C42
0.0262	1.00	C43
-0.0823	1.00	C44
-0.0579	1.00	C45
0.0676	1.00	C46
0.1149	1.00	C47

Table B-5

0.5771* XO +0.8077 * YO – 0.1205 * ZO = 8.2036
4.7106 * x + 7.5563 * y + 2.8976 * z = 8.2036

Deviation	Weight	Name
-0.0023	1.00	C1
0.0032	1.00	C2
-0.0028	1.00	C3
0.0015	1.00	C4
0.0004	1.00	C5

Table B-6

0.5692 * XO +0.8105 * YO – 0.1379 * ZO = 4.8214
4.6462 * x + 7.5955 * y + 3.0979 * z = 4.8214

Deviation	Weight	Name
0.0015	1.00	C6
0.0057	1.00	C7
-0.0108	1.00	C8
0.0120	1.00	C9
-0.0085	1.00	C10

Table B-7

0.7028 * XO –0.6418 * YO – 0.3069 * ZO = 5.0311
5.7361 * x –7.5200 * y + 4.3720 * z = 5.0311

Deviation	Weight	Name
-0.0073	1.00	C17
0.0133	1.00	C18
-0.0146	1.00	C19
0.0101	1.00	C20
0.0015	1.00	C21

Table B-8

0.6985 * XO –0.6242 * YO – 0.3501 * ZO = 8.3183
5.7009 * x –7.3331 * y + 4.9000 * z = 8.3183

Deviation	Weight	Name
0.0479	1.00	C22
-0.0381	1.00	C23
0.0117	1.00	C24
0.0124	1.00	C25
-0.0338	1.00	C26

Table B-9

0.5927 * XO +0.7951 * YO – 0.1283 * ZO = 4.3803
4.8379 * x + 7.4063 * y + 3.0077 * z = 4.3803

Deviation	Weight	Name
-0.0150	1.00	C27
0.0154	1.00	C28
-0.0110	1.00	C29
0.0037	1.00	C30
0.0070	1.00	C31

Table B-10

0.5641* XO +0.8139 * YO – 0.1392 * ZO = 7.9375
4.6040 * x + 7.6370 * y + 3.1078 * z = 7.9375

Deviation	Weight	Name
0.0090	1.00	C32
-0.0119	1.00	C33
0.0101	1.00	C34
-0.0045	1.00	C35
0.0027	1.00	C36

Table B-11

0.7118 * XO –0.6233 * YO – 0.3237 * ZO = -0.3885
5.8102 * x –7.3412 * y + 4.6023 * z = -0.3885

Deviation	Weight	Name
0.0007	1.00	C43
-0.0005	1.00	C44
-0.0000	1.00	C45
0.0005	1.00	C46
-0.0008	1.00	C47

Table B-12

0.6881* XO –0.6403 * YO – 0.3414 * ZO = -3.8563
5.6163 * x –7.4853 * y + 4.7679 * z = -3.8563

Deviation	Weight	Name
-0.0349	1.00	C48
0.0269	1.00	C49
-0.0023	1.00	C50
-0.0198	1.00	C51
0.0302	1.00	C52

Table B-13

0.7722 * XO – 0.6157 * YO – 0.1570 * ZO = 4.9119
6.3025 * x –7.3422 * y + 2.6816 * z = 4.9119

Deviation	Weight	Name
-0.0332	1.00	C12
0.0500	1.00	C13
-0.0501	1.00	C14
0.0343	1.00	C15
-0.0009	1.00	C16

Table B-14

0.7995 * XO –0.5724 * YO – 0.1818 * ZO = -0.9642
6.5259 * x –6.9325 * y + 3.0543 * z = -0.9642

Deviation	Weight	Name
0.0477	1.00	C38
-0.1119	1.00	C39
-0.1300	1.00	C40
-0.0941	1.00	C41
0.0283	1.00	C42

Table B-15

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
2	0	-16	109	85	23
3	0	-16	85	25	35
1	1	-16	50	46	49
2	1	-16	87	12	30
3	1	-16	0	13	1
1	2	-16	0	37	1
2	2	-16	0	85	1
3	2	-16	88	70	34
3	-1	-15	80	74	32
4	-1	-15	72	25	48
5	-1	-15	61	71	61
1	0	-15	0	31	1
2	0	-15	130	93	17
3	0	-15	0	21	1
4	0	-15	77	53	31
5	0	-15	69	52	40
1	1	-15	0	2	1
2	1	-15	51	32	51
3	1	-15	74	71	40
4	1	-15	85	72	31
5	1	-15	110	91	23
1	2	-15	48	29	47
2	2	-15	0	24	1
3	2	-15	29	20	28
4	2	-15	80	58	29
5	2	-15	0	23	1
1	3	-15	57	62	57
2	3	-15	88	18	25
3	3	-15	0	26	1
4	3	-15	101	47	25
1	4	-15	0	34	1
2	4	-15	67	83	53
3	4	-15	52	17	51
4	4	-15	64	41	63
1	5	-15	84	74	31
2	5	-15	0	55	1
3	5	-15	67	88	66
2	-6	-14	33	7	32
3	-6	-14	49	54	49
0	-5	-14	98	53	31
1	-5	-14	121	96	22
2	-5	-14	65	57	54
3	-5	-14	43	57	43
-1	-4	-14	69	32	68
0	-4	-14	89	11	40
1	-4	-14	55	26	55
2	-4	-14	54	90	54
-1	-3	-14	26	51	25
0	-3	-14	69	34	69
-1	-2	-14	16	14	16
2	-1	-14	75	15	32
3	-1	-14	59	59	47
4	-1	-14	73	7	33
5	-1	-14	51	95	50
6	-1	-14	71	86	36
7	-1	-14	25	12	24
1	0	-14	35	30	35
2	0	-14	0	43	1
3	0	-14	58	52	38
4	0	-14	29	74	29
5	0	-14	52	50	51
6	0	-14	62	62	46
7	0	-14	0	32	1
-3	1	-14	0	9	1
-2	1	-14	77	15	39
0	1	-14	2	32	2
1	1	-14	116	127	18
2	1	-14	30	39	29
3	1	-14	65	59	44
4	1	-14	0	15	1
5	1	-14	89	72	27
6	1	-14	0	32	1
7	1	-14	114	88	22
-3	2	-14	93	64	30
-2	2	-14	114	65	25
0	2	-14	92	81	22
1	2	-14	0	38	1
2	2	-14	58	84	51
3	2	-14	31	62	30
4	2	-14	0	38	1
5	2	-14	56	36	56
6	2	-14	0	35	1
-3	3	-14	59	26	59
0	3	-14	48	66	48
1	3	-14	0	66	1
2	3	-14	30	53	29
3	3	-14	93	84	21
-2	-6	-11	13	79	12
-1	-6	-11	0	27	1
0	-6	-11	102	105	17
4	3	-14	77	73	31
5	3	-14	74	30	30
6	3	-14	72	35	39
-3	4	-14	108	73	29
0	4	-14	64	46	42
1	4	-14	36	26	36
2	4	-14	86	64	24
3	4	-14	50	29	49
4	4	-14	95	81	23
5	4	-14	0	41	1
0	5	-14	94	50	24
1	5	-14	79	68	33
2	5	-14	0	33	1
3	5	-14	70	63	40
4	5	-14	100	101	27
5	5	-14	95	41	30
0	6	-14	50	24	50
1	6	-14	97	118	27
2	6	-14	55	18	54
3	6	-14	68	24	50
4	6	-14	0	61	1
0	7	-14	66	32	66
1	7	-14	58	43	58
2	7	-14	60	45	59
1	-7	-13	0	43	1
2	-7	-13	66	18	42
3	-7	-13	19	48	18
4	-7	-13	0	44	1
0	-6	-13	0	36	1
1	-6	-13	92	70	26
2	-6	-13	74	85	32
3	-6	-13	35	42	35
4	-6	-13	41	42	40
5	-6	-13	31	11	31
6	-6	-13	0	15	1
-2	-5	-13	87	44	47
-1	-5	-13	145	126	19
0	-5	-13	0	44	1
1	-5	-13	43	34	43
2	-5	-13	47	39	46
3	-5	-13	103	119	21
4	-5	-13	0	10	1
5	-5	-13	113	95	18
-2	-4	-13	101	65	30
-1	-4	-13	18	63	17
0	-4	-13	72	71	40
1	-4	-13	34	51	33
2	-4	-13	0	27	1
3	-4	-13	50	45	49
4	-4	-13	106	81	18
-2	-3	-13	82	8	47
-1	-3	-13	122	123	25
0	-3	-13	58	63	58
1	-3	-13	76	65	30
2	-3	-13	0	30	1
-1	-2	-13	69	88	58
0	-2	-13	125	110	18
1	-2	-13	49	56	49
-1	-1	-13	63	36	62
1	-1	-13	125	90	16
2	-1	-13	21	69	20
3	-1	-13	67	80	33
4	-1	-13	106	47	19
5	-1	-13	71	64	36
6	-1	-13	53	24	52
7	-1	-13	124	56	18
8	-1	-13	0	48	1
-4	0	-13	67	86	66
-3	0	-13	117	110	18
-2	0	-13	69	69	38
0	0	-13	42	33	41
1	0	-13	0	22	1
2	0	-13	104	95	17
3	0	-13	88	89	20
4	0	-13	43	59	42
5	0	-13	0	46	1
6	0	-13	0	67	1
7	0	-13	0	46	1
8	0	-13	117	120	20
-4	1	-13	22	42	22
-3	1	-13	73	72	37
-2	1	-13	83	51	26
0	1	-13	34	45	33
1	1	-13	0	49	1
2	1	-13	70	61	20
3	1	-13	123	111	14
4	1	-13	139	109	13
-3	1	-11	74	72	23
-2	1	-11	139	156	11
-1	1	-11	22	11	21
5	1	-13	57	65	40
6	1	-13	0	36	1
7	1	-13	104	30	24
8	1	-13	50	49	50
-4	2	-13	0	13	1
-3	2	-13	113	84	19
-2	2	-13	77	46	34
0	2	-13	41	59	40
1	2	-13	26	36	25
2	2	-13	55	55	48
3	2	-13	57	52	41
4	2	-13	53	78	53
5	2	-13	119	91	18
6	2	-13	0	42	1
7	2	-13	73	92	41
-4	3	-13	57	60	57
-3	3	-13	0	21	1
-2	3	-13	96	63	23
0	3	-13	103	108	16
1	3	-13	72	51	26
2	3	-13	20	19	20
3	3	-13	35	45	34
4	3	-13	0	45	1
5	3	-13	103	59	20
6	3	-13	56	52	55
7	3	-13	0	32	1
-4	4	-13	0	19	1
-3	4	-13	96	70	25
0	4	-13	57	39	41
1	4	-13	152	136	14
2	4	-13	63	43	45
3	4	-13	30	30	30
4	4	-13	72	68	30
5	4	-13	56	77	55
6	4	-13	83	62	26
7	4	-13	98	65	25
-4	5	-13	122	82	23
-3	5	-13	0	55	1
0	5	-13	98	119	21
1	5	-13	67	59	35
2	5	-13	147	147	14
3	5	-13	48	37	47
4	5	-13	38	29	38
5	5	-13	59	38	58
6	5	-13	70	74	50
0	6	-13	0	43	1
1	6	-13	48	83	48
2	6	-13	37	37	37
3	6	-13	97	108	21
4	6	-13	75	25	30
5	6	-13	53	33	52
0	7	-13	83	2	29
1	7	-13	46	41	45
2	7	-13	107	99	22
3	7	-13	0	19	1
4	7	-13	43	78	43
0	8	-13	0	19	1
1	8	-13	0	10	1
2	8	-13	35	8	35
3	8	-13	10	52	9
1	-8	-12	83	23	37
2	-8	-12	78	63	31
3	-8	-12	53	41	53
4	-8	-12	89	60	23
5	-8	-12	57	26	56
-1	-7	-12	132	98	20
0	-7	-12	50	45	50
1	-7	-12	20	29	19
2	-7	-12	74	39	29
3	-7	-12	85	68	23
4	-7	-12	0	18	1
5	-7	-12	0	63	1
6	-7	-12	0	37	1
-2	-6	-12	97	33	33
-1	-6	-12	33	32	33
0	-6	-12	110	79	22
1	-6	-12	0	12	1
2	-6	-12	74	33	31
3	-6	-12	71	54	27
4	-6	-12	79	94	22
5	-6	-12	63	17	37
6	-6	-12	73	90	29
7	-6	-12	110	44	19
-3	-5	-12	0	30	1
-2	-5	-12	0	38	1
-1	-5	-12	143	115	18
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4	-5	-12	0	28	1
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6	-5	-12	77	29	25
-2	-4	-12	67	57	66
-1	-4	-12	77	14	39
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1	-4	-12	92	98	19
2	-4	-12	144	129	13
3	-4	-12	85	84	21
4	-4	-12	37	50	36
5	-4	-12	71	33	29
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-1	-3	-12	98	74	23
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1	-3	-12	122	111	16
2	-3	-12	74	66	22
3	-3	-12	104	91	16
4	-3	-12	37	36	37
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4	-2	-12	38	56	37
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-4	-1	-12	0	18	1
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1	-1	-12	19	21	19
2	-1	-12	62	36	28
3	-1	-12	123	134	12
4	-1	-12	114	108	13
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6	-1	-12	0	55	1
7	-1	-12	62	23	61
8	-1	-12	89	28	28
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3	0	-12	75	54	24
4	0	-12	136	134	14
5	0	-12	121	126	15
6	0	-12	30	50	29
7	0	-12	95	76	25
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3	1	-12	76	79	24
4	1	-12	100	99	16
5	1	-12	132	121	13
6	1	-12	93	113	20
7	1	-12	80	86	24
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6	2	-12	0	51	1
7	2	-12	117	88	19
8	2	-12	76	31	38
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3	-4	-10	50	63	49
4	-4	-10	0	15	1
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0	3	-12	167	165	10
1	3	-12	0	18	1
2	3	-12	114	110	14
3	3	-12	39	45	39
4	3	-12	77	57	22
5	3	-12	72	51	24
6	3	-12	42	58	41
7	3	-12	58	77	57
8	3	-12	133	89	19
-5	4	-12	100	50	27
-4	4	-12	112	74	20
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0	4	-12	84	51	21
1	4	-12	138	121	14
2	4	-12	65	20	30
3	4	-12	112	105	16
4	4	-12	71	20	29
5	4	-12	41	55	40
6	4	-12	59	58	59
7	4	-12	56	52	56
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2	5	-12	57	65	31
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5	5	-12	0	19	1
6	5	-12	19	38	18
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1	6	-12	173	157	12
2	6	-12	48	21	48
3	6	-12	74	76	29
4	6	-12	40	45	39
5	6	-12	127	124	15
6	6	-12	57	60	57
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0	7	-12	86	74	26
1	7	-12	82	88	24
2	7	-12	76	48	28
3	7	-12	0	23	1
4	7	-12	82	82	31
5	7	-12	35	38	35
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1	8	-12	126	107	17
2	8	-12	87	71	27
3	8	-12	86	29	26
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2	9	-12	113	43	19
3	9	-12	0	44	1
2	-9	-11	0	34	1
3	-9	-11	104	77	18
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1	-8	-11	40	64	39
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3	-8	-11	0	29	1
4	-8	-11	0	43	1
5	-8	-11	53	5	52
6	-8	-11	64	69	38
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3	-7	-11	49	59	49
4	-7	-11	0	51	1
5	-7	-11	102	83	16
6	-7	-11	68	19	30
7	-7	-11	134	88	16
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2	2	-10	184	185	9
3	2	-10	55	36	24

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
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3	-6	-11	81	97	20
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5	-6	-11	56	47	39
6	-6	-11	0	84	1
7	-6	-11	0	3	1
8	-6	-11	64	65	48
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-2	-5	-11	0	81	1
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0	-5	-11	59	14	39
1	-5	-11	84	101	19
2	-5	-11	80	63	23
3	-5	-11	169	180	10
4	-5	-11	75	102	20
5	-5	-11	48	24	47
6	-5	-11	0	30	1
7	-5	-11	113	84	19
8	-5	-11	85	44	28
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-2	-4	-11	80	92	34
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0	-4	-11	0	28	1
1	-4	-11	43	26	42
2	-4	-11	89	92	18
3	-4	-11	164	129	10
4	-4	-11	50	50	49
5	-4	-11	96	112	17
6	-4	-11	109	35	17
7	-4	-11	81	43	22
-2	-3	-11	203	184	14
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0	-3	-11	103	89	17
1	-3	-11	78	33	28
2	-3	-11	57	74	31
3	-3	-11	89	93	15
4	-3	-11	125	136	12
5	-3	-11	28	46	27
-2	-2	-11	21	65	20
-1	-2	-11	226	219	10
0	-2	-11	66	64	26
1	-2	-11	201	187	10
2	-2	-11	0	31	1
3	-2	-11	97	103	10
4	-2	-11	118	111	9
5	-2	-11	101	108	16
6	-2	-11	83	66	23
7	-2	-11	82	97	24
-6	-1	-11	121	79	25
-5	-1	-11	0	7	1
-4	-1	-11	220	215	12
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-2	-1	-11	40	34	40
-1	-1	-11	28	48	28
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1	-1	-11	111	78	9
2	-1	-11	136	141	12
3	-1	-11	13	48	12
4	-1	-11	0	66	1
5	-1	-11	92	143	15
6	-1	-11	105	105	15
7	-1	-11	49	50	49
8	-1	-11	136	107	17
9	-1	-11	10	50	9
-6	0	-11	32	10	32
-5	0	-11	139	116	16
-4	0	-11	0	47	1
-3	0	-11	141	158	12
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-1	0	-11	52	50	22
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1	0	-11	202	205	6
2	0	-11	82	87	17
3	0	-11	194	201	8
4	0	-11	0	25	1
5	0	-11	0	27	1
6	0	-11	84	96	22
7	0	-11	109	91	19
8	0	-11	0	62	1
9	0	-11	147	85	18
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-5	1	-11	39	29	38
-4	1	-11	144	153	14
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1	8	-10	0	55	1
2	8	-10	119	108	16
3	8	-10	0	29	1
4	8	-10	81	71	25
5	8	-10	58	25	57
0	1	-11	0	43	1
1	1	-11	64	79	22
2	1	-11	203	207	9
3	1	-11	26	45	25
4	1	-11	190	180	11
5	1	-11	0	10	1
6	1	-11	111	101	18
7	1	-11	28	73	28
8	1	-11	150	139	15
9	1	-11	28	45	28
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6	2	-11	65	41	29
7	2	-11	36	35	36
8	2	-11	72	48	37
9	2	-11	134	85	16
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3	3	-11	102	95	16
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7	3	-11	89	76	23
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3	4	-11	66	66	23
4	4	-11	0	21	1
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6	4	-11	48	41	47
7	4	-11	90	58	24
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6	6	-11	53	31	52
7	6	-11	101	90	25
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3	-2	-10	131	121	7
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6	-2	-10	55	73	37
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-6	-1	-10	45	34	44
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6	6	-9	160	152	13
7	6	-9	0	46	1
8	6	-9	0	33	1
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6	2	-10	154	155	11
7	2	-10	108	105	16
8	2	-10	106	82	19
-7	3	-10	0	19	1
-6	3	-10	0	35	1
-5	3	-10	142	158	14
-4	3	-10	120	122	15
-3	3	-10	89	65	21
-2	3	-10	42	74	41
-1	3	-10	58	55	19
0	3	-10	113	117	12
1	3	-10	192	194	8
2	3	-10	37	45	37
3	3	-10	86	87	14
4	3	-10	0	45	1
5	3	-10	56	41	34
6	3	-10	93	101	20
7	3	-10	53	53	53
8	3	-10	33	68	33
-7	4	-10	19	26	18
-6	4	-10	26	42	26
-5	4	-10	0	22	1
-4	4	-10	194	215	11
-3	4	-10	74	71	23
-2	4	-10	130	132	13
-1	4	-10	116	126	10
0	4	-10	143	146	11
1	4	-10	163	162	10
2	4	-10	3	44	3
3	4	-10	216	212	9
4	4	-10	19	31	18
5	4	-10	35	11	35
6	4	-10	0	43	1
7	4	-10	157	149	14
8	4	-10	90	78	25
-6	5	-10	44	12	44
-5	5	-10	45	72	45
-4	5	-10	64	30	34
-3	5	-10	243	260	9
-2	5	-10	181	179	7
-1	5	-10	154	151	10
0	5	-10	139	135	10
1	5	-10	52	54	32
2	5	-10	72	79	19
3	5	-10	100	121	14
4	5	-10	57	39	36
5	5	-10	133	111	14
6	5	-10	68	29	28
7	5	-10	30	40	30
8	5	-10	40	54	40
-6	6	-10	32	53	31
-5	6	-10	0	16	1
-4	6	-10	49	55	48
-3	6	-10	59	41	45
-2	6	-10	195	219	9
-1	6	-10	29	31	28
0	6	-10	135	142	12
1	6	-10	60	44	22
2	6	-10	47	50	47
3	6	-10	138	152	12
4	6	-10	145	152	12
5	6	-10	46	46	46
6	6	-10	96	77	21
7	6	-10	116	79	17
-6	7	-10	0	49	1
-5	7	-10	71	34	36
-4	7	-10	53	19	52
-3	7	-10	88	92	20
-2	7	-10	13	23	13
-1	7	-10	159	145	12
0	7	-10	40	43	39
1	7	-10	188	166	11
2	7	-10	0	15	1
3	7	-10	178	153	11
4	7	-10	59	63	32
5	7	-10	154	137	13
6	7	-10	91	71	25
7	7	-10	77	40	48
-5	8	-10	0	9	1
-4	8	-10	101	73	29
-2	8	-10	123	146	15
-1	8	-10	0	14	1
4	-8	-8	89	83	14
5	-8	-8	45	10	45
6	-8	-8	0	46	1
7	-8	-8	85	79	23
8	-8	-8	0	7	1
-4	-7	-8	97	86	20

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-5	9	-10	104	81	27
-2	9	-10	0	31	1
-1	9	-10	70	62	34
0	9	-10	30	41	30
1	9	-10	141	157	14
2	9	-10	0	34	1
3	9	-10	0	58	1
4	9	-10	56	18	55
5	9	-10	25	11	25
-2	10	-10	0	51	1
-1	10	-10	0	11	1
0	10	-10	0	61	1
1	10	-10	16	20	16
2	10	-10	82	75	29
3	10	-10	71	46	45
-2	11	-10	0	32	1
-1	11	-10	0	59	1
0	11	-10	73	7	47
1	11	-10	43	42	42
0	-10	-9	70	15	43
1	-10	-9	96	71	21
2	-10	-9	0	28	1
3	-10	-9	35	57	35
4	-10	-9	56	37	52
5	-10	-9	49	50	49
-2	-9	-9	102	88	22
-1	-9	-9	0	45	1
0	-9	-9	66	52	52
1	-9	-9	0	53	1
2	-9	-9	89	97	17
3	-9	-9	49	74	49
4	-9	-9	70	85	21
5	-9	-9	51	56	51
6	-9	-9	50	48	50
7	-9	-9	59	20	46
-3	-8	-9	0	35	1
-2	-8	-9	16	29	15
-1	-8	-9	120	137	18
0	-8	-9	38	13	38
1	-8	-9	42	37	42
2	-8	-9	0	36	1
3	-8	-9	49	51	49
4	-8	-9	104	83	13
5	-8	-9	157	152	11
6	-8	-9	41	5	40
7	-8	-9	77	49	24
8	-8	-9	95	56	26
-4	-7	-9	90	41	34
-3	-7	-9	0	26	1
-2	-7	-9	61	57	55
-1	-7	-9	0	34	1
0	-7	-9	207	221	9
1	-7	-9	44	19	44
2	-7	-9	114	130	11
3	-7	-9	98	106	14
4	-7	-9	55	27	24
5	-7	-9	123	104	13
6	-7	-9	89	104	15
7	-7	-9	63	30	32
8	-7	-9	78	55	30
-4	-6	-9	37	33	36
-3	-6	-9	112	121	22
-2	-6	-9	71	55	26
-1	-6	-9	77	79	23
0	-6	-9	56	37	28
1	-6	-9	174	176	11
2	-6	-9	135	133	11
3	-6	-9	102	91	13
4	-6	-9	0	36	1
5	-6	-9	110	101	13
6	-6	-9	0	22	1
7	-6	-9	86	89	21
8	-6	-9	0	9	1
9	-6	-9	93	24	29
-3	-5	-9	48	41	47
-2	-5	-9	47	67	47
-1	-5	-9	0	11	1
0	-5	-9	136	140	11
1	-5	-9	40	69	39
2	-5	-9	325	331	7
3	-5	-9	94	98	13
-3	-2	-8	143	145	10
-2	-2	-8	144	134	7
-1	-2	-8	30	37	29
0	-2	-8	198	197	4
1	-2	-8	245	237	7
2	-2	-8	198	199	5
3	-2	-8	54	70	12
4	-2	-8	102	86	26
5	-2	-8	71	69	10
-3	-4	-9	208	209	11
-2	-4	-9	60	80	33
-1	-4	-9	17	48	17
0	-4	-9	78	8	24
1	-4	-9	68	50	21
2	-4	-9	64	25	18
3	-4	-9	209	241	8
4	-4	-9	97	110	13
5	-4	-9	93	113	12
6	-4	-9	77	63	19
7	-4	-9	95	74	17
8	-4	-9	0	54	1
9	-4	-9	72	79	42
-7	-3	-9	21	60	20
-6	-3	-9	33	63	33
-5	-3	-9	124	83	18
-4	-3	-9	11	33	11
-3	-3	-9	102	91	11
-2	-3	-9	134	136	13
-1	-3	-9	66	38	20
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1	-3	-9	15	4	15
2	-3	-9	222	232	7
3	-3	-9	163	159	9
4	-3	-9	57	81	21
5	-3	-9	128	119	10
6	-3	-9	70	60	18
7	-3	-9	80	81	20
8	-3	-9	156	154	13
-7	-2	-9	44	19	43
-6	-2	-9	121	100	20
-5	-2	-9	76	107	27
-4	-2	-9	64	58	33
-3	-2	-9	172	155	11
-2	-2	-9	145	140	7
-1	-2	-9	311	321	4
0	-2	-9	133	121	8
1	-2	-9	130	138	9
2	-2	-9	0	11	1
3	-2	-9	346	352	4
4	-2	-9	34	31	34
5	-2	-9	320	333	6
6	-2	-9	148	134	7
7	-2	-9	116	117	9
-7	-1	-9	86	60	34
-6	-1	-9	120	107	19
-5	-1	-9	166	166	13
-4	-1	-9	214	230	10
-3	-1	-9	0	9	1
-2	-1	-9	35	26	35
-1	-1	-9	163	155	6
0	-1	-9	314	316	3
1	-1	-9	177	187	9
2	-1	-9	153	152	6
3	-1	-9	16	10	16
4	-1	-9	92	79	8
5	-1	-9	25	67	25
6	-1	-9	78	98	16
7	-1	-9	145	106	10
8	-1	-9	98	75	18
-7	0	-9	40	22	39
-6	0	-9	125	110	19
-5	0	-9	65	73	42
-4	0	-9	271	281	8
-3	0	-9	40	31	40
-2	0	-9	0	17	1
-1	0	-9	144	141	10
0	0	-9	249	235	3
1	0	-9	164	171	5
2	0	-9	158	154	6
3	0	-9	24	24	23
4	0	-9	20	37	20
5	0	-9	294	292	7
6	0	-9	81	98	14
7	0	-9	136	130	13
8	0	-9	117	66	16
-7	1	-9	82	15	37
-6	1	-9	105	106	17
-5	1	-9	166	148	12
-4	1	-9	94	88	18
-3	1	-9	147	152	11
-1	3	-8	301	320	4
0	3	-8	35	42	34
1	3	-8	365	374	6
2	3	-8	65	49	14
3	3	-8	46	31	28
4	3	-8	91	81	14
5	3	-8	282	278	7
6	3	-8	41	69	40
7	3	-8	249	243	9
4	1	-9	157	161	9
5	1	-9	92	68	13
6	1	-9	93	88	15
7	1	-9	114	125	14
8	1	-9	74	82	27
-7	2	-9	66	56	54
-6	2	-9	77	70	24
-5	2	-9	55	62	55
-4	2	-9	232	233	9
-3	2	-9	81	76	16
-2	2	-9	168	155	6
-1	2	-9	32	10	31
0	2	-9	43	44	35
1	2	-9	32	37	32
2	2	-9	279	278	7
3	2	-9	145	141	10
4	2	-9	262	270	7
5	2	-9	40	51	40
6	2	-9	36	74	36
7	2	-9	136	145	13
8	2	-9	76	78	27
-7	3	-9	177	135	15
-6	3	-9	50	37	50
-5	3	-9	60	69	36
-4	3	-9	73	47	21
-3	3	-9	195	203	9
-2	3	-9	149	142	6
-1	3	-9	232	236	7
0	3	-9	88	78	11
1	3	-9	66	77	14
2	3	-9	143	147	8
3	3	-9	135	126	9
4	3	-9	103	93	12
5	3	-9	148	150	11
6	3	-9	53	50	52
7	3	-9	74	57	25
8	3	-9	128	117	15
-7	4	-9	80	9	31
-6	4	-9	96	126	23
-5	4	-9	79	94	24
-4	4	-9	76	36	23
-3	4	-9	0	8	1
-2	4	-9	229	231	10
-1	4	-9	0	49	1
0	4	-9	152	169	9
1	4	-9	0	49	1
2	4	-9	82	97	16
3	4	-9	189	188	9
4	4	-9	168	191	10
5	4	-9	0	42	1
6	4	-9	180	171	10
7	4	-9	22	12	21
8	4	-9	43	25	43
-7	5	-9	136	89	18
-6	5	-9	0	51	1
-5	5	-9	174	178	12
-4	5	-9	0	41	1
-3	5	-9	70	53	22
-2	5	-9	0	21	1
-1	5	-9	276	278	6
0	5	-9	46	42	27
1	5	-9	304	305	7
2	5	-9	115	103	11
3	5	-9	0	22	1
4	5	-9	74	83	18
5	5	-9	158	138	12
6	5	-9	60	58	40
7	5	-9	161	138	12
8	5	-9	67	73	49
-7	6	-9	83	13	27
-6	6	-9	77	97	28
-5	6	-9	0	75	1
-4	6	-9	215	232	9
-3	6	-9	68	21	23
-2	6	-9	22	37	21
-1	6	-9	121	113	12
0	6	-9	0	40	1
1	6	-9	42	66	42
2	6	-9	134	122	13
3	6	-9	54	61	28
4	6	-9	156	149	10
-6	9	-8	106	104	21
-5	9	-8	53	55	53
-3	9	-8	97	86	19
-2	9	-8	0	47	1
-1	9	-8	99	84	17
0	9	-8	85	85	20
1	9	-8	142	146	13
2	9	-8	0	21	1
3	9	-8	0	37	1
-5	7	-9	88	104	21
-4	7	-9	87	71	20
-3	7	-9	154	143	13
-2	7	-9	44	39	44
-1	7	-9	126	105	12
0	7	-9	47	27	47
1	7	-9	276	281	8
2	7	-9	88	82	16
3	7	-9	143	151	13
4	7	-9	58	72	47
5	7	-9	78	47	23
6	7	-9	77	36	29
7	7	-9	150	128	16
-6	8	-9	0	22	1
-5	8	-9	109	55	19
-4	8	-9	146	131	15
-2	8	-9	153	177	12
-1	8	-9	41	46	41
0	8	-9	102	83	15
1	8	-9	0	35	1
2	8	-9	173	168	13
3	8	-9	76	70	21
4	8	-9	80	85	24
5	8	-9	44	42	43
6	8	-9	92	20	23
7	8	-9	0	22	1
-5	9	-9	0	8	1
-2	9	-9	136	103	14
-1	9	-9	88	93	20
0	9	-9	57	80	56
1	9	-9	93	81	19
2	9	-9	60	79	46
3	9	-9	117	125	17
4	9	-9	0	22	1
5	9	-9	122	79	20
6	9	-9	47	19	47
-2	10	-9	132	132	18
-1	10	-9	95	67	22
0	10	-9	149	123	15
1	10	-9	21	37	21
2	10	-9	68	5	36
3	10	-9	49	21	49
4	10	-9	116	83	21
-2	11	-9	0	72	1
-1	11	-9	0	40	1
0	11	-9	116	97	22
1	11	-9	70	19	39
2	11	-9	0	29	1
0	-11	-8	112	65	20
1	-11	-8	42	3	42
2	-11	-8	0	34	1
3	-11	-8	66	28	27
4	-11	-8	81	45	21
-2	-10	-8	0	19	1
-1	-10	-8	93	75	26
0	-10	-8	49	48	49
1	-10	-8	73	81	25
2	-10	-8	56	13	31
3	-10	-8	21	14	21
4	-10	-8	86	49	19
5	-10	-8	9	86	9
6	-10	-8	75	32	26
-3	-9	-8	69	38	43
-2	-9	-8	51	50	51
-1	-9	-8	0	8	1
0	-9	-8	159	161	11
1	-9	-8	70	43	22
2	-9	-8	69	58	22
3	-9	-8	28	51	28
4	-9	-8	22	54	21
5	-9	-8	46	62	46
6	-9	-8	170	155	11
7	-9	-8	48	9	48
-4	-8	-8	27	55	26
-3	-8	-8	125	102	16
-2	-8	-8	79	28	25
-1	-8	-8	89	69	18
0	-8	-8	0	16	1
1	-8	-8	197	215	9
2	-8	-8	14	50	14
3	-8	-8	162	170	9
8	-7	-7	65	36	39
9	-7	-7	59	42	59
-4	-6	-7	120	125	12
-3	-6	-7	46	28	45
-2	-6	-7	119	89	14
-1	-6	-7	116	101	11
0	-6	-7	208	210	9
1	-6	-7	210	209	7
2	-6	-7	53	66	22
-3	-7	-8	62	80	33
-2	-7	-8	203	197	10
-1	-7	-8	35	44	34
0	-7	-8	38	34	38
1	-7	-8	0	58	1
2	-7	-8	131	125	11
3	-7	-8	0	41	1
4	-7	-8	38	40	37
5	-7	-8	63	50	19
6	-7	-8	81	94	19
7	-7	-8	89	57	19
8	-7	-8	86	91	24
9	-7	-8	22	44	22
-4	-6	-8	87	62	24
-3	-6	-8	135	147	14
-2	-6	-8	144	135	12
-1	-6	-8	149	158	11
0	-6	-8	68	46	17
1	-6	-8	65	59	19
2	-6	-8	96	82	15
3	-6	-8	322	332	7
4	-6	-8	104	72	13
5	-6	-8	120	116	11
6	-6	-8	41	16	40
7	-6	-8	106	89	15
8	-6	-8	0	41	1
9	-6	-8	128	99	18
-4	-5	-8	90	75	18
-3	-5	-8	39	23	38
-2	-5	-8	235	223	9
-1	-5	-8	157	161	10
0	-5	-8	261	272	7
1	-5	-8	53	28	23
2	-5	-8	40	61	40
3	-5	-8	93	109	10
4	-5	-8	89	92	12
5	-5	-8	98	110	14
6	-5	-8	121	95	12
7	-5	-8	82	47	18
8	-5	-8	62	72	34
9	-5	-8	0	40	1
10	-5	-8	45	27	44
-7	-4	-8	0	33	1
-6	-4	-8	103	127	25
-5	-4	-8	40	54	40
-4	-4	-8	61	54	47
-3	-4	-8	96	104	17
-2	-4	-8	152	150	10
-1	-4	-8	70	57	22
0	-4	-8	286	282	7
1	-4	-8	87	80	12
2	-4	-8	109	109	11
3	-4	-8	276	276	7
4	-4	-8	182	197	8
5	-4	-8	175	175	9
6	-4	-8	129	123	11
7	-4	-8	89	89	20
8	-4	-8	24	58	23
9	-4	-8	78	92	31
10	-4	-8	0	55	1
-7	-3	-8	122	106	23
-6	-3	-8	0	41	1
-5	-3	-8	197	181	13
-4	-3	-8	104	101	16
-3	-3	-8	60	47	16
-2	-3	-8	172	166	7
-1	-3	-8	142	136	6
0	-3	-8	285	292	6
1	-3	-8	261	252	7
2	-3	-8	148	140	9
3	-3	-8	54	63	19
4	-3	-8	95	80	11
5	-3	-8	30	47	29
6	-3	-8	246	258	8
7	-3	-8	130	121	13
8	-3	-8	109	100	17
9	-3	-8	46	9	46
-7	-2	-8	118	38	24
-6	-2	-8	142	159	16
-5	-2	-8	107	76	18
-4	-2	-8	210	220	9
-8	-1	-7	52	69	52
-7	-1	-7	166	131	14
-6	-1	-7	56	43	55
-5	-1	-7	198	197	10
-4	-1	-7	42	31	41
-3	-1	-7	143	137	9
-2	-1	-7	73	57	9
-1	-1	-7	568	564	8
0	-1	-7	20	25	20

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
6	-2	-8	35	45	35
7	-2	-8	143	136	12
8	-2	-8	182	168	12
-8	-1	-8	0	29	1
-7	-1	-8	85	73	30
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1	-1	-8	297	288	4
2	-1	-8	196	204	8
3	-1	-8	226	234	4
4	-1	-8	146	147	6
5	-1	-8	242	242	9
6	-1	-8	175	172	6
7	-1	-8	0	25	1
8	-1	-8	63	53	31
-8	0	-8	0	76	1
-7	0	-8	69	26	41
-6	0	-8	132	143	14
-5	0	-8	30	13	30
-4	0	-8	74	54	20
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-2	0	-8	285	294	5
-1	0	-8	133	133	5
0	0	-8	188	198	8
1	0	-8	85	89	7
2	0	-8	261	261	4
3	0	-8	303	308	4
4	0	-8	219	229	10
5	0	-8	45	41	19
6	0	-8	136	137	10
7	0	-8	154	144	11
8	0	-8	151	150	12
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-4	1	-8	72	59	19
-3	1	-8	267	267	7
-2	1	-8	26	49	25
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1	1	-8	13	15	13
2	1	-8	91	84	7
3	1	-8	331	350	5
4	1	-8	103	118	10
5	1	-8	416	411	6
6	1	-8	58	80	26
7	1	-8	75	42	21
8	1	-8	123	117	13
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-2	2	-8	148	152	12
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2	2	-8	27	25	27
3	2	-8	91	93	11
4	2	-8	186	195	8
5	2	-8	117	99	12
6	2	-8	121	105	12
7	2	-8	59	54	31
8	2	-8	59	31	37
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-3	4	-7	192	206	11
-2	4	-7	368	366	4
-1	4	-7	302	316	4
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1	4	-7	8	56	7
2	4	-7	354	362	6
3	4	-7	195	200	7
4	4	-7	215	221	7
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6	4	-7	162	151	10
7	4	-7	129	140	11
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0	4	-8	169	172	7
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2	4	-8	366	378	6
3	4	-8	70	67	15
4	4	-8	101	95	11
5	4	-8	44	38	44
6	4	-8	93	91	14
7	4	-8	107	99	16
8	4	-8	128	123	16
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-7	5	-8	61	59	60
-6	5	-8	52	70	51
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4	5	-8	119	117	11
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6	5	-8	74	80	24
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1	6	-8	56	74	25
2	6	-8	271	276	7
3	6	-8	0	47	1
4	6	-8	143	135	11
5	6	-8	90	80	16
6	6	-8	45	32	44
7	6	-8	0	33	1
-7	7	-8	68	70	39
-6	7	-8	97	74	23
-5	7	-8	36	59	36
-4	7	-8	87	67	19
-3	7	-8	103	97	17
-2	7	-8	165	177	9
-1	7	-8	72	45	17
0	7	-8	28	46	28
1	7	-8	31	40	30
2	7	-8	163	163	10
3	7	-8	176	162	10
4	7	-8	148	147	12
5	7	-8	117	129	16
6	7	-8	60	70	42
7	7	-8	32	51	32
-7	8	-8	146	133	19
-6	8	-8	0	69	1
-5	8	-8	95	97	22
-4	8	-8	59	29	58
-2	8	-8	96	89	16
-1	8	-8	208	234	9
0	8	-8	141	151	12
1	8	-8	219	218	9
2	8	-8	53	48	40
3	8	-8	0	30	1
4	8	-8	109	112	15
5	8	-8	0	71	1
6	8	-8	102	85	21
7	8	-8	100	59	24
6	9	-7	63	14	63
-6	10	-7	0	13	1
-3	10	-7	127	130	12
-2	10	-7	0	28	1
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0	10	-7	22	33	22
1	10	-7	98	87	19
2	10	-7	47	38	46
3	10	-7	138	106	15
4	10	-7	64	44	39
5	10	-7	31	56	31
-3	11	-7	0	36	1
4	9	-8	0	7	1
5	9	-8	71	74	35
6	9	-8	56	26	55
-2	10	-8	18	45	18
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1	10	-8	181	179	13
2	10	-8	68	77	32
3	10	-8	87	39	25
4	10	-8	71	31	38
5	10	-8	38	42	38
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1	11	-8	58	7	57
2	11	-8	69	66	41
3	11	-8	0	67	1
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0	12	-8	49	17	48
1	12	-8	103	56	26
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0	-11	-7	30	50	30
1	-11	-7	63	31	32
2	-11	-7	83	81	20
3	-11	-7	0	18	1
4	-11	-7	50	40	50
5	-11	-7	27	26	26
-3	-10	-7	68	24	50
-2	-10	-7	43	31	42
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0	-10	-7	0	12	1
1	-10	-7	130	134	12
2	-10	-7	76	27	20
3	-10	-7	123	124	11
4	-10	-7	68	65	21
5	-10	-7	0	36	1
6	-10	-7	86	65	18
7	-10	-7	85	97	27
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3	-9	-7	0	28	1
4	-9	-7	164	170	10
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6	-9	-7	14	6	14
7	-9	-7	25	20	25
8	-9	-7	49	58	48
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-3	-8	-7	102	70	19
-2	-8	-7	139	139	13
-1	-8	-7	154	170	12
0	-8	-7	103	113	14
1	-8	-7	94	89	13
2	-8	-7	29	14	29
3	-8	-7	149	168	9
4	-8	-7	158	173	11
5	-8	-7	58	72	23
6	-8	-7	48	68	48
7	-8	-7	0	43	1
8	-8	-7	86	41	25
9	-8	-7	153	107	17
-4	-7	-7	0	12	1
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-2	-7	-7	162	156	11
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3	-7	-7	70	81	15
4	-7	-7	162	187	9
5	-7	-7	3	26	3
6	-7	-7	118	127	12
7	-7	-7	0	40	1
6	-7	-6	102	104	12
7	-7	-6	77	87	21
8	-7	-6	63	69	39
9	-7	-6	85	100	31
-4	-6	-6	178	181	10
-3	-6	-6	81	91	18
-2	-6	-6	252	268	8
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3	-6	-6	159	160	8
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5	-6	-7	103	113	12
6	-6	-7	44	30	44
7	-6	-7	117	112	14
8	-6	-7	100	69	17
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10	-6	-7	0	12	1
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-3	-5	-7	176	166	11
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2	-5	-7	213	221	7
3	-5	-7	207	213	7
4	-5	-7	54	33	19
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6	-5	-7	192	186	9
7	-5	-7	118	120	13
8	-5	-7	50	58	49
9	-5	-7	85	81	27
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-7	-4	-7	0	32	1
-6	-4	-7	149	146	14
-5	-4	-7	0	22	1
-4	-4	-7	223	191	9
-3	-4	-7	0	40	1
-2	-4	-7	98	98	10
-1	-4	-7	70	80	16
0	-4	-7	38	38	38
1	-4	-7	68	86	14
2	-4	-7	290	298	6
3	-4	-7	8	37	7
4	-4	-7	122	133	9
5	-4	-7	104	88	11
6	-4	-7	68	77	20
7	-4	-7	261	267	8
8	-4	-7	138	121	14
9	-4	-7	109	71	17
10	-4	-7	66	27	65
-8	-3	-7	58	31	57
-7	-3	-7	37	57	36
-6	-3	-7	88	21	26
-5	-3	-7	112	150	16
-4	-3	-7	74	91	23
-3	-3	-7	210	192	6
-2	-3	-7	120	109	17
-1	-3	-7	20	29	20
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2	-3	-7	222	227	6
3	-3	-7	482	484	6
4	-3	-7	143	142	9
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6	-3	-7	93	73	13
7	-3	-7	90	109	17
8	-3	-7	124	110	13
9	-3	-7	147	143	15
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-8	-2	-7	90	82	36
-7	-2	-7	50	35	49
-6	-2	-7	134	130	16
-5	-2	-7	91	93	18
-4	-2	-7	49	48	48
-3	-2	-7	18	28	18
-2	-2	-7	460	452	4
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2	-2	-7	212	213	4
3	-2	-7	56	82	10
4	-2	-7	231	256	4
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6	-2	-7	149	145	6
7	-2	-7	4	65	4
8	-2	-7	26	52	25
9	-2	-7	50	33	49
5	-2	-6	145	150	6
6	-2	-6	275	258	5
7	-2	-6	62	34	22
8	-2	-6	163	159	12
9	-2	-6	37	48	36
10	-2	-6	75	48	31
-8	-1	-6	95	105	25
-7	-1	-6	53	53	52
-6	-1	-6	73	77	26
-5	-1	-6	206	192	9
-4	-1	-6	167	154	10
-3	-1	-6	306	304	6
1	-1	-7	160	168	5
2	-1	-7	152	148	5
3	-1	-7	152	149	5
4	-1	-7	218	219	4
5	-1	-7	326	338	4
6	-1	-7	60	40	14
7	-1	-7	65	40	13
8	-1	-7	77	71	14
-8	0	-7	61	10	61
-7	0	-7	68	66	42
-6	0	-7	243	250	10
-5	0	-7	89	96	17
-4	0	-7	162	157	10
-3	0	-7	78	83	14
-2	0	-7	336	323	5
-1	0	-7	58	49	7
0	0	-7	666	647	3
1	0	-7	22	24	21
2	0	-7	71	68	7
3	0	-7	26	23	26
4	0	-7	89	100	7
5	0	-7	118	114	6
6	0	-7	166	173	6
7	0	-7	99	70	12
8	0	-7	74	71	22
-8	1	-7	0	39	1
-7	1	-7	0	25	1
-6	1	-7	117	100	15
-5	1	-7	197	197	8
-4	1	-7	168	179	10
-3	1	-7	0	44	1
-2	1	-7	58	53	10
-1	1	-7	267	270	5
0	1	-7	425	427	4
1	1	-7	462	468	3
2	1	-7	92	97	7
3	1	-7	161	168	5
4	1	-7	25	33	24
5	1	-7	355	360	6
6	1	-7	144	124	9
7	1	-7	172	163	10
8	1	-7	123	117	12
-8	2	-7	0	31	1
-7	2	-7	65	37	33
-6	2	-7	70	80	27
-5	2	-7	251	266	8
-4	2	-7	175	174	9
-3	2	-7	273	273	7
-2	2	-7	203	211	8
-1	2	-7	36	57	20
0	2	-7	111	115	6
1	2	-7	266	252	4
2	2	-7	484	486	3
3	2	-7	295	309	6
4	2	-7	200	209	7
5	2	-7	162	145	9
6	2	-7	210	211	8
7	2	-7	174	188	9
-8	3	-7	125	124	18
-7	3	-7	105	110	20
-6	3	-7	65	23	31
-5	3	-7	16	32	15
-4	3	-7	120	126	12
-3	3	-7	182	191	8
-2	3	-7	37	39	22
-1	3	-7	116	121	5
0	3	-7	183	190	6
1	3	-7	257	277	5
2	3	-7	66	36	13
3	3	-7	359	362	6
4	3	-7	124	121	10
5	3	-7	121	122	11
6	3	-7	119	87	11
7	3	-7	132	112	12
-8	4	-7	0	34	1
-7	4	-7	69	81	31
-6	4	-7	101	98	18
-5	4	-7	103	106	14
2	3	-6	265	253	6
3	3	-6	344	348	5
4	3	-6	168	171	7
5	3	-6	301	306	6
6	3	-6	121	119	9
7	3	-6	179	177	10
-7	4	-6	0	30	1
-6	4	-6	0	29	1
-7	4	-6	95	110	20
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-5	4	-6	203	210	8
-4	4	-6	150	150	10

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-8	5	-7	140	108	17
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-6	5	-7	181	209	11
-5	5	-7	105	118	14
-4	5	-7	132	141	11
-3	5	-7	74	90	10
-2	5	-7	125	131	6
-1	5	-7	120	122	9
0	5	-7	220	225	6
1	5	-7	210	226	7
2	5	-7	14	43	13
3	5	-7	156	159	9
4	5	-7	75	57	15
5	5	-7	191	192	8
6	5	-7	31	41	30
7	5	-7	0	42	1
-8	6	-7	65	13	52
-7	6	-7	130	114	17
-6	6	-7	45	40	44
-5	6	-7	175	160	10
-4	6	-7	11	40	10
-3	6	-7	73	66	11
-2	6	-7	62	73	13
-1	6	-7	272	292	7
0	6	-7	48	48	27
1	6	-7	207	212	7
2	6	-7	17	30	17
3	6	-7	162	139	9
4	6	-7	99	93	13
5	6	-7	178	174	10
6	6	-7	181	160	10
7	6	-7	138	125	13
-8	7	-7	0	35	1
-7	7	-7	2	23	2
-6	7	-7	186	198	12
-5	7	-7	63	51	37
-4	7	-7	246	248	8
-3	7	-7	22	20	21
-2	7	-7	51	69	28
-1	7	-7	96	88	13
0	7	-7	171	172	9
1	7	-7	174	183	9
2	7	-7	210	211	8
3	7	-7	0	17	1
4	7	-7	0	36	1
5	7	-7	122	111	15
6	7	-7	148	128	14
7	7	-7	57	59	56
-7	8	-7	56	45	55
-6	8	-7	58	63	51
-5	8	-7	138	142	13
-4	8	-7	0	25	1
-3	8	-7	150	136	10
-2	8	-7	139	127	12
-1	8	-7	0	15	1
0	8	-7	56	39	26
1	8	-7	172	197	9
2	8	-7	41	59	40
3	8	-7	142	138	12
4	8	-7	18	22	18
5	8	-7	0	37	1
6	8	-7	122	69	17
7	8	-7	105	91	21
-7	9	-7	29	9	28
-6	9	-7	0	29	1
-5	9	-7	57	43	56
-3	9	-7	46	54	45
-2	9	-7	193	219	9
-1	9	-7	33	23	32
0	9	-7	44	16	44
1	9	-7	92	96	17
2	9	-7	183	181	11
3	9	-7	47	91	47
4	9	-7	148	139	12
5	9	-7	51	38	51
6	8	-6	36	34	35
-7	9	-6	120	114	18
-6	9	-6	146	155	13
-5	9	-6	0	28	1
-3	9	-6	139	136	13
-2	9	-6	89	104	18
-1	9	-6	0	39	1
0	9	-6	245	252	9
1	9	-6	44	9	43
2	9	-6	0	18	1
3	9	-6	49	53	49
4	9	-6	104	123	18
5	9	-6	72	22	30
6	9	-6	100	69	24
-6	10	-6	112	111	21
-2	11	-7	100	123	21
-1	11	-7	78	90	25
0	11	-7	139	122	14
1	11	-7	70	8	33
2	11	-7	29	50	28
3	11	-7	39	21	38
4	11	-7	137	126	18
-3	12	-7	0	31	1
-2	12	-7	0	8	1
-1	12	-7	64	54	64
0	12	-7	102	78	21
1	12	-7	104	49	26
2	12	-7	61	22	61
0	-12	-6	0	42	1
1	-12	-6	0	44	1
2	-12	-6	86	50	20
3	-12	-6	83	78	22
4	-12	-6	0	10	1
-2	-11	-6	82	64	29
-1	-11	-6	0	27	1
0	-11	-6	33	41	33
1	-11	-6	0	7	1
2	-11	-6	17	53	17
3	-11	-6	0	15	1
4	-11	-6	123	122	13
5	-11	-6	78	62	22
6	-11	-6	33	7	32
-3	-10	-6	110	55	20
-2	-10	-6	47	74	46
-1	-10	-6	114	103	15
0	-10	-6	105	86	16
1	-10	-6	0	22	1
2	-10	-6	29	22	28
3	-10	-6	60	75	26
4	-10	-6	46	81	46
5	-10	-6	126	119	14
6	-10	-6	65	34	32
7	-10	-6	49	29	49
-4	-9	-6	0	20	1
-3	-9	-6	2	47	2
-2	-9	-6	68	70	26
-1	-9	-6	135	138	14
0	-9	-6	170	146	10
1	-9	-6	119	142	10
2	-9	-6	69	25	17
3	-9	-6	0	8	1
4	-9	-6	142	138	11
5	-9	-6	189	217	9
6	-9	-6	115	112	13
7	-9	-6	107	115	16
8	-9	-6	34	24	34
-4	-8	-6	142	119	14
-3	-8	-6	70	36	31
-2	-8	-6	49	48	49
-1	-8	-6	96	86	18
0	-8	-6	185	188	9
1	-8	-6	102	104	11
2	-8	-6	110	108	10
3	-8	-6	0	34	1
4	-8	-6	19	29	18
5	-8	-6	95	90	14
6	-8	-6	0	22	1
7	-8	-6	74	92	20
8	-8	-6	58	91	58
9	-8	-6	0	41	1
-4	-7	-6	71	57	26
-3	-7	-6	192	205	10
-2	-7	-6	32	41	32
-1	-7	-6	60	59	19
0	-7	-6	128	128	12
1	-7	-6	151	143	9
2	-7	-6	153	164	8
3	-7	-6	28	72	28
4	-7	-6	36	49	36
5	-7	-6	33	57	33
0	-8	-5	86	84	14
1	-8	-5	138	126	10
2	-8	-5	145	165	8
3	-8	-5	0	37	1
4	-8	-5	199	203	8
5	-8	-5	46	57	45
6	-8	-5	26	25	25
7	-8	-5	91	68	20
8	-8	-5	95	80	23
9	-8	-5	91	71	30
-4	-7	-5	0	24	1
-3	-7	-5	197	184	10
-2	-7	-5	46	40	46
-1	-7	-5	213	219	7
0	-7	-5	19	39	18
4	-6	-6	167	180	8
5	-6	-6	58	61	18
6	-6	-6	8	35	7
7	-6	-6	123	126	14
8	-6	-6	72	104	26
9	-6	-6	0	28	1
10	-6	-6	48	37	48
-7	-5	-6	60	101	60
-6	-5	-6	84	18	25
-5	-5	-6	0	51	1
-4	-5	-6	0	48	1
-3	-5	-6	268	256	5
-2	-5	-6	61	54	19
-1	-5	-6	298	274	7
0	-5	-6	90	117	11
1	-5	-6	47	30	26
2	-5	-6	41	56	29
3	-5	-6	76	77	12
4	-5	-6	179	200	8
5	-5	-6	72	95	17
6	-5	-6	30	58	29
7	-5	-6	134	138	13
8	-5	-6	109	64	18
9	-5	-6	68	18	68
10	-5	-6	97	84	31
-8	-4	-6	51	41	50
-7	-4	-6	134	155	17
-6	-4	-6	98	117	19
-5	-4	-6	59	36	29
-4	-4	-6	61	38	23
-3	-4	-6	315	305	4
-2	-4	-6	138	125	5
-1	-4	-6	353	353	8
0	-4	-6	188	195	8
1	-4	-6	175	173	7
2	-4	-6	108	103	8
3	-4	-6	371	364	6
4	-4	-6	128	119	10
5	-4	-6	160	161	9
6	-4	-6	102	93	13
7	-4	-6	71	85	26
8	-4	-6	125	115	16
9	-4	-6	112	71	20
10	-4	-6	39	42	38
-7	-3	-6	130	157	17
-6	-3	-6	0	54	1
-5	-3	-6	131	132	13
-4	-3	-6	0	19	1
-3	-3	-6	36	42	36
-2	-3	-6	89	94	7
-1	-3	-6	358	370	4
0	-3	-6	25	31	25
1	-3	-6	353	350	6
2	-3	-6	140	138	8
3	-3	-6	240	247	6
4	-3	-6	102	95	8
5	-3	-6	457	463	6
6	-3	-6	72	76	15
7	-3	-6	184	186	9
8	-3	-6	17	17	17
9	-3	-6	60	42	59
10	-3	-6	71	46	50
-8	-2	-6	0	20	1
-7	-2	-6	127	122	15
-6	-2	-6	298	274	9
-5	-2	-6	69	62	23
-4	-2	-6	253	254	7
-3	-2	-6	116	105	7
-2	-2	-6	155	158	6
-1	-2	-6	187	185	4
0	-2	-6	553	560	7
1	-2	-6	331	320	5
2	-2	-6	333	339	4
3	-2	-6	169	160	4
4	-2	-6	136	133	5
-2	-3	-5	159	161	8
-1	-3	-5	38	16	14
0	-3	-5	94	95	4
1	-3	-5	478	479	5
2	-3	-5	322	325	5
3	-3	-5	559	546	5
4	-3	-5	81	78	10
5	-3	-5	0	16	1
6	-3	-5	0	29	1
7	-3	-5	217	224	9
8	-3	-5	13	40	13
9	-3	-5	163	168	12
10	-3	-5	76	56	30
11	-3	-5	0	14	1
-9	-2	-5	89	60	37
-2	-1	-6	121	106	11
-1	-1	-6	161	159	3
0	-1	-6	119	123	4
1	-1	-6	347	355	4
2	-1	-6	186	167	4
3	-1	-6	125	136	5
4	-1	-6	152	135	7
5	-1	-6	187	174	5
6	-1	-6	0	43	1
7	-1	-6	132	132	7
8	-1	-6	0	19	1
9	-1	-6	115	115	15
-9	0	-6	87	68	34
-8	0	-6	0	15	1
-7	0	-6	112	71	16
-6	0	-6	40	30	40
-5	0	-6	85	63	15
-4	0	-6	212	217	8
-3	0	-6	315	337	6
-2	0	-6	370	379	4
-1	0	-6	41	43	9
0	0	-6	173	178	3
1	0	-6	438	417	15
2	0	-6	434	432	4
3	0	-6	270	267	3
4	0	-6	289	298	13
5	0	-6	155	158	9
6	0	-6	263	261	5
7	0	-6	0	48	1
8	0	-6	199	189	10
-9	1	-6	78	49	46
-8	1	-6	178	185	15
-7	1	-6	72	85	29
-6	1	-6	89	81	18
-5	1	-6	84	76	15
-4	1	-6	211	212	7
-3	1	-6	216	214	4
-2	1	-6	517	509	16
-1	1	-6	440	446	8
0	1	-6	65	73	5
1	1	-6	47	55	8
2	1	-6	45	27	11
3	1	-6	362	366	3
4	1	-6	285	285	10
5	1	-6	199	210	7
6	1	-6	46	34	16
7	1	-6	89	108	13
-9	2	-6	51	56	51
-8	2	-6	0	9	1
-7	2	-6	216	236	9
-6	2	-6	131	125	12
-5	2	-6	62	55	22
-4	2	-6	83	82	14
-3	2	-6	230	243	4
-2	2	-6	227	240	3
-1	2	-6	355	338	5
0	2	-6	267	257	9
1	2	-6	211	203	3
2	2	-6	118	122	18
3	2	-6	242	243	7
4	2	-6	185	187	4
5	2	-6	346	335	6
6	2	-6	82	68	14
7	2	-6	118	97	11
-9	3	-6	0	14	1
-8	3	-6	101	98	20
-7	3	-6	0	15	1
-6	3	-6	248	241	9
-5	3	-6	75	80	17
-4	3	-6	124	104	10
-3	3	-6	24	22	24
-2	3	-6	138	137	11
-1	3	-6	244	266	8
0	3	-6	454	455	5
1	3	-6	347	347	5
5	1	-5	378	373	7
6	1	-5	254	246	16
7	1	-5	128	113	7
-9	2	-5	85	76	29
-8	2	-5	0	27	1
-7	2	-5	0	55	1
-6	2	-5	55	38	33
-5	2	-5	254	274	7
-4	2	-5	0	37	1
-3	2	-5	216	222	8
-2	2	-5	119	114	4
-1	2	-5	172	182	9
0	2	-5	142	155	4
1	2	-5	644	632	2
2	2	-5	245	255	5
-3	4	-6	136	126	11
-2	4	-6	42	53	14
-1	4	-6	272	282	4
0	4	-6	271	250	5
1	4	-6	468	481	5
2	4	-6	385	391	5
3	4	-6	138	132	9
4	4	-6	75	61	13
5	4	-6	113	110	9
6	4	-6	180	166	9
7	4	-6	149	119	10
-9	5	-6	103	23	23
-8	5	-6	102	58	21
-7	5	-6	49	46	48
-6	5	-6	134	137	14
-5	5	-6	0	17	1
-4	5	-6	348	359	7
-3	5	-6	49	55	14
-2	5	-6	169	173	5
-1	5	-6	138	135	8
0	5	-6	370	368	6
1	5	-6	189	203	7
2	5	-6	393	401	6
3	5	-6	24	13	23
4	5	-6	0	13	1
5	5	-6	80	74	16
6	5	-6	131	126	10
7	5	-6	152	149	12
-9	6	-6	88	85	30
-8	6	-6	69	33	40
-7	6	-6	92	103	21
-6	6	-6	53	64	53
-5	6	-6	118	116	12
-4	6	-6	98	80	14
-3	6	-6	304	316	4
-2	6	-6	50	44	14
-1	6	-6	31	36	31
0	6	-6	96	80	10
1	6	-6	312	323	6
2	6	-6	77	84	14
3	6	-6	241	253	7
4	6	-6	56	63	23
5	6	-6	43	49	42
6	6	-6	82	80	20
7	6	-6	184	169	10
-8	7	-6	131	143	18
-7	7	-6	63	7	33
-6	7	-6	5	50	5
-5	7	-6	59	13	30
-4	7	-6	172	183	9
-3	7	-6	148	139	6
-2	7	-6	212	226	7
-1	7	-6	102	97	11
0	7	-6	53	52	17
1	7	-6	42	12	41
2	7	-6	181	200	8
3	7	-6	58	71	26
4	7	-6	235	239	7
5	7	-6	46	30	45
6	7	-6	32	33	32
7	7	-6	81	78	23
-8	8	-6	92	64	25
-7	8	-6	188	208	12
-6	8	-6	91	66	23
-5	8	-6	98	76	15
-4	8	-6	0	23	1
-3	8	-6	170	174	10
-2	8	-6	71	82	19
-1	8	-6	222	222	8
0	8	-6	31	61	30
1	8	-6	48	27	25
2	8	-6	68	33	19
3	8	-6	110	102	13
4	8	-6	46	27	46
5	8	-6	191	189	10
-8	7	-5	19	15	19
-7	7	-5	134	135	14
-6	7	-5	173	163	10
-5	7	-5	89	94	15
-4	7	-5	73	81	12
-3	7	-5	44	36	43
-2	7	-5	178	182	9
-1	7	-5	111	99	10
0	7	-5	258	261	7
1	7	-5	72	87	15
2	7	-5	126	135	8
3	7	-5	47	57	33
4	7	-5	134	122	11
5	7	-5	43	66	43
6	7	-5	197	205	10

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-3	10	-6	101	83	19
-2	10	-6	40	41	39
-1	10	-6	151	149	14
0	10	-6	99	52	17
1	10	-6	224	209	10
2	10	-6	59	37	34
4	10	-6	0	22	1
5	10	-6	151	107	15
6	10	-6	103	30	29
-3	11	-6	76	82	33
-2	11	-6	73	75	35
-1	11	-6	0	40	1
0	11	-6	79	101	29
1	11	-6	159	119	14
2	11	-6	98	92	17
3	11	-6	84	18	27
4	11	-6	45	27	44
-3	12	-6	125	63	22
-2	12	-6	136	135	18
-1	12	-6	79	20	33
0	12	-6	68	49	44
1	12	-6	93	83	25
2	12	-6	0	56	1
3	12	-6	128	91	19
-1	-12	-5	76	57	30
0	-12	-5	63	73	31
1	-12	-5	40	45	39
2	-12	-5	22	14	21
3	-12	-5	27	10	26
4	-12	-5	0	15	1
5	-12	-5	57	74	48
-3	-11	-5	90	78	25
-2	-11	-5	69	13	37
-1	-11	-5	89	79	22
0	-11	-5	90	74	21
1	-11	-5	124	132	12
2	-11	-5	86	86	20
3	-11	-5	88	46	16
4	-11	-5	0	46	1
5	-11	-5	66	55	28
6	-11	-5	84	83	22
7	-11	-5	0	31	1
-4	-10	-5	37	80	36
-3	-10	-5	0	10	1
-2	-10	-5	28	24	27
-1	-10	-5	72	27	32
0	-10	-5	105	92	15
1	-10	-5	129	135	10
2	-10	-5	168	167	8
3	-10	-5	72	87	16
4	-10	-5	0	36	1
5	-10	-5	113	132	12
6	-10	-5	107	110	17
7	-10	-5	125	104	15
8	-10	-5	87	80	26
-4	-9	-5	42	60	41
-3	-9	-5	205	179	12
-2	-9	-5	48	15	47
-1	-9	-5	0	15	1
0	-9	-5	112	110	12
1	-9	-5	166	181	8
2	-9	-5	72	81	15
3	-9	-5	238	248	7
4	-9	-5	10	40	10
5	-9	-5	8	13	7
6	-9	-5	75	40	18
7	-9	-5	55	74	47
8	-9	-5	58	33	57
-4	-8	-5	145	138	13
-3	-8	-5	0	69	1
-2	-8	-5	258	249	8
-1	-8	-5	49	35	28
-3	-11	-4	154	134	14
-2	-11	-4	24	2	23
-1	-11	-4	0	26	1
0	-11	-4	0	21	1
1	-11	-4	99	85	15
2	-11	-4	109	84	12
3	-11	-4	128	121	10
4	-11	-4	0	61	1
5	-11	-4	0	27	1
6	-11	-4	100	93	21
7	-11	-4	61	49	51
-4	-10	-4	85	73	27
-3	-10	-4	78	42	29
-2	-10	-4	197	199	10
-1	-10	-4	41	33	40
0	-10	-4	133	114	12
1	-10	-4	72	42	17
2	-10	-4	133	147	10

h	k	l	10Fo	10Fc	10s
1	-7	-5	77	103	13
2	-7	-5	50	34	20
3	-7	-5	235	253	6
4	-7	-5	67	63	14
5	-7	-5	151	153	9
6	-7	-5	117	110	12
7	-7	-5	59	40	32
8	-7	-5	70	37	33
9	-7	-5	112	87	21
10	-7	-5	19	18	19
-7	-6	-5	41	53	41
-6	-6	-5	145	152	15
-5	-6	-5	141	115	13
-4	-6	-5	20	45	20
-3	-6	-5	120	111	12
-2	-6	-5	370	370	7
-1	-6	-5	129	118	9
0	-6	-5	360	343	6
1	-6	-5	115	102	9
2	-6	-5	26	41	26
3	-6	-5	45	13	22
4	-6	-5	150	178	8
5	-6	-5	112	115	10
6	-6	-5	177	180	9
7	-6	-5	87	92	19
8	-6	-5	37	50	37
9	-6	-5	107	79	19
10	-6	-5	74	24	39
-8	-5	-5	67	41	67
-7	-5	-5	94	79	26
-6	-5	-5	108	124	17
-5	-5	-5	192	177	10
-4	-5	-5	197	197	6
-3	-5	-5	152	170	7
-2	-5	-5	77	78	10
-1	-5	-5	207	215	4
0	-5	-5	139	131	8
1	-5	-5	354	357	6
2	-5	-5	16	43	15
3	-5	-5	0	13	1
4	-5	-5	89	101	10
5	-5	-5	239	231	7
6	-5	-5	80	77	16
7	-5	-5	163	148	11
8	-5	-5	53	63	47
9	-5	-5	50	18	50
10	-5	-5	56	56	56
-8	-4	-5	59	23	58
-7	-4	-5	89	58	28
-6	-4	-5	176	162	12
-5	-4	-5	163	172	10
-4	-4	-5	134	122	9
-3	-4	-5	85	72	9
-2	-4	-5	0	47	1
-1	-4	-5	117	118	5
0	-4	-5	234	238	6
1	-4	-5	247	252	5
2	-4	-5	566	566	5
3	-4	-5	181	187	7
4	-4	-5	0	36	1
5	-4	-5	63	45	15
6	-4	-5	407	409	7
7	-4	-5	116	132	11
8	-4	-5	168	158	12
9	-4	-5	74	65	30
10	-4	-5	0	64	1
-8	-3	-5	53	70	53
-7	-3	-5	0	23	1
-6	-3	-5	125	104	13
-5	-3	-5	144	154	11
-4	-3	-5	214	230	7
-3	-3	-5	306	310	13
-7	-5	-4	101	61	23
-6	-5	-4	52	52	51
-5	-5	-4	0	20	1
-4	-5	-4	246	243	7
-3	-5	-4	197	202	5
-2	-5	-4	238	246	4
-1	-5	-4	51	60	9
0	-5	-4	19	25	18
1	-5	-4	220	224	5
2	-5	-4	221	224	6
3	-5	-4	524	528	5
4	-5	-4	161	169	7
5	-5	-4	44	20	36
6	-5	-4	115	106	11
7	-5	-4	283	313	8
8	-5	-4	42	69	41
9	-5	-4	169	147	14
10	-5	-4	17	57	17

h	k	l	10Fo	10Fc	10s
-8	-2	-5	108	105	21
-7	-2	-5	81	82	25
-6	-2	-5	41	37	41
-5	-2	-5	72	54	19
-4	-2	-5	123	113	11
-3	-2	-5	360	348	6
-2	-2	-5	554	547	5
-1	-2	-5	295	307	4
0	-2	-5	0	25	1
2	-2	-5	314	333	3
3	-2	-5	328	346	6
4	-2	-5	266	287	7
5	-2	-5	98	100	6
6	-2	-5	113	107	11
7	-2	-5	0	19	1
8	-2	-5	75	70	20
9	-2	-5	0	33	1
10	-2	-5	52	53	52
11	-2	-5	65	44	65
-9	-1	-5	82	25	36
-8	-1	-5	160	151	16
-7	-1	-5	32	82	32
-6	-1	-5	61	64	26
-5	-1	-5	64	56	22
-4	-1	-5	90	100	12
-3	-1	-5	148	157	8
-2	-1	-5	629	614	3
-1	-1	-5	403	390	4
0	-1	-5	387	389	2
1	-1	-5	316	308	3
2	-1	-5	92	86	4
3	-1	-5	370	368	4
4	-1	-5	186	192	4
5	-1	-5	360	351	4
6	-1	-5	82	76	15
7	-1	-5	21	7	20
8	-1	-5	23	31	22
9	-1	-5	179	177	13
10	-1	-5	107	61	20
-9	0	-5	78	23	41
-8	0	-5	0	19	1
-7	0	-5	218	238	10
-6	0	-5	77	54	19
-5	0	-5	121	115	11
-4	0	-5	177	176	8
-3	0	-5	347	354	5
-2	0	-5	431	436	3
-1	0	-5	743	720	6
0	0	-5	473	491	5
1	0	-5	35	36	9
2	0	-5	269	248	3
3	0	-5	78	75	9
4	0	-5	233	236	3
5	0	-5	309	311	3
6	0	-5	223	210	6
7	0	-5	130	114	16
8	0	-5	60	17	32
9	0	-5	0	49	1
-9	1	-5	0	19	1
-8	1	-5	96	80	24
-7	1	-5	21	35	21
-6	1	-5	288	294	8
-5	1	-5	94	88	13
-4	1	-5	314	313	6
-3	1	-5	21	23	21
-2	1	-5	244	240	3
-1	1	-5	25	29	24
0	1	-5	624	633	3
1	1	-5	58	63	5
2	1	-5	277	268	9
3	1	-5	299	279	3
4	1	-5	253	251	5
-2	-1	-4	138	149	4
-1	-1	-4	149	151	4
0	-1	-4	674	629	9
1	-1	-4	149	157	3
2	-1	-4	299	314	3
3	-1	-4	200	190	12
4	-1	-4	163	153	4
5	-1	-4	233	239	10
6	-1	-4	146	147	8
7	-1	-4	198	187	7
8	-1	-4	128	118	12
9	-1	-4	0	9	1
10	-1	-4	25	39	25
11	-1	-4	58	74	57
-9	0	-4	94	90	32
-8	0	-4	92	53	21
-7	0	-4	53	29	53
-6	0	-4	0	25	1

h	k	l	10Fo	10Fc	10s
3	2	-5	518	530	3
4	2	-5	177	190	7
5	2	-5	204	208	6
6	2	-5	205	207	12
7	2	-5	203	195	9
-9	3	-5	0	54	1
-8	3	-5	125	129	16
-7	3	-5	0	34	1
-6	3	-5	48	82	36
-5	3	-5	37	34	37
-4	3	-5	463	478	6
-3	3	-5	131	118	10
-2	3	-5	404	407	12
-1	3	-5	199	192	4
0	3	-5	295	311	5
1	3	-5	135	122	7
2	3	-5	518	549	5
3	3	-5	44	58	23
4	3	-5	205	202	6
5	3	-5	53	32	17
6	3	-5	82	87	13
7	3	-5	162	157	10
-9	4	-5	105	90	20
-8	4	-5	37	54	36
-7	4	-5	188	182	11
-6	4	-5	38	44	38
-5	4	-5	81	93	12
-4	4	-5	29	38	29
-3	4	-5	478	501	3
-2	4	-5	107	103	6
-1	4	-5	258	285	8
0	4	-5	24	35	23
1	4	-5	485	470	5
2	4	-5	177	176	6
3	4	-5	444	466	5
4	4	-5	107	93	9
5	4	-5	114	118	10
6	4	-5	61	48	20
7	4	-5	73	62	22
-9	5	-5	0	48	1
-8	5	-5	144	144	15
-7	5	-5	117	76	13
-6	5	-5	96	73	15
-5	5	-5	89	84	15
-4	5	-5	149	164	9
-3	5	-5	163	170	5
-2	5	-5	559	547	9
-1	5	-5	216	218	6
0	5	-5	330	329	5
1	5	-5	47	29	18
2	5	-5	216	227	6
3	5	-5	67	70	13
4	5	-5	221	232	7
5	5	-5	99	88	11
6	5	-5	66	68	21
-9	6	-5	58	49	58
-8	6	-5	75	97	26
-7	6	-5	166	155	11
-6	6	-5	168	177	10
-5	6	-5	19	47	19
-4	6	-5	157	159	7
-3	6	-5	188	191	7
-2	6	-5	152	147	6
-1	6	-5	318	343	6
0	6	-5	139	141	8
1	6	-5	222	236	6
2	6	-5	101	98	9
3	6	-5	134	143	9
4	6	-5	0	10	1
5	6	-5	324	308	7
6	6	-5	27	17	26
-9	7	-5	60	43	59
-10	4	-4	58	79	57
-9	4	-4	30	51	29
-8	4	-4	52	65	51
-7	4	-4	163	153	10
-6	4	-4	179	186	8
-5	4	-4	153	166	9
-4	4	-4	35	32	34
-3	4	-4	136	126	5
-2	4	-4	248	247	10
-1	4	-4	528	517	4
0	4	-4	283	314	5
1	4	-4	560	591	4
2	4	-4	112	115	7
3	4	-4	202	207	3
4	4	-4	0	37	1
5	4	-4	326	311	6
6	4	-4	60	30	17
-9	5	-4	70	75	32

h	k	l	10Fo	10Fc	10s
-8	8	-5	0	30	1
-7	8	-5	0	21	1
-6	8	-5	184	174	11
-5	8	-5	91	104	17
-4	8	-5	123	119	8
-3	8	-5	135	131	11
-2	8	-5	82	61	15
-1	8	-5	130	132	11
0	8	-5	14	15	14
1	8	-5	257	257	8
2	8	-5	170	161	10
3	8	-5	133	137	9
4	8	-5	121	129	14
5	8	-5	164	161	12
6	8	-5	0	21	1
-7	9	-5	0	30	1
-6	9	-5	0	24	1
-5	9	-5	120	120	13
-4	9	-5	141	132	12
-3	9	-5	175	171	9
-2	9	-5	170	186	10
-1	9	-5	55	15	28
0	9	-5	127	101	14
1	9	-5	82	78	18
2	9	-5	167	144	11
3	9	-5	142	115	11
4	9	-5	134	115	13
5	9	-5	54	26	53
6	9	-5	64	43	50
-4	10	-5	140	123	13
-3	10	-5	90	101	18
-2	10	-5	180	191	10
-1	10	-5	86	81	21
0	10	-5	112	77	17
1	10	-5	191	186	12
2	10	-5	173	156	12
3	10	-5	142	138	12
4	10	-5	136	96	14
5	10	-5	46	20	46
6	10	-5	81	40	36
-4	11	-5	85	66	28
-3	11	-5	171	165	11
-2	11	-5	136	114	14
-1	11	-5	204	196	11
0	11	-5	62	82	43
1	11	-5	68	71	31
2	11	-5	68	73	37
3	11	-5	107	84	17
4	11	-5	105	100	22
5	11	-5	36	37	35
-4	12	-5	21	45	21
-3	12	-5	82	18	32
-2	12	-5	85	85	28
-1	12	-5	0	27	1
0	12	-5	77	76	29
1	12	-5	46	39	46
2	12	-5	34	27	33
3	12	-5	95	19	22
-3	13	-5	0	8	1
-2	13	-5	0	32	1
-1	13	-5	133	71	21
0	13	-5	0	33	1
2	-13	-4	70	36	27
3	-13	-4	41	28	41
-1	-12	-4	89	42	23
0	-12	-4	92	56	19
1	-12	-4	0	50	1
2	-12	-4	125	122	14
3	-12	-4	74	61	23
4	-12	-4	66	49	29
5	-12	-4	70	46	32
6	-12	-4	88	39	24
1	9	-4	38	57	38
2	9	-4	130	120	12
3	9	-4	109	90	14
4	9	-4	172	146	10
5	9	-4	161	128	12
6	9	-4	0	31	1
-4	10	-4	75	62	29
-3	10	-4	75	30	25
-2	10	-4	195	191	12
-1	10	-4	109	114	14
0	10	-4	232	236	8
1	10	-4	122	95	14
2	10	-4	45	54	45
3	10	-4	67	33	31
4	10	-4	107	102	15
5	10	-4	50	69	49
-4	11	-4	58	31	58
-3	11	-4	61	57	50

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
3	-10	-4	43	7	42
4	-10	-4	224	233	7
5	-10	-4	35	42	34
6	-10	-4	32	45	31
7	-10	-4	71	43	28
8	-10	-4	75	69	35
-4	-9	-4	0	44	1
-3	-9	-4	103	103	17
-2	-9	-4	51	49	51
-1	-9	-4	188	192	8
0	-9	-4	93	95	13
1	-9	-4	149	150	10
2	-9	-4	34	16	33
3	-9	-4	147	155	10
4	-9	-4	74	85	15
5	-9	-4	210	236	8
6	-9	-4	60	25	27
7	-9	-4	34	56	33
8	-9	-4	93	58	24
9	-9	-4	20	69	20
-4	-8	-4	54	53	53
-3	-8	-4	60	78	26
-2	-8	-4	106	109	14
-1	-8	-4	74	71	15
0	-8	-4	192	196	8
1	-8	-4	94	93	11
2	-8	-4	0	32	1
3	-8	-4	6	9	6
4	-8	-4	141	140	8
5	-8	-4	25	28	25
6	-8	-4	180	156	11
7	-8	-4	29	21	28
8	-8	-4	70	45	38
9	-8	-4	78	55	41
-4	-7	-4	102	100	15
-3	-7	-4	120	113	12
-2	-7	-4	105	109	13
-1	-7	-4	207	203	7
0	-7	-4	95	93	10
1	-7	-4	231	235	6
2	-7	-4	29	30	29
3	-7	-4	38	24	33
4	-7	-4	72	67	12
5	-7	-4	70	91	15
6	-7	-4	62	71	22
7	-7	-4	208	210	11
8	-7	-4	0	35	1
9	-7	-4	0	85	1
10	-7	-4	0	12	1
-8	-6	-4	59	30	59
-7	-6	-4	34	49	33
-6	-6	-4	69	61	37
-5	-6	-4	150	143	13
-4	-6	-4	195	193	6
-3	-6	-4	53	55	17
-2	-6	-4	186	190	6
-1	-6	-4	26	32	25
0	-6	-4	182	195	7
1	-6	-4	201	203	6
2	-6	-4	437	445	6
3	-6	-4	131	144	7
4	-6	-4	206	196	7
5	-6	-4	141	131	9
6	-6	-4	91	91	15
7	-6	-4	71	68	22
8	-6	-4	146	123	13
9	-6	-4	99	64	22
10	-6	-4	30	25	30
-8	-5	-4	115	88	22
-3	-8	-3	78	87	16
-2	-8	-3	112	103	12
-1	-8	-3	98	101	11
0	-8	-3	98	96	10
1	-8	-3	190	203	7
2	-8	-3	193	193	7
3	-8	-3	209	222	7
4	-8	-3	103	83	10
5	-8	-3	45	45	37
6	-8	-3	77	47	18
7	-8	-3	22	61	21
8	-8	-3	136	133	14
9	-8	-3	48	20	47
-7	-7	-3	18	43	17
-6	-7	-3	79	64	29
-5	-7	-3	0	33	1
-4	-7	-3	179	168	6
-3	-7	-3	187	197	6
-2	-7	-3	96	102	11
-1	-7	-3	171	177	8
0	-7	-3	133	139	8
-8	-4	-4	74	64	35
-7	-4	-4	182	159	12
-6	-4	-4	0	51	1
-5	-4	-4	83	88	17
-4	-4	-4	0	36	1
-3	-4	-4	382	381	4
-2	-4	-4	347	348	4
-1	-4	-4	393	391	3
0	-4	-4	38	17	24
1	-4	-4	107	106	7
2	-4	-4	494	493	5
3	-4	-4	464	465	5
4	-4	-4	466	464	5
5	-4	-4	203	207	7
6	-4	-4	84	79	13
7	-4	-4	0	10	1
8	-4	-4	123	120	12
9	-4	-4	40	15	39
10	-4	-4	84	82	27
11	-4	-4	78	71	43
-9	-3	-4	0	25	1
-8	-3	-4	146	138	15
-7	-3	-4	170	168	13
-6	-3	-4	188	193	10
-5	-3	-4	91	100	15
-4	-3	-4	64	77	18
-3	-3	-4	55	58	12
-2	-3	-4	475	468	9
-1	-3	-4	239	247	3
0	-3	-4	559	537	2
1	-3	-4	0	6	1
2	-3	-4	18	31	17
3	-3	-4	209	228	5
4	-3	-4	431	429	5
5	-3	-4	152	158	8
6	-3	-4	199	201	7
7	-3	-4	50	60	29
8	-3	-4	40	15	39
9	-3	-4	111	123	15
10	-3	-4	49	46	48
11	-3	-4	82	66	39
-9	-2	-4	62	70	62
-8	-2	-4	96	58	22
-7	-2	-4	234	235	10
-6	-2	-4	46	46	45
-5	-2	-4	151	135	9
-4	-2	-4	144	130	8
-3	-2	-4	125	103	8
-2	-2	-4	48	48	9
-1	-2	-4	467	473	3
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2	-2	-4	99	113	6
3	-2	-4	160	169	6
4	-2	-4	83	82	12
5	-2	-4	399	412	5
6	-2	-4	211	206	7
7	-2	-4	203	210	9
8	-2	-4	131	133	12
9	-2	-4	29	45	28
10	-2	-4	88	109	28
11	-2	-4	0	31	1
-9	-1	-4	0	44	1
-8	-1	-4	62	10	44
-7	-1	-4	0	11	1
-6	-1	-4	271	281	7
-5	-1	-4	76	48	14
-4	-1	-4	489	480	6
-3	-1	-4	0	36	1
10	-4	-3	110	102	17
11	-4	-3	0	48	1
-9	-3	-3	0	9	1
-8	-3	-3	40	68	40
-7	-3	-3	0	14	1
-6	-3	-3	217	237	9
-5	-3	-3	172	152	9
-4	-3	-3	455	451	6
-3	-3	-3	66	54	8
-2	-3	-3	47	42	10
-1	-3	-3	16	22	15
0	-3	-3	425	422	2
1	-3	-3	75	59	7
2	-3	-3	796	783	4
3	-3	-3	54	66	10
4	-3	-3	28	52	28
5	-3	-3	107	107	8
6	-3	-3	250	248	7
7	-3	-3	113	105	12
8	-3	-3	164	154	11
9	-3	-3	61	69	43
-5	0	-4	193	213	8
-4	0	-4	36	10	36
-3	0	-4	519	536	5
-2	0	-4	29	14	16
-1	0	-4	121	134	3
0	0	-4	136	132	3
1	0	-4	661	650	8
2	0	-4	189	194	3
3	0	-4	390	369	5
4	0	-4	58	59	7
5	0	-4	251	239	4
6	0	-4	241	228	4
7	0	-4	211	204	12
8	0	-4	65	75	26
9	0	-4	158	158	13
10	0	-4	7	52	7
-9	1	-4	24	94	24
-8	1	-4	101	98	17
-7	1	-4	0	11	1
-6	1	-4	105	106	12
-5	1	-4	52	23	22
-4	1	-4	588	575	6
-3	1	-4	196	196	4
-2	1	-4	488	472	3
-1	1	-4	0	28	1
0	1	-4	98	81	3
1	1	-4	75	65	3
2	1	-4	472	468	3
3	1	-4	126	112	5
4	1	-4	565	562	3
5	1	-4	85	89	7
6	1	-4	78	75	9
7	1	-4	160	165	9
8	1	-4	246	247	8
-10	2	-4	84	38	33
-9	2	-4	129	118	17
-8	2	-4	174	150	13
-7	2	-4	280	287	8
-6	2	-4	93	100	14
-5	2	-4	61	37	15
-4	2	-4	106	99	10
-3	2	-4	449	477	7
-2	2	-4	53	50	24
-1	2	-4	295	277	3
0	2	-4	16	30	16
1	2	-4	220	228	4
2	2	-4	155	146	6
3	2	-4	526	523	2
4	2	-4	53	48	12
5	2	-4	359	349	3
6	2	-4	28	25	28
7	2	-4	59	52	21
-10	3	-4	43	14	42
-9	3	-4	31	52	31
-8	3	-4	90	96	19
-7	3	-4	87	85	17
-6	3	-4	242	236	8
-5	3	-4	19	27	19
-4	3	-4	42	44	22
-3	3	-4	404	411	3
-2	3	-4	416	415	6
-1	3	-4	117	110	4
0	3	-4	570	582	4
1	3	-4	72	80	7
2	3	-4	121	122	6
3	3	-4	101	99	5
4	3	-4	356	367	3
5	3	-4	0	31	1
6	3	-4	160	147	9
-8	1	-3	111	113	17
-7	1	-3	99	101	14
-6	1	-3	258	263	8
-5	1	-3	152	180	9
-4	1	-3	33	64	32
-3	1	-3	83	82	8
-2	1	-3	494	492	2
-1	1	-3	131	140	3
0	1	-3	1046	1006	4
1	1	-3	161	172	2
2	1	-3	198	196	3
3	1	-3	130	140	4
4	1	-3	548	547	3
5	1	-3	163	161	5
6	1	-3	357	353	4
7	1	-3	118	105	11
8	1	-3	96	93	13
9	1	-3	0	61	1
-10	2	-3	0	61	1
-9	2	-3	25	13	24
-8	2	-3	111	130	16
-8	5	-4	58	22	37
-7	5	-4	41	73	40
-6	5	-4	173	148	10
-5	5	-4	190	207	7
-4	5	-4	282	291	9
-3	5	-4	31	23	31
-2	5	-4	71	75	6
-1	5	-4	360	332	5
0	5	-4	552	581	5
1	5	-4	443	439	5
2	5	-4	424	440	5
3	5	-4	31	28	30
4	5	-4	40	38	28
5	5	-4	30	34	30
6	5	-4	186	172	9
-9	6	-4	69	43	39
-8	6	-4	95	71	19
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-6	6	-4	66	64	25
-5	6	-4	69	76	20
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-3	6	-4	228	234	4
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1	6	-4	266	296	6
2	6	-4	276	290	6
3	6	-4	135	136	8
4	6	-4	59	73	18
5	6	-4	230	249	7
6	6	-4	77	79	21
-9	7	-4	75	82	37
-8	7	-4	92	83	23
-7	7	-4	60	38	43
-6	7	-4	107	123	13
-5	7	-4	63	36	24
-4	7	-4	174	183	6
-3	7	-4	240	235	5
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-1	7	-4	6	28	6
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1	7	-4	181	177	8
2	7	-4	168	166	8
3	7	-4	264	276	7
4	7	-4	250	252	7
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6	7	-4	92	117	16
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3	8	-4	0	40	1
4	8	-4	195	185	8
5	8	-4	114	89	14
6	8	-4	83	35	19
-6	9	-4	0	59	1
-5	9	-4	106	116	14
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-3	9	-4	179	167	11
-2	9	-4	56	89	32
-1	9	-4	177	179	9
0	9	-4	126	119	11
5	5	-3	71	59	13
6	5	-3	126	103	10
-9	6	-3	0	18	1
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-7	6	-3	62	67	25
-6	6	-3	40	47	40
-5	6	-3	177	164	8
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1	6	-3	129	131	8
2	6	-3	179	181	7
3	6	-3	229	225	7
4	6	-3	201	207	7
5	6	-3	273	253	7
6	6	-3	99	92	12
-9	7	-3	39	49	38
-8	7	-3	66	35	36
-7	7	-3	189	201	10
-2	11	-4	0	16	1
-1	11	-4	196	174	12
0	11	-4	36	30	36
1	11	-4	225	210	10
2	11	-4	0	25	1
3	11	-4	0	43	1
4	11	-4	12	21	12
5	11	-4	89	94	30
-4	12	-4	117	110	20
-3	12	-4	54	52	54
-2	12	-4	63	61	51
-1	12	-4	0	32	1
0	12	-4	126	113	14
1	12	-4	0	31	1
2	12	-4	102	105	21
3	12	-4	0	24	1
-4	13	-4	73	26	48
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-2	13	-4	0	13	1
-1	13	-4	59	28	59
0	13	-4	0	33	1
1	13	-4	93	67	30
2	-13	-3	0	21	1
3	-13	-3	102	79	18
4	-13	-3	38	16	37
0	-12	-3	86	80	21
1	-12	-3	0	13	1
2	-12	-3	51	38	50
3	-12	-3	32	20	32
4	-12	-3	76	54	25
5	-12	-3	0	52	1
6	-12	-3	105	65	18
-2	-11	-3	45	41	44
-1	-11	-3	143	139	11
0	-11	-3	16	57	16
1	-11	-3	151	146	9
2	-11	-3	22	22	21
3	-11	-3	22	66	21
4	-11	-3	40	33	40
5	-11	-3	150	143	11
6	-11	-3	0	27	1
7	-11	-3	100	61	19
-3	-10	-3	48	52	48
-2	-10	-3	80	58	23
-1	-10	-3	82	61	16
0	-10	-3	231	235	7
1	-10	-3	80	91	16
2	-10	-3	204	201	7
3	-10	-3	0	9	1
4	-10	-3	114	105	13
5	-10	-3	39	54	39
6	-10	-3	197	205	10
7	-10	-3	73	48	27
8	-10	-3	0	43	1
-4	-9	-3	202	197	11
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3	-9	-3	107	94	9
4	-9	-3	82	77	14
5	-9	-3	145	126	11
6	-9	-3	0	28	1
7	-9	-3	147	134	13
8	-9	-3	0	35	1
9	-9	-3	25	32	24
-4	-8	-3	136	138	12
-4	13	-3	66	18	65
-3	13	-3	0	49	1
-2	13	-3	0	27	1
-1	13	-3	93	93	26
0	13	-3	38	37	38
1	13	-3	76	59	28
4	-13	-2	57	14	56
1	-12	-2	67	82	24
2	-12	-2	94	83	16
3	-12	-2	0	54	1
4	-12	-2	20	39	20
5	-12	-2	61	32	42
6	-12	-2	85	92	27
-1	-11	-2	0	17	1
0	-11	-2	67	50	23
1	-11	-2	229	232	8
2	-11	-2	97	83	13
3	-11	-2	123	118	12
4	-11	-2	70	53	20
5	-11	-2	0	46	1
6	-11	-2	69	64	33

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
1	-7	-3	46	36	17
2	-7	-3	174	188	6
3	-7	-3	221	220	6
4	-7	-3	163	170	9
5	-7	-3	147	154	10
6	-7	-3	0	22	1
7	-7	-3	32	58	31
8	-7	-3	77	76	24
9	-7	-3	144	126	14
10	-7	-3	81	35	38
-8	-6	-3	34	16	34
-7	-6	-3	132	120	17
-6	-6	-3	13	22	12
-5	-6	-3	112	93	14
-4	-6	-3	107	108	7
-3	-6	-3	285	288	5
-2	-6	-3	246	245	5
-1	-6	-3	331	331	4
0	-6	-3	95	96	8
1	-6	-3	142	164	7
2	-6	-3	104	107	8
3	-6	-3	208	215	6
4	-6	-3	290	290	6
5	-6	-3	153	156	9
6	-6	-3	123	105	10
7	-6	-3	109	97	13
8	-6	-3	115	101	17
9	-6	-3	49	31	48
10	-6	-3	75	79	37
-8	-5	-3	71	100	44
-7	-5	-3	0	42	1
-6	-5	-3	256	261	9
-5	-5	-3	75	75	19
-4	-5	-3	137	144	7
-3	-5	-3	102	106	7
-2	-5	-3	467	477	8
-1	-5	-3	357	355	3
0	-5	-3	656	646	3
1	-5	-3	183	191	6
2	-5	-3	169	172	7
4	-5	-3	99	108	10
5	-5	-3	225	230	6
6	-5	-3	193	193	9
7	-5	-3	0	64	1
8	-5	-3	58	42	28
9	-5	-3	112	113	15
10	-5	-3	61	35	61
-9	-4	-3	76	64	43
-8	-4	-3	29	23	29
-7	-4	-3	146	144	15
-6	-4	-3	51	51	51
-5	-4	-3	263	260	8
-4	-4	-3	54	39	21
-3	-4	-3	186	186	5
-2	-4	-3	257	250	4
-1	-4	-3	218	224	3
0	-4	-3	166	172	5
1	-4	-3	464	458	5
2	-4	-3	337	339	4
3	-4	-3	74	92	9
4	-4	-3	106	106	8
5	-4	-3	365	372	6
6	-4	-3	87	99	11
7	-4	-3	322	304	7
8	-4	-3	0	25	1
9	-4	-3	0	7	1
-4	-6	-2	96	85	14
-3	-6	-2	168	165	12
-2	-6	-2	217	222	5
-1	-6	-2	263	265	4
0	-6	-2	170	185	4
1	-6	-2	613	618	7
2	-6	-2	217	231	6
3	-6	-2	334	325	6
4	-6	-2	139	133	9
5	-6	-2	97	89	11
6	-6	-2	139	119	12
7	-6	-2	260	257	8
8	-6	-2	75	78	21
9	-6	-2	65	69	34
10	-6	-2	75	41	40
-9	-5	-2	123	21	24
-8	-5	-2	74	92	41
-7	-5	-2	0	38	1
-6	-5	-2	52	69	43
-5	-5	-2	82	91	19
-4	-5	-2	306	287	7
-3	-5	-2	26	24	25
-2	-5	-2	170	179	5
-1	-5	-2	161	150	5
10	-3	-3	0	18	1
11	-3	-3	70	70	63
-9	-2	-3	161	147	16
-8	-2	-3	0	60	1
-7	-2	-3	73	68	24
-6	-2	-3	30	32	30
-5	-2	-3	174	173	9
-4	-2	-3	180	177	7
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0	-2	-3	52	47	5
1	-2	-3	601	586	4
2	-2	-3	216	224	4
3	-2	-3	450	488	4
4	-2	-3	212	220	5
5	-2	-3	101	93	9
6	-2	-3	65	73	16
7	-2	-3	49	76	29
8	-2	-3	115	92	13
9	-2	-3	130	129	13
10	-2	-3	0	11	1
11	-2	-3	0	28	1
-9	-1	-3	80	40	34
-8	-1	-3	129	112	15
-7	-1	-3	33	38	32
-6	-1	-3	44	52	43
-5	-1	-3	131	124	10
-4	-1	-3	300	315	6
-3	-1	-3	317	289	5
-2	-1	-3	648	635	3
-1	-1	-3	222	212	3
0	-1	-3	319	282	5
1	-1	-3	177	172	2
2	-1	-3	510	492	3
3	-1	-3	180	189	3
4	-1	-3	500	481	3
5	-1	-3	34	42	14
6	-1	-3	118	105	7
7	-1	-3	162	170	10
8	-1	-3	146	113	12
9	-1	-3	74	59	27
10	-1	-3	98	99	22
11	-1	-3	40	26	39
-10	0	-3	73	4	56
-9	0	-3	155	122	15
-8	0	-3	218	217	10
-7	0	-3	140	133	11
-6	0	-3	172	156	10
-5	0	-3	25	6	24
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1	0	-3	39	47	6
2	0	-3	152	161	3
3	0	-3	604	604	7
4	0	-3	179	185	6
5	0	-3	699	684	3
6	0	-3	76	75	7
7	0	-3	60	71	18
8	0	-3	41	62	40
9	0	-3	216	235	10
10	0	-3	79	27	32
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3	-2	-2	334	340	4
4	-2	-2	180	187	6
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6	-2	-2	153	130	9
7	-2	-2	164	164	9
8	-2	-2	0	34	1
9	-2	-2	111	112	17
10	-2	-2	0	27	1
11	-2	-2	90	89	29
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-2	2	-3	217	216	3
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1	2	-3	488	495	4
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3	2	-3	238	236	3
4	2	-3	96	106	4
5	2	-3	460	459	3
6	2	-3	141	143	5
7	2	-3	161	175	10
8	2	-3	75	75	20
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5	8	-3	149	133	11
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-2	9	-3	66	37	22
-1	9	-3	114	108	11
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1	9	-3	237	242	8
2	9	-3	0	17	1
3	9	-3	173	144	11
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2	8	-2	191	183	9
3	8	-2	26	36	25
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-2	-9	-2	204	193	9
-1	-9	-2	60	43	21
0	-9	-2	249	250	7
1	-9	-2	25	36	24
2	-9	-2	132	138	10
3	-9	-2	157	153	8
4	-9	-2	225	240	8
5	-9	-2	130	129	11
6	-9	-2	72	73	23
7	-9	-2	50	71	50
8	-9	-2	45	7	45
9	-9	-2	125	96	21
-7	-8	-2	135	122	19
-6	-8	-2	70	17	33
-5	-8	-2	159	154	13
-4	-8	-2	57	66	26
-3	-8	-2	99	93	11
-2	-8	-2	0	33	1
-1	-8	-2	174	181	8
0	-8	-2	137	128	8
1	-8	-2	92	90	9
2	-8	-2	93	80	10
3	-8	-2	69	73	12
4	-8	-2	140	147	10
5	-8	-2	169	165	9
6	-8	-2	164	153	11
7	-8	-2	63	15	32
8	-8	-2	0	25	1
9	-8	-2	0	48	1
-8	-7	-2	0	48	1
-7	-7	-2	73	25	40
-6	-7	-2	139	147	14
-5	-7	-2	19	24	18
-4	-7	-2	0	29	1
-3	-7	-2	209	215	5
-2	-7	-2	241	236	5
-1	-7	-2	33	45	33
0	-7	-2	519	492	6
1	-7	-2	53	45	16
2	-7	-2	76	94	10
3	-7	-2	123	119	8
4	-7	-2	103	96	11
5	-7	-2	122	119	11
6	-7	-2	177	176	9
7	-7	-2	85	108	19
8	-7	-2	69	91	32
9	-7	-2	100	52	25
10	-7	-2	0	25	1
-8	-6	-2	85	35	33
-7	-6	-2	82	85	28
-6	-6	-2	31	22	31
-5	-6	-2	231	239	9
-2	-9	-1	33	55	33
-1	-9	-1	113	101	11
0	-9	-1	261	259	6
1	-9	-1	68	98	13
2	-9	-1	71	75	14
3	-9	-1	28	54	28
4	-9	-1	40	40	40
5	-9	-1	73	81	20
6	-9	-1	187	189	11
7	-9	-1	56	16	56
8	-9	-1	24	68	24
9	-9	-1	75	70	44
-7	-8	-1	47	41	47
-6	-8	-1	58	31	57
-5	-8	-1	213	210	11
-4	-8	-1	49	47	19
-3	-8	-1	128	112	11
-2	-8	-1	4	8	3
-1	-8	-1	26	18	26
0	-8	-1	61	78	16
1	-8	-1	328	338	6
2	-8	-1	27	30	27
3	-8	-1	196	193	7
4	-8	-1	137	129	9

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
0	-5	-2	314	311	3
1	-5	-2	145	164	4
2	-5	-2	702	720	5
3	-5	-2	35	36	23
4	-5	-2	233	240	6
5	-5	-2	143	135	9
6	-5	-2	182	184	8
7	-5	-2	85	112	14
8	-5	-2	226	230	10
9	-5	-2	0	7	1
10	-5	-2	72	21	33
-9	-4	-2	96	96	29
-8	-4	-2	30	96	29
-7	-4	-2	137	116	15
-6	-4	-2	130	107	11
-5	-4	-2	105	110	11
-4	-4	-2	236	237	7
-3	-4	-2	702	705	8
-2	-4	-2	475	473	3
-1	-4	-2	54	58	7
0	-4	-2	154	167	5
1	-4	-2	468	465	4
2	-4	-2	221	220	5
3	-4	-2	666	658	5
4	-4	-2	61	51	13
5	-4	-2	57	30	14
6	-4	-2	158	136	10
7	-4	-2	235	228	8
8	-4	-2	93	105	20
9	-4	-2	155	162	13
10	-4	-2	0	30	1
11	-4	-2	17	53	16
-9	-3	-2	67	34	67
-8	-3	-2	188	184	13
-7	-3	-2	95	115	18
-6	-3	-2	139	139	11
-5	-3	-2	0	25	1
-4	-3	-2	129	135	8
-3	-3	-2	74	100	6
-2	-3	-2	634	624	3
-1	-3	-2	377	374	2
0	-3	-2	326	328	4
1	-3	-2	280	273	4
2	-3	-2	429	425	4
3	-3	-2	281	259	5
4	-3	-2	433	442	5
5	-3	-2	172	161	7
6	-3	-2	105	121	11
7	-3	-2	78	69	14
8	-3	-2	59	76	25
9	-3	-2	40	25	40
10	-3	-2	75	92	28
11	-3	-2	0	25	1
-9	-2	-2	82	29	31
-8	-2	-2	200	183	12
-7	-2	-2	160	157	12
-6	-2	-2	156	149	10
-5	-2	-2	179	189	8
-4	-2	-2	141	159	8
-3	-2	-2	109	113	7
-2	-2	-2	469	476	8
-1	-2	-2	41	36	5
0	-2	-2	31	47	30
-9	-4	-1	25	27	25
-8	-4	-1	79	99	31
-7	-4	-1	158	144	11
-6	-4	-1	176	172	11
-5	-4	-1	133	133	11
-4	-4	-1	152	152	8
-3	-4	-1	301	308	4
-2	-4	-1	47	32	8
-1	-4	-1	282	290	4
0	-4	-1	111	106	4
1	-4	-1	295	296	2
2	-4	-1	254	256	5
3	-4	-1	323	298	5
4	-4	-1	187	179	6
5	-4	-1	449	421	6
6	-4	-1	141	154	9
7	-4	-1	167	157	10
8	-4	-1	0	31	1
9	-4	-1	120	137	16
10	-4	-1	27	23	27
-9	-3	-1	40	74	39
-8	-3	-1	25	39	25
-7	-3	-1	171	173	10
-6	-3	-1	162	165	9
-5	-3	-1	310	303	7
-4	-3	-1	198	213	6
-3	-3	-1	171	177	6
3	-1	-2	186	165	3
4	-1	-2	366	347	3
5	-1	-2	53	45	8
6	-1	-2	361	372	6
7	-1	-2	28	21	28
8	-1	-2	94	74	14
9	-1	-2	41	43	40
10	-1	-2	60	108	51
11	-1	-2	0	21	1
-10	0	-2	76	32	43
-9	0	-2	89	40	29
-8	0	-2	40	46	40
-7	0	-2	0	39	1
-6	0	-2	153	150	9
-5	0	-2	285	301	6
-4	0	-2	518	551	5
-3	0	-2	211	207	5
-2	0	-2	202	208	4
-1	0	-2	630	628	6
0	0	-2	1155	1142	6
1	0	-2	1739	1658	12
2	0	-2	530	505	14
3	0	-2	94	83	5
4	0	-2	67	70	8
5	0	-2	511	499	3
6	0	-2	106	89	15
7	0	-2	259	267	7
8	0	-2	73	100	18
9	0	-2	5	27	5
10	0	-2	0	45	1
11	0	-2	105	44	22
-10	1	-2	15	39	15
-9	1	-2	182	156	13
-8	1	-2	58	35	29
-7	1	-2	36	45	35
-6	1	-2	193	191	8
-5	1	-2	287	287	6
-4	1	-2	470	461	5
-3	1	-2	351	355	4
-2	1	-2	260	246	2
-1	1	-2	267	279	5
0	1	-2	707	656	13
1	1	-2	1107	1048	4
2	1	-2	747	733	2
3	1	-2	459	457	3
4	1	-2	431	420	6
5	1	-2	63	58	7
6	1	-2	165	164	7
7	1	-2	148	157	9
8	1	-2	140	145	12
9	1	-2	88	103	20
10	1	-2	23	29	22
-10	2	-2	118	105	24
-9	2	-2	41	61	41
-8	2	-2	187	188	10
-7	2	-2	176	157	11
-6	2	-2	114	107	11
-5	2	-2	91	70	11
-3	2	-2	72	59	4
-2	2	-2	255	254	4
-1	2	-2	778	778	4
0	2	-2	117	107	5
1	2	-2	28	35	12
-7	0	-1	48	43	48
-6	0	-1	142	134	9
-5	0	-1	122	117	9
-4	0	-1	506	493	5
-3	0	-1	325	301	4
-2	0	-1	382	371	3
0	0	-1	355	333	1
1	0	-1	118	135	2
2	0	-1	727	674	3
3	0	-1	239	265	2
4	0	-1	617	594	7
5	0	-1	306	307	7
6	0	-1	81	110	12
7	0	-1	128	142	10
8	0	-1	98	110	14
9	0	-1	119	128	14
10	0	-1	114	132	18
11	0	-1	0	11	1
-10	1	-1	0	16	1
-9	1	-1	192	189	12
-8	1	-1	53	50	38
-7	1	-1	212	218	8
-6	1	-1	99	89	12
-5	1	-1	226	241	6
-4	1	-1	126	140	7
-3	1	-1	389	375	4
-2	1	-1	13	23	13
6	3	-2	148	137	8
7	3	-2	66	57	17
8	3	-2	86	86	16
-10	4	-2	64	41	40
-9	4	-2	67	54	32
-8	4	-2	156	160	11
-7	4	-2	71	87	16
-6	4	-2	239	257	7
-5	4	-2	214	203	7
-4	4	-2	222	209	4
-3	4	-2	533	469	3
-2	4	-2	604	585	4
-1	4	-2	53	43	7
0	4	-2	569	580	4
1	4	-2	366	349	4
2	4	-2	64	66	9
3	4	-2	245	252	3
4	4	-2	256	274	3
5	4	-2	49	54	18
6	4	-2	222	232	7
7	4	-2	35	38	35
-10	5	-2	68	64	39
-9	5	-2	0	35	1
-8	5	-2	54	53	38
-7	5	-2	215	226	7
-6	5	-2	265	277	7
-5	5	-2	269	273	4
-4	5	-2	68	64	8
-3	5	-2	0	16	1
-2	5	-2	181	173	4
-1	5	-2	701	664	5
0	5	-2	33	28	33
2	5	-2	90	88	8
3	5	-2	130	141	4
4	5	-2	259	268	8
5	5	-2	227	225	5
-10	6	-2	70	45	36
-9	6	-2	62	76	37
-8	6	-2	34	33	33
-7	6	-2	54	75	33
-6	6	-2	168	155	9
-5	6	-2	0	7	1
-4	6	-2	471	461	4
-3	6	-2	57	49	10
-2	6	-2	51	28	19
-1	6	-2	64	65	14
0	6	-2	532	537	6
1	6	-2	98	95	9
2	6	-2	440	447	5
3	6	-2	99	89	10
4	6	-2	184	182	8
5	6	-2	85	82	13
-8	7	-2	61	30	33
-7	7	-2	41	73	41
-6	7	-2	55	39	35
-5	7	-2	157	132	6
-4	7	-2	62	54	13
-3	7	-2	352	340	4
-2	7	-2	81	83	14
-1	7	-2	102	90	11
0	7	-2	164	146	8
1	7	-2	403	412	6
2	7	-2	59	75	16
-3	4	-1	35	37	12
-2	4	-1	209	198	3
-1	4	-1	176	180	5
0	4	-1	557	497	4
1	4	-1	212	209	5
2	4	-1	677	667	4
3	4	-1	270	273	4
4	4	-1	151	172	5
5	4	-1	59	62	9
6	4	-1	85	83	12
7	4	-1	40	36	40
8	4	-1	154	160	11
-10	5	-1	0	50	1
-9	5	-1	136	132	13
-8	5	-1	131	132	12
-7	5	-1	81	87	16
-6	5	-1	76	42	13
-5	5	-1	87	91	7
-4	5	-1	333	326	7
-3	5	-1	635	625	6
-2	5	-1	268	258	3
-1	5	-1	190	173	5
0	5	-1	99	100	8
1	5	-1	445	467	5
2	5	-1	42	41	16
3	5	-1	408	419	5
4	5	-1	14	4	13
4	9	-2	42	48	41
5	9	-2	109	109	16
-5	10	-2	48	55	47
-4	10	-2	114	98	16
-3	10	-2	226	228	10
-2	10	-2	216	199	9
-1	10	-2	188	199	10
0	10	-2	262	256	8
1	10	-2	104	99	14
2	10	-2	49	59	48
3	10	-2	59	31	25
4	10	-2	175	166	12
5	10	-2	107	69	19
-5	11	-2	60	63	59
-4	11	-2	0	39	1
-3	11	-2	56	23	56
-2	11	-2	47	72	46
-1	11	-2	134	132	13
0	11	-2	182	195	10
1	11	-2	109	113	18
2	11	-2	49	28	49
3	11	-2	34	31	33
4	11	-2	62	35	50
-5	12	-2	109	99	22
-4	12	-2	0	21	1
-3	12	-2	89	22	27
-2	12	-2	48	60	47
-1	12	-2	79	48	26
0	12	-2	118	119	16
1	12	-2	130	112	16
2	12	-2	103	79	18
3	12	-2	26	28	25
4	12	-2	103	46	28
-4	13	-2	122	79	21
-3	13	-2	152	108	16
-2	13	-2	24	40	24
-1	13	-2	79	8	30
0	13	-2	127	75	17
1	13	-2	86	45	25
2	13	-2	38	53	37
5	-13	-1	44	19	43
3	-12	-1	67	68	29
4	-12	-1	69	65	26
5	-12	-1	73	41	29
6	-12	-1	55	37	55
1	-11	-1	47	31	47
2	-11	-1	149	132	9
3	-11	-1	45	45	45
4	-11	-1	136	133	11
5	-11	-1	139	98	12
6	-11	-1	115	102	19
7	-11	-1	82	71	32
-1	-10	-1	227	211	7
0	-10	-1	136	120	9
1	-10	-1	167	189	8
2	-10	-1	0	9	1
3	-10	-1	0	12	1
4	-10	-1	180	177	8
5	-10	-1	186	191	11
6	-10	-1	164	140	11
7	-10	-1	91	96	24
8	-10	-1	72	40	47
-3	-9	-1	109	89	13
3	10	-1	92	88	17
4	10	-1	22	52	22
-5	11	-1	53	36	53
-4	11	-1	228	232	11
-3	11	-1	37	74	37
-2	11	-1	196	177	10
-1	11	-1	55	9	55
0	11	-1	0	30	1
1	11	-1	108	88	15
2	11	-1	136	120	14
3	11	-1	104	90	16
4	11	-1	117	91	17
-5	12	-1	81	48	35
-4	12	-1	0	29	1
-3	12	-1	53	72	53
-2	12	-1	104	104	18
-1	12	-1	100	111	19
0	12	-1	10	47	10
1	12	-1	78	73	25
2	12	-1	37	37	37
3	12	-1	118	99	16
-5	13	-1	14	13	13
-4	13	-1	0	57	1
-3	13	-1	113	79	22
-2	13	-1	152	123	16
-1	13	-1	0	35	1
0	13	-1	88	67	23
5	-8	-1	157	139	11
6	-8	-1	0	56	1
7	-8	-1	196	180	10
8	-8	-1	80	88	27
9	-8	-1	89	89	35
-8	-7	-1	103	81	25
-7	-7	-1	27	38	27
-6	-7	-1	62	43	45
-5	-7	-1	58	46	31
-4	-7	-1	172	167	13
-3	-7	-1	144	141	6
-2	-7	-1	259	272	4
-1	-7	-1	80	80	8
0	-7	-1	15	39	14
1	-7	-1	79	81	6
2	-7	-1	355	362	5
3	-7	-1	0	10	1
4	-7	-1	238	247	7
5	-7	-1	0	52	1
6	-7	-1	80	100	17
7	-7	-1	38	20	38
8	-7	-1	188	171	12
9	-7	-1	0	35	1
10	-7	-1	82	53	32
-8	-6	-1	60	58	60
-7	-6	-1	54	81	54
-6	-6	-1	51	69	50
-5	-6	-1	65	29	24
-4	-6	-1	243	255	8
-3	-6	-1	365	381	4
-2	-6	-1	258	261	4
-1	-6	-1	385	379	3
0	-6	-1	24	27	24
1	-6	-1	135	140	4
2	-6	-1	84	78	4
3	-6	-1	510	514	5
4	-6	-1	120	119	8
5	-6	-1	162	180	9
6	-6	-1	64	65	17
7	-6	-1	126	114	11
8	-6	-1	104	105	16
9	-6	-1	200	174	12
10	-6	-1	0	19	1
-9	-5	-1	82	45	41
-8	-5	-1	105	118	21
-7	-5	-1	166	170	11
-6	-5	-1	107	112	15
-5	-5	-1	153	146	9
-4	-5	-1	99	92	11
-3	-5	-1	37	36	20
-2	-5	-1	932	909	10
-1	-5	-1	480	485	3
0	-5	-1	559	575	8
1	-5	-1	51	60	7
2	-5	-1	194	200	5
3	-5	-1	49	63	15
4	-5	-1	421	422	6
5	-5	-1	96	82	10
6	-5	-1	209	201	7
7	-5	-1	98	108	13
8	-5	-1	82	98	19
9	-5	-1	0	53	1
10	-5	-1	98	74	23
-1	-7	0	349	359	17
0	-7	0	376	387	15
1	-7	0	42	33	12
2	-7	0	87	82	5
3	-7	0	24	35	23
4	-7	0	378	378	6
5	-7	0	166	147	9
6	-7	0	216	225	8
7	-7	0	20	31	20
8	-7	0	63	56	37
9	-7	0	62	45	59
10	-7	0	72	54	51
-8	-6	0	0	45	1
-7	-6	0	96	117	22
-6	-6	0	150	143	12
-5	-6	0	190	186	10
-4	-6	0	84	75	15
-3	-6	0	81	88	7
-2	-6	0	127	123	6
-1	-6	0	433	444	3
0	-6	0	602	614	12
1	-6	0	464	484	15
2	-6	0	297	293	3
3	-6	0	81	100	10
4	-6	0	153	164	8
5	-6	0	189	183	7
6	-6	0	102	85	12

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-2	-3	-1	295	278	7
-1	-3	-1	372	370	2
0	-3	-1	235	250	2
1	-3	-1	162	165	2
3	-3	-1	49	51	9
4	-3	-1	59	48	10
5	-3	-1	232	227	6
6	-3	-1	332	313	7
7	-3	-1	169	156	10
8	-3	-1	180	179	11
9	-3	-1	31	15	30
10	-3	-1	0	31	1
11	-3	-1	0	25	1
-10	-2	-1	83	48	48
-9	-2	-1	76	67	40
-8	-2	-1	111	125	17
-7	-2	-1	44	55	44
-6	-2	-1	203	209	8
-5	-2	-1	174	170	8
-4	-2	-1	632	615	5
-3	-2	-1	456	456	4
-2	-2	-1	149	145	3
-1	-2	-1	906	926	4
0	-2	-1	981	925	3
1	-2	-1	349	318	3
2	-2	-1	613	600	4
3	-2	-1	267	230	4
4	-2	-1	0	44	1
5	-2	-1	238	240	5
6	-2	-1	0	12	1
7	-2	-1	149	159	9
8	-2	-1	0	31	1
9	-2	-1	88	61	21
10	-2	-1	31	29	30
11	-2	-1	61	63	61
-10	-1	-1	0	15	1
-9	-1	-1	207	160	13
-8	-1	-1	133	108	13
-7	-1	-1	127	120	13
-6	-1	-1	22	34	21
-5	-1	-1	276	277	6
-4	-1	-1	179	202	6
-3	-1	-1	521	529	4
-2	-1	-1	216	224	4
-1	-1	-1	70	62	3
0	-1	-1	486	491	7
1	-1	-1	909	873	3
2	-1	-1	1085	1045	4
3	-1	-1	373	378	4
4	-1	-1	411	396	5
5	-1	-1	174	181	7
6	-1	-1	222	217	7
7	-1	-1	51	53	24
8	-1	-1	188	197	9
9	-1	-1	152	147	11
10	-1	-1	67	74	33
11	-1	-1	73	46	42
-10	0	-1	98	96	26
-9	0	-1	43	68	43
-8	0	-1	180	205	11
6	-3	0	117	107	10
7	-3	0	151	150	9
8	-3	0	106	98	14
9	-3	0	177	156	12
10	-3	0	40	51	39
-10	-2	0	78	57	43
-9	-2	0	0	59	1
-8	-2	0	298	278	9
-7	-2	0	70	46	18
-6	-2	0	220	223	8
-5	-2	0	148	122	8
-4	-2	0	328	324	5
-3	-2	0	43	53	15
-2	-2	0	192	184	5
-1	-2	0	708	690	3
0	-2	0	871	864	8
1	-2	0	403	400	3
2	-2	0	716	683	4
3	-2	0	217	214	4
4	-2	0	339	352	5
5	-2	0	200	199	6
6	-2	0	196	200	7
7	-2	0	63	87	20
8	-2	0	79	86	17
9	-2	0	49	110	48
10	-2	0	94	86	20
-10	-1	0	32	48	32
-9	-1	0	54	10	53
-8	-1	0	0	43	1
-7	-1	0	198	189	9
-1	1	-1	1684	1603	8
0	1	-1	86	107	3
1	1	-1	159	167	3
2	1	-1	27	21	20
3	1	-1	595	585	3
4	1	-1	371	345	3
5	1	-1	623	597	4
6	1	-1	99	108	10
7	1	-1	0	37	1
8	1	-1	195	203	9
9	1	-1	75	83	24
10	1	-1	95	92	23
-10	2	-1	0	31	1
-9	2	-1	39	9	38
-8	2	-1	156	134	11
-7	2	-1	58	61	22
-6	2	-1	414	412	6
-5	2	-1	66	63	13
-4	2	-1	244	240	2
-3	2	-1	268	251	2
-2	2	-1	287	256	12
-1	2	-1	548	543	7
0	2	-1	1018	951	4
1	2	-1	763	768	3
2	2	-1	48	56	5
3	2	-1	74	76	8
4	2	-1	353	355	7
5	2	-1	119	117	9
6	2	-1	213	237	7
7	2	-1	33	58	33
8	2	-1	95	98	15
9	2	-1	96	94	19
10	2	-1	31	46	30
-10	3	-1	100	46	22
-9	3	-1	82	94	24
-8	3	-1	66	61	24
-7	3	-1	108	97	11
-6	3	-1	103	101	11
-5	3	-1	390	397	20
-4	3	-1	129	118	6
-3	3	-1	181	162	3
-2	3	-1	354	338	7
-1	3	-1	247	254	2
0	3	-1	131	132	5
1	3	-1	75	59	6
2	3	-1	259	251	4
3	3	-1	146	161	6
4	3	-1	39	42	10
5	3	-1	403	409	3
6	3	-1	70	73	15
7	3	-1	301	317	7
8	3	-1	15	59	15
9	3	-1	0	44	1
-10	4	-1	138	73	16
-9	4	-1	62	81	32
-8	4	-1	83	73	16
-7	4	-1	0	34	1
-6	4	-1	372	394	6
-5	4	-1	326	334	11
-4	4	-1	800	782	7
-11	2	0	66	65	65
-10	2	0	114	86	20
-9	2	0	124	110	15
-8	2	0	102	86	13
-7	2	0	105	87	11
-6	2	0	198	200	7
-5	2	0	192	199	3
-4	2	0	334	352	2
-3	2	0	222	214	2
-2	2	0	747	683	2
-1	2	0	406	400	16
0	2	0	887	864	4
1	2	0	695	690	3
2	2	0	190	184	7
3	2	0	44	53	6
4	2	0	329	324	4
5	2	0	135	122	9
6	2	0	199	223	8
7	2	0	68	46	17
8	2	0	250	278	8
9	2	0	47	59	46
10	2	0	96	57	23
-11	3	0	0	65	1
-10	3	0	16	51	16
-9	3	0	164	156	12
-8	3	0	87	97	15
-7	3	0	155	150	9
-6	3	0	103	107	9
-5	3	0	224	232	3
-4	3	0	333	338	3
5	5	-1	98	83	8
6	5	-1	73	68	14
-9	6	-1	105	85	17
-8	6	-1	61	44	31
-7	6	-1	162	181	9
-6	6	-1	183	192	8
-5	6	-1	85	75	8
-4	6	-1	362	364	4
-3	6	-1	250	250	13
-2	6	-1	571	546	5
-1	6	-1	115	102	8
0	6	-1	61	75	13
1	6	-1	176	175	7
2	6	-1	614	621	5
3	6	-1	138	129	8
4	6	-1	420	432	13
5	6	-1	36	10	29
-7	7	-1	184	177	9
-6	7	-1	158	139	9
-5	7	-1	189	189	13
-4	7	-1	77	86	9
-3	7	-1	256	250	4
-2	7	-1	273	254	6
-1	7	-1	283	293	6
0	7	-1	116	115	10
1	7	-1	131	115	9
2	7	-1	63	62	17
3	7	-1	139	150	9
4	7	-1	111	85	10
5	7	-1	209	187	9
-5	8	-1	161	154	10
-4	8	-1	66	69	11
-3	8	-1	0	41	1
-2	8	-1	80	58	12
-1	8	-1	206	194	8
0	8	-1	206	210	8
1	8	-1	132	103	10
2	8	-1	53	50	21
3	8	-1	116	103	11
4	8	-1	178	170	9
5	8	-1	125	114	12
-5	9	-1	173	170	10
-4	9	-1	188	187	9
-3	9	-1	64	62	22
-2	9	-1	74	75	20
-1	9	-1	28	59	28
0	9	-1	204	199	9
1	9	-1	221	203	8
2	9	-1	68	48	18
3	9	-1	82	45	16
4	9	-1	55	59	34
5	9	-1	166	141	12
-5	10	-1	244	241	10
-4	10	-1	6	54	6
-3	10	-1	86	76	18
-2	10	-1	69	25	24
-1	10	-1	94	55	15
0	10	-1	117	91	14
1	10	-1	273	247	8
2	10	-1	66	74	24
-3	6	0	99	100	5
-2	6	0	311	293	5
-1	6	0	486	484	5
0	6	0	610	614	5
1	6	0	449	444	5
2	6	0	131	123	8
3	6	0	73	88	11
4	6	0	70	74	8
5	6	0	185	186	13
6	6	0	146	143	10
-5	7	0	163	147	7
-4	7	0	387	378	4
-3	7	0	25	35	25
-2	7	0	83	82	10
-1	7	0	25	33	24
0	7	0	403	387	6
1	7	0	365	359	6
2	7	0	302	302	6
3	7	0	173	176	7
4	7	0	69	69	31
-6	8	0	0	34	1
-5	8	0	123	121	11
-4	8	0	77	85	14
-3	8	0	192	190	8
-2	8	0	15	54	15
-1	8	0	82	85	12
0	8	0	87	86	12
1	8	0	238	226	7
2	8	0	128	129	11
3	8	0	0	46	1
1	13	-1	16	37	16
2	13	-1	0	40	1
4	-12	0	54	19	54
5	-12	0	97	100	20
6	-12	0	47	44	47
2	-11	0	177	148	9
3	-11	0	0	41	1
4	-11	0	91	91	15
5	-11	0	86	62	18
6	-11	0	109	82	18
7	-11	0	0	35	1
0	-10	0	34	35	33
1	-10	0	303	300	6
2	-10	0	56	58	23
3	-10	0	189	167	9
4	-10	0	0	17	1
5	-10	0	35	16	34
6	-10	0	75	47	24
7	-10	0	146	137	16
8	-10	0	37	28	37
-7	-9	0	37	48	37
-6	-9	0	109	27	20
-5	-9	0	46	39	46
-4	-9	0	192	185	11
-2	-9	0	217	194	8
-1	-9	0	159	143	8
0	-9	0	45	31	32
1	-9	0	17	6	16
2	-9	0	201	218	7
3	-9	0	44	63	32
4	-9	0	327	327	7
5	-9	0	38	33	38
6	-9	0	8	47	7
7	-9	0	48	23	48
8	-9	0	104	66	20
9	-9	0	81	28	36
-7	-8	0	138	92	16
-6	-8	0	12	77	12
-5	-8	0	62	75	33
-4	-8	0	168	157	10
-3	-8	0	55	45	19
-2	-8	0	135	129	6
-1	-8	0	211	226	15
0	-8	0	83	86	12
1	-8	0	79	85	11
2	-8	0	59	54	14
3	-8	0	175	190	8
4	-8	0	107	85	11
5	-8	0	153	121	10
6	-8	0	54	34	31
7	-8	0	106	97	18
8	-8	0	37	37	37
9	-8	0	162	135	15
-8	-7	0	42	26	42
-7	-7	0	131	118	17
-6	-7	0	97	85	18
-5	-7	0	91	92	17
-4	-7	0	64	69	21
-3	-7	0	173	176	5
-2	-7	0	285	302	4
4	-10	1	65	54	27
5	-10	1	231	241	9
6	-10	1	59	64	59
7	-10	1	66	71	56
8	-10	1	58	41	58
-7	-9	1	123	96	19
-6	-9	1	17	68	17
-5	-9	1	129	140	14
-4	-9	1	60	59	31
-3	-9	1	70	45	18
-2	-9	1	0	48	1
-1	-9	1	185	202	8
0	-9	1	207	199	8
1	-9	1	51	59	21
2	-9	1	64	75	18
3	-9	1	72	62	14
4	-9	1	201	187	8
5	-9	1	174	170	10
6	-9	1	164	150	10
7	-9	1	121	98	15
8	-9	1	24	22	23
9	-9	1	0	59	1
-7	-8	1	72	22	38
-6	-8	1	101	123	19
-5	-8	1	117	114	14
-4	-8	1	196	170	10
-3	-8	1	103	103	13
-2	-8	1	51	50	15
-1	-8	1	101	103	7
0	-8	1	198	210	16
7	-6	0	160	152	11
8	-6	0	0	62	1
9	-6	0	0	62	1
10	-6	0	0	17	1
-9	-5	0	57	68	57
-8	-5	0	53	20	53
-7	-5	0	117	118	17
-6	-5	0	110	87	13
-5	-5	0	275	285	8
-4	-5	0	64	64	17
-3	-5	0	458	472	6
-2	-5	0	363	389	5
-1	-5	0	125	137	5
0	-5	0	274	282	8
1	-5	0	537	529	6
2	-5	0	384	370	5
3	-5	0	282	286	5
4	-5	0	38	39	23
5	-5	0	97	101	10
6	-5	0	393	387	7
7	-5	0	134	126	10
8	-5	0	200	206	10
9	-5	0	88	60	23
10	-5	0	49	50	48
-9	-4	0	61	20	60
-8	-4	0	166	161	12
-7	-4	0	74	111	24
-6	-4	0	100	81	12
-5	-4	0	198	203	8
-4	-4	0	439	437	6
-3	-4	0	190	189	4
-2	-4	0	366	368	3
-1	-4	0	152	144	4
0	-4	0	377	359	17
1	-4	0	203	216	5
2	-4	0	336	341	4
3	-4	0	365	351	5
4	-4	0	51	32	13
5	-4	0	135	139	8
6	-4	0	64	64	19
7	-4	0	236	237	9
8	-4	0	110	109	17
9	-4	0	86	103	25
10	-4	0	0	29	1
-10	-3	0	79	25	44
-9	-3	0	123	104	21
-8	-3	0	46	19	45
-7	-3	0	150	127	14
-6	-3	0	69	92	20
-5	-3	0	202	209	8
-4	-3	0	116	115	9
-3	-3	0	557	561	5
-2	-3	0	110	106	4
-1	-3	0	284	281	2
0	-3	0	403	416	7
1	-3	0	351	363	3
2	-3	0	362	353	4
3	-3	0	499	493	4
4	-3	0	329	338	5
5	-3	0	223	232	6
1	-5	1	188	173	4
2	-5	1	263	258	4
3	-5	1	630	625	5
4	-5	1	348	326	6
5	-5	1	80	91	11
6	-5	1	0	42	1
7	-5	1	85	87	17
8	-5	1	152	132	13
9	-5	1	152	132	14
10	-5	1	110	50	23
-9	-4	1	54	59	54
-8	-4	1	168	160	15
-7	-4	1	20	36	19
-6	-4	1	89	83	15
-5	-4	1	76	62	14
-4	-4	1	181	172	8
-3	-4	1	275	273	6
-2	-4	1	683	667	7
-1	-4	1	211	209	3
0	-4	1	521	497	2
1	-4	1	178	180	7
2	-4	1	202	198	4
3	-4	1	24	37	24
4	-4	1	821	782	5
5	-4	1	329	334	6
6	-4	1	394	394	7
7	-4	1	0	34	1
8	-4	1	82	73	21
9	-4	1	93	81	19
10	-4	1	0	73	1

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-6	-1	0	19	59	18
-5	-1	0	313	331	6
-4	-1	0	66	59	9
-3	-1	0	163	181	5
-2	-1	0	347	342	4
-1	-1	0	1021	952	7
0	-1	0	305	302	3
1	-1	0	285	250	2
2	-1	0	715	685	4
3	-1	0	448	409	4
4	-1	0	254	255	5
5	-1	0	587	584	5
6	-1	0	100	89	11
7	-1	0	32	39	31
8	-1	0	45	25	45
9	-1	0	104	108	17
10	-1	0	0	55	1
-10	0	0	76	23	36
-9	0	0	105	104	21
-8	0	0	94	108	19
-7	0	0	0	17	1
-5	0	0	137	156	8
-4	0	0	304	338	5
-3	0	0	149	156	6
-2	0	0	887	870	4
-1	0	0	42	35	4
1	0	0	47	35	4
2	0	0	909	870	9
3	0	0	157	156	2
4	0	0	338	338	3
5	0	0	166	156	3
6	0	0	311	326	6
7	0	0	0	17	1
8	0	0	121	108	12
9	0	0	119	104	14
10	0	0	21	23	20
-10	1	0	63	55	48
-9	1	0	111	108	16
-8	1	0	0	25	1
-7	1	0	0	39	1
-6	1	0	73	89	13
-5	1	0	587	584	4
-4	1	0	252	255	4
-3	1	0	461	409	11
-2	1	0	690	685	10
-1	1	0	293	250	1
0	1	0	298	302	2
1	1	0	1019	952	4
2	1	0	350	342	3
3	1	0	168	181	10
4	1	0	50	59	7
5	1	0	343	331	11
6	1	0	48	59	23
7	1	0	177	189	8
8	1	0	32	43	31
9	1	0	47	11	47
10	1	0	73	48	33
5	-1	1	239	241	6
6	-1	1	83	89	11
7	-1	1	204	218	8
8	-1	1	47	50	46
9	-1	1	171	189	12
-10	0	1	161	132	16
-9	0	1	155	128	14
-8	0	1	113	110	15
-7	0	1	170	142	9
-6	0	1	103	110	11
-5	0	1	308	307	6
-4	0	1	600	594	5
-3	0	1	233	265	4
-2	0	1	726	674	4
-1	0	1	134	135	3
2	0	1	368	371	3
3	0	1	326	301	4
4	0	1	489	493	5
5	0	1	105	117	8
6	0	1	119	134	9
7	0	1	53	43	23
8	0	1	197	205	9
9	0	1	0	68	1
10	0	1	81	96	29
-11	1	1	0	46	1
-10	1	1	0	75	1
-9	1	1	133	147	15
-8	1	1	183	197	10
-7	1	1	24	53	23
-6	1	1	212	217	7
-5	1	1	178	181	7
-4	1	1	414	396	7
-3	1	1	366	378	4
-3	3	0	516	493	4
-2	3	0	384	353	4
-1	3	0	354	363	4
0	3	0	391	416	4
1	3	0	284	280	4
2	3	0	107	106	6
3	3	0	531	561	4
4	3	0	130	115	6
5	3	0	214	209	4
6	3	0	79	92	13
7	3	0	118	127	12
8	3	0	41	19	40
9	3	0	97	104	19
10	3	0	64	25	52
-10	4	0	0	29	1
-9	4	0	69	103	29
-8	4	0	117	109	13
-7	4	0	244	237	7
-6	4	0	70	64	12
-5	4	0	139	139	5
-4	4	0	54	32	14
-3	4	0	365	351	9
-2	4	0	349	341	11
-1	4	0	208	216	5
0	4	0	366	359	4
1	4	0	160	144	5
2	4	0	357	368	4
3	4	0	173	189	5
4	4	0	440	437	13
5	4	0	198	203	6
6	4	0	54	81	19
7	4	0	119	111	12
8	4	0	162	161	10
9	4	0	65	20	41
-10	5	0	10	50	9
-9	5	0	27	60	26
-8	5	0	211	206	8
-7	5	0	156	126	9
-6	5	0	378	387	6
-5	5	0	111	101	7
-4	5	0	24	39	23
-3	5	0	288	286	6
-2	5	0	397	370	5
-1	5	0	562	529	5
0	5	0	288	282	5
1	5	0	131	137	6
2	5	0	377	389	5
3	5	0	460	472	5
4	5	0	55	64	9
5	5	0	278	285	4
6	5	0	89	87	13
7	5	0	100	118	15
-8	6	0	66	63	23
-7	6	0	178	152	9
-6	6	0	86	85	13
-5	6	0	177	183	5
-4	6	0	171	164	4
8	3	1	23	39	22
9	3	1	68	74	32
10	3	1	0	23	1
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-10	4	1	25	23	25
-9	4	1	138	138	13
-8	4	1	54	31	31
-7	4	1	159	157	9
-6	4	1	151	154	5
-5	4	1	442	421	3
-4	4	1	187	179	4
-3	4	1	316	298	3
-2	4	1	268	256	7
-1	4	1	302	296	4
0	4	1	118	106	6
1	4	1	289	290	4
2	4	1	38	31	15
3	4	1	303	308	4
4	4	1	148	152	5
5	4	1	148	133	8
6	4	1	162	172	9
7	4	1	126	144	12
8	4	1	83	99	23
9	4	1	69	27	38
-9	5	1	75	54	21
-8	5	1	121	98	11
-7	5	1	107	108	11
-6	5	1	188	201	5
-5	5	1	85	82	9
-4	5	1	433	422	18
-3	5	1	63	63	12
-2	5	1	195	200	6
-1	5	1	62	60	11
4	8	0	155	157	9
-6	9	0	29	47	28
-5	9	0	82	33	19
-4	9	0	342	327	7
-3	9	0	82	63	18
-2	9	0	201	218	9
-1	9	0	37	7	36
0	9	0	0	31	1
1	9	0	149	143	11
2	9	0	209	194	8
3	9	0	69	85	19
4	9	0	194	185	9
-6	10	0	0	47	1
-5	10	0	0	16	1
-4	10	0	0	17	1
-3	10	0	175	167	10
-2	10	0	34	58	33
-1	10	0	309	300	8
0	10	0	27	35	27
1	10	0	0	28	1
2	10	0	75	55	18
3	10	0	137	138	12
4	10	0	73	66	23
-6	11	0	79	82	28
-5	11	0	0	62	1
-4	11	0	100	91	17
-3	11	0	44	41	43
-2	11	0	149	148	12
-1	11	0	60	85	41
0	11	0	262	232	9
1	11	0	47	13	47
2	11	0	53	53	53
3	11	0	68	50	34
4	11	0	188	160	10
-5	12	0	120	100	19
-4	12	0	0	19	1
-3	12	0	0	21	1
-2	12	0	91	99	20
-1	12	0	174	153	15
0	12	0	30	56	29
1	12	0	138	121	14
2	12	0	0	29	1
3	12	0	0	37	1
-5	13	0	65	46	64
-4	13	0	103	82	24
-3	13	0	0	30	1
-2	13	0	83	15	28
-1	13	0	0	47	1
0	13	0	0	68	1
1	13	0	0	41	1
6	-12	1	0	32	1
4	-11	1	233	232	8
5	-11	1	0	36	1
6	-11	1	106	67	20
7	-11	1	95	50	27
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3	-10	1	74	76	16
1	9	1	99	101	13
2	9	1	68	55	21
3	9	1	91	89	13
4	9	1	182	171	10
-6	10	1	127	140	14
-5	10	1	182	191	11
-4	10	1	187	177	11
-3	10	1	27	12	26
-2	10	1	10	9	10
-1	10	1	208	189	9
0	10	1	109	120	12
1	10	1	230	211	9
2	10	1	55	37	43
3	10	1	80	53	19
4	10	1	48	85	47
-6	11	1	100	102	20
-5	11	1	72	98	31
-4	11	1	96	132	19
-3	11	1	0	45	1
-2	11	1	150	132	11
-1	11	1	43	31	42
0	11	1	145	116	14
1	11	1	43	50	42
2	11	1	152	152	12
3	11	1	0	47	1
-6	12	1	0	37	1
-5	12	1	0	41	1
-4	12	1	54	65	53
-3	12	1	49	68	49
-2	12	1	95	79	20
-1	12	1	84	34	25
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1	12	1	102	81	19
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2	-8	1	60	58	10
3	-8	1	40	41	29
4	-8	1	54	69	21
5	-8	1	151	154	9
6	-8	1	103	105	14
7	-8	1	149	140	13
8	-8	1	0	12	1
9	-8	1	0	47	1
-8	-7	1	19	38	18
-7	-7	1	65	33	42
-6	-7	1	0	33	1
-5	-7	1	199	187	10
-4	-7	1	81	85	17
-3	-7	1	145	150	6
-2	-7	1	76	62	13
-1	-7	1	129	115	5
0	-7	1	107	116	5
1	-7	1	283	293	7
2	-7	1	260	254	7
3	-7	1	253	250	6
4	-7	1	86	85	11
5	-7	1	199	189	8
6	-7	1	155	139	10
7	-7	1	175	177	11
8	-7	1	132	130	13
9	-7	1	103	103	23
-9	-6	1	0	16	1
-8	-6	1	138	125	17
-7	-6	1	95	85	20
-6	-6	1	49	73	49
-5	-6	1	0	10	1
-4	-6	1	396	432	7
-3	-6	1	142	129	11
-2	-6	1	604	621	3
-1	-6	1	176	175	7
0	-6	1	61	75	7
1	-6	1	95	102	5
2	-6	1	560	546	3
3	-6	1	250	250	5
4	-6	1	360	364	5
5	-6	1	74	75	12
6	-6	1	182	192	10
7	-6	1	205	181	10
8	-6	1	61	44	33
9	-6	1	76	85	27
10	-6	1	67	52	66
-9	-5	1	39	87	39
-8	-5	1	53	39	52
-7	-5	1	187	186	12
-6	-5	1	40	68	39
-5	-5	1	58	83	23
-4	-5	1	0	4	1
-3	-5	1	403	419	3
-2	-5	1	36	41	36
-1	-5	1	450	467	3
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7	-8	2	94	79	18
8	-8	2	148	156	15
9	-8	2	83	62	35
-8	-7	2	62	33	62
-7	-7	2	136	161	17
-6	-7	2	85	72	21
-5	-7	2	109	108	15
-4	-7	2	22	66	22
-3	-7	2	295	319	7
-2	-7	2	88	75	10
-1	-7	2	394	412	14
0	-7	2	155	146	8
1	-7	2	91	90	6
2	-7	2	87	83	12
3	-7	2	350	340	6
4	-7	2	49	54	22
5	-7	2	153	132	9
6	-7	2	65	39	20
7	-7	2	60	73	33
8	-7	2	0	29	1
9	-7	2	59	76	58
-9	-6	2	76	8	57
-8	-6	2	104	103	24
-7	-6	2	0	44	1
-6	-6	2	224	230	9
-5	-6	2	63	82	26
-4	-6	2	193	181	9
-3	-6	2	92	89	6
-2	-6	2	431	447	3
-1	-6	2	102	95	4
0	-6	2	521	537	18
1	-6	2	65	65	7
2	-6	2	0	28	1
-10	-3	1	0	23	1
-9	-3	1	98	44	24
-8	-3	1	0	59	1
-7	-3	1	308	317	8
-6	-3	1	68	73	17
-5	-3	1	408	409	6
-4	-3	1	24	42	24
-3	-3	1	144	161	7
-2	-3	1	259	251	3
-1	-3	1	62	58	4
0	-3	1	120	132	3
1	-3	1	238	254	3
2	-3	1	342	338	4
3	-3	1	188	162	5
4	-3	1	127	118	7
5	-3	1	396	397	6
6	-3	1	112	101	10
7	-3	1	101	97	13
8	-3	1	82	61	19
9	-3	1	77	94	22
10	-3	1	71	46	34
-10	-2	1	0	46	1
-9	-2	1	96	94	25
-8	-2	1	87	98	18
-7	-2	1	68	58	24
-6	-2	1	232	237	8
-5	-2	1	103	117	10
-4	-2	1	347	355	5
-3	-2	1	73	76	9
-2	-2	1	46	55	13
-1	-2	1	772	768	2
0	-2	1	1038	951	16
1	-2	1	524	543	3
2	-2	1	279	256	4
3	-2	1	275	251	5
4	-2	1	256	240	5
5	-2	1	75	63	12
6	-2	1	432	412	6
7	-2	1	58	61	26
8	-2	1	105	134	15
9	-2	1	0	9	1
10	-2	1	84	31	27
-10	-1	1	70	92	47
-9	-1	1	96	83	22
-8	-1	1	196	203	9
-7	-1	1	59	37	25
-6	-1	1	102	108	12
-5	-1	1	623	597	5
-4	-1	1	374	345	5
-3	-1	1	596	585	4
-2	-1	1	0	21	1
-1	-1	1	166	167	4
0	-1	1	81	107	2
1	-1	1	1692	1603	5
2	-1	1	28	22	13
3	-1	1	398	375	4
4	-1	1	138	140	7
-4	-3	2	365	370	6
-3	-3	2	371	373	5
-2	-3	2	308	333	5
-1	-3	2	268	279	8
0	-3	2	39	66	6
1	-3	2	248	255	3
2	-3	2	253	252	4
3	-3	2	530	534	5
4	-3	2	89	94	9
5	-3	2	0	43	1
6	-3	2	73	86	15
7	-3	2	278	277	8
8	-3	2	0	39	1
9	-3	2	111	140	16
10	-3	2	45	15	44
-10	-2	2	0	8	1
-9	-2	2	199	188	12
-8	-2	2	151	141	14
-7	-2	2	181	182	10
-6	-2	2	130	121	11
-5	-2	2	91	93	11
-3	-2	2	166	147	6
-2	-2	2	231	220	4
-1	-2	2	10	36	9
0	-2	2	118	107	3
1	-2	2	786	778	3
2	-2	2	248	254	4
3	-2	2	69	59	8
4	-2	2	673	672	5
5	-2	2	65	70	12
6	-2	2	127	107	9
7	-2	2	155	157	10
8	-2	2	190	188	10

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-2	1	1	1090	1045	12
-1	1	1	912	873	7
0	1	1	491	491	2
1	1	1	69	62	3
2	1	1	217	224	6
3	1	1	535	529	4
4	1	1	186	202	5
5	1	1	269	277	6
6	1	1	0	34	1
7	1	1	127	120	11
8	1	1	82	108	18
9	1	1	159	160	13
10	1	1	46	15	46
-11	2	1	105	63	26
-10	2	1	23	29	22
-9	2	1	46	61	46
-8	2	1	59	31	28
-7	2	1	151	159	10
-6	2	1	31	12	30
-5	2	1	240	240	5
-4	2	1	46	44	12
-3	2	1	267	230	9
-2	2	1	630	600	2
-1	2	1	355	318	5
0	2	1	988	925	4
1	2	1	905	926	4
2	2	1	153	145	4
3	2	1	457	456	8
4	2	1	609	615	3
5	2	1	161	170	7
6	2	1	197	209	7
7	2	1	20	55	20
8	2	1	131	125	13
9	2	1	24	67	24
10	2	1	33	48	33
-11	3	1	25	25	25
-10	3	1	0	31	1
-9	3	1	0	15	1
-8	3	1	167	179	9
-7	3	1	160	156	8
-6	3	1	313	313	5
-5	3	1	225	227	4
-4	3	1	67	49	19
-3	3	1	54	51	6
-2	3	1	395	379	5
-1	3	1	168	165	4
0	3	1	231	250	4
1	3	1	376	369	4
2	3	1	276	277	4
3	3	1	176	177	3
4	3	1	199	213	3
5	3	1	278	303	6
6	3	1	154	165	8
7	3	1	166	173	10
0	1	2	1276	1205	4
1	1	2	534	502	3
2	1	2	148	160	2
3	1	2	36	39	12
4	1	2	289	291	5
5	1	2	288	295	5
6	1	2	113	133	10
7	1	2	180	188	8
8	1	2	57	76	30
9	1	2	63	71	35
10	1	2	0	42	1
-11	2	2	117	89	20
-10	2	2	40	27	39
-9	2	2	95	112	20
-8	2	2	0	34	1
-7	2	2	162	164	9
-6	2	2	134	130	5
-5	2	2	426	446	5
-4	2	2	177	187	4
-3	2	2	326	340	5
-2	2	2	182	172	2
-1	2	2	392	401	3
0	2	2	33	47	10
1	2	2	9	36	9
2	2	2	474	476	3
3	2	2	116	113	4
4	2	2	164	159	3
5	2	2	178	189	7
6	2	2	143	149	8
7	2	2	141	157	11
8	2	2	167	183	10
9	2	2	70	29	33
10	2	2	0	2	1
-11	3	2	44	25	43
-10	3	2	161	92	14
-9	3	2	85	25	19
0	5	1	575	575	5
1	5	1	479	485	5
2	5	1	906	909	5
3	5	1	26	36	26
4	5	1	106	92	10
5	5	1	143	146	8
6	5	1	112	112	12
7	5	1	168	170	10
8	5	1	109	118	17
-6	6	1	79	65	10
-5	6	1	176	180	5
-4	6	1	125	119	7
-3	6	1	516	514	3
-2	6	1	73	78	10
-1	6	1	138	140	7
0	6	1	38	27	25
1	6	1	392	379	6
2	6	1	260	261	6
3	6	1	378	381	6
4	6	1	250	255	5
5	6	1	0	29	1
6	6	1	92	69	16
7	6	1	93	81	17
-6	7	1	83	100	15
-5	7	1	34	51	33
-4	7	1	238	247	7
-3	7	1	0	10	1
-2	7	1	360	362	6
-1	7	1	86	81	11
0	7	1	0	39	1
1	7	1	65	80	14
2	7	1	285	272	6
3	7	1	148	141	9
4	7	1	176	167	8
5	7	1	16	46	16
6	7	1	0	43	1
-6	8	1	75	56	18
-5	8	1	135	139	10
-4	8	1	140	129	9
-3	8	1	194	193	8
-2	8	1	0	30	1
-1	8	1	334	338	7
0	8	1	96	79	12
1	8	1	0	18	1
2	8	1	0	8	1
3	8	1	124	112	11
4	8	1	71	47	18
-6	9	1	195	189	10
-5	9	1	75	82	20
-4	9	1	46	40	46
-3	9	1	45	54	45
-2	9	1	86	75	16
-1	9	1	119	98	12
0	9	1	253	259	7
5	5	2	97	91	12
6	5	2	92	70	15
7	5	2	43	38	43
8	5	2	109	93	18
9	5	2	58	21	58
-6	6	2	139	119	9
-5	6	2	91	89	11
-4	6	2	142	133	8
-3	6	2	344	325	6
-2	6	2	217	231	6
0	6	2	180	185	6
1	6	2	262	265	6
2	6	2	234	222	6
3	6	2	151	165	8
4	6	2	75	85	14
5	6	2	230	239	8
6	6	2	0	22	1
7	6	2	56	85	55
8	6	2	0	35	1
-6	7	2	187	175	9
-5	7	2	98	119	13
-4	7	2	89	96	12
-3	7	2	122	119	9
-2	7	2	102	94	9
-1	7	2	30	45	29
0	7	2	517	492	6
1	7	2	46	45	25
2	7	2	234	236	6
3	7	2	220	215	7
4	7	2	27	29	27
5	7	2	32	24	32
6	7	2	143	147	12
-6	8	2	165	153	10
-5	8	2	154	165	10
-4	8	2	158	147	9
-3	8	2	68	73	16
2	12	1	80	77	26
3	12	1	151	132	16
-5	13	1	100	19	27
-4	13	1	65	84	51
-3	13	1	43	22	43
-2	13	1	77	105	29
-1	13	1	6	69	6
0	13	1	65	22	52
1	13	1	27	27	26
5	-11	2	72	63	31
6	-11	2	130	114	17
7	-11	2	112	55	25
-6	-10	2	60	76	59
-5	-10	2	71	69	29
-4	-10	2	149	166	13
-3	-10	2	41	31	41
3	-10	2	237	228	8
4	-10	2	101	98	14
5	-10	2	72	55	25
6	-10	2	110	79	17
7	-10	2	144	127	16
8	-10	2	89	96	31
-7	-9	2	37	40	37
-6	-9	2	56	12	56
-5	-9	2	113	109	17
-4	-9	2	0	48	1
-3	-9	2	165	188	10
-2	-9	2	35	31	35
-1	-9	2	129	122	11
0	-9	2	0	59	1
1	-9	2	100	115	16
2	-9	2	132	132	7
3	-9	2	173	162	9
4	-9	2	90	80	16
5	-9	2	50	63	49
6	-9	2	22	70	21
7	-9	2	116	114	19
8	-9	2	80	102	30
9	-9	2	129	50	19
-8	-8	2	131	85	20
-7	-8	2	26	20	25
-6	-8	2	49	45	49
-5	-8	2	54	25	53
-4	-8	2	183	184	10
-3	-8	2	0	36	1
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1	-8	2	75	77	9
2	-8	2	191	195	6
3	-8	2	175	168	6
4	-8	2	306	295	6
5	-8	2	44	75	43
6	-8	2	0	35	1
-1	13	2	120	104	19
0	13	2	76	60	34
7	-11	3	52	64	51
-6	-10	3	21	29	20
-5	-10	3	0	28	1
-4	-10	3	87	89	21
-3	-10	3	54	42	42
-2	-10	3	201	227	9
-1	-10	3	24	49	23
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5	-10	3	27	56	27
6	-10	3	120	77	16
7	-10	3	35	30	35
8	-10	3	90	55	36
-7	-9	3	111	68	21
-6	-9	3	33	42	32
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-4	-9	3	26	19	25
-3	-9	3	158	144	11
-2	-9	3	30	17	29
-1	-9	3	222	242	7
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2	-9	3	0	37	1
3	-9	3	132	123	7
4	-9	3	66	89	24
5	-9	3	185	177	10
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-3	-8	3	34	73	34
3	-6	2	37	49	26
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6	-6	2	171	155	9
7	-6	2	83	75	16
8	-6	2	0	33	1
9	-6	2	53	76	53
10	-6	2	14	45	14
-9	-5	2	0	27	1
-8	-5	2	0	33	1
-7	-5	2	210	209	12
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2	-5	2	176	173	5
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4	-5	2	54	64	15
5	-5	2	288	273	7
6	-5	2	278	277	7
7	-5	2	222	226	9
8	-5	2	50	53	49
9	-5	2	0	35	1
10	-5	2	88	64	35
-9	-4	2	138	90	19
-8	-4	2	64	51	38
-7	-4	2	50	38	49
-6	-4	2	224	232	9
-5	-4	2	53	54	29
-4	-4	2	255	274	7
-3	-4	2	250	252	6
-2	-4	2	72	66	6
-1	-4	2	366	349	5
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1	-4	2	45	43	9
2	-4	2	609	585	4
3	-4	2	515	469	5
4	-4	2	217	209	5
5	-4	2	202	203	7
6	-4	2	258	257	7
7	-4	2	78	87	18
8	-4	2	169	160	10
9	-4	2	63	53	41
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-7	-3	2	92	57	15
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-5	-3	2	262	265	7
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-5	-5	3	76	59	16
-4	-5	3	236	224	8
-3	-5	3	316	329	6
-2	-5	3	231	247	3
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6	-5	3	162	169	9
7	-5	3	180	175	10
8	-5	3	0	45	1
9	-5	3	180	147	13
10	-5	3	46	44	45
-9	-4	3	115	108	22
-8	-4	3	103	94	20
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-6	-4	3	43	73	42
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-3	-4	3	248	247	6
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0	-4	3	235	225	4
1	-4	3	108	93	5
2	-4	3	430	418	4
3	-4	3	594	558	5
4	-4	3	765	739	5
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6	-4	3	93	97	14
7	-4	3	48	44	48
8	-4	3	119	121	15
9	-2	2	69	61	29
10	-2	2	158	105	15
-10	-1	2	38	29	37
-9	-1	2	46	103	45
-8	-1	2	181	145	11
-7	-1	2	168	157	10
-6	-1	2	165	164	9
-5	-1	2	57	58	18
-4	-1	2	435	420	5
-3	-1	2	464	457	4
-2	-1	2	746	733	4
-1	-1	2	1114	1048	4
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1	-1	2	274	279	3
2	-1	2	265	246	4
3	-1	2	359	355	4
4	-1	2	468	461	5
5	-1	2	279	286	6
6	-1	2	175	191	8
7	-1	2	39	45	38
8	-1	2	42	35	42
9	-1	2	145	156	13
10	-1	2	0	39	1
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-10	0	2	51	45	50
-9	0	2	59	27	47
-8	0	2	109	100	14
-7	0	2	272	267	8
-6	0	2	74	89	14
-5	0	2	503	499	5
-4	0	2	69	70	10
-3	0	2	118	84	6
-2	0	2	516	505	3
-1	0	2	1712	1658	5
0	0	2	198	208	4
1	0	2	195	207	5
2	0	2	527	551	5
3	0	2	282	301	6
4	0	2	154	150	8
5	0	2	7	39	7
6	0	2	72	46	21
7	0	2	39	40	39
8	0	2	0	32	1
-11	1	2	60	21	60
-10	1	2	139	108	17
-9	1	2	47	43	47
-8	1	2	74	74	19
-7	1	2	28	21	27
-6	1	2	369	372	3
-5	1	2	37	45	30
-4	1	2	367	347	4
-3	1	2	185	165	5
-2	1	2	275	269	3
-1	1	2	676	609	3
-2	-1	3	216	196	5
-1	-1	3	167	172	4
1	-1	3	132	140	4
2	-1	3	487	492	4
3	-1	3	97	82	6
4	-1	3	67	64	11
5	-1	3	169	180	8
6	-1	3	266	263	7
7	-1	3	125	101	11
8	-1	3	107	113	14
9	-1	3	53	46	47
10	-1	3	72	12	45
-11	0	3	142	92	20
-10	0	3	0	27	1
-9	0	3	237	235	9
-8	0	3	55	62	41
-7	0	3	64	71	18
-6	0	3	89	75	12
-5	0	3	711	684	5
-4	0	3	182	185	7
-3	0	3	612	604	4
-2	0	3	162	161	5
-1	0	3	49	47	7
2	0	3	294	302	4
3	0	3	549	516	5
4	0	3	65	54	10
5	0	3	7	7	7
6	0	3	167	156	9
7	0	3	133	133	10
8	0	3	199	217	10
9	0	3	99	122	18
10	0	3	0	4	1
-11	1	3	0	26	1
-10	1	3	93	99	25
-9	1	3	39	59	39
-8	1	3	98	113	14

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-8	3	2	88	76	15
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-6	3	2	129	121	5
-5	3	2	152	161	4
-4	3	2	418	442	5
-3	3	2	287	259	6
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-1	3	2	274	273	4
0	3	2	335	328	4
1	3	2	371	374	4
2	3	2	625	624	4
3	3	2	94	100	5
4	3	2	143	135	4
5	3	2	0	25	1
6	3	2	132	139	10
7	3	2	98	115	15
8	3	2	181	184	12
9	3	2	65	34	45
-10	4	2	103	30	20
-9	4	2	168	162	11
-8	4	2	125	106	11
-7	4	2	220	228	7
-6	4	2	139	136	5
-5	4	2	33	30	17
-4	4	2	47	51	9
-3	4	2	677	658	6
-2	4	2	230	220	5
-1	4	2	465	465	4
0	4	2	164	167	6
1	4	2	54	58	9
2	4	2	474	474	4
3	4	2	687	705	4
4	4	2	229	238	13
5	4	2	112	110	9
6	4	2	102	107	13
7	4	2	106	116	12
8	4	2	90	96	21
9	4	2	35	96	35
-8	5	2	229	230	7
-7	5	2	131	112	9
-6	5	2	185	184	9
-5	5	2	140	135	5
-4	5	2	243	240	7
-3	5	2	17	36	16
-2	5	2	713	720	5
-1	5	2	157	164	6
0	5	2	315	311	5
1	5	2	157	150	6
2	5	2	181	178	6
3	5	2	35	24	35
4	5	2	299	287	4
3	3	3	66	54	8
4	3	3	452	451	9
5	3	3	166	152	8
6	3	3	221	237	8
7	3	3	53	14	37
8	3	3	75	68	27
9	3	3	0	9	1
-8	4	3	54	25	25
-7	4	3	298	304	6
-6	4	3	109	99	7
-5	4	3	360	372	3
-4	4	3	99	107	5
-3	4	3	100	92	4
-2	4	3	328	339	4
-1	4	3	466	458	4
0	4	3	170	172	6
1	4	3	203	224	5
2	4	3	250	250	5
3	4	3	194	186	6
4	4	3	36	39	19
5	4	3	265	260	8
6	4	3	38	51	38
7	4	3	142	144	11
8	4	3	0	23	1
9	4	3	66	64	60
-6	5	3	204	193	6
-5	5	3	225	230	10
-4	5	3	121	108	9
-3	5	3	287	278	5
-2	5	3	180	172	6
-1	5	3	204	191	6
0	5	3	663	646	5
1	5	3	350	355	5
2	5	3	475	477	5
3	5	3	109	106	9
4	5	3	162	144	8
5	5	3	74	75	18
6	5	3	267	261	8
7	5	3	30	42	30
-2	8	2	52	80	20
-1	8	2	66	90	18
0	8	2	149	128	9
1	8	2	172	181	8
2	8	2	0	33	1
3	8	2	100	93	13
4	8	2	71	66	20
5	8	2	154	154	12
-6	9	2	30	72	29
-5	9	2	120	129	12
-4	9	2	243	240	8
-3	9	2	163	153	9
-2	9	2	161	138	10
-1	9	2	27	36	26
0	9	2	248	250	8
1	9	2	64	43	19
2	9	2	201	193	9
3	9	2	93	68	16
-6	10	2	71	60	29
-5	10	2	80	64	21
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-3	10	2	104	135	14
-2	10	2	166	155	11
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1	10	2	114	104	14
2	10	2	102	75	16
3	10	2	189	185	10
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-5	11	2	0	46	1
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-2	11	2	92	83	20
-1	11	2	225	232	10
0	11	2	0	50	1
1	11	2	0	17	1
2	11	2	107	75	19
3	11	2	131	97	15
-6	12	2	96	93	28
-5	12	2	46	32	46
-4	12	2	88	39	24
-3	12	2	83	54	22
-2	12	2	81	83	21
-1	12	2	59	82	34
0	12	2	121	101	16
1	12	2	65	59	38
2	12	2	0	22	1
3	12	2	0	45	1
-4	13	2	13	14	12
-3	13	2	0	21	1
-2	13	2	50	42	50
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-1	9	3	204	204	8
0	9	3	98	90	12
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2	9	3	0	25	1
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-6	10	3	199	205	11
-5	10	3	36	54	35
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-2	10	3	198	201	9
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0	10	3	251	235	9
1	10	3	70	61	21
2	10	3	78	58	22
3	10	3	97	52	20
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-6	11	3	61	27	60
-5	11	3	161	143	12
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-3	11	3	30	66	30
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0	11	3	59	57	30
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2	11	3	26	41	25
3	11	3	0	49	1
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9	-8	3	76	49	36
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3	1	3	301	289	3
4	1	3	291	315	6
5	1	3	126	124	8
6	1	3	31	52	30
7	1	3	0	38	1
8	1	3	76	112	21
9	1	3	27	40	27
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-2	2	3	217	224	2
-1	2	3	594	586	4
0	2	3	60	47	7
1	2	3	197	202	4
2	2	3	0	15	1
3	2	3	801	795	3
4	2	3	173	177	5
5	2	3	170	173	9
6	2	3	28	32	28
7	2	3	53	68	35
8	2	3	52	60	52
9	2	3	119	147	16
-10	3	3	60	18	44
-9	3	3	90	69	20
-8	3	3	170	154	10
-7	3	3	131	105	9
-6	3	3	252	248	5
-5	3	3	109	107	8
-4	3	3	42	52	20
-3	3	3	70	66	7
-2	3	3	787	783	4
-1	3	3	64	59	7
0	3	3	427	422	4
1	3	3	0	23	1
2	3	3	51	42	9
9	1	4	62	44	52
-11	2	4	54	31	53
-10	2	4	132	108	16
-9	2	4	51	45	51
-8	2	4	146	133	10
-7	2	4	216	210	5
-6	2	4	197	206	5
-5	2	4	398	412	10
-4	2	4	77	82	6
-3	2	4	163	169	4
-2	2	4	113	113	4
-1	2	4	379	385	10
0	2	4	129	122	6
1	2	4	470	473	4
2	2	4	41	48	12
3	2	4	117	103	5
4	2	4	142	130	9
5	2	4	139	134	9
6	2	4	28	46	27
7	2	4	237	235	9
8	2	4	63	58	31
9	2	4	58	70	58
-9	3	4	113	123	16
-8	3	4	24	15	23
-7	3	4	47	60	16
-6	3	4	193	201	5
-5	3	4	151	158	9
-4	3	4	438	429	3
-3	3	4	208	228	4
-2	3	4	42	30	13
-1	3	4	0	7	1
0	3	4	558	537	4
1	3	4	244	247	4
2	3	4	476	468	4
3	3	4	59	58	10
4	3	4	85	77	12
5	3	4	80	100	12
6	3	4	184	193	10
7	3	4	162	168	11

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
8	5	3	108	100	20
-7	6	3	79	97	17
-6	6	3	97	105	13
-5	6	3	153	156	8
-4	6	3	297	290	6
-3	6	3	218	215	6
-2	6	3	108	107	9
-1	6	3	169	164	7
0	6	3	103	96	9
1	6	3	323	331	6
2	6	3	250	245	6
3	6	3	277	288	6
5	6	3	83	93	18
6	6	3	0	22	1
7	6	3	114	120	18
8	6	3	0	16	1
-7	7	3	23	58	22
-6	7	3	0	22	1
-5	7	3	154	154	9
-4	7	3	156	170	8
-3	7	3	227	220	7
-2	7	3	173	188	7
-1	7	3	43	36	19
0	7	3	135	139	9
1	7	3	178	177	7
2	7	3	107	102	11
3	7	3	195	197	7
5	7	3	51	33	50
6	7	3	48	64	48
7	7	3	40	43	39
-7	8	3	28	61	28
-6	8	3	76	46	20
-5	8	3	26	45	26
-4	8	3	89	83	12
-3	8	3	215	222	7
-2	8	3	190	193	8
-1	8	3	193	203	8
0	8	3	104	96	11
1	8	3	124	102	10
2	8	3	100	103	12
3	8	3	115	87	12
5	8	3	90	87	19
6	8	3	40	24	39
-7	9	3	119	134	15
-6	9	3	0	28	1
-5	9	3	145	126	10
-4	9	3	70	77	19
-3	9	3	120	94	10
-7	7	4	185	210	9
-6	7	4	81	71	15
-5	7	4	76	91	16
-4	7	4	56	67	20
-3	7	4	42	24	33
-2	7	4	0	30	1
-1	7	4	231	235	7
0	7	4	79	93	10
1	7	4	214	203	7
2	7	4	134	109	9
3	7	4	123	113	10
5	7	4	156	153	12
6	7	4	70	75	31
7	7	4	37	14	37
-7	8	4	0	21	1
-6	8	4	169	156	11
-5	8	4	32	28	31
-4	8	4	140	140	11
-3	8	4	25	9	25
-2	8	4	51	31	26
-1	8	4	93	93	11
0	8	4	203	196	8
1	8	4	84	71	14
2	8	4	157	109	10
3	8	4	54	78	33
5	8	4	110	106	17
6	8	4	122	122	23
-7	9	4	97	55	19
-6	9	4	20	25	20
-5	9	4	226	236	9
-4	9	4	89	85	15
-3	9	4	161	155	8
-2	9	4	45	16	37
-1	9	4	156	150	11
0	9	4	110	95	11
1	9	4	204	192	9
2	9	4	56	49	27
3	9	4	106	103	15
5	9	4	61	74	60
-7	10	4	36	44	36
-6	10	4	61	45	37
-5	10	4	40	42	39
-2	13	3	0	21	1
-1	13	3	61	31	42
0	13	3	30	33	29
-5	-11	4	94	94	26
-4	-11	4	0	21	1
-3	-11	4	0	43	1
-2	-11	4	42	25	42
-6	-10	4	46	35	45
-5	-10	4	90	69	21
-4	-10	4	102	102	15
-3	-10	4	34	33	33
-2	-10	4	63	54	25
-1	-10	4	110	95	13
0	-10	4	203	236	10
1	-10	4	108	114	12
2	-10	4	177	191	11
7	-10	4	43	39	43
-7	-9	4	0	52	1
-6	-9	4	33	31	33
-5	-9	4	115	128	16
-4	-9	4	145	146	15
-3	-9	4	103	90	14
-2	-9	4	113	120	12
-1	-9	4	53	57	25
0	-9	4	120	119	10
1	-9	4	166	179	10
2	-9	4	69	89	18
3	-9	4	171	167	10
4	-9	4	34	27	33
5	-9	4	130	116	13
6	-9	4	56	59	55
7	-9	4	221	204	11
8	-9	4	71	5	45
-7	-8	4	0	41	1
-6	-8	4	0	35	1
-5	-8	4	68	89	24
-4	-8	4	178	185	11
-3	-8	4	34	40	33
-2	-8	4	99	90	12
-1	-8	4	47	39	30
0	-8	4	46	52	28
1	-8	4	104	114	11
2	-8	4	262	258	7
3	-8	4	93	91	8
4	-8	4	122	119	11
5	-8	4	34	33	33
6	-8	4	104	86	15
7	-8	4	113	108	19
-7	-9	5	35	23	34
-6	-9	5	0	43	1
-5	-9	5	39	26	38
-4	-9	5	108	115	16
-3	-9	5	127	115	13
-2	-9	5	132	144	12
-1	-9	5	52	77	31
0	-9	5	102	101	10
1	-9	5	0	15	1
2	-9	5	170	186	10
3	-9	5	169	171	10
4	-9	5	137	132	12
6	-9	5	25	24	25
7	-9	5	93	30	26
8	-9	5	97	51	29
-7	-8	5	107	111	22
-6	-8	5	66	21	33
-5	-8	5	161	161	12
-4	-8	5	101	129	16
-3	-8	5	134	137	11
-2	-8	5	153	161	9
-1	-8	5	227	257	8
0	-8	5	0	15	1
1	-8	5	127	132	8
2	-8	5	66	61	21
3	-8	5	133	131	11
4	-8	5	127	119	10
5	-8	5	92	104	14
6	-8	5	186	174	11
7	-8	5	52	21	52
8	-8	5	37	30	37
-8	-7	5	66	52	65
-7	-7	5	31	79	31
-6	-7	5	203	205	11
-5	-7	5	65	66	33
-4	-7	5	124	122	11
-3	-7	5	54	57	28
-2	-7	5	133	135	9
-1	-7	5	83	87	12
0	-7	5	255	262	7
1	-7	5	85	99	14
2	-7	5	199	182	6
-9	-5	4	72	20	52
-8	-5	4	86	73	28
-7	-5	4	94	79	19
-6	-5	4	194	172	11
-5	-5	4	43	34	43
-4	-5	4	34	38	33
-3	-5	4	32	28	32
-2	-5	4	412	440	5
-1	-5	4	452	439	5
0	-5	4	567	581	12
1	-5	4	356	332	3
2	-5	4	85	75	8
3	-5	4	10	23	10
4	-5	4	292	291	6
5	-5	4	206	207	8
6	-5	4	160	148	10
7	-5	4	79	73	18
8	-5	4	24	22	23
9	-5	4	61	75	49
-10	-4	4	0	45	1
-9	-4	4	0	10	1
-8	-4	4	84	75	27
-7	-4	4	185	181	11
-6	-4	4	24	30	23
-5	-4	4	307	311	7
-4	-4	4	0	37	1
-3	-4	4	210	207	7
-2	-4	4	87	115	11
-1	-4	4	573	591	5
0	-4	4	285	314	3
1	-4	4	534	517	3
2	-4	4	251	247	5
3	-4	4	140	126	8
4	-4	4	0	33	1
5	-4	4	164	166	8
6	-4	4	189	186	9
7	-4	4	147	153	12
8	-4	4	95	65	19
9	-4	4	12	51	12
-10	-3	4	10	70	10
-9	-3	4	39	29	38
-8	-3	4	72	83	27
-7	-3	4	52	60	48
-6	-3	4	150	147	11
-5	-3	4	0	31	1
-4	-3	4	340	367	6
-3	-3	4	103	99	9
-2	-3	4	119	122	8
-9	-4	5	50	62	50
-8	-4	5	68	41	34
-7	-4	5	84	62	23
-6	-4	5	54	48	39
-5	-4	5	118	118	13
-4	-4	5	103	93	11
-3	-4	5	436	466	6
-2	-4	5	170	176	8
-1	-4	5	463	470	5
0	-4	5	0	35	1
1	-4	5	275	285	4
2	-4	5	113	103	7
3	-4	5	489	501	5
4	-4	5	16	38	15
5	-4	5	84	93	12
6	-4	5	26	44	25
7	-4	5	193	182	10
8	-4	5	43	55	42
9	-4	5	111	90	20
-10	-3	5	0	55	1
-9	-3	5	79	53	34
-8	-3	5	188	174	13
-7	-3	5	150	157	12
-6	-3	5	85	88	16
-5	-3	5	0	33	1
-4	-3	5	198	202	7
-3	-3	5	72	58	12
-2	-3	5	532	549	5
-1	-3	5	136	122	8
0	-3	5	301	311	2
1	-3	5	189	192	4
2	-3	5	417	407	4
3	-3	5	130	118	8
4	-3	5	470	478	5
5	-3	5	46	35	24
6	-3	5	75	82	17
7	-3	5	50	34	50
8	-3	5	123	129	14
9	-3	5	97	54	24
-10	-2	5	57	33	56
-9	-2	5	82	78	29
-8	-2	5	61	66	41
-2	-1	4	485	468	4
-1	-1	4	74	65	7
1	-1	4	44	28	10
2	-1	4	486	472	4
3	-1	4	195	196	6
4	-1	4	584	575	5
5	-1	4	33	23	33
6	-1	4	101	107	10
7	-1	4	0	12	1
8	-1	4	75	98	24
9	-1	4	83	94	25
-11	0	4	142	27	23
-10	0	4	52	52	51
-9	0	4	161	158	15
-8	0	4	42	75	41
-7	0	4	211	204	8
-6	0	4	229	228	8
-5	0	4	249	239	7
-4	0	4	90	59	9
-3	0	4	399	369	4
-2	0	4	203	194	5
-1	0	4	660	650	4
2	0	4	0	14	1
4	0	4	31	10	31
5	0	4	194	213	7
6	0	4	15	25	14
7	0	4	42	29	42
8	0	4	83	53	21
9	0	4	98	90	19
-11	1	4	0	74	1
-10	1	4	46	39	45
-9	1	4	98	9	16
-8	1	4	125	118	13
-7	1	4	187	187	8
-6	1	4	161	148	9
-5	1	4	248	239	6
-4	1	4	166	153	7
-3	1	4	208	190	5
-2	1	4	312	314	3
-1	1	4	156	157	4
1	1	4	147	151	4
2	1	4	145	149	4
3	1	4	12	36	12
4	1	4	494	480	5
5	1	4	50	48	20
6	1	4	260	281	7
7	1	4	60	11	28
8	1	4	50	10	49
-1	0	5	35	35	16
2	0	5	435	436	4
3	0	5	350	354	12
4	0	5	185	176	8
5	0	5	133	115	9
6	0	5	61	54	23
7	0	5	240	238	9
8	0	5	0	19	1
9	0	5	0	22	1
-11	1	5	23	82	22
-10	1	5	77	61	33
-9	1	5	195	177	12
-8	1	5	43	31	42
-7	1	5	0	7	1
-6	1	5	89	76	12
-5	1	5	363	351	6
-4	1	5	195	192	6
-3	1	5	401	368	4
-2	1	5	83	86	8
-1	1	5	303	308	3
1	1	5	406	390	4
2	1	5	647	614	4
3	1	5	149	157	4
4	1	5	107	101	8
5	1	5	8	56	7
6	1	5	57	64	23
7	1	5	62	82	28
8	1	5	144	151	14
9	1	5	98	25	24
-10	2	5	35	53	35
-9	2	5	56	33	39
-8	2	5	101	70	14
-7	2	5	37	18	37
-6	2	5	111	107	6
-5	2	5	114	100	8
-4	2	5	289	287	5
-3	2	5	343	346	4
-2	2	5	341	333	4
-1	2	5	20	32	19
0	2	5	0	25	1
1	2	5	313	307	4
2	2	5	576	547	4
8	3	4	131	138	16
9	3	4	0	25	1
-7	4	4	28	10	27
-6	4	4	73	79	8
-5	4	4	213	207	7
-4	4	4	468	464	3
-3	4	4	465	465	5
-2	4	4	502	493	5
-1	4	4	118	106	7
0	4	4	32	17	26
1	4	4	399	391	5
2	4	4	347	348	5
3	4	4	385	381	5
4	4	4	60	37	18
5	4	4	104	88	14
6	4	4	54	51	36
7	4	4	152	159	13
8	4	4	45	64	45
-7	5	4	289	313	6
-6	5	4	108	106	10
-5	5	4	0	20	1
-4	5	4	161	169	7
-3	5	4	520	528	5
-2	5	4	211	224	6
-1	5	4	224	224	6
0	5	4	0	25	1
1	5	4	48	60	15
2	5	4	254	246	5
3	5	4	205	202	6
5	5	4	57	21	33
6	5	4	79	52	20
7	5	4	54	61	53
8	5	4	48	88	48
-7	6	4	49	68	45
-6	6	4	100	91	12
-5	6	4	145	131	8
-4	6	4	209	196	7
-3	6	4	135	144	8
-2	6	4	453	445	6
-1	6	4	207	203	6
0	6	4	185	195	7
1	6	4	13	32	12
2	6	4	189	190	7
3	6	4	61	55	19
5	6	4	155	143	11
6	6	4	42	61	41
7	6	4	21	49	21
8	6	4	69	30	50
-2	5	5	37	43	24
-1	5	5	349	357	5
0	5	5	129	131	8
1	5	5	206	215	6
2	5	5	80	78	12
3	5	5	157	170	8
5	5	5	183	177	11
6	5	5	153	124	13
7	5	5	92	79	24
8	5	5	33	41	33
-7	6	5	51	92	35
-6	6	5	160	180	8
-5	6	5	113	115	10
-4	6	5	160	178	7
-3	6	5	0	13	1
-2	6	5	51	41	18
-1	6	5	104	102	10
0	6	5	343	343	6
1	6	5	121	118	9
2	6	5	386	370	6
3	6	5	102	111	11
4	6	5	111	115	15
6	6	5	152	152	13
7	6	5	0	53	1
-7	7	5	65	40	25
-6	7	5	124	110	12
-5	7	5	148	153	10
-4	7	5	45	63	28
-3	7	5	252	253	7
-2	7	5	45	34	31
-1	7	5	102	103	10
0	7	5	13	39	12
1	7	5	205	219	7
2	7	5	28	40	28
3	7	5	186	184	9
5	7	5	0	30	1
6	7	5	35	27	35
7	7	5	129	82	22
-7	8	5	69	69	27
-6	8	5	40	25	40
-5	8	5	90	57	16
-4	8	5	198	203	8

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-4	10	4	217	233	9
-3	10	4	0	7	1
-2	10	4	126	147	13
-1	10	4	63	42	27
0	10	4	106	114	14
1	10	4	0	33	1
2	10	4	195	199	10
3	10	4	0	42	1
-7	11	4	89	49	27
-6	11	4	96	93	21
-5	11	4	27	28	27
-4	11	4	49	61	48
-3	11	4	121	121	14
-2	11	4	75	84	25
-1	11	4	88	85	19
0	11	4	65	21	31
1	11	4	50	26	50
2	11	4	0	2	1
-6	12	4	0	39	1
-5	12	4	84	46	29
-4	12	4	41	49	41
-3	12	4	122	61	16
-2	12	4	132	122	17
-1	12	4	84	50	25
0	12	4	24	56	23
1	12	4	55	42	55
2	12	4	73	51	40
-5	-11	5	64	37	64
-4	-11	5	82	100	33
-3	-11	5	0	84	1
-2	-11	5	48	73	47
-1	-11	5	42	71	41
0	-11	5	100	82	16
1	-11	5	185	196	11
-6	-10	5	0	40	1
-5	-10	5	35	20	35
-4	-10	5	71	96	28
-3	-10	5	122	139	14
-2	-10	5	175	156	11
-1	-10	5	177	186	9
0	-10	5	77	77	20
1	-10	5	76	81	21
2	-10	5	191	191	11
3	-10	5	98	101	19
4	-10	5	144	122	12
1	12	5	93	57	26
-3	-12	6	133	91	18
-2	-12	6	58	56	57
-4	-11	6	45	27	44
-3	-11	6	86	18	23
-2	-11	6	104	92	19
-1	-11	6	120	119	15
0	-11	6	101	101	18
1	-11	6	51	40	51
2	-11	6	57	75	56
-6	-10	6	0	30	1
-5	-10	6	128	107	16
-4	-10	6	0	22	1
-3	-10	6	27	69	26
-2	-10	6	32	37	31
-1	-10	6	227	209	10
0	-10	6	0	52	1
1	-10	6	139	149	14
2	-10	6	18	41	17
3	-10	6	85	83	26
4	-10	6	50	79	50
5	-10	6	105	85	21
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-4	-9	6	114	123	14
-3	-9	6	44	53	43
-2	-9	6	0	18	1
-1	-9	6	0	9	1
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3	-9	6	148	136	11
4	-9	6	74	103	24
-7	-8	6	78	51	42
-6	-8	6	46	34	46
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-4	-8	6	77	27	19
-3	-8	6	119	102	13
-2	-8	6	73	33	17
-1	-8	6	0	27	1
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1	-8	6	210	222	8
2	-8	6	79	82	18
3	-8	6	168	174	10
6	-8	6	67	66	29
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7	-6	5	168	155	12
8	-6	5	95	97	21
9	-6	5	0	49	1
-9	-5	5	65	42	65
-8	-5	5	128	120	19
-7	-5	5	120	105	18
-6	-5	5	74	68	22
-5	-5	5	82	88	19
-4	-5	5	225	232	7
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1	-5	5	228	218	4
2	-5	5	563	547	4
3	-5	5	165	170	7
4	-5	5	170	164	9
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6	-5	5	69	73	22
7	-5	5	93	76	18
8	-5	5	131	144	13
9	-5	5	92	48	26
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1	-5	6	133	135	7
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3	-5	6	53	56	18
4	-5	6	368	359	6
5	-5	6	55	17	25
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7	-5	6	0	46	1
8	-5	6	24	58	24
9	-5	6	26	23	26
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-7	-4	6	135	119	15
-6	-4	6	173	166	10
-5	-4	6	98	110	16
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5	-4	6	221	210	7
6	-4	6	0	45	1
7	-4	6	113	110	15
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9	-4	6	26	30	25
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3	-2	5	226	222	6
4	-2	5	35	37	35
5	-2	5	275	274	6
6	-2	5	32	38	32
7	-2	5	58	55	28
8	-2	5	46	27	46
9	-2	5	55	75	54
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5	-1	5	79	88	12
6	-1	5	295	294	8
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9	-1	5	0	19	1
-11	0	5	107	52	29
-10	0	5	123	102	17
-9	0	5	47	49	46
-8	0	5	0	18	1
-7	0	5	107	114	13
-6	0	5	223	210	7
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8	-1	6	191	185	11
9	-1	6	4	49	4
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-6	0	6	283	261	8
-5	0	6	164	158	8
-4	0	6	303	298	6
-3	0	6	275	267	5
-2	0	6	445	432	5
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2	0	6	377	379	5
3	0	6	330	337	3
4	0	6	228	217	7
5	0	6	65	63	17
6	0	6	32	30	32
7	0	6	36	71	35
8	0	6	52	15	51
9	0	6	81	68	30
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-6	1	6	0	43	1
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-2	1	6	191	167	6
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2	1	6	124	105	6
3	1	6	312	304	3
4	1	6	165	154	7
5	1	6	187	192	10
6	1	6	79	77	19
7	1	6	61	53	45
8	1	6	92	105	28
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-8	2	6	180	159	10
-7	2	6	23	34	23
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-4	2	6	143	133	8
3	2	5	352	348	4
4	2	5	108	113	10
5	2	5	68	54	16
6	2	5	0	37	1
7	2	5	68	82	27
8	2	5	94	105	24
9	2	5	17	60	16
-8	3	5	0	40	1
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-6	3	5	0	29	1
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-3	3	5	570	546	12
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0	3	5	88	95	8
1	3	5	0	16	1
2	3	5	165	161	6
3	3	5	295	310	4
4	3	5	231	230	7
5	3	5	153	154	9
6	3	5	75	104	22
7	3	5	0	23	1
8	3	5	97	70	23
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-4	4	5	29	36	28
-3	4	5	169	187	6
-2	4	5	567	566	5
-1	4	5	242	252	5
0	4	5	236	238	5
1	4	5	125	118	8
2	4	5	44	46	19
3	4	5	66	71	12
4	4	5	123	122	11
5	4	5	159	172	11
6	4	5	159	162	11
7	4	5	68	58	31
8	4	5	0	23	1
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-6	5	5	35	77	34
-5	5	5	217	231	6
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-3	5	5	29	13	28
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-7	5	6	27	58	26
-6	5	6	90	96	11
-5	5	6	188	200	7
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-2	5	6	73	56	13
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1	5	6	285	274	6
2	5	6	42	54	38
5	5	6	76	51	27
6	5	6	0	18	1
7	5	6	113	101	24
-8	6	6	104	104	16
-7	6	6	134	126	10
-6	6	6	41	35	41
-5	6	6	77	61	13
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-3	6	6	147	160	9
-2	6	6	245	251	6
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1	6	6	153	153	9
2	6	6	261	268	7
5	6	6	30	2	29
6	6	6	25	39	25
7	6	6	0	39	1
-8	7	6	109	69	17
-7	7	6	111	87	14
-6	7	6	105	104	12
-5	7	6	0	57	1
-4	7	6	68	49	18
-3	7	6	70	72	17
-2	7	6	161	164	8
-1	7	6	149	143	9
0	7	6	130	128	10
1	7	6	72	59	15
2	7	6	46	41	42
5	7	6	150	130	15
6	7	6	100	35	29
-8	8	6	129	91	16
-7	8	6	86	92	24
-6	8	6	0	22	1
-5	8	6	116	90	14
-3	8	5	35	37	34
-2	8	5	161	165	9
-1	8	5	124	126	10
0	8	5	73	84	15
1	8	5	46	35	42
2	8	5	252	249	8
5	8	5	84	24	25
6	8	5	15	56	14
-7	9	5	76	74	27
-6	9	5	48	40	47
-5	9	5	0	13	1
-4	9	5	46	40	46
-3	9	5	240	248	8
-2	9	5	106	81	12
-1	9	5	172	181	9
0	9	5	99	110	13
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2	9	5	0	15	1
5	9	5	90	117	28
-7	10	5	129	104	14
-6	10	5	86	110	21
-5	10	5	125	132	13
-4	10	5	56	36	27
-3	10	5	66	87	22
-2	10	5	180	167	10
-1	10	5	150	135	13
0	10	5	110	92	15
1	10	5	66	27	28
2	10	5	89	24	19
-7	11	5	88	30	28
-6	11	5	67	83	37
-5	11	5	36	55	36
-4	11	5	38	46	38
-3	11	5	24	46	23
-2	11	5	101	86	15
-1	11	5	151	132	13
0	11	5	58	74	42
1	11	5	76	80	25
2	11	5	54	13	54
-5	12	5	41	74	41
-4	12	5	60	14	54
-3	12	5	71	10	37
-2	12	5	0	14	1
-1	12	5	46	45	45
0	12	5	74	73	31
-2	-12	7	0	22	1
-1	-12	7	71	49	37
0	-12	7	86	78	30
-4	-11	7	89	126	27
-3	-11	7	0	21	1
-2	-11	7	0	50	1
-1	-11	7	0	8	1
0	-11	7	117	122	17
1	-11	7	72	90	34
2	-11	7	109	123	18
3	-11	7	62	36	57
4	-11	7	30	57	30
-5	-10	7	67	56	38
-4	-10	7	0	44	1
-3	-10	7	126	106	15
-2	-10	7	47	39	47
-1	-10	7	94	87	22
0	-10	7	0	33	1
1	-10	7	201	224	12
2	-10	7	65	28	29
3	-10	7	120	130	18
4	-10	7	53	11	53
5	-10	7	17	41	17
-6	-9	7	44	14	43
-5	-9	7	0	38	1
-4	-9	7	132	139	14
-3	-9	7	106	91	15
-2	-9	7	170	181	10
-1	-9	7	86	96	19
0	-9	7	0	16	1
1	-9	7	43	23	43
2	-9	7	202	219	12
3	-9	7	0	54	1
4	-9	7	170	167	12
-7	-8	7	51	91	51
-6	-8	7	112	69	18
-5	-8	7	66	37	39
-4	-8	7	0	22	1
-3	-8	7	139	138	12
-2	-8	7	66	59	23
-1	-8	7	179	197	8
0	-8	7	58	39	28
1	-8	7	0	15	1
2	-8	7	148	127	11
3	-8	7	133	136	12

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
7	-8	6	207	208	12
8	-8	6	73	64	47
-8	-7	6	116	111	24
-7	-7	6	74	78	44
-6	-7	6	34	33	33
-5	-7	6	70	30	26
-4	-7	6	208	239	9
-3	-7	6	83	71	16
-2	-7	6	196	200	9
-1	-7	6	0	12	1
0	-7	6	46	52	46
1	-7	6	98	97	15
2	-7	6	218	226	10
4	-7	6	210	183	8
5	-7	6	66	13	23
6	-7	6	66	50	31
7	-7	6	29	6	28
8	-7	6	141	143	18
-8	-6	6	60	9	60
-7	-6	6	171	169	15
-6	-6	6	70	80	23
-5	-6	6	79	49	21
-4	-6	6	69	63	17
-3	-6	6	248	253	7
-2	-6	6	99	84	12
-1	-6	6	315	323	7
0	-6	6	92	80	10
1	-6	6	0	36	1
2	-6	6	36	44	35
3	-6	6	312	316	6
4	-6	6	63	80	17
5	-6	6	119	116	10
6	-6	6	79	64	17
7	-6	6	115	103	14
8	-6	6	0	33	1
9	-6	6	103	85	26
-9	-5	6	0	44	1
-8	-5	6	89	101	27
-7	-5	6	146	149	16
-6	-5	6	123	126	11
-5	-5	6	76	74	19
-4	-5	6	0	13	1
2	-5	7	131	131	8
3	-5	7	94	90	10
4	-5	7	154	141	9
5	-5	7	118	118	11
6	-5	7	196	209	11
7	-5	7	50	69	49
8	-5	7	82	108	33
-9	-4	7	0	35	1
-8	-4	7	110	102	21
-7	-4	7	117	140	17
-6	-4	7	153	151	14
-5	-4	7	184	196	10
-4	-4	7	210	221	9
-3	-4	7	184	200	9
-2	-4	7	355	362	6
-1	-4	7	57	56	16
0	-4	7	179	171	8
1	-4	7	305	316	4
2	-4	7	366	366	5
3	-4	7	207	206	7
4	-4	7	97	100	11
5	-4	7	116	106	11
6	-4	7	118	98	13
7	-4	7	106	81	15
8	-4	7	48	33	48
-10	-3	7	116	41	27
-9	-3	7	149	120	18
-8	-3	7	71	45	42
-7	-3	7	113	112	16
-6	-3	7	95	87	16
-5	-3	7	140	122	10
-4	-3	7	135	121	10
-3	-3	7	353	362	6
-2	-3	7	33	36	33
-1	-3	7	267	277	10
0	-3	7	176	190	4
1	-3	7	128	121	7
2	-3	7	51	39	16
3	-3	7	188	191	7
4	-3	7	133	126	8
5	-3	7	27	32	27
6	-3	7	48	23	42
7	-3	7	103	110	18
8	-3	7	127	124	16
-10	-2	7	62	40	62
-9	-2	7	71	42	42
-8	-2	7	227	203	11
-7	-2	7	201	189	12
3	-3	6	0	22	1
4	-3	6	112	104	9
5	-3	6	89	80	12
6	-3	6	231	241	8
7	-3	6	53	15	41
8	-3	6	88	98	19
9	-3	6	0	14	1
-10	-2	6	153	122	16
-9	-2	6	79	54	30
-8	-2	6	158	152	14
-7	-2	6	90	97	19
-6	-2	6	0	68	1
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-4	-2	6	188	187	8
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3	-2	6	233	243	5
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6	-2	6	152	125	10
7	-2	6	215	236	9
8	-2	6	0	9	1
9	-2	6	38	56	38
-10	-1	6	0	56	1
-9	-1	6	164	158	12
-8	-1	6	31	77	31
-7	-1	6	109	108	13
-6	-1	6	56	35	27
-5	-1	6	233	210	9
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-1	-1	6	56	55	10
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2	-1	6	503	510	5
3	-1	6	213	214	7
4	-1	6	197	212	7
5	-1	6	79	76	15
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-3	0	7	0	23	1
-2	0	7	52	68	16
-1	0	7	37	24	20
2	0	7	322	323	5
3	0	7	89	83	12
4	0	7	161	157	10
5	0	7	81	96	16
6	0	7	224	250	8
7	0	7	44	66	43
8	0	7	0	10	1
-9	1	7	86	82	24
-8	1	7	80	71	21
-7	1	7	65	39	23
-6	1	7	0	39	1
-5	1	7	341	338	6
-4	1	7	234	219	6
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-2	1	7	149	148	8
-1	1	7	176	168	6
2	1	7	53	57	15
3	1	7	128	138	9
4	1	7	28	31	27
5	1	7	198	197	10
6	1	7	48	43	48
7	1	7	121	131	16
8	1	7	83	70	30
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-7	2	7	84	65	23
-6	2	7	167	145	8
-5	2	7	71	44	16
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-2	2	7	230	213	6
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2	2	7	436	452	5
4	2	7	63	48	21
5	2	7	87	93	16
6	2	7	134	130	14
7	2	7	62	35	48
8	2	7	77	82	37
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-7	3	7	102	109	12
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-5	3	7	273	283	6
-4	3	7	135	142	7
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-2	2	6	325	339	4
-1	2	6	329	320	3
0	2	6	554	560	5
1	2	6	184	185	5
2	2	6	148	158	6
3	2	6	113	105	7
4	2	6	263	254	8
5	2	6	49	62	42
6	2	6	284	274	8
7	2	6	128	123	14
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4	3	6	43	19	43
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7	3	6	169	157	13
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-5	8	7	26	72	25
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-3	8	6	76	34	17
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1	8	6	101	86	12
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5	8	6	80	69	30
-8	9	6	87	24	30
-7	9	6	121	115	17
-6	9	6	137	112	13
-5	9	6	204	217	9
-4	9	6	156	138	11
-3	9	6	62	8	21
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0	9	6	154	146	11
1	9	6	152	138	11
2	9	6	25	70	24
-7	10	6	70	29	32
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-1	10	6	0	21	1
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1	10	6	90	103	19
2	10	6	87	74	23
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-5	11	6	80	62	21
-4	11	6	82	122	21
-3	11	6	40	15	39
-2	11	6	59	53	35
-1	11	6	44	7	44
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1	11	6	76	27	33
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-3	12	6	122	78	17
-2	12	6	80	50	26
-1	12	6	26	44	26
0	12	6	32	42	32
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-6	-9	8	24	26	24
-5	-9	8	74	74	36
-4	-9	8	90	7	20
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-2	-9	8	44	21	44
-1	-9	8	133	146	14
0	-9	8	107	85	17
1	-9	8	60	84	35
2	-9	8	0	47	1
3	-9	8	91	86	20
4	-9	8	115	114	17
-7	-8	8	63	59	62
-6	-8	8	99	85	26
-5	-8	8	77	71	30
-4	-8	8	138	112	14
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-1	-8	8	215	218	9
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1	-8	8	230	234	9
2	-8	8	121	89	13
3	-8	8	205	198	13
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-2	-7	8	157	163	11
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2	-7	8	185	177	11
-8	-6	8	122	109	25
-7	-6	8	0	33	1
-6	-6	8	27	32	26
-5	-6	8	60	80	40
-4	-6	8	140	135	11
-3	-6	8	44	47	43
-2	-6	8	265	276	8
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1	-6	8	197	194	9
5	-6	8	78	48	21
6	-6	8	0	32	1
7	-6	8	99	93	23
8	-6	8	109	48	23
-9	-5	8	71	44	66
-8	-7	7	40	60	40
-7	-7	7	90	60	27
-6	-7	7	147	128	14
-5	-7	7	109	111	18
-4	-7	7	0	36	1
-3	-7	7	52	17	28
-2	-7	7	204	211	9
-1	-7	7	168	183	10
0	-7	7	177	172	10
1	-7	7	86	88	15
2	-7	7	77	69	21
5	-7	7	59	51	31
6	-7	7	192	198	11
7	-7	7	0	23	1
8	-7	7	0	35	1
-8	-6	7	87	74	37
-7	-6	7	115	125	19
-6	-6	7	170	160	15
-5	-6	7	175	174	12
-4	-6	7	94	93	15
-3	-6	7	122	139	10
-2	-6	7	0	30	1
-1	-6	7	209	212	8
0	-6	7	39	49	38
1	-6	7	284	292	7
3	-6	7	61	67	15
4	-6	7	0	40	1
5	-6	7	169	160	10
6	-6	7	53	40	53
7	-6	7	127	114	15
8	-6	7	0	13	1
-9	-5	7	0	61	1
-8	-5	7	0	24	1
-7	-5	7	0	42	1
-6	-5	7	61	41	44
-5	-5	7	203	192	9
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0	-5	7	241	225	7
1	-5	7	136	122	11
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-2	-3	8	37	49	37
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1	-3	8	312	320	5
2	-3	8	156	164	8
3	-3	8	41	22	33
4	-3	8	72	64	16
5	-3	8	144	142	10
6	-3	8	146	142	12
7	-3	8	30	45	29
8	-3	8	63	26	62
-10	-2	8	89	69	36
-9	-2	8	61	95	61
-8	-2	8	74	31	31
-7	-2	8	75	54	24
-6	-2	8	131	105	14
-5	-2	8	107	99	14
-4	-2	8	197	195	9
-3	-2	8	100	93	13
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-1	-2	8	80	104	12
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3	-2	8	40	57	40
4	-2	8	93	63	12
5	-2	8	0	36	1
6	-2	8	273	281	9
7	-2	8	13	47	12
8	-2	8	39	93	38
-10	-1	8	116	75	24
-9	-1	8	51	54	50
-8	-1	8	125	117	14
-7	-1	8	0	42	1
-6	-1	8	44	80	43
-5	-1	8	418	411	7
-4	-1	8	100	118	13
-3	-1	8	332	350	6
-2	-1	8	100	84	10
-1	-1	8	31	15	31
1	-1	8	501	499	5
2	-1	8	62	49	15
3	-1	8	273	267	7
4	-1	8	83	59	13
5	-1	8	22	10	22
6	-1	8	0	25	1
7	-1	8	139	131	15

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
-6	-2	7	226	211	8
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-4	-2	7	208	209	8
-3	-2	7	284	309	7
-2	-2	7	491	486	6
-1	-2	7	255	252	6
0	-2	7	118	115	5
1	-2	7	66	57	8
2	-2	7	209	211	6
3	-2	7	266	273	6
4	-2	7	185	174	8
5	-2	7	256	266	7
6	-2	7	85	80	14
7	-2	7	0	37	1
8	-2	7	5	31	4
-10	-1	7	62	92	62
-9	-1	7	69	81	40
-8	-1	7	145	117	13
-7	-1	7	186	163	11
-6	-1	7	143	124	11
-5	-1	7	375	360	7
-4	-1	7	48	33	24
-3	-1	7	172	168	8
-2	-1	7	101	97	9
-1	-1	7	454	468	5
1	-1	7	276	270	5
2	-1	7	64	53	13
3	-1	7	59	43	16
4	-1	7	182	179	8
5	-1	7	194	197	8
6	-1	7	89	100	17
7	-1	7	47	24	47
8	-1	7	0	39	1
-10	0	7	63	57	63
-9	0	7	74	31	30
-8	0	7	58	71	50
-7	0	7	0	70	1
-6	0	7	206	173	9
-5	0	7	131	114	11
1	2	8	51	37	16
2	2	8	149	134	8
3	2	8	156	145	11
4	2	8	226	221	9
5	2	8	67	76	26
6	2	8	167	159	13
7	2	8	0	38	1
-8	3	8	96	100	16
-7	3	8	118	121	12
-6	3	8	245	258	7
-5	3	8	18	47	18
-4	3	8	64	80	14
-3	3	8	0	64	1
-2	3	8	149	140	7
-1	3	8	237	252	6
0	3	8	303	292	6
1	3	8	137	136	8
2	3	8	159	166	8
4	3	8	93	101	17
5	3	8	212	181	11
6	3	8	30	41	30
7	3	8	121	106	20
-8	4	8	63	58	32
-7	4	8	72	89	20
-6	4	8	129	123	11
-5	4	8	161	175	8
-4	4	8	191	197	7
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-2	4	8	109	109	9
-1	4	8	64	80	15
0	4	8	277	282	6
1	4	8	71	57	13
2	4	8	155	150	9
4	4	8	14	54	13
5	4	8	62	54	43
6	4	8	139	127	16
7	4	8	30	34	30
-8	5	8	80	72	22
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-4	5	8	85	92	12
-3	5	8	97	109	12
-2	5	8	59	61	15
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0	5	8	254	272	6
1	5	8	169	161	8
2	5	8	235	223	7
4	5	8	80	75	25
5	5	8	0	22	1
6	5	8	108	82	26
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0	3	7	109	105	8
1	3	7	23	28	22
2	3	7	115	109	8
4	3	7	95	91	13
5	3	7	180	150	12
6	3	7	26	21	26
7	3	7	86	57	29
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-3	4	7	27	37	27
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2	4	7	108	98	10
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-3	5	7	211	213	7
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-1	5	7	351	358	6
0	5	7	37	14	37
1	5	7	193	201	7
2	5	7	63	54	17
5	5	7	218	185	12
6	5	7	0	17	1
7	5	7	80	49	43
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0	9	8	168	162	11
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-5	10	8	89	85	23
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0	10	8	78	48	23
1	10	8	116	75	17
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0	11	8	78	65	30
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1	-11	9	110	40	25
2	-11	9	124	72	22
3	-11	9	22	36	21
-4	-10	9	82	83	31
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-2	-10	9	0	5	1
-1	-10	9	34	37	34
0	-10	9	118	123	20
1	-10	9	35	68	35
2	-10	9	142	132	15
3	-10	9	0	39	1
4	-10	9	91	46	29
5	-10	9	102	78	33
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0	-11	8	0	18	1
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2	-11	8	155	136	16
3	-11	8	0	39	1
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3	-10	8	108	57	22
4	-10	8	89	15	26
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-1	1	9	180	187	7
1	1	9	168	155	7
2	1	9	0	26	1
3	1	9	49	9	32
4	1	9	231	230	8
5	1	9	186	166	13
6	1	9	93	107	21
7	1	9	48	60	48
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2	2	9	167	140	10
3	2	9	180	155	10
4	2	9	65	58	29
5	2	9	128	107	14
6	2	9	100	101	24
7	2	9	96	20	29
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-7	3	9	98	81	15
-6	3	9	52	60	35
-5	3	9	100	119	13
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-3	3	9	149	159	8
-2	3	9	237	232	7
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4	3	9	37	33	36
5	3	9	94	83	21
6	3	9	34	63	33
-8	4	9	51	54	50
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-6	4	9	69	63	19
-5	4	9	127	113	10
-4	4	9	95	110	11
-3	4	9	244	241	7
-2	4	9	0	25	1
-1	4	9	0	51	1
0	4	9	0	8	1
1	4	9	75	48	15
4	4	9	110	67	17
5	4	9	82	88	34
6	4	9	50	41	49
-8	5	9	164	142	13
-7	5	9	48	60	47
-6	5	9	128	133	16
-5	5	9	63	54	30
8	-1	8	39	22	39
-10	0	8	81	112	31
-9	0	8	118	89	18
-8	0	8	172	150	12
-7	0	8	163	144	13
-6	0	8	167	137	10
-5	0	8	0	41	1
-4	0	8	226	229	8
-3	0	8	304	308	6
-2	0	8	264	261	6
-1	0	8	106	89	8
2	0	8	288	294	6
3	0	8	90	91	14
4	0	8	67	54	21
5	0	8	0	13	1
6	0	8	142	143	13
7	0	8	45	26	45
8	0	8	9	76	8
-8	1	8	55	53	55
-7	1	8	32	25	32
-6	1	8	207	172	9
-5	1	8	258	242	8
-4	1	8	160	147	8
-3	1	8	222	234	7
-2	1	8	208	204	6
-1	1	8	288	288	5
2	1	8	157	153	7
3	1	8	360	353	7
4	1	8	71	62	18
5	1	8	125	128	13
6	1	8	33	43	33
7	1	8	116	73	19
8	1	8	71	29	47
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-4	2	8	109	86	9
-3	2	8	60	70	14
-2	2	8	211	198	6
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0	8	9	61	13	29
1	8	9	156	137	14
-7	9	9	48	20	48
-6	9	9	0	48	1
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-3	9	9	97	74	17
-2	9	9	112	97	13
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0	9	9	84	52	25
1	9	9	0	45	1
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-4	10	9	50	37	49
-3	10	9	51	57	51
-2	10	9	35	28	35
-1	10	9	92	71	19
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-1	-11	10	0	42	1
0	-11	10	0	7	1
1	-11	10	79	59	54
2	-11	10	0	32	1
-3	-10	10	69	46	51
-2	-10	10	84	75	34
-1	-10	10	68	20	42
0	-10	10	76	61	38
1	-10	10	70	11	47
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4	-10	10	29	48	29
-5	-9	10	51	12	51
-4	-9	10	0	18	1
-3	-9	10	26	58	25
-2	-9	10	37	34	37
-1	-9	10	159	157	12
0	-9	10	81	41	32
1	-9	10	73	62	32
2	-9	10	45	31	44
3	-9	10	136	106	18
4	-9	10	0	39	1
-6	-8	10	91	78	38
-5	-8	10	48	25	48
-4	-8	10	65	71	45
-3	-8	10	56	29	56
-2	-8	10	109	108	19
-1	-8	10	58	55	58
0	-8	10	180	171	13
1	-8	10	0	14	1
2	-8	10	155	146	15
3	-8	10	85	36	31
-7	-7	10	94	40	37

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

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-8	6	8	43	41	43
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-6	6	8	78	16	17
-5	6	8	117	115	10
-4	6	8	78	72	16
-3	6	8	321	332	7
-2	6	8	57	82	20
-1	6	8	71	59	14
0	6	8	23	46	22
1	6	8	172	158	9
2	6	8	154	135	10
5	6	8	15	22	15
-8	7	8	95	91	21
-7	7	8	98	57	18
-6	7	8	94	94	16
-5	7	8	38	50	37
-4	7	8	60	40	24
-3	7	8	38	41	37
-2	7	8	125	125	10
-1	7	8	46	58	31
0	7	8	0	34	1
1	7	8	75	44	18
5	7	8	52	49	52
-8	8	8	0	7	1
-7	8	8	95	79	23
-6	8	8	0	46	1
-5	8	8	39	9	39
-4	8	8	78	83	18
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-2	8	8	42	50	42
-1	8	8	212	215	8
0	8	8	0	16	1
1	8	8	75	69	19
-7	9	8	95	9	25
-6	9	8	151	155	16
-5	9	8	16	62	16
-1	-4	10	166	162	9
0	-4	10	158	146	11
1	-4	10	122	126	13
5	-4	10	27	22	26
6	-4	10	56	42	55
7	-4	10	91	26	28
-9	-3	10	0	39	1
-8	-3	10	68	68	55
-7	-3	10	98	53	24
-6	-3	10	96	101	22
-5	-3	10	0	41	1
-4	-3	10	70	45	21
-3	-3	10	97	87	13
-2	-3	10	43	45	42
-1	-3	10	198	194	9
0	-3	10	92	117	14
3	-3	10	55	65	27
4	-3	10	114	122	12
5	-3	10	149	158	11
6	-3	10	0	35	1
7	-3	10	35	19	35
-9	-2	10	39	38	39
-8	-2	10	34	82	34
-7	-2	10	103	105	19
-6	-2	10	151	155	13
-5	-2	10	117	110	14
-4	-2	10	44	57	44
-3	-2	10	0	36	1
-2	-2	10	166	185	10
-1	-2	10	138	144	11
0	-2	10	230	252	9
1	-2	10	309	307	6
2	-2	10	57	37	22
3	-2	10	0	35	1
4	-2	10	89	78	14
5	-2	10	161	153	12
6	-2	10	107	114	19
7	-2	10	84	63	28
-9	-1	10	0	43	1
-8	-1	10	60	71	60
-7	-1	10	48	59	48
-6	-1	10	134	128	14
-5	-1	10	136	136	10
-4	-1	10	276	281	7
-3	-1	10	40	64	39
-2	-1	10	90	85	12
-1	-1	10	192	195	9
0	-1	10	177	165	8
1	-1	10	126	119	9
2	-1	10	84	64	16
3	-1	10	136	131	11
4	-1	10	0	19	1
5	-1	10	56	41	39
6	-1	10	105	95	18
-1	-8	9	0	35	1
0	-8	9	87	83	21
1	-8	9	34	46	33
2	-8	9	188	177	12
3	-8	9	100	79	26
-7	-7	9	95	128	25
-6	-7	9	59	36	59
-5	-7	9	0	47	1
-4	-7	9	81	72	24
-3	-7	9	147	151	11
-2	-7	9	69	82	25
-1	-7	9	262	281	9
0	-7	9	56	27	33
1	-7	9	99	106	16
2	-7	9	0	39	1
-8	-6	9	0	33	1
-7	-6	9	94	46	23
-6	-6	9	166	152	15
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1	-6	9	90	113	15
2	-6	9	40	37	40
-8	-5	9	93	72	30
-7	-5	9	160	138	13
-6	-5	9	66	58	44
-5	-5	9	129	138	13
-4	-5	9	72	83	22
-3	-5	9	12	22	11
-2	-5	9	84	103	16
-1	-5	9	297	305	8
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-4	3	10	0	50	1
-3	3	10	66	59	15
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0	3	10	162	150	9
1	3	10	95	72	11
4	3	10	202	194	12
5	3	10	102	119	20
6	3	10	82	82	43
-9	4	10	0	29	1
-8	4	10	71	34	34
-7	4	10	122	123	14
-6	4	10	0	38	1
-5	4	10	141	144	10
-4	4	10	0	15	1
-3	4	10	61	63	18
-2	4	10	0	11	1
-1	4	10	258	241	8
0	4	10	72	41	15
1	4	10	243	226	8
4	4	10	90	53	25
5	4	10	61	86	60
-9	5	10	81	44	34
-8	5	10	72	30	36
-7	5	10	76	48	34
-6	5	10	105	97	18
-5	5	10	29	40	28
-4	5	10	113	120	14
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-2	5	10	78	99	13
-1	5	10	66	67	17
0	5	10	164	170	9
1	5	10	64	63	23
4	5	10	60	20	60
5	5	10	17	26	16
-8	6	10	0	84	1
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1	6	10	141	143	12
4	6	10	97	28	30
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-7	7	10	79	54	28
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7	-2	9	80	56	30
8	-2	9	70	65	47
-10	-1	9	46	19	46
-9	-1	9	89	74	29
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-7	-1	9	126	125	14
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-5	-1	9	58	68	24
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4	-1	9	79	88	17
5	-1	9	166	148	10
6	-1	9	101	106	20
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-7	0	9	153	130	13
-6	0	9	135	98	11
-5	0	9	297	292	7
-4	0	9	43	37	42
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-2	0	9	159	154	8
-1	0	9	167	171	8
2	0	9	0	17	1
3	0	9	0	31	1
4	0	9	294	281	8
5	0	9	75	73	25
6	0	9	106	110	16
7	0	9	96	22	26
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-7	-3	11	86	77	38
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-4	8	9	91	83	16
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-2	8	9	54	36	30
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4	-1	11	184	153	11
5	-1	11	91	29	21
6	-1	11	68	58	41
-4	0	11	42	25	42
-3	0	11	189	201	9
-2	0	11	86	87	15
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0	0	11	0	29	1
2	0	11	9	42	8
3	0	11	158	158	11
4	0	11	0	47	1
5	0	11	124	116	18
6	0	11	0	10	1
-1	1	11	85	78	13
1	1	11	63	48	21
2	1	11	14	34	14
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4	1	11	197	215	11
5	1	11	62	7	62
6	1	11	110	79	24
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3	2	11	49	15	49
4	2	11	89	49	29
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1	-7	10	161	145	14
2	-7	10	0	23	1
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-5	-6	10	57	45	57
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-3	-6	10	139	152	14
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-2	-7	12	39	48	39
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-6	-6	12	75	60	41
-5	-6	12	152	124	16
-4	-6	12	47	45	46
-3	-6	12	69	76	37
-2	-6	12	20	21	19
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0	-6	12	76	43	28
1	-6	12	148	121	15
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-6	-5	12	0	38	1
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-1	-5	12	59	54	49
0	-5	12	94	102	24
1	-5	12	68	54	32
2	-5	12	141	138	14
-7	-4	12	28	52	28
-6	-4	12	82	58	30
-5	-4	12	24	55	23
-4	-4	12	0	20	1
-3	-4	12	106	105	17

Table B-15, Continued

Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s
7	-1	10	77	39	44
-6	0	10	80	54	20
-5	0	10	257	252	8
-4	0	10	70	79	18
-3	0	10	261	276	7
-2	0	10	53	32	25
-1	0	10	171	167	9
2	0	10	70	67	17
3	0	10	51	52	51
4	0	10	43	59	42
5	0	10	90	77	21
6	0	10	66	67	35
7	0	10	117	59	24
-3	1	10	48	36	29
-2	1	10	253	268	7
-1	1	10	53	37	21
1	1	10	9	52	9
3	1	10	246	233	9
4	1	10	155	125	12
5	1	10	99	61	22
6	1	10	71	34	38
-8	2	10	0	23	1
-1	2	10	150	141	9
0	2	10	42	44	38
1	2	10	91	91	10
3	2	10	217	209	9
4	2	10	82	77	24
5	2	10	71	57	33
6	2	10	0	45	1
-9	3	10	57	13	56
-8	3	10	99	113	19
-7	3	10	81	102	20
-6	3	10	68	75	22
-2	0	12	0	35	1
-1	0	12	188	170	10
0	0	12	154	135	11
1	0	12	140	125	12
2	0	12	45	19	44
3	0	12	88	79	19
4	0	12	47	29	47
5	0	12	33	17	33
0	1	12	83	90	14
2	1	12	192	189	10
3	1	12	92	30	22
4	1	12	0	18	1
5	1	12	65	24	64
-8	2	12	75	80	39
-7	2	12	81	5	24
-3	2	12	123	97	10
-2	2	12	53	56	26
-1	2	12	0	44	1
0	2	12	41	43	40
3	2	12	213	188	12
4	2	12	68	29	45
5	2	12	107	60	30
-8	3	12	58	62	58
-7	3	12	115	80	18
-6	3	12	0	25	1
-5	3	12	65	40	22
-4	3	12	0	35	1
-3	3	12	76	91	18
-2	3	12	80	66	15
-1	3	12	72	111	18
0	3	12	84	66	16
3	3	12	98	71	23
4	3	12	0	52	1
-8	4	12	56	30	55
-7	4	12	0	22	1
-6	4	12	120	106	14
-5	4	12	55	33	30
-4	4	12	0	50	1
-3	4	12	103	84	14
-2	4	12	123	129	12
-1	4	12	114	98	15
0	4	12	113	126	13
3	4	12	83	59	37
4	4	12	86	73	44
-7	5	12	89	93	28
-6	5	12	48	29	47
-5	5	12	103	107	16
-4	5	12	0	28	1
-3	5	12	40	19	40
-2	5	12	25	54	24
-1	5	12	128	116	11
0	5	12	103	77	15
-7	6	12	27	44	27
-6	6	12	92	90	21
-5	6	12	0	17	1
-4	6	12	98	94	16
-3	6	12	64	54	25
-1	7	10	60	51	26
0	7	10	68	40	23
1	7	10	0	55	1
-7	8	10	0	2	1
-6	8	10	0	59	1
-5	8	10	52	69	52
-4	8	10	0	58	1
-3	8	10	72	78	23
-2	8	10	55	46	28
-1	8	10	150	135	12
0	8	10	98	58	17
-6	9	10	27	24	27
-5	9	10	40	49	39
-4	9	10	23	21	22
-3	9	10	78	53	21
-2	9	10	82	64	19
-1	9	10	80	60	24
0	9	10	9	26	9
-3	10	10	68	11	33
-2	10	10	0	23	1
-1	10	10	81	84	28
-2	-10	11	42	16	42
-1	-10	11	83	15	35
0	-10	11	130	63	21
1	-10	11	62	46	61
2	-10	11	75	66	41
-4	-9	11	0	28	1
-3	-9	11	72	44	43
-2	-9	11	0	20	1
-1	-9	11	58	64	57
0	-9	11	0	30	1
1	-9	11	129	103	18
2	-9	11	81	44	44
-1	6	12	0	11	1
0	6	12	74	79	22
-6	7	12	70	37	41
-5	7	12	69	63	32
-4	7	12	44	18	44
-3	7	12	52	68	51
-2	7	12	30	39	30
-1	7	12	40	29	39
0	7	12	45	45	44
-4	8	12	57	60	36
-3	8	12	66	41	31
-2	8	12	72	63	27
-1	8	12	80	23	28
-3	-8	13	59	52	59
-2	-8	13	65	8	65
-1	-8	13	51	10	50
0	-8	13	0	19	1
1	-8	13	92	70	32
-4	-7	13	72	78	39
-3	-7	13	0	19	1
-2	-7	13	132	99	17
-1	-7	13	77	41	43
0	-7	13	73	2	47
1	-7	13	0	39	1
2	-7	13	0	45	1
-5	-6	13	78	33	37
-4	-6	13	42	25	42
-3	-6	13	57	108	57
-2	-6	13	0	37	1
-1	-6	13	82	83	31
0	-6	13	14	43	13
1	-6	13	89	33	30
2	-6	13	16	27	16
3	-6	13	113	77	29
-6	-5	13	35	74	34
-5	-5	13	86	38	28
-4	-5	13	0	29	1
-3	-5	13	54	37	54
-2	-5	13	180	147	13
-1	-5	13	29	59	29
0	-5	13	134	119	16
1	-5	13	84	13	28
2	-5	13	83	59	34
-7	-4	13	45	65	44
-6	-4	13	27	62	27
-5	-4	13	108	77	22
-4	-4	13	0	68	1
-3	-4	13	20	30	20
-2	-4	13	0	43	1
-1	-4	13	155	136	14
0	-4	13	79	39	29
1	-4	13	118	127	15
2	-4	13	0	36	1
-7	-3	13	0	32	1
-6	-3	13	98	52	25
-5	-3	13	89	59	25
-4	-3	13	75	45	29
-5	-3	11	89	45	22
-4	-3	11	92	88	15
-3	-3	11	73	95	19
-2	-3	11	85	86	17
-1	-3	11	166	145	10
0	-3	11	86	110	15
5	-3	11	0	13	1
6	-3	11	115	101	18
-9	-2	11	105	85	32
-8	-2	11	16	48	15
-7	-2	11	58	35	57
-6	-2	11	47	41	47
-5	-2	11	162	155	12
-4	-2	11	88	83	15
-3	-2	11	197	199	9
-2	-2	11	57	74	26
-1	-2	11	120	111	13
0	-2	11	73	14	18
2	-2	11	78	42	18
3	-2	11	100	94	14
4	-2	11	57	67	37
5	-2	11	0	56	1
6	-2	11	0	47	1
-7	-1	11	55	73	55
-6	-1	11	120	101	16
-5	-1	11	0	10	1
-4	-1	11	190	180	9
-3	-1	11	0	45	1
-2	-1	11	202	207	9
-1	-1	11	40	79	40
0	-1	11	0	42	1
1	-1	11	44	11	43
2	-1	11	160	156	9
-2	-3	13	0	19	1
-1	-3	13	60	51	30
0	-3	13	113	108	16
1	-3	13	121	113	17
-6	-2	13	63	42	56
-5	-2	13	99	91	21
-4	-2	13	72	78	30
-3	-2	13	70	52	26
-2	-2	13	77	55	24
-1	-2	13	90	36	18
0	-2	13	99	59	18
1	-2	13	137	106	17
-3	-1	13	127	111	13
-2	-1	13	86	61	19
-1	-1	13	47	49	47
0	-1	13	72	45	25
1	-1	13	132	118	14
3	0	13	121	110	17
4	0	13	42	86	41
0	1	13	65	65	25
2	1	13	0	16	1
3	1	13	56	68	56
4	1	13	85	68	34
-8	2	13	63	28	62
-7	2	13	88	51	27
-6	2	13	99	99	20
-5	2	13	0	22	1
-4	2	13	80	55	17
-3	2	13	0	36	1
-2	2	13	77	83	19
-1	2	13	59	56	25
0	2	13	110	110	13
2	2	13	21	24	21
3	2	13	0	13	1
4	2	13	92	69	32
-7	3	13	0	24	1
-6	3	13	0	34	1
-5	3	13	114	111	15
-4	3	13	0	9	1
-3	3	13	48	57	47
-2	3	13	45	30	45
-1	3	13	38	65	37
0	3	13	59	63	28
3	3	13	0	30	1
-7	4	13	121	46	19
-6	4	13	100	89	20
-5	4	13	0	31	1
-4	4	13	103	81	14
-3	4	13	0	45	1
-2	4	13	47	27	46
-1	4	13	85	51	19
0	4	13	82	71	18
-6	5	13	0	46	1
-5	5	13	84	95	28
-4	5	13	0	10	1
-3	5	13	132	119	12
-2	5	13	0	39	1
0	4	11	13	28	13
1	4	11	105	96	14
4	4	11	80	25	40
-8	5	11	0	44	1
-7	5	11	0	83	1
-6	5	11	42	30	42
-5	5	11	0	24	1
-4	5	11	140	102	13
-3	5	11	175	180	9
-2	5	11	62	63	23
-1	5	11	98	101	12
0	5	11	0	14	1
4	5	11	25	61	25
-8	6	11	34	65	33
-7	6	11	0	3	1
-6	6	11	103	84	18
-5	6	11	45	47	45
-4	6	11	41	26	41
-3	6	11	89	97	15
-2	6	11	163	152	11
-1	6	11	98	93	13
0	6	11	106	105	13
-7	7	11	122	88	17
-6	7	11	42	19	41
-5	7	11	84	83	23
-4	7	11	0	51	1
-3	7	11	49	59	49
-2	7	11	0	25	1
-1	7	11	41	42	41
0	7	11	52	54	51
-6	8	11	56	69	55
-5	8	11	77	5	23
-4	8	11	38	43	37
-5	6	13	6	11	6
-4	6	13	0	42	1
-3	6	13	28	42	27
-2	6	13	103	85	17
-1	6	13	108	70	16
-4	7	13	8	44	7
-3	7	13	74	48	24
-2	7	13	64	18	32
-1	7	13	0	44	1
-2	-7	14	55	45	55
-1	-7	14	6	43	6
0	-7	14	83	32	43
-4	-6	14	115	61	24
-3	-6	14	0	24	1
-2	-6	14	37	18	37
-1	-6	14	152	118	18
0	-6	14	82	24	39
1	-6	14	118	57	26
2	-6	14	0	10	1
-5	-5	14	78	41	43
-4	-5	14	98	101	24
-3	-5	14	0	62	1
-2	-5	14	0	33	1
-1	-5	14	0	68	1
0	-5	14	47	50	46
1	-5	14	0	29	1
2	-5	14	71	45	56
-6	-4	14	41	37	40
-5	-4	14	67	41	66
-4	-4	14	109	81	19
-3	-4	14	78	29	33
-2	-4	14	111	64	23
-1	-4	14	70	26	42
0	-4	14	75	46	34
1	-4	14	130	89	17
2	-4	14	73	18	52
-6	-3	14	93	35	32
-5	-3	14	50	29	50
-4	-3	14	81	73	29
-3	-3	14	88	83	23
-2	-3	14	54	54	53
-1	-3	14	79	66	29
0	-3	14	45	66	45
1	-3	14	60	30	60
2	-3	14	64	62	52
-3	-2	14	0	62	1
-2	-2	14	88	84	25
-1	-2	14	39	38	39
0	-2	14	106	81	20
1	-2	14	74	25	33
0	-1	14	75	32	28
1	-1	14	129	105	20
-1	1	14	85	69	17
3	1	14	94	56	26
-6	2	14	35	25	34
-5	2	14	0	9	1
-4	2	14	57	75	38
-2	-4	12	0	20	1
-1	-4	12	134	121	13
0	-4	12	36	51	35
1	-4	12	98	81	18
-8	-3	12	160	89	18
-7	-3	12	82	77	32
-6	-3	12	0	57	1
-5	-3	12	79	51	26
-4	-3	12	97	57	18
-3	-3	12	0	45	1
-2	-3	12	143	110	12
-1	-3	12	51	19	51
0	-3	12	180	165	12
1	-3	12	0	25	1
-7	-2	12	102	88	27
-6	-2	12	0	51	1
-5	-2	12	35	63	34
-4	-2	12	40	26	40
-3	-2	12	132	112	12
-2	-2	12	110	83	15
-1	-2	12	202	218	9
0	-2	12	109	94	12
5	-2	12	131	118	18
-5	-1	12	136	121	14
-4	-1	12	113	99	13
-3	-1	12	98	79	14
-2	-1	12	137	117	11
-1	-1	12	70	27	23
0	-1	12	178	138	10
2	-1	12	97	81	14
3	-1	12	41	25	41
4	-1	12	76	47	29
5	-1	12	9	54	9
-2	2	14	82	74	17
-1	2	14	28	31	28
2	2	14	86	90	32
-6	3	14	89	77	23
-5	3	14	78	93	23
-4	3	14	64	23	27
-3	3	14	112	76	14
-2	3	14	0	46	1
-1	3	14	0	49	1
0	3	14	0	18	1
-5	4	14	77	28	26
-4	4	14	28	58	28
-3	4	14	0	21	1
-2	4	14	113	90	15
-1	4	14	0	26	1
-4	5	14	0	5	1
-3	5	14	61	57	35
-2	5	14	74	57	23
-1	5	14	95	96	18
-3	6	14	24	54	23
-2	6	14	18	8	18
-3	-5	15	73	88	73
-2	-5	15	53	55	53
-1	-5	15	107	74	27
0	-5	15	57	38	57
-4	-4	15	29	41	28
-3	-4	15	62	18	62
-2	-4	15	25	83	24
-1	-4	15	57	34	56
0	-4	15	72	38	44
1	-4	15	80	13	42
-4	-3	15	25	47	25
-3	-3	15	0	26	1
-2	-3	15	77	18	39
-1	-3	15	39	62	39
0	-3	15	95	49	30
1	-3	15	96	63	27
2	-3	15	61	20	61
0	-2	15	53	61	52
1	-2	15	70	9	45
2	-2	15	78	40	52
-2	1	15	42	41	41
-1	1	15	73	86	34
-5	2	15	81	73	27
-4	2	15	0	29	1
-3	2	15	36	35	35
-2	2	15	31	67	30
-1	2	15	109	67	16
-4	3	15	12	12	12
-3	3	15	0	24	1
-2	3	15	54	22	53
-1	3	15	83	43	24
-3	4	15	57	20	56
-2	4	15	39	46	38

Table B-15, Continued
Observed and Calculated Structure Factors for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-2	6	12	0	33	1	-3	-3	13	0	46	1	-1	5	13	68	34	25	-3	2	14	0	21	1						

APPENDIX C

Crystallography Data for 1,6-diferrocenylhexane

Equations of Mean Plane for 1,6-diferrocenylhexane

Table C-1

-0.2261 * XO + 0.6969* YO + 0.6806 * ZO = 4.7724
-2.8817 * x + 5.8496 * y –7.2697 * z = 4.7724

Deviation	Weight	Name
0.0044	1.00	C1
-0.0060	1.00	C2
0.0053	1.00	C3
-0.0024	1.00	C4
-0.0014	1.00	C5

Table C-2

-0.2333 * XO + 0.7141 * YO + 0.6601 * ZO = 1.6922
-2.9738* x + 5.9936 * y –7.0773 * z = 1.6922

Deviation	Weight	Name
-0.0040	1.00	C6
0.0037	1.00	C7
-0.0019	1.00	C8
-0.0006	1.00	C9
0.0028	1.00	C10

Table C-3
Observed and Calculated Structure Factor Tables for 1,6-diferrocenylhexane

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	0	0	472	449	8	7	5	0	65	65	3	4	1	1	524	502	5	-7	4	1	3	1	3	-7	7	1	135	136	3
2	0	0	1175	1141	4	8	5	0	23	12	11	5	1	1	247	233	1	-6	4	1	165	171	2	-6	7	1	31	16	18
3	0	0	1485	1540	5	9	5	0	118	101	4	6	1	1	627	618	1	-5	4	1	146	150	2	-5	7	1	95	92	3
4	0	0	78	81	3	10	5	0	50	34	8	7	1	1	209	204	1	-4	4	1	177	175	2	-4	7	1	155	150	2
5	0	0	565	547	3	11	5	0	62	63	7	8	1	1	350	350	2	-3	4	1	115	114	2	-3	7	1	50	51	5
6	0	0	319	321	3	12	5	0	0	24	1	9	1	1	358	371	2	-2	4	1	151	146	1	-2	7	1	140	138	2
7	0	0	195	207	3	13	5	0	0	7	1	10	1	1	72	69	3	-1	4	1	180	187	1	-1	7	1	131	140	2
8	0	0	464	476	3	14	5	0	41	32	16	11	1	1	180	184	2	0	4	1	339	332	2	0	7	1	200	210	2
9	0	0	122	132	10	0	6	0	323	321	8	12	1	1	83	73	4	1	4	1	89	76	2	1	7	1	164	157	3
10	0	0	295	309	5	1	6	0	104	106	2	13	1	1	79	64	6	2	4	1	114	116	2	2	7	1	0	15	1
11	0	0	168	188	4	2	6	0	251	242	3	14	1	1	92	86	4	3	4	1	215	211	2	3	7	1	219	211	4
12	0	0	36	42	9	3	6	0	176	175	2	15	1	1	48	20	7	4	4	1	98	103	2	4	7	1	134	140	2
13	0	0	113	129	8	4	6	0	52	42	3	16	1	1	52	46	8	5	4	1	187	197	2	5	7	1	26	18	13
14	0	0	58	57	11	5	6	0	195	189	4	-16	2	1	0	16	1	6	4	1	31	9	5	6	7	1	164	161	2
15	0	0	60	46	14	6	6	0	106	113	3	-15	2	1	27	0	18	7	4	1	48	47	3	7	7	1	94	109	3
16	0	0	61	61	18	7	6	0	33	6	14	-14	2	1	29	17	16	8	4	1	93	95	2	8	7	1	67	72	5
1	1	0	80	66	1	8	6	0	165	158	4	-13	2	1	21	3	21	9	4	1	17	6	17	9	7	1	109	94	3
2	1	0	523	500	1	9	6	0	63	62	7	-12	2	1	51	43	5	10	4	1	35	31	17	10	7	1	24	5	24
3	1	0	187	168	1	10	6	0	87	91	5	-11	2	1	47	42	4	11	4	1	2	8	2	11	7	1	37	41	21
4	1	0	164	163	1	11	6	0	74	74	7	-10	2	1	36	36	6	12	4	1	27	21	26	12	7	1	46	36	45
5	1	0	106	99	2	12	6	0	0	7	1	-9	2	1	25	28	9	13	4	1	24	7	24	-12	8	1	59	17	19
6	1	0	138	140	2	13	6	0	65	55	14	-8	2	1	142	153	2	14	4	1	0	17	1	-11	8	1	55	40	12
7	1	0	87	88	2	14	6	0	14	35	14	-7	2	1	82	57	1	15	4	1	30	27	30	-10	8	1	0	7	1
8	1	0	117	115	1	1	7	0	39	50	5	-6	2	1	79	63	2	-15	5	1	58	57	12	-9	8	1	68	59	8
9	1	0	16	4	15	2	7	0	112	110	3	-5	2	1	82	81	1	-14	5	1	37	19	17	-8	8	1	113	99	4
10	1	0	0	6	1	3	7	0	85	75	3	-4	2	1	32	45	2	-13	5	1	66	75	8	-7	8	1	0	9	1
11	1	0	56	54	4	4	7	0	116	109	3	-3	2	1	153	150	2	-12	5	1	106	104	5	-6	8	1	163	178	4
12	1	0	42	39	7	5	7	0	50	41	5	-2	2	1	230	203	1	-11	5	1	44	8	9	-5	8	1	107	93	4
13	1	0	21	14	21	6	7	0	125	124	3	-1	2	1	142	118	1	-10	5	1	154	169	3	-4	8	1	101	88	4
14	1	0	13	5	13	7	7	0	84	84	3	0	2	1	500	469	3	-9	5	1	106	96	2	-3	8	1	129	139	3
15	1	0	0	8	1	8	7	0	61	59	5	1	2	1	773	754	7	-8	5	1	136	133	3	-2	8	1	41	31	14
16	1	0	27	4	26	9	7	0	73	69	7	2	2	1	40	56	1	-7	5	1	208	210	3	-1	8	1	61	72	5
0	2	0	578	544	9	10	7	0	0	23	1	3	2	1	264	247	1	-6	5	1	73	76	3	0	8	1	93	100	4
1	2	0	315	328	2	11	7	0	0	14	1	4	2	1	236	224	1	-5	5	1	357	358	3	1	8	1	9	4	9
2	2	0	580	588	3	12	7	0	47	48	15	5	2	1	86	82	1	-4	5	1	277	278	4	2	8	1	149	163	3
3	2	0	555	520	4	13	7	0	0	10	1	6	2	1	160	140	1	-3	5	1	158	145	2	3	8	1	65	52	5
4	2	0	7	31	6	0	8	0	158	144	6	7	2	1	168	182	1	-2	5	1	501	518	3	4	8	1	151	141	10
5	2	0	532	535	2	1	8	0	67	79	5	8	2	1	72	67	3	-1	5	1	199	186	2	5	8	1	113	122	3
6	2	0	413	403	2	2	8	0	146	151	4	9	2	1	4	22	3	0	5	1	434	420	5	6	8	1	54	63	6
7	2	0	58	61	2	3	8	0	143	141	5	10	2	1	31	33	7	1	5	1	510	531	2	7	8	1	99	97	5
8	2	0	455	461	2	4	8	0	0	26	1	11	2	1	62	56	3	2	5	1	51	55	2	8	8	1	18	19	17
9	2	0	124	130	2	5	8	0	146	140	5	12	2	1	26	9	12	3	5	1	384	372	3	9	8	1	32	21	17
10	2	0	138	147	2	6	8	0	105	100	4	13	2	1	27	16	16	4	5	1	334	334	5	10	8	1	31	41	30
11	2	0	219	228	5	7	8	0	67	73	5	14	2	1	0	5	1	5	5	1	133	142	2	11	8	1	62	28	11
12	2	0	40	4	6	8	8	0	107	106	4	15	2	1	0	9	1	6	5	1	269	270	2	-10	9	1	64	43	21
13	2	0	114	118	5	9	8	0	23	4	22	16	2	1	0	0	1	7	5	1	78	67	4	-9	9	1	82	53	12
14	2	0	69	53	5	10	8	0	80	56	8	-16	3	1	37	22	17	8	5	1	141	145	2	-8	9	1	29	34	29
15	2	0	52	32	6	11	8	0	48	38	15	-15	3	1	56	64	6	9	5	1	168	176	4	-7	9	1	112	107	5
16	2	0	57	51	7	1	9	0	84	90	6	-14	3	1	38	18	8	10	5	1	0	22	1	-6	9	1	52	24	12
1	3	0	54	52	1	2	9	0	105	83	12	-13	3	1	102	93	3	11	5	1	128	133	9	-5	9	1	108	111	6
2	3	0	232	216	3	3	9	0	53	42	10	-12	3	1	111	113	3	12	5	1	70	61	7	-4	9	1	93	96	6
3	3	0	57	53	1	4	9	0	134	145	4	-11	3	1	77	90	7	13	5	1	16	28	16	-3	9	1	26	35	25
4	3	0	111	113	1	5	9	0	18	27	18	-10	3	1	191	200	2	14	5	1	62	60	9	-2	9	1	129	126	6
5	3	0	58	48	2	6	9	0	92	98	9	-9	3	1	77	85	3	-14	6	1	26	27	26	-1	9	1	57	68	15
6	3	0	243	251	2	7	9	0	71	59	7	-8	3	1	213	207	2	-13	6	1	38	29	16	0	9	1	59	61	9
7	3	0	54	48	2	8	9	0	42	21	16	-7	3	1	501	515	2	-12	6	1	19	8	19	1	9	1	140	135	4
8	3	0	84	70	2	9	9	0	0	30	1	-6	3	1	12	8	12	-11	6	1	86	71	6	2	9	1	42	33	11
9	3	0	51	49	5	10	9	0	25	24	25	-5	3	1	578	556	3	-10	6	1	51	67	9	3	9	1	118	124	4
10	3	0	48	38	4	0 1	0	0	33	21	32	-4	3	1	703	690	3	-9	6	1	49	40	13	4	9	1	95	87	5
11	3	0	30	17	8	1 1	0	0	71	33	9	-3	3	1	189	176	1	-8	6	1	140	143	2	5	9	1	58	60	8
12	3	0	0	3	1	2 1	0	0	34	17	33	-2	3	1	785	760	3	-7	6	1	60	49	3	6	9	1	106	95	5
13	3	0	0	3	1	3 1	0	0	60	60	12	-1	3	1	64	48	1	-6	6	1	97	79	3	7	9	1	5	9	5
14	3	0	50	20	9	4 1	0	0	41	12	22	0	3	1	245	238	1	-5	6	1	59	63	3	8	9	1	87	68	6
15	3	0	24	5	24	5 1	0	0	78	66	18	1	3	1	290	307	3	-4	6	1	83	83	2	9	9	1	0	34	1
16	3	0	29	15	28	6 1	0	0	52	34	15	2	3	1	33	15	2	-3	6	1	123	122	1	-7	10	1	57	5	14
0	4	0	769	773	6	7 1	0	0	55	43	16	3	3	1	619	600	3	-2	6	1	77	79	2	-6	10	1	74	51	18
1	4	0	234	215	1	-17	1	1	47	25	20	4	3	1	283	279	2	-1	6	1	110	113	2	-5	10	1	45	24	18
2	4	0	506	462	1	-16	1	1	65	32	8	5	3	1	112	112	1	0	6	1	196	196	2	-4	10	1	61	52	11
3	4	0	701	707	4	-15	1	1	61	76	6	6	3	1	487	503	5	1	6	1	29	16	5	-3	10	1	62	59	11
4	4	0	69	68	1	-14	1	1	33	21	10	7	3	1	151	149	1	2	6	1	118	114	2	-2	10	1	14	1	13
5	4	0	509	512	3	-13	1	1	120	130	3	8	3	1	231	240	3	3	6	1	156	164	2	-1	10	1	50	66	15
6	4	0	361	353	3	-12	1	1	122	142	3	9	3	1	245	246	2	4	6	1	58	72	3	0	10	1	76	68	9
7	4	0	217	210	2	-11	1	1	59	58	5	10	3	1	29	20	8	5	6	1	45	42	5	1	10	1	58	24	13
8	4	0	256	267	1	-10	1	1	298	307	6	11	3	1	192	204	3	6	6	1	55	49	4	2	10	1	92	89	7
9	4	0	93	88	2	-9	1	1	140	148	2	12	3	1	110	113	4	7	6	1	87	74	3	3	10	1	57	44	11
10	4	0	164	174	2	-8	1	1	248	256	3	13	3	1	75	62	9	8	6	1	0	12	1	4	10	1	57	54	30
11	4	0	149	163	3	-7	1	1	279	287	1	14	3	1	78	85	12	9	6	1	43	42	11	5	10	1	71	65	8
12	4	0	39	33	10	-6	1	1	56	60	1	15	3	1	47	20	10	10	6	1	66	44	8	6	10	1	0	9	1
13	4	0	117	115	5	-5	1	1	421	440	1	16	3	1	70	34	13	11	6	1	25	16	25	7	10	1	47	34	16
14	4	0	52	43	9	-4	1	1	452	432	3	-15	4	1	0	5	1	12	6	1	26	27	26	-17	0	2	75	43	16
15	4	0	33	34	25	-3	1	1	210	216	2	-14	4	1	0	23	1	13	6	1	64	43	10	-16	0	2	0	20	1
1	5	0	211	214	2	-2	1	1	1606	1593	4	-13	4	1	36	36	13	-13	7	1	50	46	13	-15	0	2	51	65	10
2	5	0	194	203	1	-1	1	1	605	582	8	-12	4	1	22	19	22	-12	7	1	51	46	12	-14	0	2	111	117	6
3	5	0	48	21	2	0	1	1	994	956	5	-11	4	1	49	56	5	-11	7	1	16	18	16	-13	0	2	0	20	1
4	5	0	130	131	2	1	1	1	1420	1393	11	-10	4	1	96	102	3	-10	7	1	109	102	7	-12	0	2	180	196	3
5	5	0	151	145	2	2	1	1	208	196	1	-9	4	1	94	94	3	-9	7	1	46	57	11	-11	0	2	178	209	3
6	5	0	67	59	3	3	1	1	494	476	4	-8	4	1	121	109	2	-8	7	1	119	112	3	-10	0	2	116	128	5
-9	0	2	310	326	12	11	2	2	74	67	3	3	5	2	141	147	3	10	8	2	44	37	16	4	2	3	103	101	2
-8	0	2	94	89	3	12	2	2	125	134	3	4	5	2	104	101	2	11	8	2	56	12	18	5	2	3	25	16	3
-7	0	2	143	173	3	13	2	2	57	33	8	5	5	2	118	119	2	-10	9	2	61	35	22	6	2	3	107	110	1
-6	0	2	261	252	3	14	2	2	70	61	17	6	5	2	79	89	4	-7	9	2	61	54	10	7	2	3	31	28	4

Table C-3, Continued
Observed and Calculated Structure Factor Tables for 1,6-diferrocenylhexane

h	k	l	10Fo	10Fc	10s
-5	0	2	144	174	2
-4	0	2	955	936	5
-3	0	2	94	72	1
-2	0	2	215	201	2
-1	0	2	1755	1781	3
0	0	2	237	241	4
1	0	2	532	505	7
2	0	2	561	576	3
3	0	2	191	191	5
4	0	2	778	751	1
5	0	2	318	293	1
6	0	2	597	589	1
7	0	2	570	562	4
8	0	2	65	46	5
9	0	2	378	369	2
10	0	2	103	94	4
11	0	2	102	120	4
12	0	2	95	88	14
13	0	2	36	19	35
14	0	2	81	70	6
15	0	2	79	66	18
16	0	2	0	5	1
-17	1	2	43	8	42
-16	1	2	0	8	1
-15	1	2	24	2	24
-14	1	2	16	2	15
-13	1	2	31	24	11
-12	1	2	49	17	5
-11	1	2	31	25	14
-10	1	2	0	14	1
-9	1	2	21	11	9
-8	1	2	36	35	4
-7	1	2	35	33	4
-6	1	2	151	142	2
-5	1	2	164	150	1
-4	1	2	7	10	7
-3	1	2	93	95	1
-2	1	2	357	351	1
-1	1	2	466	431	2
0	1	2	339	328	2
1	1	2	998	981	7
2	1	2	256	256	2
3	1	2	34	24	2
4	1	2	47	39	1
5	1	2	76	75	1
6	1	2	76	72	1
7	1	2	60	50	2
8	1	2	49	44	2
9	1	2	0	2	1
10	1	2	30	19	6
11	1	2	63	59	5
12	1	2	21	10	20
13	1	2	24	23	23
14	1	2	24	7	24
15	1	2	35	2	13
16	1	2	0	2	1
-16	2	2	37	19	12
-15	2	2	80	57	6
-14	2	2	65	70	5
-13	2	2	22	27	22
-12	2	2	160	155	4
-11	2	2	36	36	6
-10	2	2	120	124	2
-9	2	2	258	255	2
-8	2	2	40	49	4
-7	2	2	330	332	2
-6	2	2	424	426	2
-5	2	2	108	107	2
-4	2	2	545	519	2
-3	2	2	363	361	2
-2	2	2	371	373	3
-1	2	2	61	54	2
0	2	2	120	91	2
1	2	2	51	27	3
2	2	2	44	47	9
3	2	2	98	93	1
4	2	2	451	473	3
5	2	2	110	102	1
6	2	2	192	188	1
7	2	2	397	408	2
8	2	2	34	33	4
9	2	2	202	206	1
10	2	2	146	138	2
-2	5	3	46	47	2
-1	5	3	374	370	1
0	5	3	436	443	5
1	5	3	103	106	4
2	5	3	407	410	6
3	5	3	221	236	4
4	5	3	201	209	5
5	5	3	284	285	3
15	2	2	75	63	24
16	2	2	32	0	31
-16	3	2	33	13	14
-15	3	2	29	22	28
-14	3	2	25	16	18
-13	3	2	16	32	16
-12	3	2	33	25	27
-11	3	2	53	64	4
-10	3	2	93	92	3
-9	3	2	30	31	6
-8	3	2	126	129	2
-7	3	2	115	112	2
-6	3	2	151	154	1
-5	3	2	180	180	2
-4	3	2	39	47	2
-3	3	2	145	144	2
-2	3	2	186	177	2
-1	3	2	203	206	2
0	3	2	9	15	9
1	3	2	199	192	1
2	3	2	193	196	1
3	3	2	45	54	2
4	3	2	95	87	2
5	3	2	230	228	1
6	3	2	70	58	2
7	3	2	34	33	4
8	3	2	44	45	5
9	3	2	99	94	3
10	3	2	23	23	16
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15	3	2	47	15	12
-15	4	2	47	50	11
-14	4	2	79	75	6
-13	4	2	0	7	1
-12	4	2	113	101	3
-11	4	2	104	93	3
-10	4	2	95	83	3
-9	4	2	154	173	2
-8	4	2	147	130	3
-7	4	2	319	315	2
-6	4	2	446	440	1
-5	4	2	56	60	3
-4	4	2	692	679	2
-3	4	2	319	310	2
-2	4	2	400	396	1
-1	4	2	640	642	1
0	4	2	36	25	2
1	4	2	507	491	3
2	4	2	559	557	4
3	4	2	200	197	3
4	4	2	421	435	2
5	4	2	161	162	3
6	4	2	286	296	4
7	4	2	206	212	4
8	4	2	61	53	3
9	4	2	208	216	2
10	4	2	144	138	3
11	4	2	77	75	6
12	4	2	127	135	5
13	4	2	0	34	1
14	4	2	48	43	13
15	4	2	55	47	21
-15	5	2	29	11	29
-14	5	2	0	7	1
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-12	5	2	44	47	8
-11	5	2	30	19	10
-10	5	2	129	126	4
-9	5	2	39	4	5
-8	5	2	103	112	2
-7	5	2	67	60	3
-6	5	2	21	26	7
-5	5	2	130	127	1
-4	5	2	133	126	2
-3	5	2	80	83	2
-2	5	2	283	273	2
-1	5	2	11	4	11
0	5	2	284	286	3
1	5	2	133	134	1
2	5	2	173	184	1
9	8	3	61	50	8
10	8	3	26	4	26
-7	9	3	48	34	48
-6	9	3	119	113	12
-5	9	3	38	47	20
-4	9	3	74	82	7
-3	9	3	149	156	8
-2	9	3	42	45	16
7	5	2	81	54	3
8	5	2	111	96	3
9	5	2	39	44	7
10	5	2	52	43	13
11	5	2	50	37	10
12	5	2	39	4	14
13	5	2	37	37	21
14	5	2	51	16	12
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-13	6	2	0	17	1
-12	6	2	89	96	6
-11	6	2	69	70	6
-10	6	2	82	85	4
-9	6	2	171	181	3
-8	6	2	20	12	19
-7	6	2	116	124	2
-6	6	2	156	153	2
-5	6	2	57	48	3
-4	6	2	181	184	2
-3	6	2	101	106	2
-2	6	2	186	193	1
-1	6	2	254	267	1
0	6	2	26	12	7
1	6	2	344	348	3
2	6	2	167	169	2
3	6	2	24	35	9
4	6	2	298	283	7
5	6	2	114	129	3
6	6	2	97	107	3
7	6	2	195	190	2
8	6	2	52	44	5
9	6	2	122	126	3
10	6	2	82	77	6
11	6	2	28	18	27
12	6	2	58	45	10
13	6	2	65	34	9
-13	7	2	40	34	19
-12	7	2	4	16	4
-11	7	2	62	52	8
-10	7	2	81	74	6
-9	7	2	39	13	15
-8	7	2	128	133	4
-7	7	2	99	87	3
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-5	7	2	121	114	3
-4	7	2	69	61	4
-3	7	2	116	116	2
-2	7	2	137	143	5
-1	7	2	17	3	16
0	7	2	122	125	2
1	7	2	135	132	3
2	7	2	120	126	3
3	7	2	116	116	3
4	7	2	51	47	5
5	7	2	115	105	4
6	7	2	14	22	13
7	7	2	75	67	4
8	7	2	73	62	6
9	7	2	20	9	19
10	7	2	40	29	39
11	7	2	73	59	11
12	7	2	0	1	1
-11	8	2	51	34	21
-10	8	2	70	48	13
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-3	8	2	131	148	5
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6	8	2	82	76	5
7	8	2	120	117	4
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9	8	2	80	73	5
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13	1	4	12	5	12
14	1	4	0	11	1
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-1	9	2	0	3	1
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2	9	2	95	88	5
3	9	2	136	138	4
4	9	2	24	11	23
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7	9	2	30	34	30
8	9	2	42	41	15
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4	10	2	83	64	7
5	10	2	34	15	28
6	10	2	54	40	12
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-15	1	3	24	2	24
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3	1	3	314	321	3
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5	1	3	653	659	3
6	1	3	30	22	3
7	1	3	354	354	2
8	1	3	251	252	2
9	1	3	110	111	2
10	1	3	144	140	2
11	1	3	58	39	5
12	1	3	75	71	4
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1	2	3	18	6	7
2	2	3	185	195	1
3	2	3	231	239	2
4	4	4	468	486	5
4	4	4	71	79	3
5	4	4	259	274	3
6	4	4	184	174	2
7	4	4	104	92	3
8	4	4	188	193	2
9	4	4	107	95	3
10	4	4	97	86	4
8	2	3	24	4	7
9	2	3	54	53	3
10	2	3	27	7	7
11	2	3	62	75	12
12	2	3	28	14	23
13	2	3	24	40	24
14	2	3	0	20	1
15	2	3	30	5	29
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-8	3	3	338	337	2
-7	3	3	11	17	11
-6	3	3	507	497	3
-5	3	3	338	354	2
-4	3	3	238	250	2
-3	3	3	569	565	4
-2	3	3	82	84	2
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2	3	3	643	657	4
3	3	3	240	248	3
4	3	3	224	235	4
5	3	3	305	319	3
6	3	3	0	11	1
7	3	3	205	209	2
8	3	3	122	116	3
9	3	3	53	49	4
10	3	3	157	161	2
11	3	3	81	78	6
12	3	3	101	86	5
13	3	3	104	93	11
14	3	3	20	4	20
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-10	4	3	104	120	3
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-7	4	3	91	89	2
-6	4	3	111	107	2
-5	4	3	103	105	2
-4	4	3	168	162	2
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-2	4	3	168	168	2
-1	4	3	40	39	2
0	4	3	445	438	2
1	4	3	100	117	2
2	4	3	306	295	3
3	4	3	297	298	1
4	4	3	89	92	2
5	4	3	89	88	4
6	4	3	129	127	3
7	4	3	98	98	2
8	4	3	31	36	8
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10	4	3	0	11	1
11	4	3	66	57	15
12	4	3	25	8	24
13	4	3	31	16	31
14	4	3	44	27	20
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-14	5	3	84	74	8
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-12	5	3	64	42	11
-11	5	3	120	134	3
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-9	5	3	137	143	3
-8	5	3	164	168	2
-7	5	3	18	21	12
-6	5	3	291	295	3
-5	5	3	178	178	2
-4	5	3	218	222	2
-3	5	3	371	377	3
-2	7	4	80	75	4
-1	7	4	90	85	4
0	7	4	34	21	25
1	7	4	64	62	6
2	7	4	27	26	26
3	7	4	15	25	15
4	7	4	85	89	10
5	7	4	80	58	11

Table C-3, Continued
Observed and Calculated Structure Factor Tables for 1,6-diferrocenylhexane

h	k	l	10Fo	10Fc	10s
6	5	3	36	36	6
7	5	3	226	224	4
8	5	3	149	143	3
9	5	3	70	65	4
10	5	3	147	153	3
11	5	3	69	48	7
12	5	3	47	38	27
13	5	3	43	53	22
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-13	6	3	30	22	29
-12	6	3	66	52	6
-11	6	3	37	11	20
-10	6	3	75	60	4
-9	6	3	47	48	8
-8	6	3	87	76	3
-7	6	3	45	45	4
-6	6	3	0	19	1
-5	6	3	35	36	4
-4	6	3	119	120	2
-3	6	3	36	33	5
-2	6	3	185	183	2
-1	6	3	144	142	2
0	6	3	168	175	2
1	6	3	137	136	4
2	6	3	38	26	5
3	6	3	164	166	2
4	6	3	21	35	17
5	6	3	14	14	13
6	6	3	114	108	3
7	6	3	29	38	10
8	6	3	72	81	4
9	6	3	99	79	8
10	6	3	14	8	14
11	6	3	50	44	26
12	6	3	43	36	16
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-10	7	3	54	9	9
-9	7	3	117	129	4
-8	7	3	124	123	4
-7	7	3	55	50	5
-6	7	3	116	117	2
-5	7	3	131	133	2
-4	7	3	95	91	5
-3	7	3	166	169	7
-2	7	3	70	72	3
-1	7	3	220	233	2
0	7	3	132	133	2
1	7	3	48	44	5
2	7	3	206	197	5
3	7	3	112	125	3
4	7	3	61	74	4
5	7	3	193	195	2
6	7	3	73	89	4
7	7	3	118	117	3
8	7	3	127	126	3
9	7	3	21	15	21
10	7	3	83	65	4
11	7	3	30	34	30
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-10	8	3	77	64	13
-9	8	3	38	46	37
-7	8	3	124	128	5
-6	8	3	14	14	14
-5	8	3	131	119	3
-4	8	3	91	100	5
-3	8	3	36	34	8
-2	8	3	152	147	2
-1	8	3	68	73	4
0	8	3	94	95	3
1	8	3	168	175	3
2	8	3	34	14	12
3	8	3	138	150	5
4	8	3	63	61	5
5	8	3	67	67	5
6	8	3	93	79	4
7	8	3	35	16	12
8	8	3	64	52	6
-9	2	5	67	61	3
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-7	2	5	12	12	11
-6	2	5	106	104	1
-5	2	5	45	38	2
-4	2	5	94	91	2
-3	2	5	102	97	1
-2	2	5	52	39	2
-1	2	5	137	144	1
0	2	5	25	19	3
1	2	5	24	25	3
2	2	5	191	202	1

h	k	l	10Fo	10Fc	10s
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0	9	3	146	150	5
1	9	3	28	9	18
2	9	3	141	144	6
3	9	3	77	64	10
4	9	3	64	67	6
5	9	3	73	69	6
6	9	3	28	11	28
7	9	3	83	66	7
8	9	3	36	33	17
-6	1	0	3	32	19
-5	1	0	3	52	34
-4	1	0	3	39	48
-3	1	0	3	32	5
-2	1	0	3	57	60
-1	1	0	3	62	54
0	1	0	3	50	44
1	1	0	3	73	80
2	1	0	3	20	8
3	1	0	3	57	53
4	1	0	3	44	50
5	1	0	3	41	15
6	1	0	3	36	44
-16	0	4	52	46	21
-15	0	4	60	63	25
-14	0	4	40	32	16
-13	0	4	148	146	4
-12	0	4	116	126	5
-11	0	4	140	139	4
-10	0	4	321	332	3
-9	0	4	57	40	5
-8	0	4	430	425	6
-7	0	4	289	299	2
-6	0	4	169	166	5
-5	0	4	864	863	7
-4	0	4	106	103	2
-3	0	4	487	461	7
-2	0	4	770	764	4
-1	0	4	118	119	1
0	0	4	645	602	7
1	0	4	350	362	4
2	0	4	378	381	5
3	0	4	755	748	12
4	0	4	228	227	2
5	0	4	579	570	3
6	0	4	442	452	5
7	0	4	95	92	3
8	0	4	283	282	5
9	0	4	112	112	3
10	0	4	110	109	4
11	0	4	121	131	8
12	0	4	51	43	11
13	0	4	86	87	8
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-9	1	4	71	66	4
-8	1	4	0	10	1
-7	1	4	91	88	4
-6	1	4	101	97	2
-5	1	4	201	197	1
-4	1	4	44	34	2
-3	1	4	49	60	1
-2	1	4	108	110	1
-1	1	4	38	32	2
0	1	4	342	326	2
1	1	4	62	50	2
2	1	4	115	105	2
3	1	4	98	107	1
4	1	4	9	12	8
5	1	4	32	27	3
6	1	4	93	87	2
7	1	4	57	53	3
8	1	4	13	15	13
9	1	4	29	4	6
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-6	5	5	51	54	3
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-4	5	5	239	242	3
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-2	5	5	261	274	2
-1	5	5	254	254	2
0	5	5	116	117	2

h	k	l	10Fo	10Fc	10s
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-13	2	4	124	114	3
-12	2	4	34	34	8
-11	2	4	118	122	4
-10	2	4	207	200	2
-9	2	4	0	1	1
-8	2	4	326	341	4
-7	2	4	300	305	3
-6	2	4	278	267	2
-5	2	4	419	423	5
-4	2	4	111	110	1
-3	2	4	369	371	2
-2	2	4	353	344	4
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2	2	4	288	299	4
3	2	4	655	681	7
4	2	4	66	63	1
5	2	4	250	252	1
6	2	4	290	296	4
7	2	4	18	26	12
8	2	4	152	150	3
9	2	4	116	102	2
10	2	4	66	55	4
11	2	4	137	135	4
12	2	4	46	27	25
13	2	4	83	82	14
14	2	4	59	58	10
15	2	4	33	16	32
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-12	3	4	34	38	10
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-5	3	4	95	85	2
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-2	3	4	253	241	2
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4	3	4	160	156	6
5	3	4	30	26	6
6	3	4	65	59	3
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10	3	4	31	4	11
11	3	4	46	60	10
12	3	4	56	38	11
13	3	4	0	7	1
14	3	4	21	10	20
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-13	4	4	89	86	3
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-11	4	4	92	86	4
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-8	4	4	242	232	4
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7	8	5	36	52	15
8	8	5	0	24	1
9	8	5	47	12	46
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-6	9	5	61	11	18
-5	9	5	73	61	8
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-3	9	5	0	11	1
-2	9	5	109	94	6
-1	9	5	53	53	7

h	k	l	10Fo	10Fc	10s
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12	4	4	27	5	26
13	4	4	58	57	15
14	4	4	39	38	39
-15	5	4	7	5	7
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-10	5	4	61	50	4
-9	5	4	40	39	7
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-4	5	4	73	68	3
-3	5	4	130	129	2
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1	5	4	239	243	2
2	5	4	28	22	7
3	5	4	0	5	1
4	5	4	163	165	2
5	5	4	69	73	3
6	5	4	69	73	3
7	5	4	148	138	3
8	5	4	22	13	22
9	5	4	111	111	3
10	5	4	32	26	13
11	5	4	0	22	1
12	5	4	42	27	15
13	5	4	23	15	22
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-12	6	4	26	18	25
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-9	6	4	33	28	10
-8	6	4	131	142	3
-7	6	4	118	114	3
-6	6	4	74	62	3
-5	6	4	196	199	2
-4	6	4	61	58	4
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-2	6	4	167	173	2
-1	6	4	46	36	7
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1	6	4	45	48	4
2	6	4	73	76	5
3	6	4	177	176	6
4	6	4	46	47	7
5	6	4	175	180	2
6	6	4	170	165	7
7	6	4	18	22	18
8	6	4	155	160	3
9	6	4	80	79	4
10	6	4	43	45	9
11	6	4	60	55	9
12	6	4	62	24	11
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-9	7	4	54	53	11
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-7	7	4	96	91	7
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1	7	4	144	148	2
2	7	4	67	70	4
3	7	4	78	68	4
4	7	4	93	89	3
5	7	4	28	18	15
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-10	2	6	87	85	3
-9	2	6	214	228	3
-8	2	6	99	95	4
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-5	2	6	18	9	9
-4	2	6	287	287	3
-3	2	6	283	285	3
-2	2	6	202	209	1
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0	2	6	155	160	2

h	k	l	10Fo	10Fc	10s
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3	8	4	121	130	3
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5	8	4	91	82	4
6	8	4	86	95	4
7	8	4	0	3	1
8	8	4	96	80	4
9	8	4	16	22	15
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3	9	4	43	22	10
4	9	4	67	65	6
5	9	4	46	44	12
6	9	4	56	32	8
7	9	4	60	48	8
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1	10	4	45	38	15
2	10	4	53	44	11
3	10	4	0	41	1
4	10	4	0	2	1
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-14	1	5	60	41	6
-13	1	5	81	77	4
-12	1	5	152	149	3
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-10	1	5	239	250	2
-9	1	5	212	219	2
-8	1	5	181	173	2
-7	1	5	448	448	3
-6	1	5	164	158	1
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-4	1	5	592	609	4
-3	1	5	44	43	2
-2	1	5	600	578	2
-1	1	5	517	512	3
0	1	5	418	432	3
1	1	5	670	663	5
2	1	5	142	143	1
3	1	5	450	446	2
4	1	5	491	502	4
5	1	5	79	86	2
6	1	5	298	299	4
7	1	5	177	181	1
8	1	5	109	122	2
9	1	5	194	194	3
10	1	5	53	55	5
11	1	5	117	117	3
12	1	5	110	117	7
13	1	5	0	9	1
14	1	5	68	65	14
-16	2	5	19	12	19
-15	2	5	20	4	20
-14	2	5	0	1	1
-13	2	5	19	20	19
-12	2	5	36	30	9
-11	2	5	0	18	1
-10	2	5	59	53	4
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-8	5	6	48	39	7
-7	5	6	75	77	5
-6	5	6	45	18	6
-5	5	6	116	122	3
-4	5	6	98	90	3
-3	5	6	60	51	4
-2	5	6	85	85	3
-1	5	6	126	119	2
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1	5	6	109	111	3
2	5	6	180	187	2

Table C-3, Continued
Observed and Calculated Structure Factor Tables for 1,6-diferrocenylhexane

h	k	l	10Fo	10Fc	10s
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6	2	5	69	68	5
7	2	5	23	19	10
8	2	5	25	3	13
9	2	5	41	22	5
10	2	5	41	42	7
11	2	5	27	10	26
12	2	5	54	33	10
13	2	5	36	7	20
14	2	5	0	1	1
-16	3	5	0	20	1
-15	3	5	79	68	5
-14	3	5	32	33	31
-13	3	5	52	63	6
-12	3	5	120	121	3
-11	3	5	17	12	17
-10	3	5	153	159	2
-9	3	5	176	180	2
-8	3	5	111	120	2
-7	3	5	315	316	3
-6	3	5	35	35	4
-5	3	5	212	228	1
-4	3	5	248	246	2
-3	3	5	21	1	6
-2	3	5	437	465	1
-1	3	5	435	426	2
0	3	5	192	189	5
1	3	5	746	772	6
2	3	5	222	236	7
3	3	5	383	397	4
4	3	5	314	324	4
5	3	5	0	14	1
6	3	5	203	207	3
7	3	5	142	145	2
8	3	5	65	58	3
9	3	5	148	162	4
10	3	5	64	56	4
11	3	5	103	101	4
12	3	5	76	73	8
13	3	5	28	29	28
14	3	5	52	49	13
-15	4	5	29	16	28
-14	4	5	30	26	18
-13	4	5	43	12	9
-12	4	5	40	24	8
-11	4	5	37	54	8
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-7	4	5	86	75	4
-6	4	5	79	69	2
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5	4	5	112	114	3
6	4	5	28	27	9
7	4	5	104	102	3
8	4	5	21	8	21
9	4	5	73	73	4
10	4	5	54	47	10
11	4	5	34	14	12
12	4	5	0	4	1
13	4	5	0	17	1
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-6	9	6	0	14	1
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2	9	6	27	37	27
3	9	6	82	62	6
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-15	1	7	29	16	29
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3	5	5	180	185	6
4	5	5	175	176	2
5	5	5	80	76	3
6	5	5	213	218	8
7	5	5	118	102	3
8	5	5	90	84	3
9	5	5	141	147	6
10	5	5	25	23	24
11	5	5	74	65	5
12	5	5	15	42	14
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-7	6	5	23	1	23
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6	6	5	27	8	14
7	6	5	95	112	4
8	6	5	68	55	5
9	6	5	53	41	7
10	6	5	27	30	26
11	6	5	37	13	19
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-9	7	5	70	68	18
-8	7	5	54	41	45
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0	8	5	86	90	4
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6	9	5	76	58	8
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-9	0	6	256	245	3
-8	0	6	45	38	11
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-4	0	6	544	558	11
-3	0	6	604	563	3
-2	0	6	216	217	2
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2	0	6	333	350	5
3	0	6	25	25	6
4	0	6	313	324	6
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6	0	6	183	183	5
7	0	6	215	221	6
8	0	6	50	40	6
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-3	1	6	22	19	5
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0	1	6	55	50	2
1	1	6	128	127	2
2	1	6	78	74	2
3	1	6	71	62	2
4	1	6	65	61	2
5	1	6	97	96	4
6	1	6	52	53	3
7	1	6	45	46	5
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9	1	6	41	29	7
10	1	6	24	3	24
11	1	6	22	19	21
12	1	6	0	2	1
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7	2	6	198	205	3
8	2	6	75	74	3
9	2	6	126	126	3
10	2	6	136	131	3
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12	2	6	93	85	9
13	2	6	44	26	26
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-3	3	6	72	81	2
-2	3	6	92	85	2
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2	3	6	62	72	5
3	3	6	92	96	2
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5	3	6	56	48	4
6	3	6	7	14	7
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-11	4	6	105	108	3
-10	4	6	43	44	10
-9	4	6	191	191	2
-8	4	6	77	69	5
-7	4	6	173	189	2
-6	4	6	196	191	2
-5	4	6	69	59	4
-4	4	6	228	244	3
-3	4	6	229	227	2
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0	4	6	181	189	2
1	4	6	242	259	2
2	4	6	265	277	6
3	4	6	46	46	4
4	4	6	205	213	6
5	4	6	144	145	4
6	4	6	81	78	5
7	4	6	180	195	2
8	4	6	77	74	4
9	4	6	106	100	3
10	4	6	106	98	3
11	4	6	42	32	9
12	4	6	57	59	12
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6	1	8	27	14	16
7	1	8	44	43	8
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-12	2	8	57	66	6
-11	2	8	62	53	7
-10	2	8	128	133	3
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-8	2	8	120	115	3
-7	2	8	170	169	3
3	5	6	98	87	3
4	5	6	97	97	3
5	5	6	66	72	4
6	5	6	64	64	5
7	5	6	46	51	6
8	5	6	72	71	7
9	5	6	23	5	22
10	5	6	28	10	20
11	5	6	57	19	15
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-9	6	6	91	107	7
-8	6	6	48	55	17
-7	6	6	85	82	5
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-5	6	6	31	32	9
-4	6	6	207	210	4
-3	6	6	148	155	2
-2	6	6	58	59	4
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0	6	6	28	15	10
1	6	6	104	97	4
2	6	6	92	83	3
3	6	6	32	17	10
4	6	6	157	155	4
5	6	6	105	87	5
6	6	6	61	63	6
7	6	6	119	114	4
8	6	6	31	33	14
9	6	6	58	56	7
10	6	6	67	46	11
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-1	7	6	24	29	20
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2	7	6	46	44	7
3	7	6	94	89	3
4	7	6	27	1	26
5	7	6	79	77	5
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7	7	6	18	20	18
8	7	6	42	35	13
9	7	6	26	6	26
-10	8	6	81	11	14
-9	8	6	51	50	25
-8	8	6	30	39	29
-7	8	6	51	43	11
-6	8	6	78	79	7
-5	8	6	41	26	9
-4	8	6	95	96	4
-3	8	6	91	80	4
-2	8	6	56	41	6
-1	8	6	105	104	4
0	8	6	49	48	7
1	8	6	68	65	5
2	8	6	123	120	4
3	8	6	38	22	11
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5	8	6	75	63	6
6	8	6	26	22	25
7	8	6	70	61	6
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-6	9	6	42	41	14
-5	8	8	24	17	24
-4	8	8	38	53	12
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-2	8	8	20	23	20
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0	8	8	38	40	7
1	8	8	13	2	12
2	8	8	76	70	4
3	8	8	53	58	5
4	8	8	0	6	1
5	8	8	79	77	4
6	8	8	11	6	10
7	8	8	72	74	5
8	8	8	23	20	23
6	5	8	35	27	12

Table C-3, Continued
Observed and Calculated Structure Factor Tables for 1,6-diferrocenylhexane

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-10	1	7	32	36	10
-9	1	7	114	114	3
-8	1	7	154	155	2
-7	1	7	35	30	6
-6	1	7	215	217	2
-5	1	7	316	307	2
-4	1	7	106	108	2
-3	1	7	400	389	2
-2	1	7	185	184	3
-1	1	7	280	277	3
0	1	7	274	295	4
1	1	7	24	24	6
2	1	7	192	198	1
3	1	7	164	174	2
4	1	7	115	120	3
5	1	7	186	190	2
6	1	7	51	40	4
7	1	7	174	175	2
8	1	7	148	145	3
9	1	7	44	36	10
10	1	7	126	121	4
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-13	2	7	11	10	11
-12	2	7	44	17	8
-11	2	7	13	17	12
-10	2	7	0	2	1
-9	2	7	36	47	8
-8	2	7	7	20	6
-7	2	7	61	48	3
-6	2	7	14	22	13
-5	2	7	48	42	3
-4	2	7	28	18	5
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-2	2	7	28	23	5
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2	2	7	22	20	9
3	2	7	30	41	6
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6	2	7	29	18	16
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-8	3	7	207	198	3
-7	3	7	22	14	17
-6	3	7	146	157	3
-5	3	7	137	126	1
-4	3	7	41	37	4
-3	3	7	250	261	4
-2	3	7	98	100	2
-1	3	7	210	222	2
0	3	7	280	289	2
1	3	7	36	26	5
2	3	7	253	265	2
3	3	7	136	142	2
7	1	9	91	78	12
8	1	9	33	28	20
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Table C-3, Continued
Observed and Calculated Structure Factor Tables for 1,6-diferrocenylhexane

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0	2	11	15	7	14
1	2	11	23	15	22
2	2	11	42	4	18
3	2	11	0	21	1
4	2	11	30	10	30
5	2	11	41	16	41
6	2	11	0	18	1
-10	3	11	46	35	17
-9	3	11	53	38	14
-8	3	11	80	81	22
-7	3	11	30	23	29
-6	3	11	89	69	7
-5	3	11	119	112	5
-4	3	11	0	19	1
-3	3	11	130	133	3
-2	3	11	117	116	4
-1	3	11	64	50	5
0	3	11	132	136	3
1	3	11	52	41	7
2	3	11	95	85	5
3	3	11	77	78	6
4	3	11	30	12	26
5	3	11	72	73	7
6	3	11	33	37	32
-9	4	11	49	14	31
-8	4	11	0	21	1
-7	4	11	0	11	1
-6	4	11	33	29	33
-5	4	11	36	18	19
-4	4	11	54	41	10
-3	4	11	0	1	1
-2	4	11	40	38	10
-1	4	11	37	31	12
0	4	11	0	5	1
1	4	11	51	24	7
2	4	11	23	26	23
3	4	11	38	2	13
4	4	11	16	28	15
5	4	11	0	9	1
-7	5	11	0	9	1
-1	0	12	61	13	16
0	0	12	101	90	10
1	0	12	68	59	16
2	0	12	38	44	37
3	0	12	81	71	13
4	0	12	12	13	11
-9	1	12	54	9	36
-8	1	12	33	12	33
-7	1	12	0	0	1
-6	1	12	0	21	1
-5	1	12	0	27	1
-4	1	12	0	5	1
-3	1	12	39	29	39
-2	1	12	47	12	19
-1	1	12	32	5	32
0	1	12	37	11	26
1	1	12	29	23	29
2	1	12	23	6	22
3	1	12	56	18	13
4	1	12	13	8	12
-9	2	12	66	21	11
-8	2	12	34	40	34
-7	2	12	75	60	12
-6	2	12	0	11	1
-5	2	12	88	71	6
-4	2	12	83	87	14
-3	2	12	55	23	14
-2	2	12	119	114	5
-1	2	12	29	52	29
0	2	12	89	74	7
1	2	12	103	84	7
2	2	12	41	11	21
3	2	12	86	68	9
-8	3	12	44	21	44
-7	3	12	0	1	1
-6	3	12	35	33	35
-5	3	12	16	17	16
-4	3	12	34	29	25
-3	3	12	37	30	17
-2	3	12	33	3	16
-1	3	12	20	18	19
0	3	12	0	15	1
1	3	12	22	6	21
2	3	12	38	15	37
3	3	12	0	15	1
-6	4	12	48	9	25
-5	4	12	71	64	11
-4	4	12	59	52	10
-3	4	12	53	36	12
-2	4	12	76	77	6
-1	4	12	35	17	24
0	4	12	49	52	9
1	4	12	39	45	21
2	4	12	15	7	15
-6	1	13	87	50	13
-1	1	13	47	49	23
0	1	13	0	18	1
1	1	13	41	53	27
-5	2	13	0	23	1
-4	2	13	36	3	36
-3	2	13	0	26	1
-1	2	13	51	8	17
0	2	13	45	12	21

APPENDIX D

Electrochemical Data for Solution and Monolayer Voltammetry

Table D-1
Solution Voltammetry Data for 1,6-diferrocenylhexane-1,6-dione

scan rate (mV/s)	E_{pa}	E_{pc}	i_{pa}	i_{pc}	ΔE_p	E°	i_{pa}/i_{pc}	Sq Rt scan rate
25	308	230	4.58	3.99	78.0	269.0	1.148	5.000
50	308	231	6.28	5.35	77.0	269.5	1.174	7.071
75	308	235	7.48	6.58	73.0	271.5	1.137	8.660
100	308	236	8.58	7.97	72.0	272.0	1.077	10.000
125	309	233	9.31	8.50	76.0	271.0	1.095	11.180
150	312	222	19.10	18.80	90.0	267.0	1.016	12.247
175	311	234	10.70	10.00	77.0	272.5	1.070	13.229
200	314	221	21.60	21.40	93.0	267.5	1.009	14.142
225	314	230	12.10	11.40	84.0	272.0	1.061	15.000
250	313	231	12.80	12.40	82.0	272.0	1.032	15.811
275	314	232	13.50	12.90	82.0	273.0	1.047	16.583
300	315	229	13.80	13.40	86.0	272.0	1.030	17.321
325	317	229	14.50	14.10	88.0	273.0	1.028	18.028
350	317	228	14.70	14.40	89.0	272.5	1.021	18.708
375	319	225	15.00	14.90	94.0	272.0	1.007	19.365
400	319	227	15.30	15.30	92.0	273.0	1.000	20.000
425	319	225	15.60	15.80	94.0	272.0	0.987	20.616
450	319	224	16.00	16.20	95.0	271.5	0.988	21.213
475	321	222	16.10	16.50	99.0	271.5	0.976	21.794
500	322	221	16.40	16.80	101.0	271.5	0.976	22.361
525	320	220	16.50	17.20	100.0	270.0	0.959	22.913
550	320	224	16.80	17.50	96.0	272.0	0.960	23.452
575	322	222	16.90	17.60	100.0	272.0	0.960	23.979
600	319	219	17.10	18.00	100.0	269.0	0.950	24.495
625	325	219	17.20	18.20	106.0	272.0	0.945	25.000
650	322	222	17.40	18.50	100.0	272.0	0.941	25.495
675	324	218	17.40	18.80	106.0	271.0	0.926	25.981
700	328	221	17.60	18.90	107.0	274.5	0.931	26.458
750	328	215	17.90	19.40	113.0	271.5	0.923	27.386
800	327	213	18.30	19.70	114.0	270.0	0.929	28.284
850	327	215	18.70	20.40	112.0	271.0	0.917	29.155
900	330	212	18.70	20.60	118.0	271.0	0.908	30.000
950	327	216	19.20	21.10	111.0	271.5	0.910	30.822
1000	329	213	19.40	21.50	116.0	271.0	0.902	31.623
					94.5	271.5		

Table D-2

Solution Voltammetry Data for 1-ferrocenylcarbonyl-2-ferrocenylcyclopentene

scan rate (mV/s)	E_{pa1}	E_{pa2}	E_{pc1}	E_{pc2}	i_{pa1}	i_{pa2}	i_{pc1}	i_{pc2}
25	119	375	307	51	3.85	3.48	3.72	3.45
50	123	374	308	49	5.06	4.48	4.93	4.49
75	121	376	308	53	6.82	5.35	5.94	5.44
100	120	373	309	51	7.34	6.13	6.86	6.24
125	119	375	307	53	7.82	6.74	7.44	6.85
150	122	377	307	51	8.44	7.20	8.04	7.48
175	124	378	307	50	9.09	7.72	8.64	8.01
200	124	380	308	51	9.69	8.18	9.14	8.54
250	126	381	306	51	10.70	8.99	10.10	9.44
300	126	381	307	47	11.60	9.72	11.00	10.30
350	127	385	305	49	12.50	10.40	11.70	11.00
400	130	386	302	46	13.30	11.00	12.40	11.70
450	130	387	302	46	14.10	11.50	13.10	12.40
500	132	388	302	44	14.70	12.00	13.60	13.00
550	128	384	307	48	15.50	12.60	14.20	13.60
600	129	389	305	45	16.20	13.20	14.60	14.10
650	133	385	303	44	16.70	13.30	15.10	14.60
700	129	392	306	42	17.20	13.60	15.40	15.00
750	135	395	298	45	17.70	13.90	15.80	15.50
800	133	396	301	46	18.20	14.20	16.20	15.90
850	131	396	299	41	18.70	14.50	16.60	16.30
900	133	389	298	40	19.10	14.80	16.90	16.80
950	140	397	301	44	19.50	14.90	17.20	17.10

ΔE_{pa1}	ΔE_{pa2}	E^0_1	E^0_2	I_{pa1}/I_{pc1}	I_{pc2}/I_{pa2}	Sq Rt scan rate
68	324	85.0	341.0	1.116	0.935	5.000
74	325	86.0	341.0	1.127	0.909	7.071
68	323	87.0	342.0	1.254	0.901	8.660
69	322	85.5	341.0	1.176	0.894	10.000
66	322	86.0	341.0	1.142	0.906	11.180
71	326	86.5	342.0	1.128	0.896	12.247
74	328	87.0	342.5	1.135	0.894	13.229
73	329	87.5	344.0	1.135	0.895	14.142
75	330	88.5	343.5	1.133	0.890	15.811
79	334	86.5	344.0	1.126	0.884	17.321
78	336	88.0	345.0	1.136	0.889	18.708
84	340	88.0	344.0	1.137	0.887	20.000
84	341	88.0	344.5	1.137	0.878	21.213
88	344	88.0	345.0	1.131	0.882	22.361
80	336	88.0	345.5	1.140	0.887	23.452
84	344	87.0	347.0	1.149	0.904	24.495
89	341	88.5	344.0	1.144	0.881	25.495
87	350	85.5	349.0	1.147	0.883	26.458
90	350	90.0	346.5	1.142	0.880	27.386
87	350	89.5	348.5	1.145	0.877	28.284
90	355	86.0	347.5	1.147	0.873	29.155
93	349	86.5	343.5	1.137	0.876	30.000
96	353	92.0	349.0	1.140	0.866	30.822
80	336	87.0	344.0			

Table D-3
Solution Voltammetry Data for 1,6-diferrocenylhexane

scan rate (mV/s)	E_{pa}	E_{pc}	i_{pa}	i_{pc}	ΔE_p	E°	i_{pa}/i_{pc}	Sq Rt Scan Rate
25	20	-50	4.52	4.19	70.0	-15.0	1.079	5.000
50	22	-52	6.34	5.75	74.0	-15.0	1.103	7.071
75	19	-50	7.41	7.04	69.0	-15.5	1.053	8.660
100	18	-52	8.61	8.19	70.0	-17.0	1.051	10.000
125	23	-49	9.69	8.92	72.0	-13.0	1.086	11.180
150	22	-49	10.50	9.69	71.0	-13.5	1.084	12.247
175	27	-46	11.30	10.60	73.0	-9.5	1.066	13.229
200	26	-46	12.10	11.20	72.0	-10.0	1.080	14.142
250	30	-45	13.40	13.00	75.0	-7.5	1.031	15.811
300	25	-53	14.70	14.40	78.0	-14.0	1.021	17.321
350	28	-53	16.20	15.50	81.0	-12.5	1.045	18.708
400	30	-52	17.10	16.70	82.0	-11.0	1.024	20.000
450	31	-53	18.30	17.70	84.0	-11.0	1.034	21.213
500	34	-53	19.10	18.60	87.0	-9.5	1.027	22.361
550	33	-48	20.10	19.70	81.0	-7.5	1.020	23.452
600	31	-56	21.10	20.40	87.0	-12.5	1.034	24.495
650	37	-54	21.80	21.30	91.0	-8.5	1.023	25.495
700	35	-51	22.50	22.30	86.0	-8.0	1.009	26.458
750	32	-51	23.50	23.10	83.0	-9.5	1.017	27.386
800	37	-50	24.10	23.70	87.0	-6.5	1.017	28.284
850	32	-57	24.90	24.50	89.0	-12.5	1.016	29.155
900	40	-50	25.60	25.30	90.0	-5.0	1.012	30.000
950	37	-56	26.40	25.90	93.0	-9.5	1.019	30.822
1000	40	-53	27.00	26.60	93.0	-6.5	1.015	31.623
					81.5	-10.5		

Table D-4
Solution Voltammetry Data for 1,6-diferrocenylhexane-1-one

scan rate (mV/s)	E_{pa1}	E_{pa2}	E_{pc1}	E_{pc2}	i_{pa1}	i_{pa2}	i_{pc1}	i_{pc2}
25	41	348	264	-31	3.05	2.91	2.56	2.94
50	47	344	260	-28	4.29	3.90	3.85	4.10
75	44	338	266	-29	5.36	4.76	4.85	5.06
100	44	339	267	-27	6.24	5.52	5.82	5.86
125	44	339	270	-28	6.98	6.21	6.60	6.54
150	44	339	267	-28	7.62	6.82	7.30	7.15
175	43	337	269	-26	8.36	7.44	8.02	7.75
200	44	338	271	-29	9.01	7.99	8.47	8.25
225	44	340	269	-28	9.22	8.27	9.00	8.75
250	44	340	270	-26	9.88	8.92	9.42	9.27
275	43	341	269	-29	10.10	9.05	9.93	9.70
300	42	341	270	-29	10.90	9.73	10.30	10.10
325	46	340	268	-29	11.30	10.10	10.80	10.50
350	61	360	251	-51	8.86	6.64	7.79	9.86
375	61	364	252	-53	9.24	6.61	7.79	10.10
400	63	364	246	-58	8.98	6.50	8.00	10.30
425	68	369	246	-58	9.29	6.52	8.01	10.60
450	66	367	246	-60	9.06	6.45	8.11	10.80
475	73	369	244	-63	9.24	6.42	8.17	11.00
500	73	367	244	-63	8.89	6.34	8.56	11.30
550	75	361	248	-64	9.01	6.45	8.99	11.80
600	74	365	249	-62	9.20	6.54	9.11	12.20
650	82	362	247	-66	9.34	6.61	9.35	12.60

ΔE_{pa1}	ΔE_{pa2}	E°_{c1}	E°_{c2}	i_{pc1}/i_{pa1}	i_{pc2}/i_{pa2}	Sq Rt scan rate
72	84	5.0	306.0	1.037	1.137	5.000
75	84	9.5	302.0	1.046	1.013	7.071
73	72	7.5	302.0	1.059	0.981	8.660
71	72	8.5	303.0	1.065	0.948	10.000
72	69	8.0	304.5	1.067	0.941	11.180
72	72	8.0	303.0	1.066	0.934	12.247
69	68	8.5	303.0	1.079	0.928	13.229
73	67	7.5	304.5	1.092	0.943	14.142
72	71	8.0	304.5	1.054	0.919	15.000
70	70	9.0	305.0	1.066	0.947	15.811
72	72	7.0	305.0	1.041	0.911	16.583
71	71	6.5	305.5	1.079	0.945	17.321
75	72	8.5	304.0	1.076	0.935	18.028
112	109	5.0	305.5	0.899	0.852	18.708
114	112	4.0	308.0	0.915	0.849	19.365
121	118	2.5	305.0	0.872	0.813	20.000
126	123	5.0	307.5	0.876	0.814	20.616
126	121	3.0	306.5	0.839	0.795	21.213
136	125	5.0	306.5	0.840	0.786	21.794
136	123	5.0	305.5	0.787	0.741	22.361
139	113	5.5	304.5	0.764	0.717	23.452
136	116	6.0	307.0	0.754	0.718	24.495
148	115	8.0	304.5	0.741	0.707	25.495
75	**84**	**7.0**	**305.0**			

Table D-5
Monolayer Voltammetry Data for Thiol -First Electrode

scan rate (mV/s)	E_{pa1}	E_{pa2}	E_{pc1}	E_{pc2}	i_{pa1}	i_{pa2}	i_{pc1}	i_{pc2}
25	322	495	446	259	0.090	0.765	0.033	0.213
26	316	492	446	264	0.125	0.089	0.976	0.253
50	321	507	442	252	0.092	1.130	1.203	0.321
75	322	522	443	248	0.122	1.462	1.537	0.431
100	326	506	443	245	0.102	1.638	1.772	0.488
125	425	529	443	245	0.127	1.806	2.035	0.557
150	323	523	443	240	0.120	2.081	2.252	0.593
175	323	530	441	237	0.159	2.017	2.400	0.662
200	319	526	442	242	0.232	3.032	3.455	1.034
250	318	531	442	238	0.278	3.195	3.955	1.173
300	315	531	441	236	0.274	3.463	4.348	1.288
350	318	534	439	234	0.319	3.405	4.675	1.383
400	317	536	439	231	0.270	3.657	4.993	1.467
450	316	537	439	229	0.323	3.708	5.267	1.517
500	315	540	438	228	0.365	3.807	5.536	1.539

ΔE_{pa}	ΔE_{pc}	i_{pa1}/i_{pc1}	i_{pa2}/i_{pc2}	E°_1	E°_2	Area 1	Area 2	Area 3	Area 4
63	236	0.421	23.454	290.5	470.5	2.44E-09	3.52E-08	3.26E-08	5.87E-09
52	228	0.493	0.091	290.0	469.0	3.05E-09	4.06E-08	4.14E-08	7.44E-09
69	255	0.287	0.939	286.5	474.5	2.50E-09	5.86E-08	5.23E-08	1.01E-08
74	274	0.284	0.951	285.0	482.5	3.46E-09	9.16E-03	7.07E-08	1.55E-08
81	261	0.208	0.934	285.5	474.5	2.87E-09	8.82E-08	7.72E-08	1.85E-08
180	284	0.229	0.887	335.0	486.0	3.91E-09	1.20E-07	9.19E-08	2.08E-08
83	283	0.201	0.924	281.5	483.0	3.57E-09	1.35E-07	1.04E-07	2.34E-08
86	295	0.240	0.840	280.0	485.5	5.50E-09	1.31E-07	1.16E-07	2.81E-08
77	284	0.224	0.878	280.5	484.0	6.62E-09	1.96E-07	1.63E-07	4.29E-08
80	293	0.237	0.808	278.0	486.5	7.78E-09	2.16E-07	1.86E-07	5.33E-08
79	295	0.213	0.796	275.5	486.0	6.73E-09	2.33E-07	2.09E-07	5.69E-08
84	300	0.231	0.728	276.0	486.5	9.13E-09	2.30E-07	2.32E-07	6.30E-08
86	305	0.184	0.732	274.0	487.5	5.96E-09	2.67E-07	2.48E-07	6.81E-08
87	308	0.213	0.704	272.5	488.0	8.40E-09	2.58E-07	2.55E-07	7.10E-08
87	312	0.237	0.688	271.5	489.0	9.65E-09	2.81E-07	2.75E-07	7.01E-08
81	284			280.5	495.5	5.99E-10	1.98E-07	1.05E-07	3.80E-08

scan rate (V/s)	Γ_1	Γ_2	Γ_3	Γ_4	FWHM	FWHM	FWHM	FWHM
0.025	1.26E-11	1.81E-10	1.68E-10	3.03E-11	54.5	112.2	83.4	61
0.050	7.87E-12	1.05E-10	1.07E-10	1.92E-11				
0.075	4.30E-12	1.01E-10	8.99E-11	1.73E-11				
0.100	4.47E-12	1.18E-05	9.11E-11	2.00E-11				
0.125	2.96E-12	9.09E-11	7.96E-11	1.91E-11				
0.150	3.36E-12	1.03E-10	7.90E-11	1.79E-11				
0.175	2.63E-12	9.96E-11	7.63E-11	1.72E-11				
0.200	3.55E-12	8.42E-11	7.45E-11	1.81E-11	59.3	189.2	95.7	96.2
0.250	3.41E-12	1.01E-10	8.42E-11	2.21E-11				
0.300	3.34E-12	9.27E-11	8.01E-11	2.29E-11				
0.350	2.48E-12	8.60E-11	7.69E-11	2.10E-11				
0.400	2.94E-12	7.43E-11	7.47E-11	2.03E-11				
0.450	1.71E-12	7.66E-11	7.10E-11	1.95E-11				
0.500	2.16E-12	6.64E-11	6.57E-11	1.83E-11	44.9	234	107.4	102.6
	3.35E-12	9.61E-11	7.93E-11	1.94E-11				
0.200	3.86E-13	1.28E-10	6.77E-11	2.45E-11				

Table D-6

MonolayerVoltammetry Data for Thiol-Second Electrode

scan rate (mV/s)	Epa_1	Epa_2	Epc_1	Epc_2	ipa_1	ipa_2	ipc_1	ipc_2
25	298	476	449	276	0.386	0.477	0.516	0.391
50	302	474	446	273	0.688	0.809	0.892	0.641
75	298	472	449	274	0.701	1.033	1.257	0.821
100	301	471	450	272	0.831	1.264	1.552	0.981
125	301	472	449	272	0.934	1.486	1.833	1.122
150	301	473	450	270	1.037	1.708	2.128	1.292
175	302	475	450	269	1.141	1.869	2.394	1.416
200	302	475	450	270	1.231	2.058	2.675	1.548
250	302	476	447	268	1.435	2.433	3.158	1.775
300	303	479	448	268	1.568	2.785	3.632	2.035
350	304	479	448	266	1.747	3.133	4.075	2.279
400	305	479	446	265	1.957	3.435	4.545	2.492
450	305	482	446	264	2.131	3.779	4.966	2.669
500	305	481	447	263	2.282	4.089	5.376	2.925

ΔEp_1	ΔEp_2	ipa_1/ipc_1	ipa_2/ipc_2	E^0_1	E^0_2	Area 1	Area 2	Area 3	Area 4
22	200	0.986	0.924	287.0	462.5	5.935E-09	2.014E-08	2.062E-08	7.959E-09
29	201	1.072	0.907	287.5	460.0	1.268E-08	3.149E-08	3.626E-08	1.437E-08
24	198	0.854	0.822	286.0	460.5	1.333E-08	3.944E-08	5.283E-08	2.009E-08
29	199	0.847	0.814	286.5	460.5	1.892E-08	4.614E-08	6.302E-08	2.577E-08
29	200	0.832	0.811	286.5	460.5	2.179E-08	5.506E-08	7.67E-08	2.835E-08
31	203	0.803	0.809	285.5	461.5	2.658E-08	6.488E-08	8.757E-08	3.651E-08
33	206	0.806	0.781	285.5	462.5	2.97E-08	7.209E-08	9.958E-08	4.025E-08
32	205	0.795	0.769	286.0	462.5	3.158E-08	7.779E-08	1.123E-07	4.185E-08
34	208	0.808	0.770	285.0	461.5	3.873E-08	9.338E-08	1.399E-07	4.944E-08
35	211	0.771	0.767	285.5	463.5	4.126E-08	1.128E-07	1.539E-07	5.783E-08
38	213	0.767	0.769	285.0	463.5	4.951E-08	1.252E-07	1.694E-07	6.734E-08
40	214	0.785	0.756	285.0	462.5	5.963E-08	1.351E-07	1.994E-07	7.484E-08
41	218	0.798	0.761	284.5	464.0	6.703E-08	1.595E-07	2.203E-07	7.902E-08
42	218	0.780	0.761	284.0	464.0	7.098E-08	1.655E-07	2.322E-07	9.055E-08
32.5	205.5			285.5	462.5	6.91E-09	5.92E-08	3.59E-08	2.94E-08

scan rate (V/s)	$\Gamma 1$	$\Gamma 2$	$\Gamma 3$	$\Gamma 4$	FWHM	FWHM	FWHM	FWHM
0.025	3.06E-11	1.04E-10	1.06E-10	4.10E-11	40.1	110.6	78.6	54.5
0.050	3.27E-11	8.12E-11	9.35E-11	3.70E-11				
0.075	2.29E-11	6.78E-11	9.08E-11	3.45E-11				
0.100	2.44E-11	5.95E-11	8.12E-11	3.34E-11				
0.125	2.25E-11	5.68E-11	7.91E-11	2.92E-11				
0.150	2.28E-11	5.58E-11	7.53E-11	3.14E-11				
0.175	2.19E-11	5.31E-11	7.34E-11	2.96E-11				
0.200	2.04E-11	5.01E-11	7.24E-11	4.70E-11	44.9	80.2	86.6	85
0.250	2.00E-11	4.82E-11	7.21E-11	2.55E-11				
0.300	1.77E-11	4.85E-11	6.61E-11	2.48E-11				
0.350	1.82E-11	4.61E-11	6.34E-11	2.48E-11				
0.400	1.92E-11	4.33E-11	6.43E-11	2.41E-11				
0.450	1.92E-11	4.57E-11	6.31E-11	2.26E-11				
0.500	1.83E-11	4.27E-11	5.99E-11	2.53E-11	54.5	107.4	85	89.8
	2.11E-11	5.16E-11	7.29E-11	2.81E-11				
0.100	1.78E-11	1.53E-10	9.26E-11	7.58E-11				

Table D-7
Monolayer Voltammetry Data for Thiol-Third Electrode

scan rate (mV/s)	E_{pa1}	E_{pa2}	E_{pc1}	E_{pc2}	i_{pa1}	i_{pa2}	i_{pc1}	i_{pc2}
25	295	468	448	270	0.319	0.375	0.433	0.258
50	298	473	444	266	0.475	0.647	0.737	0.428
75	296	471	447	268	0.647	0.854	1.043	0.569
100	296	471	447	267	0.800	1.026	1.265	0.725
125	296	473	449	265	0.943	1.213	1.503	8.508
150	298	473	448	265	1.071	1.393	1.778	0.972
175	298	476	448	264	1.227	1.540	1.996	1.115
200	299	476	446	263	1.347	1.667	2.191	1.242
250	301	476	446	263	1.579	1.995	2.686	1.457
300	302	478	444	259	1.818	2.238	3.138	1.714
350	302	476	444	258	2.036	2.505	3.505	1.933
400	304	479	444	258	2.207	2.731	3.823	2.101
450	305	480	445	258	2.383	2.942	4.179	7.839
500	306	482	444	256	2.587	3.164	4.678	2.478

ΔE_{p1}	ΔE_{p2}	i_{pa2}/i_{pc2}	i_{pa1}/i_{pc1}	E^{o}_{1}	E^{o}_{2}	Area 1	Area 2	Area 3	Area 4
25	198	1.236	0.866	282.5	458.0	6.72E-09	1.41E-08	1.94E-08	5.90E-09
32	207	1.110	0.877	282.0	458.5	1.08E-08	2.50E-08	3.37E-08	1.16E-08
28	203	1.137	0.819	282.0	459.0	1.78E-08	3.23E-08	5.00E-08	1.47E-08
29	204	1.103	0.811	281.5	459.0	2.14E-08	3.90E-08	5.76E-08	2.07E-08
31	208	0.111	0.807	280.5	461.0	2.51E-08	4.81E-08	6.38E-08	2.52E-08
33	208	1.102	0.783	281.5	460.5	3.06E-08	5.48E-08	8.19E-08	2.76E-08
34	212	1.100	0.772	281.0	462.0	3.60E-08	6.33E-08	8.78E-08	3.26E-08
36	213	1.085	0.761	281.0	461.0	3.99E-08	6.90E-08	9.94E-08	3.83E-08
38	213	1.084	0.743	282.0	461.0	4.77E-08	8.07E-08	1.25E-07	4.23E-08
43	219	1.061	0.713	280.5	461.0	5.87E-08	9.10E-08	1.51E-07	5.81E-08
44	218	1.053	0.715	280.0	460.0	6.35E-08	9.61E-08	1.66E-07	6.60E-08
46	221	1.050	0.714	281.0	461.5	6.99E-08	1.13E-07	1.80E-07	6.83E-08
47	222	0.304	0.704	281.5	462.5	7.56E-08	1.21E-07	2.03E-07	7.84E-08
50	226	1.044	0.676	281.0	463.0	8.64E-08	1.34E-07	2.19E-07	8.31E-08
36	212.5			281.3	461.0	1.68E-08	6.89E-08	7.70E-07	3.53E-08

scan rate (V/s)	C 1	C 2	C 3	C 4	FWHM	FWHM	FWHM	FWHM
0.025	3.47E-11	7.27E-11	9.98E-11	3.04E-11	38.4	89.8	83.4	65.8
0.050	2.78E-11	6.44E-11	8.70E-11	2.98E-11				
0.075	3.06E-11	5.54E-11	8.00E-11	2.53E-11				
0.100	2.76E-11	5.03E-11	7.42E-11	2.67E-11				
0.125	2.59E-11	4.96E-11	6.58E-11	2.59E-11				
0.150	2.63E-11	4.71E-11	7.04E-11	2.37E-11				
0.175	2.65E-11	4.66E-11	6.47E-11	2.40E-11				
0.200	2.57E-11	4.45E-11	6.41E-11	2.47E-11	43.3	125.0	83.4	93.0
0.250	2.46E-11	4.16E-11	6.46E-11	2.18E-11				
0.300	2.52E-11	3.91E-11	6.50E-11	2.50E-11				
0.350	2.34E-11	3.54E-11	6.11E-11	2.43E-11				
0.400	2.25E-11	3.63E-11	5.79E-11	2.20E-11				
0.450	2.17E-11	3.48E-11	5.82E-11	2.25E-11				
0.500	2.23E-11	3.46E-11	5.64E-11	2.14E-11	52.9	152.3	89.8	88.2
	2.58E-11	4.56E-11	6.48E-11	2.45E-11				
0.200	1.08E-11	4.44E-11	4.96E-10	2.28E-11				