Synthesis, Structure, and Photophysics of Polypyridophenazine Transition-Metal Complexes

Thesis by

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In Partial Fulfillment of the Requirements
for the Degree of
Doctor of Philosophy

California Institute of Technology
Pasadena, California
1994
(Submitted May, 1994)

For Lena Larson

on her 93rd birthday

Acknowledgment

I has been a wonder to work for Harry Gray. He made me a chemist.

The work presented in this thesis would not have been possible without the help of Harry, Vince Catalano, Mike Hill, Jay Winkler, Marilyn Olmsted, Max Bachrach, Michelle Arkin, Eric Stemp, Jeff Clites, Cindy Dupreur, Sam Kim, Kent Mann, and the Gray Group.

For help in un- and nonprofessional activities, I must thank Michelle, Vince, Alison McCurdy, Dan Jones, Todd Richmond, Missy Richmond, Marc Hilmeyer, Steve Buratto, the Gray Group, and The Larsons.

Abstract

The condensation of phenanthroline-5,6-dione (phendione) with polyamines is a versatile synthetic route to a wide variety of chelating ligands. Condensation with 2,3-*napthalene* diamine gives benzo[i]dipyrido[3,2-a:2',3'-c]phenazine (bdppz) a ligand containing weakly-coupled orbitals of benzophenazine (bpz) and 2,2'-bipyridinde(bpy) character. The bpy character gives Re and Ru complexes excited-state redox properties; intramolecular electron transfer (ET) takes place to the bpz portion of the ligand. The charge-separated state so produced has an extraordinarily-long 50 μs lifetime. The slow rate of charge recombination arises from a combination of extremely weak coupling between the metal center and the bpz acceptor orbital and Marcus "inverted region" behavior. Molecular orbital calculations show that only 3% the electron density in the lowest unoccupied molecular orbital lies on the bpy atoms of bdppz, effectively trapping the transferred electron on the bpz portion. The rate of charge recombination decreases with increasing driving force, showing that these rates lie in the inverted region. Comparison of forward and back ET rates shows that donor-acceptor coupling is four orders of magnitude greater for photoinduced electron transfer than it is for thermal charge recombination.

Condensation of phendione with itself or tetramines gives a series of binucleating tetrapyridophenazine ligands of incrementally-varying coordination-site separation. When a photoredox-active metal center is attached, excited-state energy and electron transfer to an acceptor metal center at the other coordination site can be studied as a function of distance. A variety of monometallic and homo- and heterodimetallic tetrapyridophenazine complexes has been synthesized. Electro- and magnetochemistry show that no ground-state interaction exists between the metals in bimetallic complexes. Excited-state energy and electron transfer, however, takes place at rates which are invariant with increasing donor-acceptor separation, indicating that a very efficient

coupling mechanism is at work. Theory and experiment have suggested that such behavior might exist in extended π-systems like those presented by these ligands.

Condensation of three equivalents of 4,5-dimethyl-1,2-phenylenediamine with hexaketocyclohexane gives the trinucleating ligand hexaazahexamethyltrinapthalene (hhtn). Attaching two photredox-active metal centers and a third catalytic center to hhtn provides means by which multielectron photocatalyzed reactions might be carried out. The coordination properties of hhtn have been examined; X-ray crystallographic structure determination shows that the ligand's constricted coordination pocket leads to distorted geometries in its mono- and dimetallic derivatives.

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Abbreviations of Ligand Names

bdppz	benzo[i]dipyrido[3,2-a:2',3'-c]phenazine
bdppzd	benzo[i]dipyrido[3,2-a:2',3'-c]phenazine-10, 15-dione
bpy	2,2'-bipyridine
bpz	benzo[a]phenazine
dppz	dipyrido[3,2-a:2',3'-c]phenazine
hhtn	5,6,11,12,17,18-hexaaza-2,3,8,9,14,15-hexamethyltrinapthalene
phen	1,10-phenanthroline
phendione	1,10-phenanthroline-5,6-doine
pz	phenazine
tatpp	5,7,12,14-tetraaza-tetrapyrido[3,2-*a*:2',3'-*c*:3",2"-*h*:2"',3"'-*j*]pentacence
tpbpz	tetrapyrido[3,2-*d*:2',3'-*f*:3",2"-*d'*:2"',3"'-*f*]biphenazine
tppz	tetrapyrido[3,2-*a*:2',3'-*c*:3",2"-*f*:2"',3"'-*h*] phenazine

Chapter 1

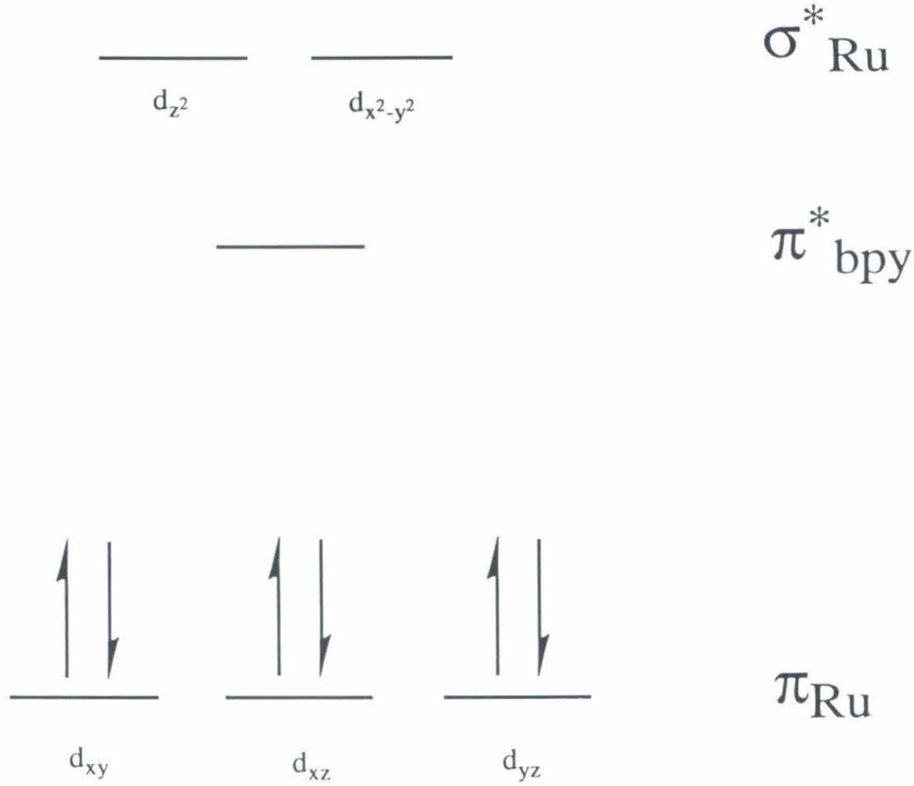
Introduction

The Modern Era of inorganic photochemistry began in 1972 with Gafney and Adamson's report that $Ru(bpy)_3^{2+}$ acts as an excited-state electron-transfer reductant.[1] The authors expressed their wish that the complex would someday find general use as a photosensitizer. To date, thousands of papers of studies of $Ru(bpy)_3^{2+}$ and its derivatives have been published. The "endearing properties"[2] of the molecule- photostability, high visible-region extinction coefficients, and a long excited-state lifetime- have made this huge body of work possible.

These qualities can be understood in terms of the MO diagram shown in figure 1.1. Octahedral symmetry splits the metal d orbitals into two sets of degenerate MOs, three nonbonding π orbitals and two antibonding σ^* orbitals. The six d electrons of Ru^{2+} fill the π MOs, giving a singlet ground state. Empty bpy π^* orbitals lie between the metal-centered orbitals, giving rise to a lowest excited state which is MLCT in character. The singlet-singlet MLCT is allowed and intense (ε=14,000 mol l^{-1} cm^{-1}) with an absorption maximum of 450 nm, giving $Ru(bpy)_3^{2+}$ complexes their characteristic orange color. Excited-state ligand dissociation is circumvented since the electron promoted does not reside in an antibonding orbital. The heavy Ru atom promotes intersystem crossing to the ^{3}MLCT state with unit efficiency; spin-forbidden radiative relaxation to the ground state is slow, giving the excited state a lifetime of 600 ns in fluid solution at room temperature.[3] $Ru(bpy)_3^{2+*}$ can participate in an exited-state reaction if the rate of inter- or intramolecular ET or energy transfer is greater than the rate of radiative decay; its long lifetime assures that such reactions are possible.

In its excited state, $Ru(bpy)_3^{2+}$ is both a better oxidant and reductant than it is in its ground state, as shown in figure 1.2. Oxidative quenching occurs by ET from the energetic ^{3}MLCT excited state; the electron gained by reductive quenching fills the hole in the LUMO vacated by the excited electron. The energy content of the excited state is the amount of energy the incoming photon has in excess of the ground-state reduction potential:

Figure 1.1. MO energy level diagram of $Ru(bpy)_3^{2+}$.


σ*Ru
d_{z^2}
$d_{x^2-y^2}$
π*bpy
πRu
d_{xy}
d_{xz}
d_{yz}

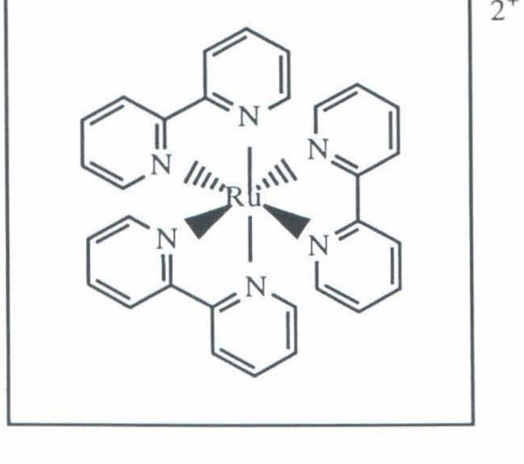
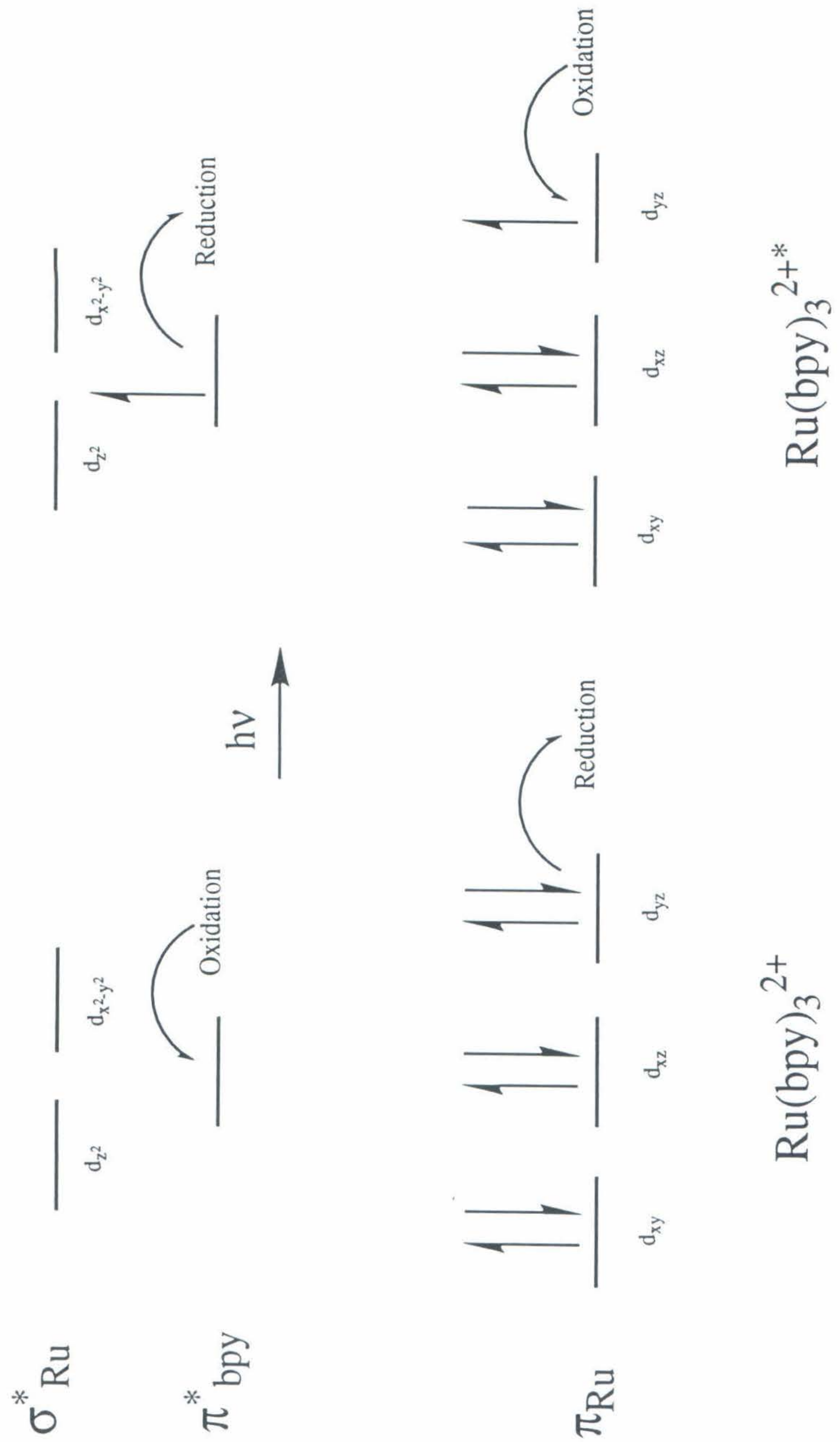

2+
N
N
N
N
N
N
Ru

Figure 1.2. Ground- and excited-state redox scheme for $Ru(bpy)_3^{2+}$.


σ*Ru
π*bpy
πRu
dz²
dx²-y²
Oxidation
dxy
dxz
dyz
Reduction
Ru(bpy)3 2+
hν
dz²
dx²-y²
Reduction
dxy
dxz
dyz
Oxidation
Ru(bpy)3 2+*

$$E(A^+/A^*)=E(A^+/A)-E_{0-0} \qquad 1$$

$$E(A^*/A^-)=E(A/A^-)+E_{0-0} \qquad 2$$

where E_{0-0} is the energy of the 0-0 transition of the emitting excited state. The relevant energies of $Ru(bpy)_3^{2+}$ are shown in a modified Latimer diagram in figure 1.3.[3] The excited state can reduce molecule A with $E^0(A/A^-) > -0.86$ V (Equation 3) and oxidize molecule A with $E^0(A^+/A) < 0.86$ V (Equation 4).

$$Ru(bpy)_3^{2+} + A + h\nu \rightarrow Ru(bpy)_3^{2+*} + A \rightarrow Ru(bpy)_3^{3+} + A^- \qquad 3$$

$$Ru(bpy)_3^{2+} + A + h\nu \rightarrow Ru(bpy)_3^{2+*} + A \rightarrow Ru(bpy)_3^{+} + A^+ \qquad 4$$

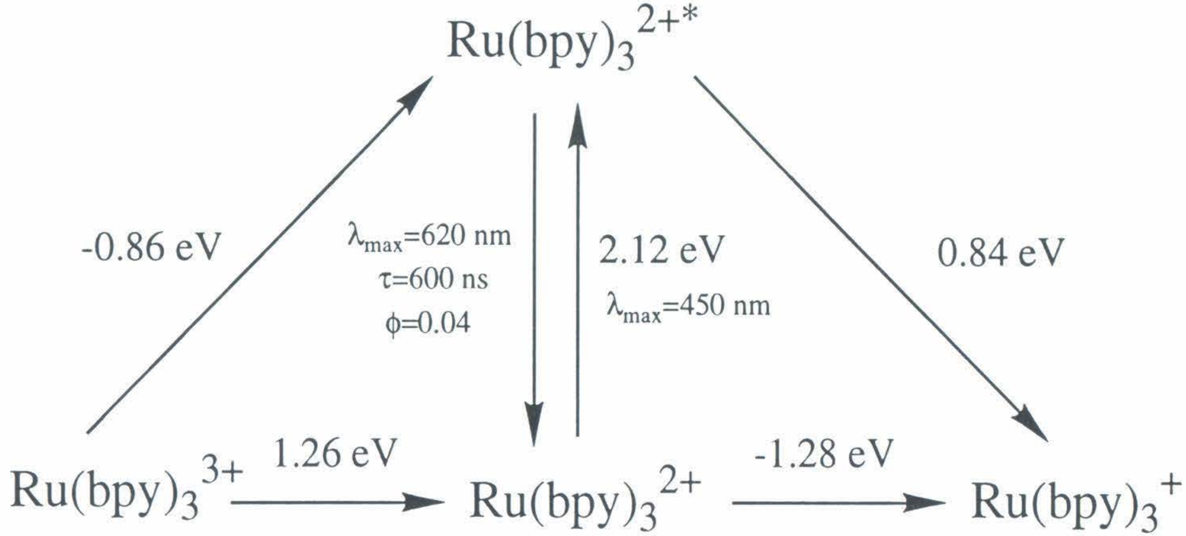
Thus light can be used to drive a reaction in a nonspontaneous direction. The state so produced is thermodynamically unstable; back reaction to $Ru(bpy)_3^{2+}$ and A is rapid. If, however, another molecule B is present which can react with the transient Ru species, net electron transfer between A and B can be effected by the photocatalytic action of $Ru(bpy)_3^{2+}$, shown in figure 1.4 This scheme is an inorganic equivalent of photosynthesis, in which chlorophyll uses light energy to reduce CO_2 to carbohydrate and, in the other half-reaction, to oxidize H_2O to O_2. The realization that photochemical energy conversion using $Ru(bpy)_3^{2+}$ was possible came in 1975,[4] in the wake of the OPEC oil embargo, an event that made Western nations aware, at least temporarily, that oil was an exhaustible resource controlled by nations with different agendas. The Energy Crisis that followed brought increased funding for research into alternative energy sources, and the next ten years saw the publication of hundreds of papers utilizing emissive coordination compounds in attempts to develop technologies to convert sunlight into more useful forms of energy. Chief among these was splitting water.

Examination of the reactions relevant to the oxidation and reduction of H_2O to O_2 and H_2 at pH 7 (Equations 5 and 6) shows that $Ru(bpy)_3^{2+*}$ is capable of performing both.

$$1/2\ H_2O \rightarrow H^+ + 1/4O_2 + e^- \qquad E^0=0.82\ V \qquad 5$$

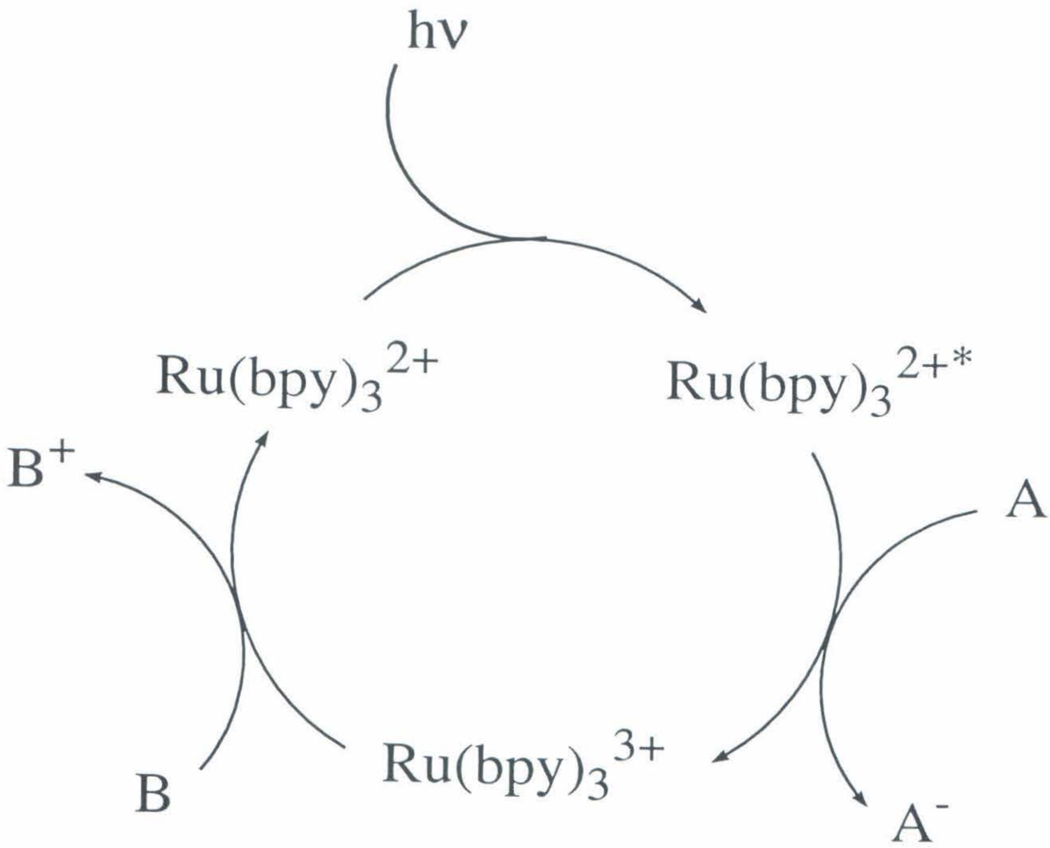
$$1/2\ H_2O + e^- \rightarrow OH^- + 1/2H_2 \qquad E^0=-0.41\ V \qquad 6$$

Figure 1.3. Modified Latimer diagram for $Ru(bpy)_3^{2+}$.



Ru(bpy)3 2+*
-0.86 eV
λmax=620 nm
τ=600 ns
φ=0.04
2.12 eV
λmax=450 nm
0.84 eV
Ru(bpy)3 3+
1.26 eV
Ru(bpy)3 2+
-1.28 eV
Ru(bpy)3 +

Figure 1.4. Electron transfer photosensitized by $Ru(bpy)_3^{2+}$.

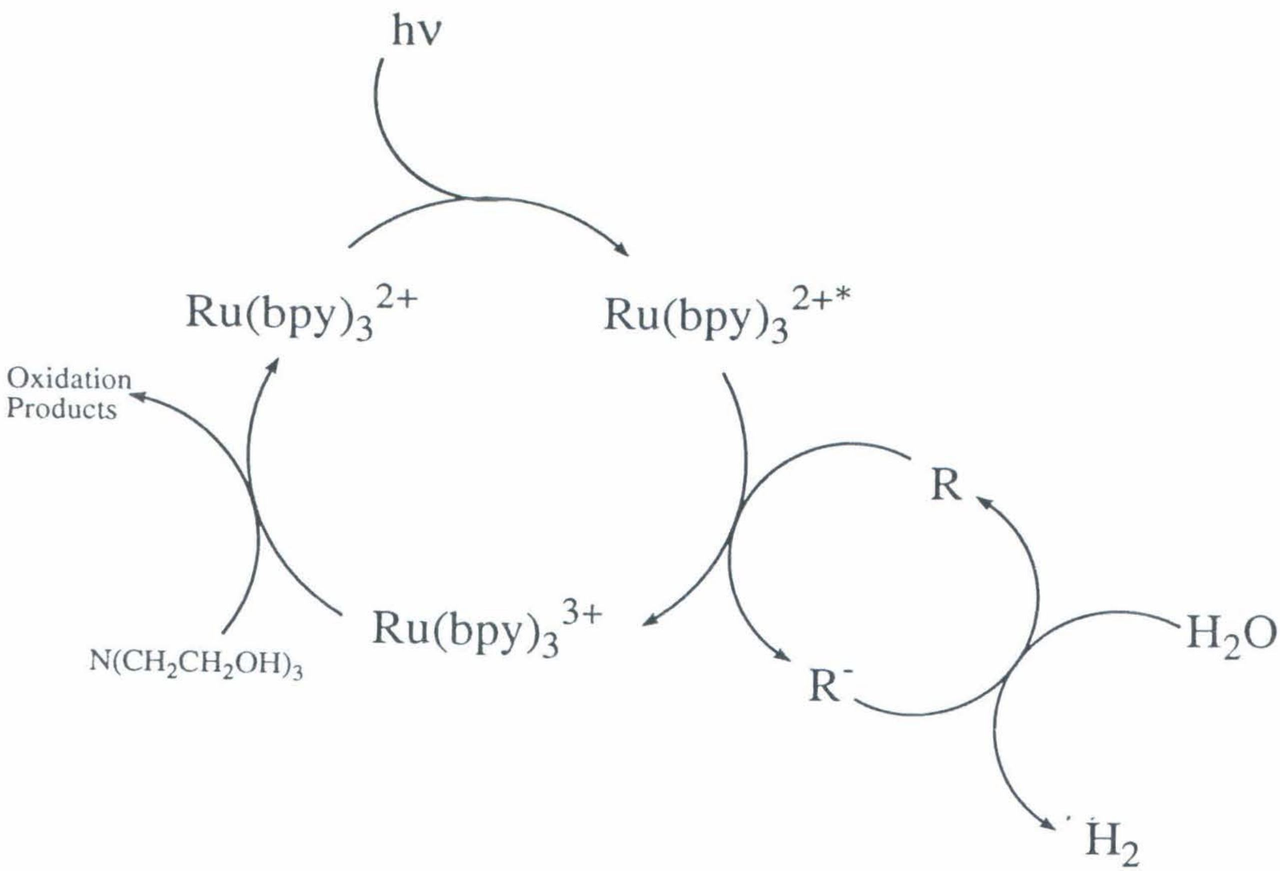

hν
Ru(bpy)3 2+
Ru(bpy)3 2+*
B+
A
B
Ru(bpy)3 3+
A-

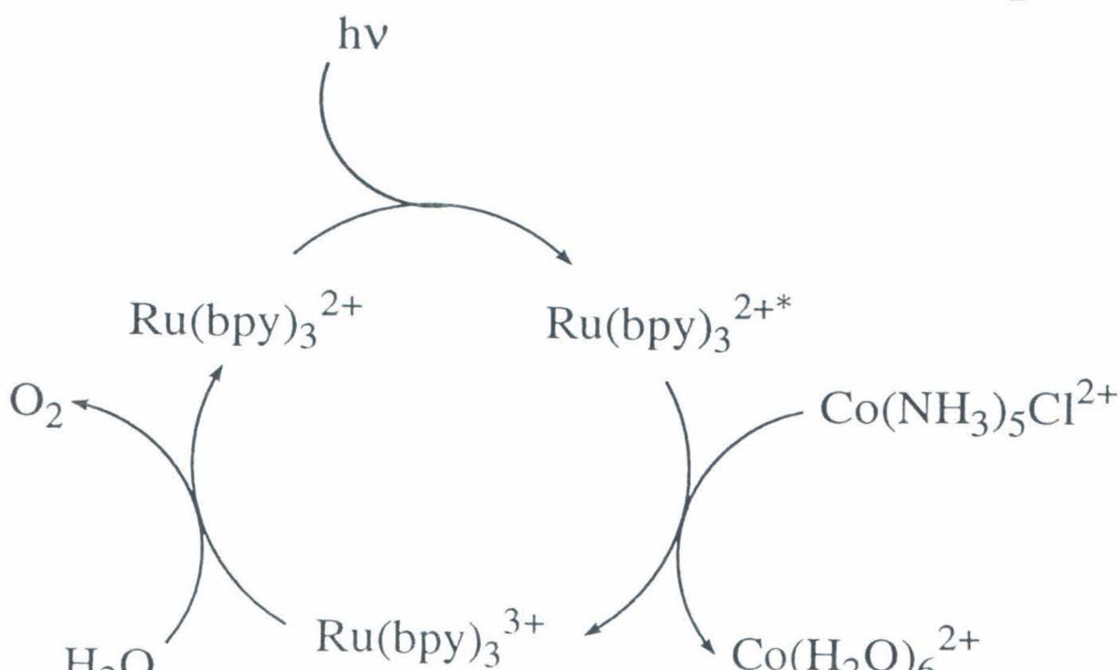
It need only be able to carry out one of the half-reactions, since the $Ru(bpy)_3^{3+}$ or $Ru(bpy)_3^{+}$ formed by ET quenching can accomplish the other half-reaction thermally. Obviously, since $Ru(bpy)_3^{2+}$ is emissive in water, water splitting does not happen. The potentials in equations 5 and 6 are for overall oxidation and reduction; $Ru(bpy)_3^{2+*}$ is not capable of direct one-electron reduction to H_2 (E^0=-2.69 V) or one-electron oxidation to hydroxyl radical (E^0=2.33 V).[5] Catalysts are needed to stabilize radical intermediates and make the rates of desirable reactions competitive with energy-wasting back reactions. Energy-conversion systems become complicated rapidly.

Work led to the development of systems that could produce either H_2 or O_2; no one has ever been able to devise a coordination-compound-based method for visible-light- induced decomposition of water into both its elements. Whether O_2- or H_2-producing, these systems share the characteristic that $Ru(bpy)_3^{2+*}$ does not react directly with H_2O, a feature shown in figure 1.5. The excited state is oxidatively quenched by a reversible relay which reduces water with the aid of a catalyst; a sacrificial electron donor such as triethanolamine prevents back ET by reducing $Ru(bpy)_3^{+}$.[6] To oxidize water, $Ru(bpy)_3^{2+*}$ transfers an electron irreversibly to an acceptor such as $Co(NH_3)_5Cl$, which is rapidly aquated. The $Ru(bpy)_3^{3+}$ so formed can then produce O_2 in the presence of a catalyst.[7]

It is difficult to envision an homogenous system that splits water; the highly-energetic species needed to perform the oxidation and reduction would be most reactive toward each other, short-circuiting the process. A possible solution to the problem is the physical separation of the components needed for each half-reaction. The next phase of research examined ET behavior in heterogenous systems, including polymers,[8] functionalized electrodes,[9] and membranes.[10] While a great deal of creativity and energy went into these studies, it appears that the initial promise $Ru(bpy)_3^{2+}$ showed as a sensitizer for photochemical energy conversion will go unfulfilled. Such is the nature of basic research.

Figure 1.5. H_2 and O_2 production with $Ru(bpy)_3^{2+}$.


hν
Ru(bpy)3 2+
Ru(bpy)3 2+*
Oxidation Products
R
H2O
Ru(bpy)3 3+
N(CH2CH2OH)3
R-
H2


hν
Ru(bpy)3 2+
Ru(bpy)3 2+*
O2
Co(NH3)5Cl 2+
Ru(bpy)3 3+
H2O
Co(H2O)6 2+

The Modern Era is far from over, however. $Ru(bpy)_3{}^{2+}$ continues to generate substantial interest; nearly 100 papers on $Ru(diimine)_3{}^{2+}$ complexes were published in 1993.[11] Inorganic photochemistry has grown to include many additional compounds which exhibit excited-state properties like those of $Ru(bpy)_3{}^{2+}$, including $[Au_2$(bis-(dicyclohexylphospino)ethane$)_3]^{2+}$[12], $Re(CO)_3(bpy)Cl$[13], [Ir(μ-pyrazolyl) (cyclooctadine)$]_2$.[14] The field continues to flourish.

In a sense, research in the area of ET employing inorganic chromophores has come full circle, through the period of energy conversion research, back to 1974, when Meyer et al. published the first paper providing direct spectroscopic evidence of the ability of $Ru(bpy)_3{}^{2+*}$ to act as an ET agent.[15] The study employed MV^{2+}, which becomes intensely colored upon reduction, to oxidatively quench the excited state. Transient absorption spectroscopy showed that $MV^{+\bullet}$ and $Ru(bpy)_3{}^{3+}$ were formed upon laser irradiation of a solution containing MV^{2+} and $Ru(bpy)_3{}^{2+}$, proving that ET had taken place. The system was now in an unstable state, and the rate of thermal ET from $MV^{+\bullet}$ back to $Ru(bpy)_3{}^{3+}$ was measured by following the decay of $MV^{+\bullet}$ absorbance. In theory, it could have been possible to measure the rate by mixing $MV^{+\bullet}$ and $Ru(bpy)_3{}^{3+}$ generated by chemical reduction and oxidation in a stopped-flow apparatus. The rate of charge recombination, 8.3×10^9 M^{-1} s^{-1}, was much faster than could be measured using stopped-flow techniques, however, and this work showed that using an ET sensitizer allowed the rates of very exothermic reactions to be measured. For reactions slow enough to be followed via mixing, photon-triggered production of the redox partners provided a much more convenient method of determination since the reactants were generated *in situ*.. It was also possible, of course, to measure the rates of photoinduced ET from the excited state by transient absorption spectroscopy and by measuring loss of emission intensity and excited-state lifetime in the presence of a quencher.

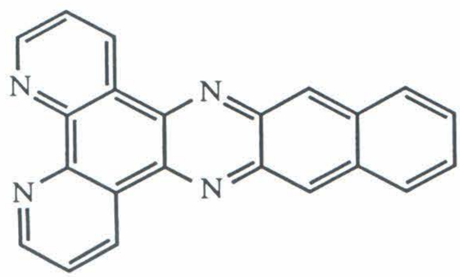
While $Ru(bpy)_3^{2+}$ will not solve the world's energy problems, it is invaluable for its use as a probe of ET properties and will continue to be for the forseeable future. Bimolecular experiments exactly like those performed twenty years ago are still providing new insight into ET phenomena.[16] Donor-acceptor pairs containing bpy-based chromophores have been covalently attached to a great number of molecular spacers to investigate the role the intervening medium plays in promoting thermal and photoinduced ET. These spacers have been biomolecules such as DNA[17] and proteins,[18] to examine reactions fundamental to life, and synthetic spacers which serve as simpler models for biological systems.[19]

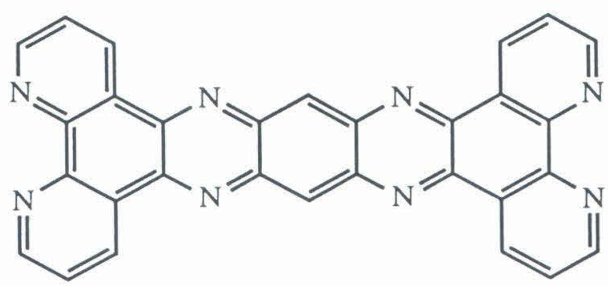
The work described in this thesis is an exploration of ET in Ru and Re polypyridophenazine-based donor-acceptor systems. The following three chapters are united by a common synthetic motif, shown in Figure 1.6 - the condensation of α-polyketones with α-polyamines to give substituted phenazines.

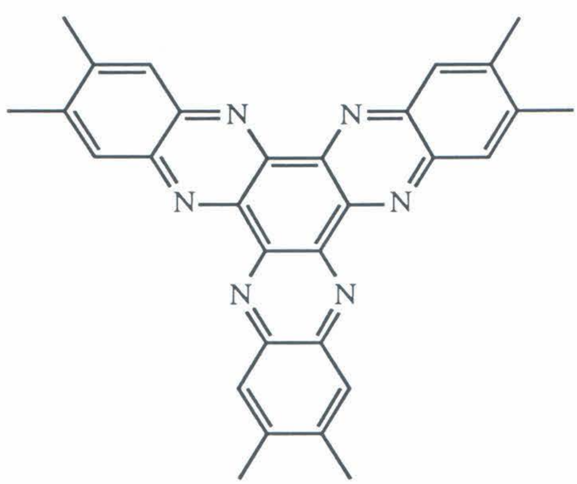
In Chapter 2, phendione is condensed with 2,3-diaminonapthalene to give bdppz, which acts as independent bpy and bpz units. The bpz portion of the molecule, which acts as an electron acceptor, is very poorly coupled to the coordinated photoactive metal center, leading to a photoinduced charge-separated state with an extraordinarily long lifetime. This lifetime is further lengthened by increasing the thermodynamic force for thermal charge recombination, pushing the kinetics deeper into the "inverted region" predicted by the Marcus theory of electron transfer.[20] Extracting the coupling matrix elements from plots of ET rate versus driving force for forward and reverse ET reveals that photoinduced ET out to the bpz portion of the molecule is electronically coupled four orders of magnitude more strongly than thermal charge recombination.

Condensation of phendione with benzenetetramine gives tatpp, a ligand with two diimine binding sites. Mono- and dimetallic compounds of tatpp and related tetradentate ligands with varying binding-site separations are synthesized in Chapter 3. Ground- and excited-state energy and electron transfer in these complexes is examined in a number of

Figure 1.6. Ligands employed in this work: bdppz, top; tatpp; middle; hhtn, bottom.







ways. Ground-state metal-metal coupling in electrochemically-generated mixed-valence $Ru^{II}Ru^{III}$ dimers is treated with Hush theory,[21] which shows that the metal centers are essentially uncoupled. This finding is independently verified by variable-temperature magnetic susceptibility measurement s, which also indicate that there is no communication between the metal atoms in dimeric Cu^{II} complexes of the ligands. Time-resolved spectroscopic studies of $Ru(bpy)_2$-spacer-M;where M is Ru, Os, or Cu; shows that photoinduced ET from Ru to M is very rapid, the result of good excited-state donor-acceptor coupling. The lack of ground-state coupling manifests itself in thermal charge recombination rates orders of magnitude lower than forward photoinduced rates. Energy and electron transfer in Ru-Os complexes appears to take place with rates that are independent of the metal-metal separation distance. This behavior has been predicted in extended, planar π systems.

Condensation of 4,5-dimethyl-1,2-phenylenediamine with hexaketocyclohexane gives hhtn, a ligand with three metal-binding sites. Re and Pd complexes of hhtn are examined in Chapter 4 in an initial investigation of the use of hhtn as platform for constructing photochemical systems capable of performing multielectron photochemistry. X-ray crystallography reveals the structures of mono- and dimetallic derivatives of the ligand to be very distorted. Based on these initial results, suggestions are made for the development of future multielectron photocatalytic systems.

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Chapter 2

Long-lived Charge Separation in Simple Molecules

Introduction

The photosynthetic reaction center is a marvel. Charge separation over a distance of 17 Å takes place on an extremely fast time scale. As shown in Figure 2.1, the crystal structure of the membrane-bound reaction center in *Rhodopseudoomonas viridis*,[1] photoinduced ET from the special pair (SP) to bacteriopheophytin (BP) takes place in 3 ps; the electron then jumps to menaquinone (MQ) in 200 ps. The charge-separated states produced have charge-recombination kinetics that are slow relative to the rate of their formation; the SP^+/BP^- state has a lifetime of 15 ns; charge recombination of SP^+/MQ^- to SP/MQ has a rate constant of 10 s^{-1}.[2] The nine-order-of-magnitude difference between the rates of charge separation and charge recombination assures that the photon energy absorbed by an organism is converted into useful chemical energy and none is lost to wasteful return to the SP/MQ state.

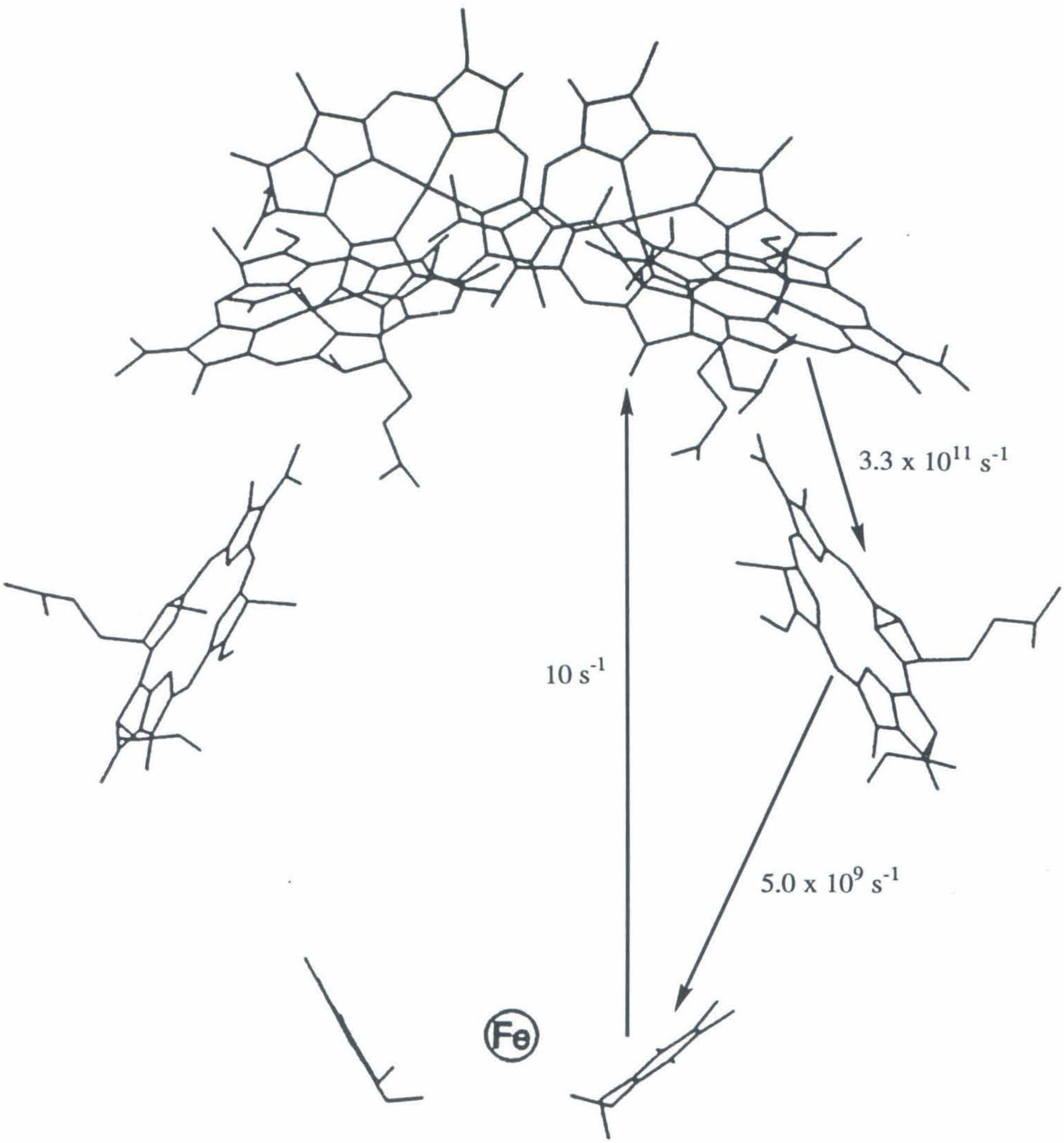
A great deal of effort has gone into elucidating the structure and photophysics of the photosynthetic reaction center. Much research has also been directed toward the construction of simple systems which model specific parts of the photosynthetic system, both to help understand biological systems and, as discussed in Chapter 1, to achieve the ends of photosynthesis artificially.[3] An understanding of the factors which govern ET rates is needed to understand the extraordinary kinetic behavior of natural systems and to devise ways to exploit these factors to design new compounds whose charge-separation properties resemble those found in organisms.

Marcus has derived a semiclassical expression for the rate of ET, given in Equation 1.[4] Examination of the equation shows that the ET rate, k_{ET}, is governed by

$$k_{ET} = \frac{2(H_{ab})^2}{h}\left(\frac{\pi^3}{\lambda RT}\right)^{1/2}\exp\left(\frac{(\Delta G^0 + \lambda)^2}{4RT\lambda}\right) \qquad 1$$

three factors: the degree of coupling between donor and acceptor, H_{ab}, the thermodynamic driving force for the reaction, $-\Delta G^0$, and the reorganization energy , λ.

Figure 2.1. X-ray crystallographic structure of the photosynthetic reaction center of *Rhodopseudoomonas viridis*. Figure from Reference 1, rates from Reference 2.


3.3 x 10^11 s^-1
10 s^-1
5.0 x 10^9 s^-1
Fe

These three parameters are shown graphically in Figure 2.2. H_{ab} is one half of the separation between the potential surfaces of the reactants and products at the crossing avoidance point, $-\Delta G^0$ is the difference between the minimum of the reactant and product energy wells, and λ is the difference between the reactant surface minimum and the product surface when $-\Delta G^0=0$. The barrier to ET, $\Delta G^{\ddagger}$, is defined as the difference in energy between the minimum of the reactant potential surface and the point where reactant and product potential surfaces intersect.

The quadratic form of the Marcus equation predicts that at fixed H_{ab} and λ k_{ET} will increase as $-\Delta G^0$, the driving force for the reaction, increases, reaching a maximum when $-\Delta G^0= \lambda$. As the reaction becomes more exothermic, k_{ET} should actually begin to fall. This surprising behavior is said to take place in the "inverted region" where $-\Delta G^0>\lambda$. The reason for the existence of the inverted region is shown graphically in Figure 2.3. The barrier to ET which exists when $-\Delta G^0=0$ vanishes when $-\Delta G^0= \lambda$ because the reactant and product surfaces now cross at the minimum of the reactant potential well. When $-\Delta G^0$ becomes greater than λ, a new barrier arises from the nesting of reactant and product potential wells. A plot of $\ln(k_{ET})$ versus $-\Delta G^0$ (Figure 2.4) is thus parabolic with a maximum at $-\Delta G^0= \lambda$. While such a relationship may be counterintuitive, the existence of the inverted region has been proven by several different researchers.[5] The relationship between k_{ET} and H_{ab} is more straightforward; since it is a pre-exponential term, increasing C at fixed $-\Delta G^0$ and λ increases k_{ET} as electron donor and electron acceptor become better-coupled. The effect is to displace the entire parabola vertically, as shown in Figure 2.5. The reorganization energy is the sum of two components, the inner-sphere reorganization energy, λ_i, which is the energy required for the changes in bond lengths and angles which accompany changes in oxidation state resulting from ET, and the solvent reorganization energy, λ_s, the energy required to reorganize solvent dipoles after ET occurs. For a given H_{ab}, increasing λ has the effect of broadening the parabola since

Figure 2.2. Graphic representation of the factors governing k_{ET}.

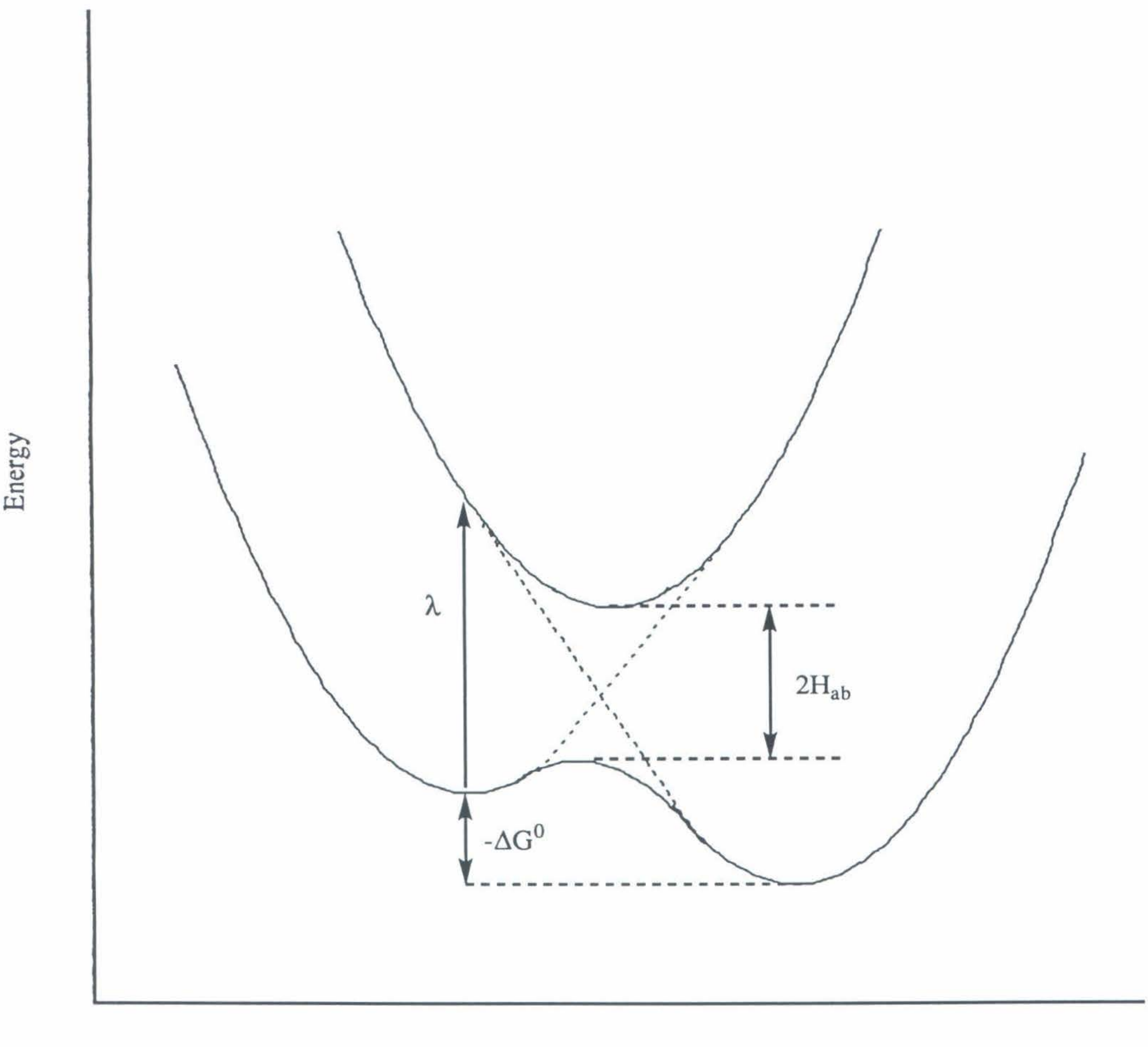

Energy
λ
2H_ab
-ΔG^0
Reaction Coordinate

Figure 2.3. Variation of $\Delta G^{\ddagger}$ with $-\Delta G^0$ at constant H_{ab} and λ.

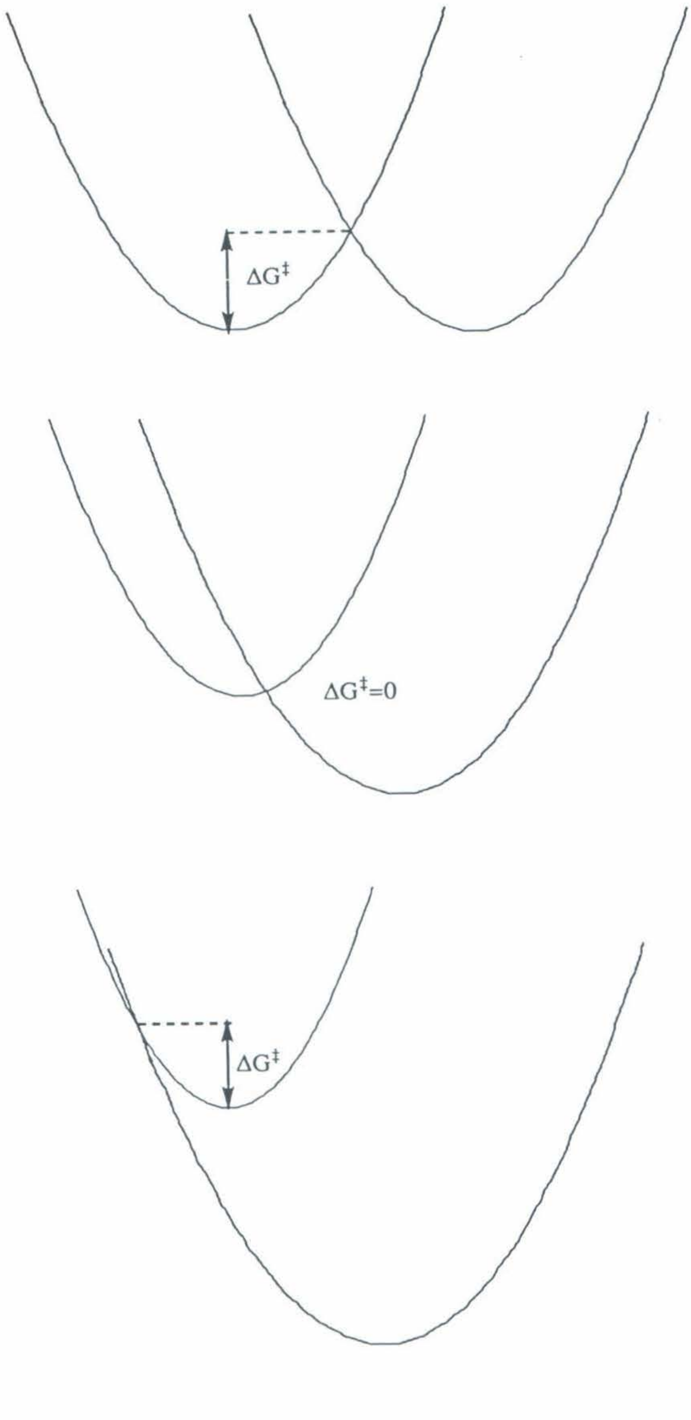

ΔG‡
ΔG‡=0
ΔG‡

Figure 2.4. Theoretical plot of $\ln(k_{ET})$ versus $-\Delta G^0$ at constant H_{ab} and λ.

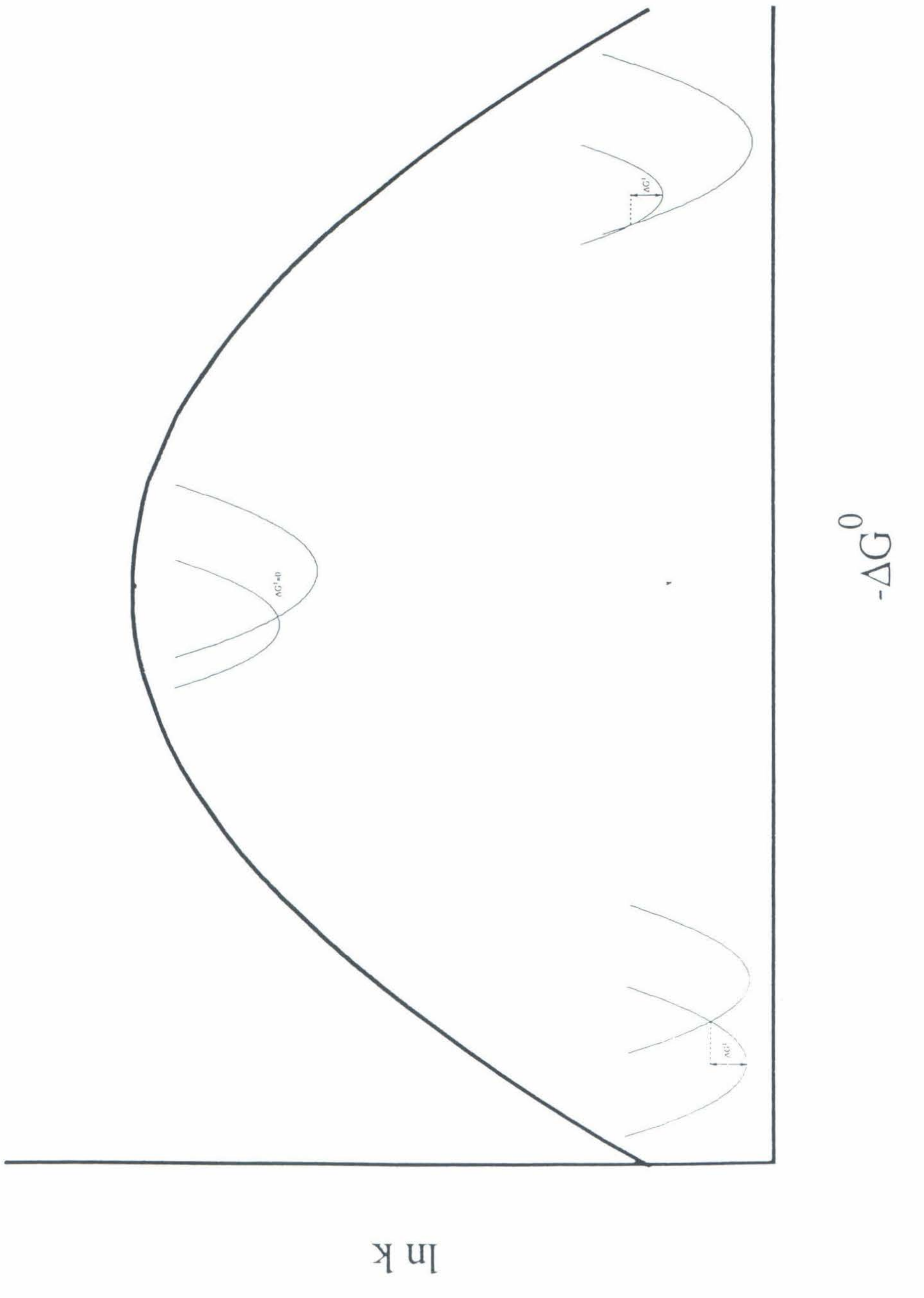
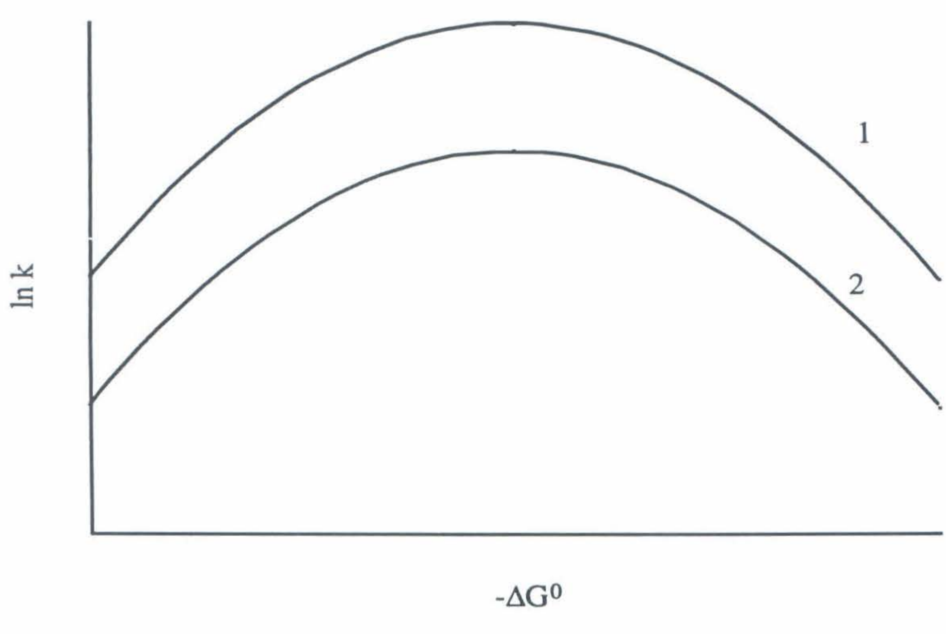

ln k
-ΔG0

Figure 2.5. Effect of increasing H_{ab} on plot of $\ln(k_{ET})$ versus $-\Delta G^0$ at constant λ. $H_{ab}(1)>H_{ab}(2)$.



1
2
ln k
-ΔG0

its maximum, at $-\Delta G^0 = \lambda$, is moved to higher energy. The effect of increasing λ on a plot of $\ln(k_{ET})$ versus $-\Delta G^0$ is shown in figure 2.6.

Marcus theory offers two explanations for the extremely long lifetime of the SP^+MQ^- state in the photosynthetic reaction center. The first is that H_{ab} is much greater for forward ET than it is for thermal charge recombination. This would be possible if excited-state photoinduced ET took place through a higher-lying, better-coupled pathway than the ground-state pathway used for the back reaction. Work in Ru-modified proteins, however, has shown that H_{ab} is the same whether photoinduced or thermal ET is operative.[6] It seems that the same should be true in the peptide framework of the reaction center.

More likely is that the fast forward reactions lie near the apex of the Marcus parabola while the back reactions occur at $-\Delta G^0 > \lambda$ and lie in the inverted region. An energy-level diagram for the reaction center of *Rhodopseudoomonas viridis* is presented in Figure 2.7. As shown by the diagram, ET from SP* to BP and from BP^- to MQ both have a driving force of about 0.3 eV. The reorganization energy of 0.3 eV required to put the rates of these reactions at the apex of the parabola seems too small compared to the λ of 1.0 eV observed in most Ru-modified proteins.[6] It must be remembered, though, that these studies employed solvent-exposed surface-bound Ru probes. λ_s generally makes a larger contribution to the overall λ than does λ_i, so that in the absence of extensive solvent reorganization λ is small. The reaction center is a membrane-bound protein, so the "solvent" is the surrounding peptide. It is unlikely that the residues near the redox centers undergo much reorganization as ET takes place, so a λ of 0.3 eV seems very plausible. The result, shown in Figure 2.8, is a narrow Marcus parabola. k_{ET} drops off very rapidly in the inverted region, and the driving force for thermal recombination of SP^+/BP^- to SP/BP of 1.0 eV puts it well into the inverted region. ET from BP^- to MQ, with $-\Delta G^0$=0.3 eV, is also rapid. Charge recombination of SP^+/MQ^- to SP/MQ, with

Figure 2.6. Effect of varying λ on plot of $\ln(k_{ET})$ versus $-\Delta G^0$ at constant H_{ab}.

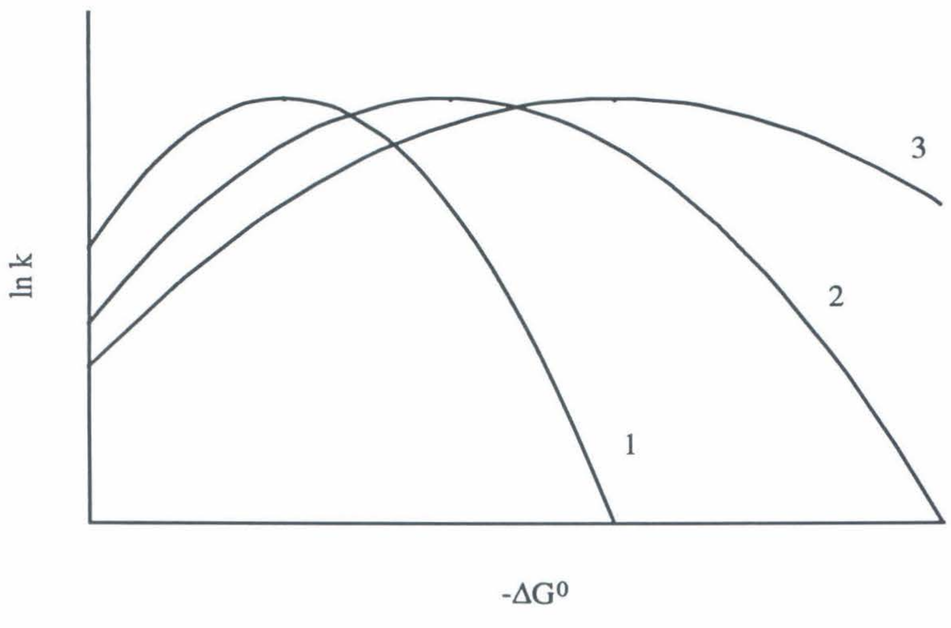

3
2
1
ln k
-ΔG⁰

Figure 2.7. Energy-level diagram for the photosynthetic reaction center of *Rhodopseudoomonas viridis*.

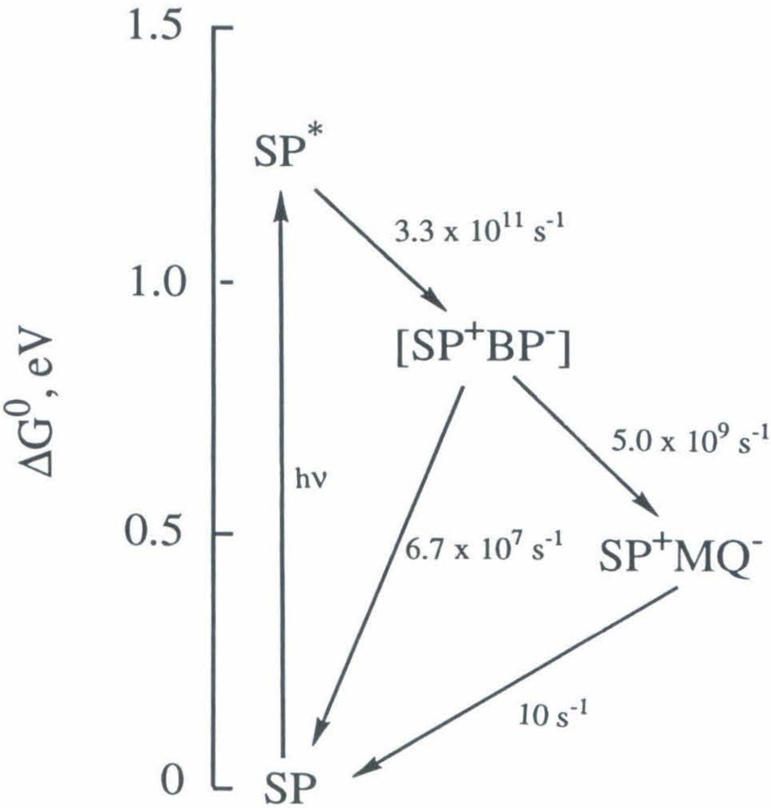
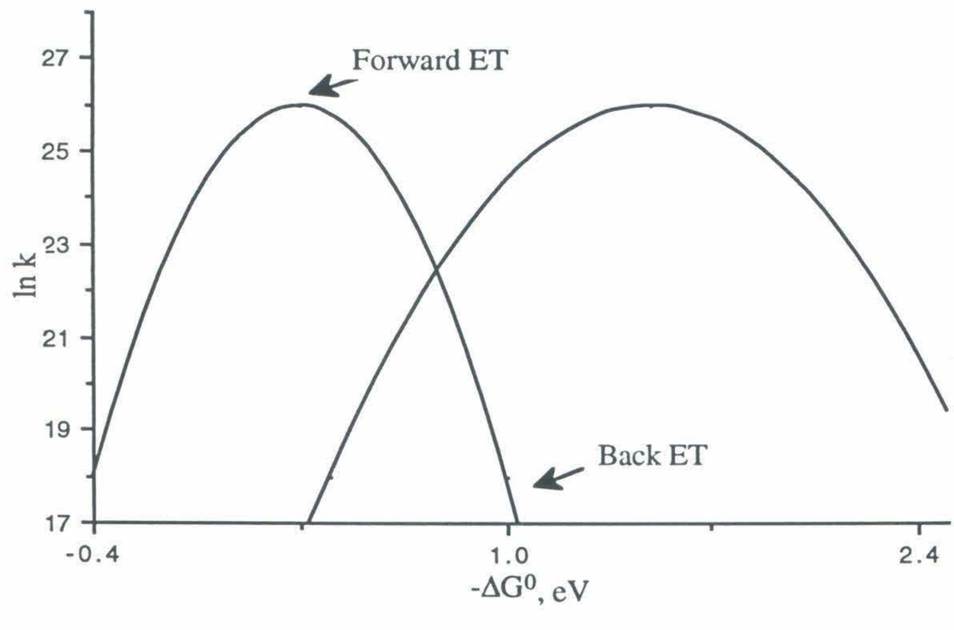

1.5
1.0
0.5
0
ΔG⁰, eV
SP*
3.3 x 10¹¹ s⁻¹
[SP⁺BP⁻]
5.0 x 10⁹ s⁻¹
hν
6.7 x 10⁷ s⁻¹
SP⁺MQ⁻
10 s⁻¹
SP

Figure 2.8. Marcus plot for the photosynthetic reaction center of *Rhodopseudoomonas viridis*. A plot for a typical model system is included for comparison.

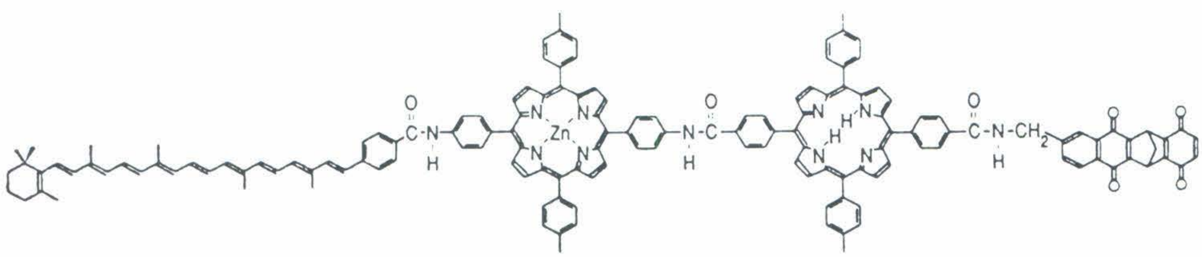

Forward ET
Back ET
ln k
27
25
23
21
19
17
-0.4
1.0
2.4
-ΔG0, eV

$-\Delta G^0$=0.6 eV, should also be in the inverted region, but inverted behavior alone cannot explain the incredibly long 100 ms lifetime of the SP^+/MQ^- state. SP and MQ lie 17 Å apart in the photosynthetic apparatus, leading to a small matrix coupling element. Also responsible is protonation of MQ^- to give a semiquinone, effectively trapping the electron.

The most straightforward approach to constructing an artificial system whose ET behavior begins to approach that of *Rhodopseudoomonas viridis* is to use the same elements present in the natural system. Several researchers have synthesized covalently-linked porphyrin-quinone compounds,[3] the most elaborate of which is the molecular pentad shown in Figure 2.9.[7] It contains all of the features of the biological system: an antenna pigment; a Zn porphyrin that serves the function of the SP; a free-base porphyrin which acts as BP; and a pair of quinones which function as MQ and ubiquinone, the final acceptor in the photosynthetic ET chain. Excitation with visible light leads to a charge-separated state with an impressively-long lifetime of 56 μs. It is likely that the long lifetime in this compound is due solely to its complexity; as in the natural system, large spatial separation leads to slow recombination. The thermodynamic driving force for recombination, 1.0 eV, is not likely to be large enough to give rise to inverted behavior in fluid solution. Thus this system does not possess all of the factors at work in the biological system.

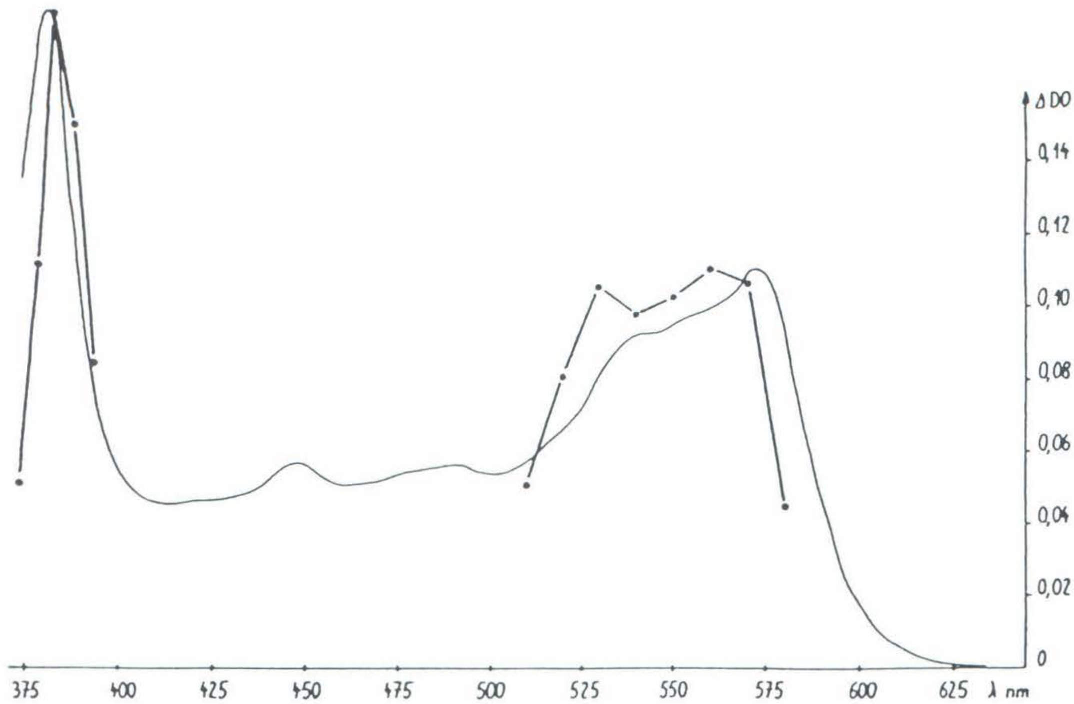
The motivation behind the work in this chapter is the belief that it may be possible to produce long-lived charge separation in a much simpler systems by taking fullest advantage of the features that give rise to the remarkable behavior of the reaction center, namely, inverted behavior and trapping the electron as a semiquinone. The price one pays for simplicity is a lack of donor-acceptor separation and the realtively large electronic coupling which results, leading to faster recombination kinetics. Work by Chambron et al. provides one possibility for the architecture of a simple intramolecular ET system.[8] The dppz ligand of $Ru(bpy)_2(dppz)^{2+}$ has both "optical" bpy and "acceptor"

Figure 2.9. Molecular pentad model of the photosynthetic reaction center. Figure from Reference 7.


O
C-N
H
N
Zn
N
N
N
N-C
H
O
N
H
N
H
N
O
C-N-CH2
H

pz orbitals which are relatively uncoupled. Optical excitation yields MLCT to the bpy portion of the ligand; intramolecular ET from the MLCT state to the pz portion of the ligand gives a charge-separated state whose spectral properties resemble those of singly-reduced pz. Superimposed spectra of reduced pz and the charge-separated state of $Ru(bpy)_2(dppz)^{2+}$ are shown in Figure 2.10. Charge separation leaves Ru in its powerfully-oxidizing 3+ state, giving the back reaction a driving force in excess of 2.0 eV, an energy regime which has produced inverted behavior in several other systems.[5] Ligands like dppz are easily accessible via condensation of phendione with ortho-diamines, allowing the synthesis of new photoredox-active ligands which retain the properties of their components. Condensation with 2,3-diamino-1,4-napthaquinone to give bdppzd (Figure 2.11) and its incorporation into excited-state ET chromophores of Re and Ru yields a system which resembles the basics of the photosynthetic reaction center: a photon-driven electron donor, a quinone acceptor, and inverted behavior. Chapter 2 presents the results of a study that began with bdppzd aimed at producing long-lived charge separation in simple compounds.

Figure 2.10. Transient absorption spectrum of $Ru(bpy)_2(dppz)^{2+}$ (dashed line) and the spectrum of reduced phenazine (solid line). Spectrum reproduced from Reference 8a.


ΔDO
0,14
0,12
0,10
0,08
0,06
0,04
0,02
0
375
400
425
450
475
500
525
550
575
600
625
λ nm

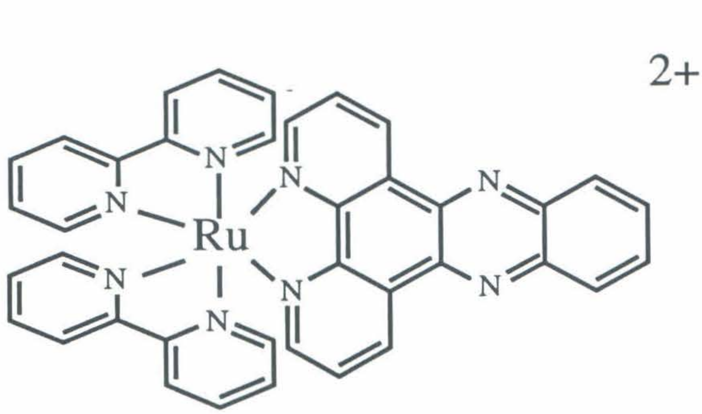
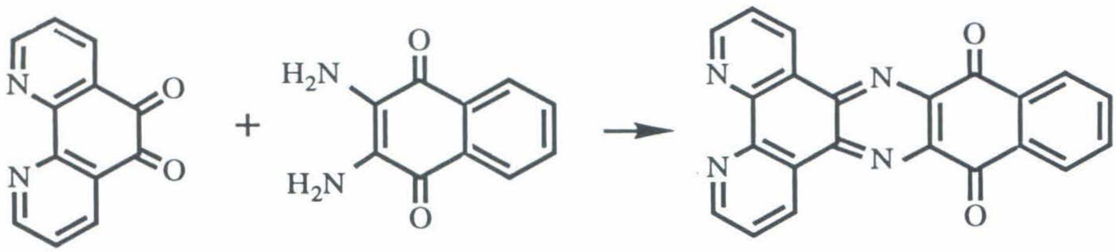

2+
Ru
N

Figure 2.11. Benzodipyridophenazinedione, bdppzd.



Experimental Section

Preparation of Compounds. Chemicals were used as received from Aldrich except 4,4'-$(CH_3)_2$-bpy, which was purchased from GFS. Phendione was prepared according to the method of Yamada.[9] Heating the reaction mixture at 120° for 4 h gave a higher yield than procedure given in the paper. 2,3-diamino-1,4-napthaquinone was synthesized from 2-amino-3-acetamino-1,4-napthaquinone[10] using the procedure of Neeff.[11] Dipyridophenazine ligands were synthesized using the procedure of Dickeson.[12] 4,4'-$(CF_3)_2$-bpy was prepared according to the procedure of Furue.[13] Ru(diimine)$_2$Cl$_2$ complexes were prepared according to Sullivan's procedure.[14] Ru(bpy)$_2$(phendione)(PF$_6$)$_2$ was synthesized using the procedure of Goss.[15] Re(CO)$_3$(bpy)Cl, Re(CO)$_3$(phen)Cl, and Re(CO)$_3$(phendione)Cl were prepared according to the procedure of Morse.[16]

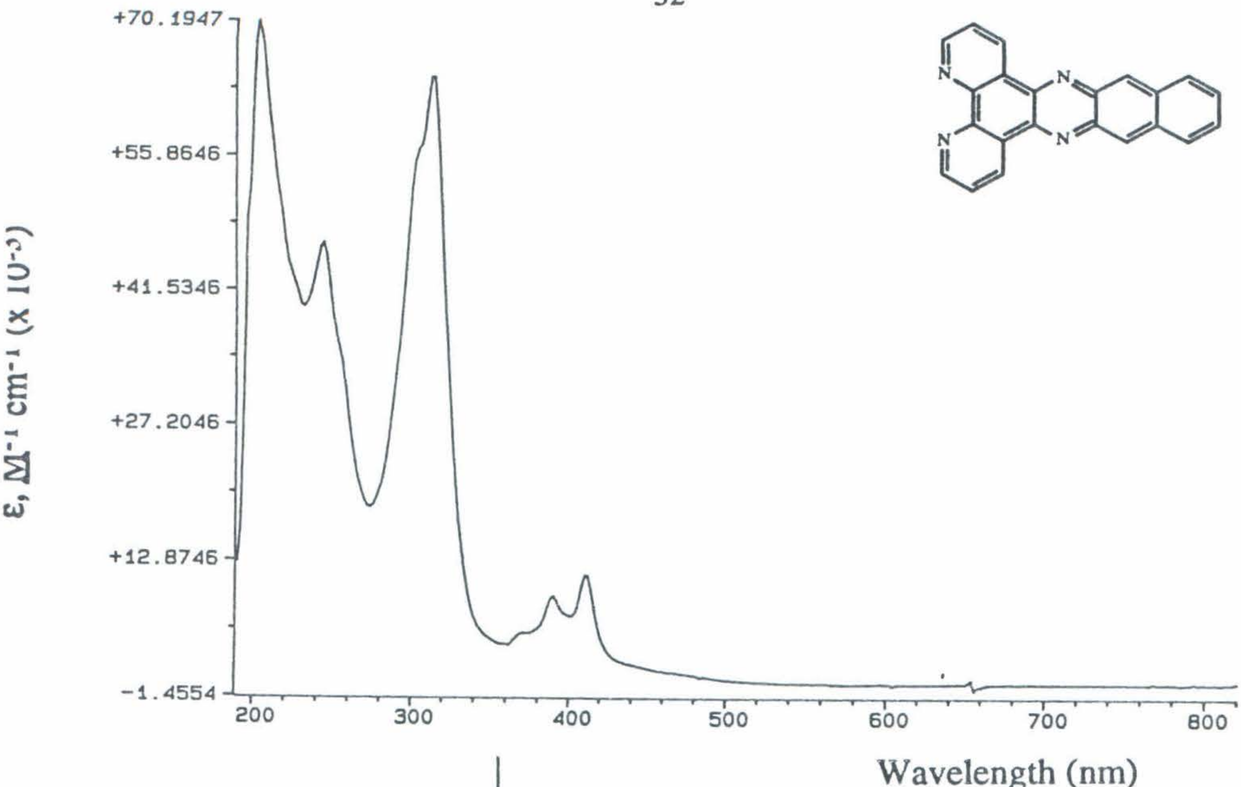
Benzo[i]dipyrido[3,2-a:2',3'-c]phenazine, bdppz. A solution of 360 mg of phendione in 25 ml of 100% ethanol was brought to boiling. 300 mg of 2,3-diamino-napthalene were added; after 30 min, the orange precipitate which formed was collected by filtration and washed with acetone and ether to give 450 mg of bdppz, mp 285 (subl). UV-Vis (CH_3CN), ^{1}H NMR (acetone-d$_6$) Figure 2.12.

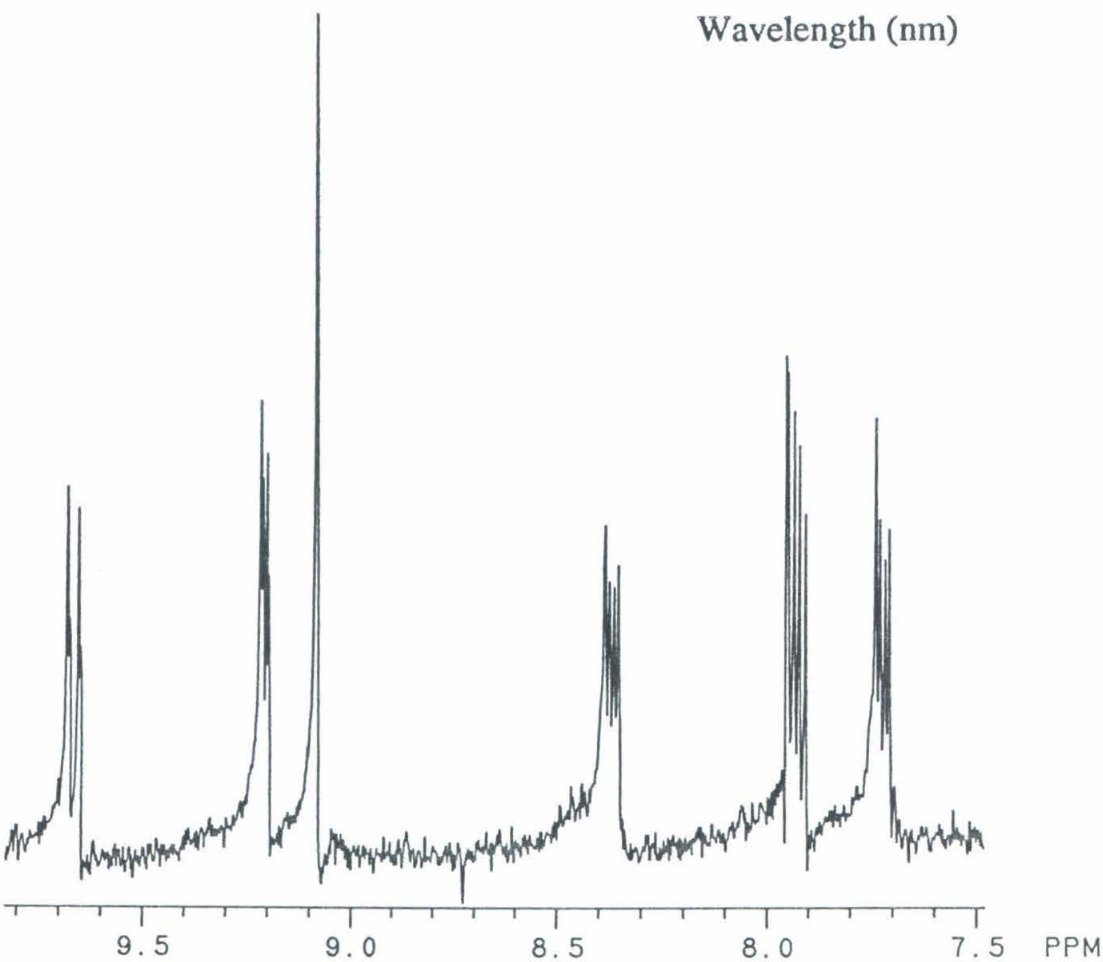
General Methods for Ru(diimine)$_2$ (X-dipyridophenazine)(PF$_6$)$_2$.

Method A: 100 mg of Ru(diimine)$_2$(phendione)(PF$_6$)$_2$ and 2 equivalents of the appropriate diamine were heated in 50 ml of refluxing 100% ethanol for 4 h. The complex which precipitated was collected and purified on neutral alumina (acetonitrile). Unreacted Ru(bpy)$_2$(phendione)(PF$_6$)$_2$ remained adsorbed to the column.

Method B: 100 mg of Ru(diimine)$_2$Cl$_2$ were added to a suspension of 1.2 equivalents of X-dipyridophenazine in 20 ml of ethylene glycol at 150°. The color quickly changed from deep red to orange. After 15 min of heating, the reaction mixture was cooled to room temperature and diluted with 20 ml of H_2O. The complex was

Figure 2.12. UV-Vis (CH_3CN), ^1H NMR (acetone-d_6) spectra of bdppz.


+70.1947
+55.8646
+41.5346
+27.2046
+12.8746
-1.4554
ε, M⁻¹ cm⁻¹ (x 10⁻³)
200
300
400
500
600
700
800
Wavelength (nm)
N
N
N
N


9.5
9.0
8.5
8.0
7.5
PPM

precipitated with a saturated aqueous solution of NH_4PF_6, collected by filtration, washed with H_2O and ether, and purified as above.

Yields were typically 70 % by either method.

$Re(CO)_3$(X-dppz)Cl. Complexes of this type were prepared by refluxing a mixture of 100 mg of $Re(CO)_3$(phendione)Cl and 1.2 equivalents of the appropriate diamine in 50 ml of 100% ethanol for 4 h. The precipitate collected after cooling was used without further purification. Yield: 80%.

$Ru(bpy)_2(Cl_2$-dppz)$(PF_6)_2$. Method A. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.13.

$Ru(bpy)_2$(bdppz)$(PF_6)_2$ [17]. Method B. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.14.

Ru(bpy)$(bdppz)_2(PF_6)_2$. Method B. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.15.

$Ru(bdppz)_3(PF_6)_2$. Method B. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.16.

$Ru(CH_3$-bpy$)_2$(bdppz)$(PF_6)_2$. Method B. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.17.

$Ru(CF_3$-bpy$)_2$(bdppz)$(PF_6)_2$. Method B. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.18.

$Ru(bpy)_2$(bdppzd)$(PF_6)_2$. Method A. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.19.

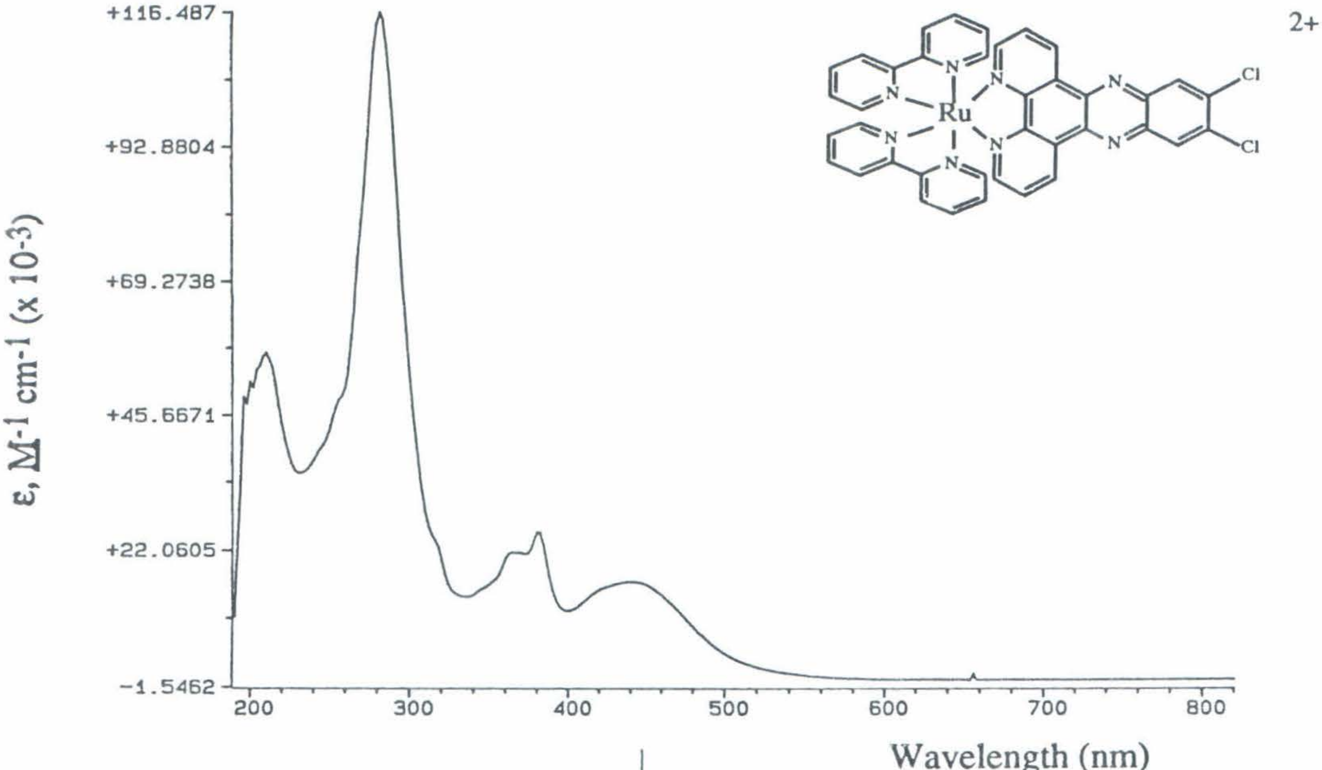
$Re(CO)_3$(dppz)Cl. UV-Vis(CH_3CN),^{1}H NMR (DMSO-d_6) Figure 2.20.

$Re(CO)_3$(bdppz)Cl. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.21.

$Re(CO)_3$(bdppzd)Cl. UV-Vis(CH_3CN),^{1}H NMR (CD_3CN) Figure 2.22.

Figure 2.13. UV-Vis(CH_3CN), ^1H NMR (CD_3CN) spectra of $Ru(bpy)_2(Cl_2dppz)(PF_6)_2$

.


2+
Cl
Cl
Ru
N
ε, M-1 cm-1 (x 10-3)
+116.487
+92.8804
+69.2738
+45.6671
+22.0605
-1.5462
200
300
400
500
600
700
800
Wavelength (nm)

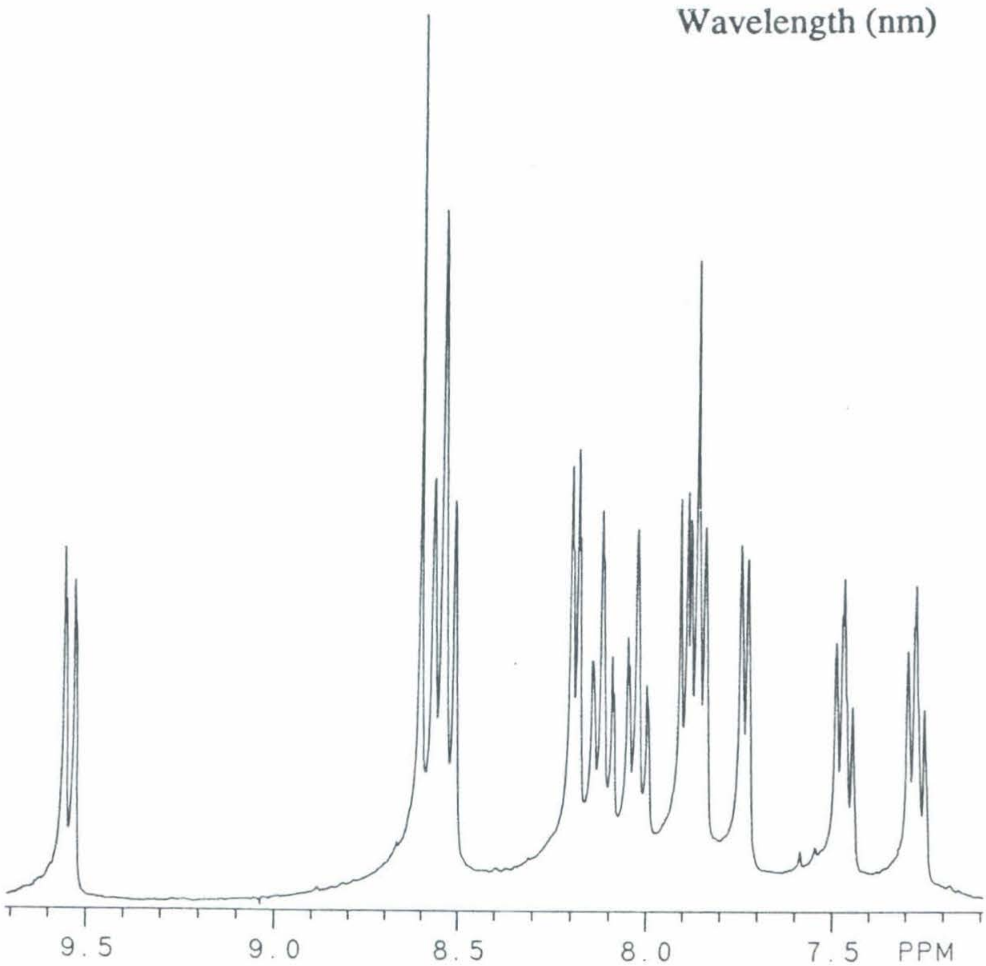
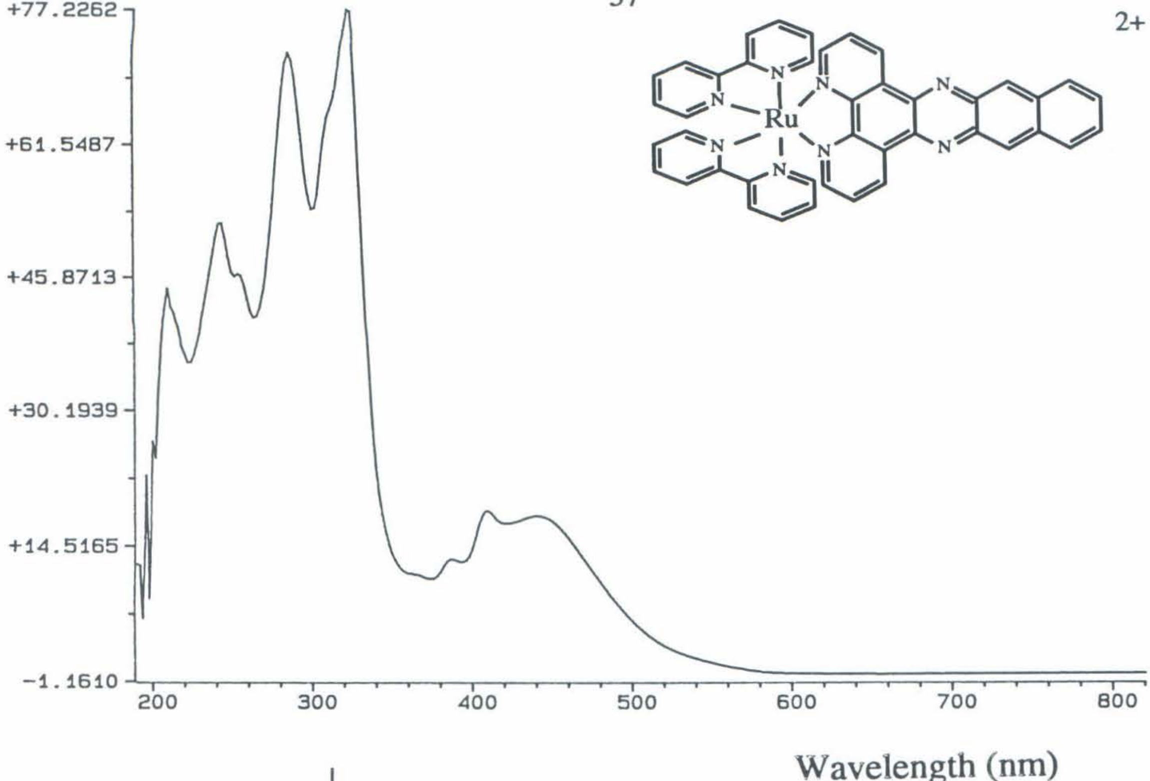

9.5
9.0
8.5
8.0
7.5
PPM

Figure 2.14. UV-Vis(CH_3CN),^1H NMR (CD_3CN) spectra of $Ru(bpy)_2(bdppz)(PF_6)_2$.

57



2+
Ru
N
+77.2262
+61.5487
+45.8713
+30.1939
+14.5165
-1.1610
200
300
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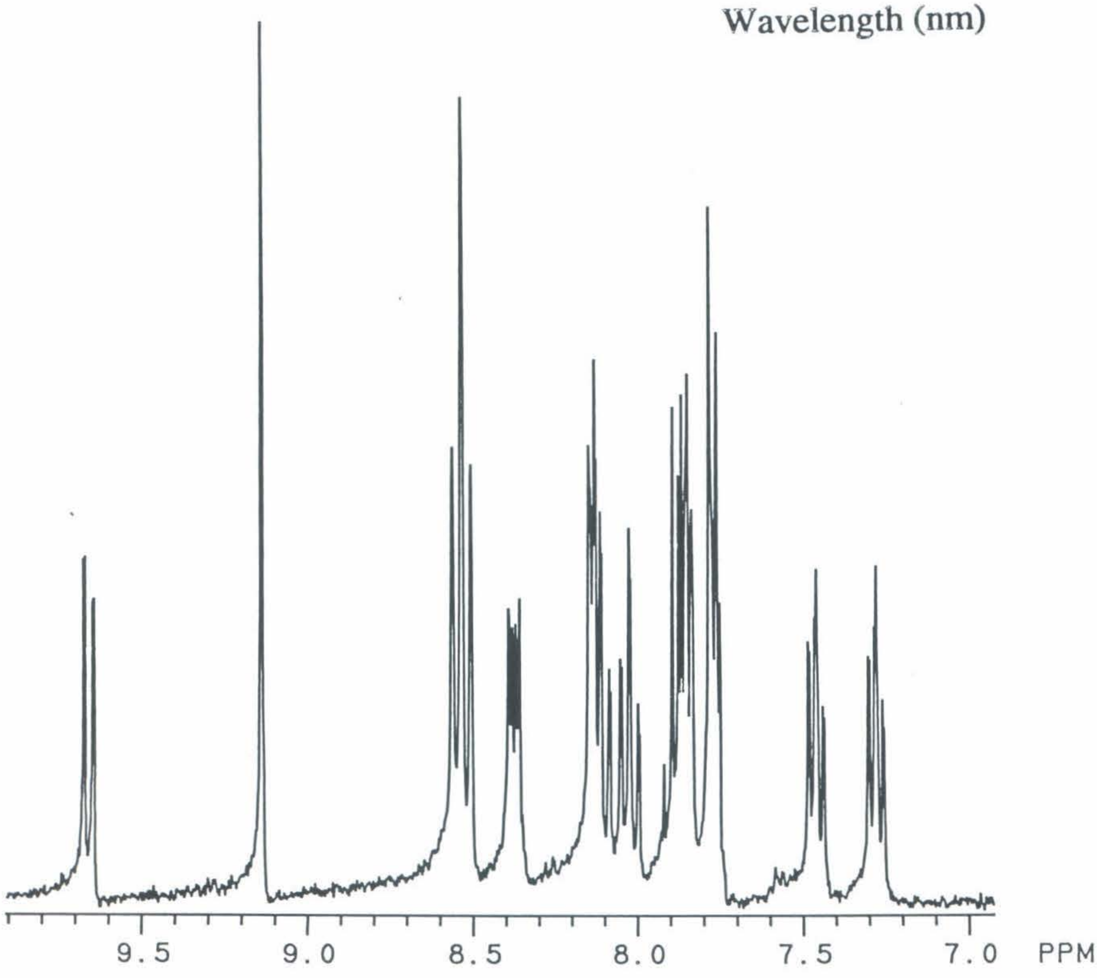
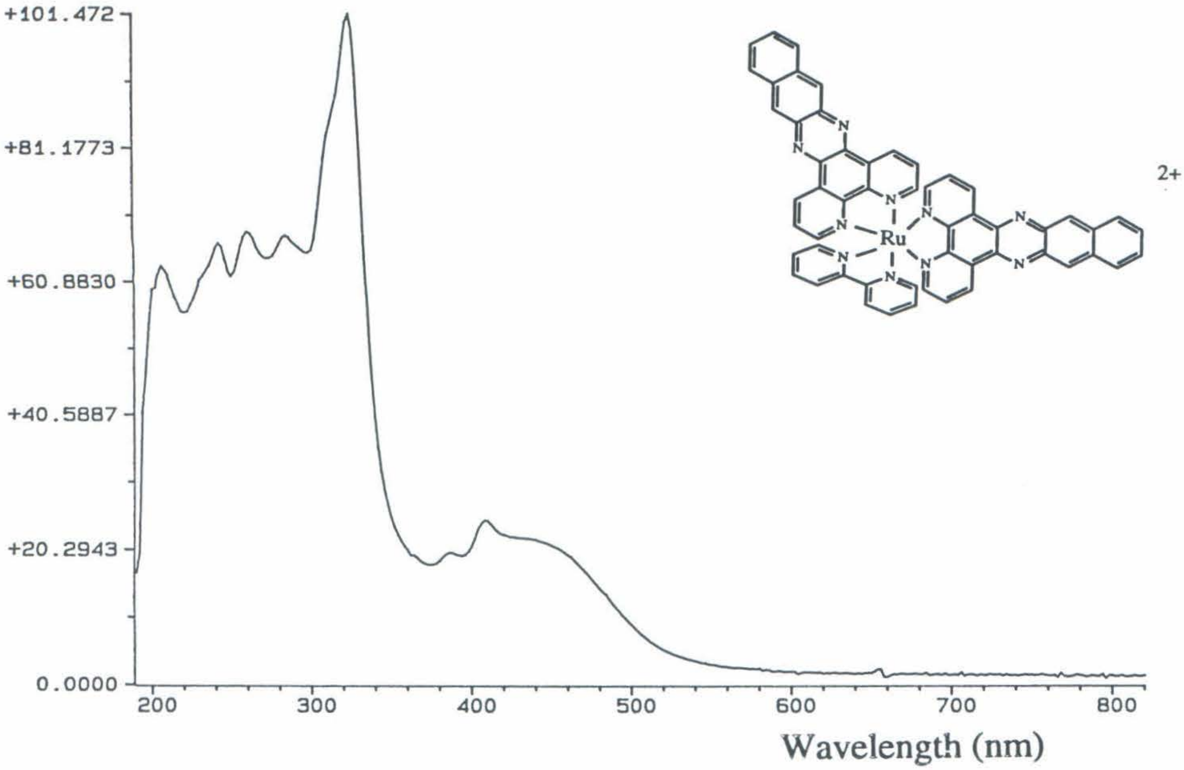
500
600
700
800
Wavelength (nm)



9.5
9.0
8.5
8.0
7.5
7.0
PPM

Figure 2.15. UV-Vis(CH_3CN),^1H NMR (CD_3CN) spectra of $Ru(bpy)(bdppz)_2(PF_6)_2$.


+101.472
+81.1773
+60.8830
+40.5887
+20.2943
0.0000
200
300
400
500
600
700
800
Wavelength (nm)
2+
Ru
N

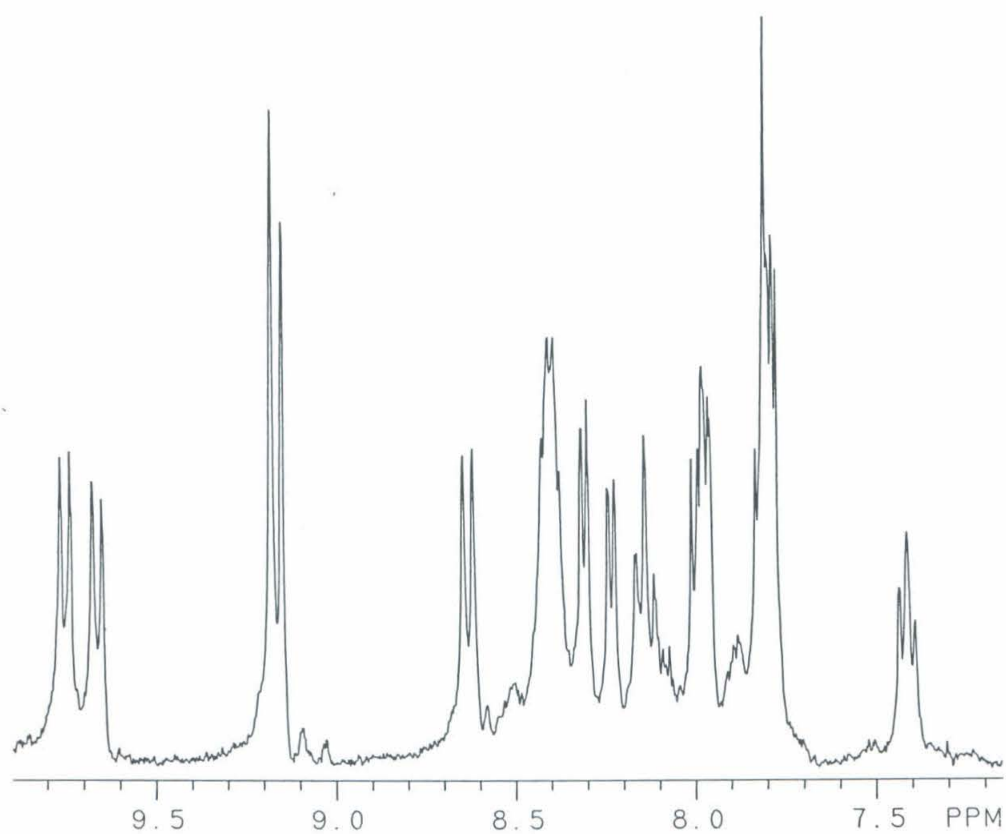
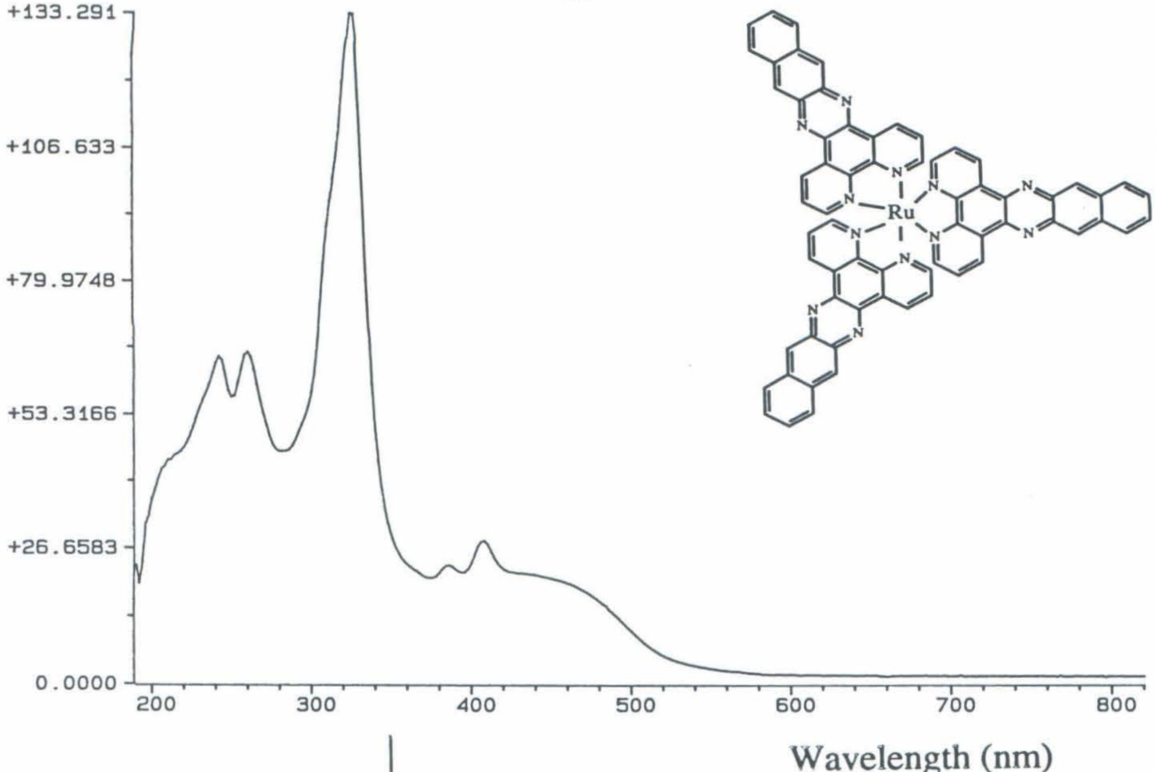

9.5
9.0
8.5
8.0
7.5
PPM

Figure 2.16. UV-Vis(CH_3CN), [1]H NMR (CD_3CN) spectra of $Ru(bdppz)_3(PF_6)_2$.


+133.291
+106.633
+79.9748
+53.3166
+26.6583
0.0000
200
300
400
500
600
700
800
Wavelength (nm)
Ru
2+

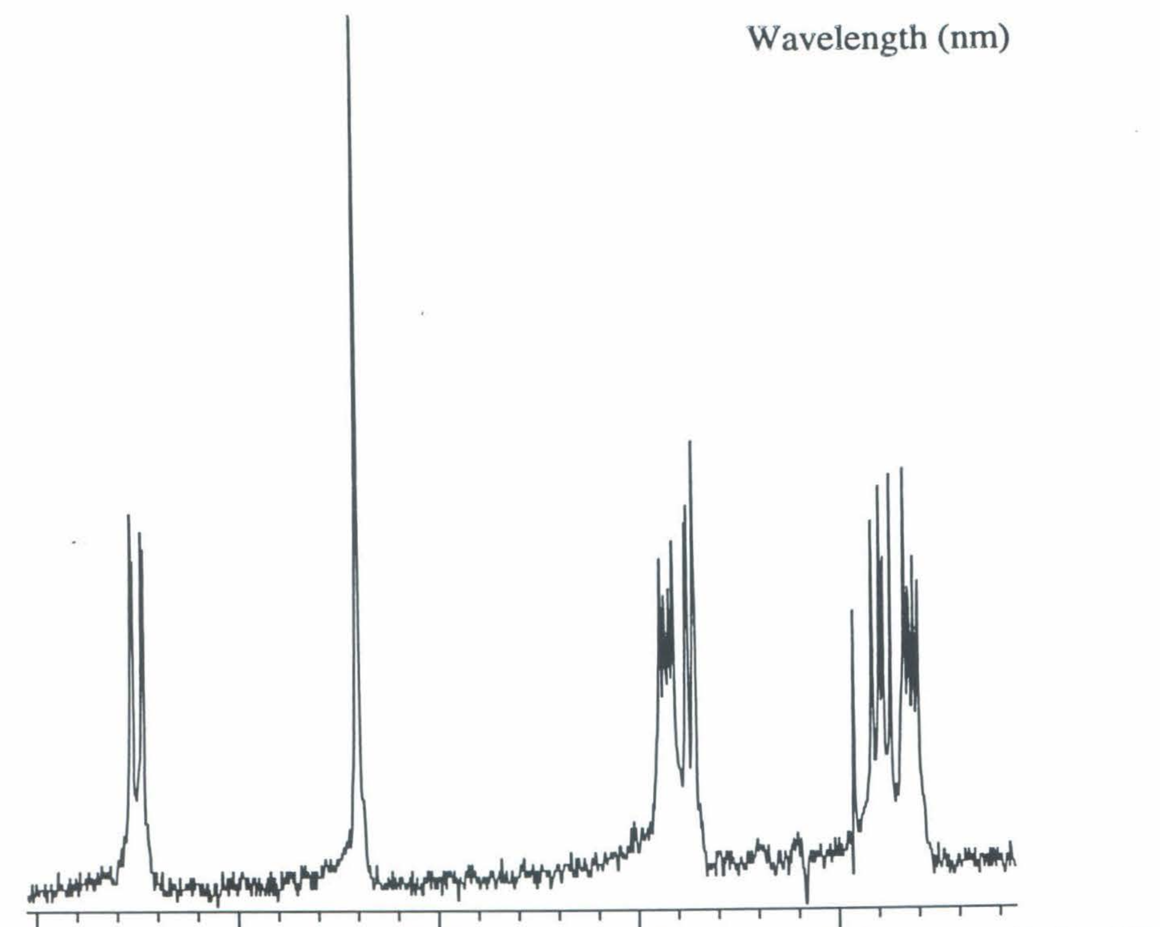
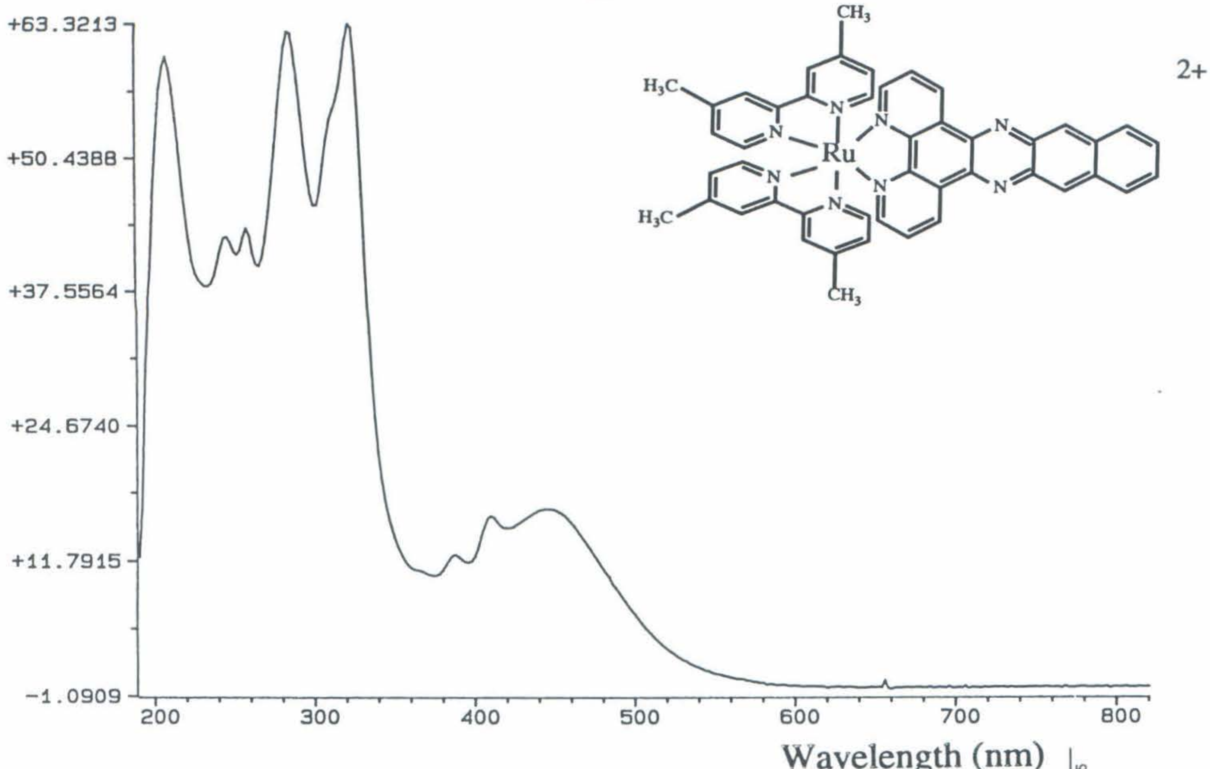

10.0
9.5
9.0
8.5
8.0
7.5 PPM

Figure 2.17. UV-Vis(CH_3CN),^1H NMR (CD_3CN) spectra of Ru(CH_3-bpy)$_2$(bdppz)(PF_6)$_2$.


+63.3213
+50.4388
+37.5564
+24.6740
+11.7915
-1.0909
200
300
400
500
600
700
800
Wavelength (nm)
CH3
H3C
H3C
CH3
N
Ru
2+

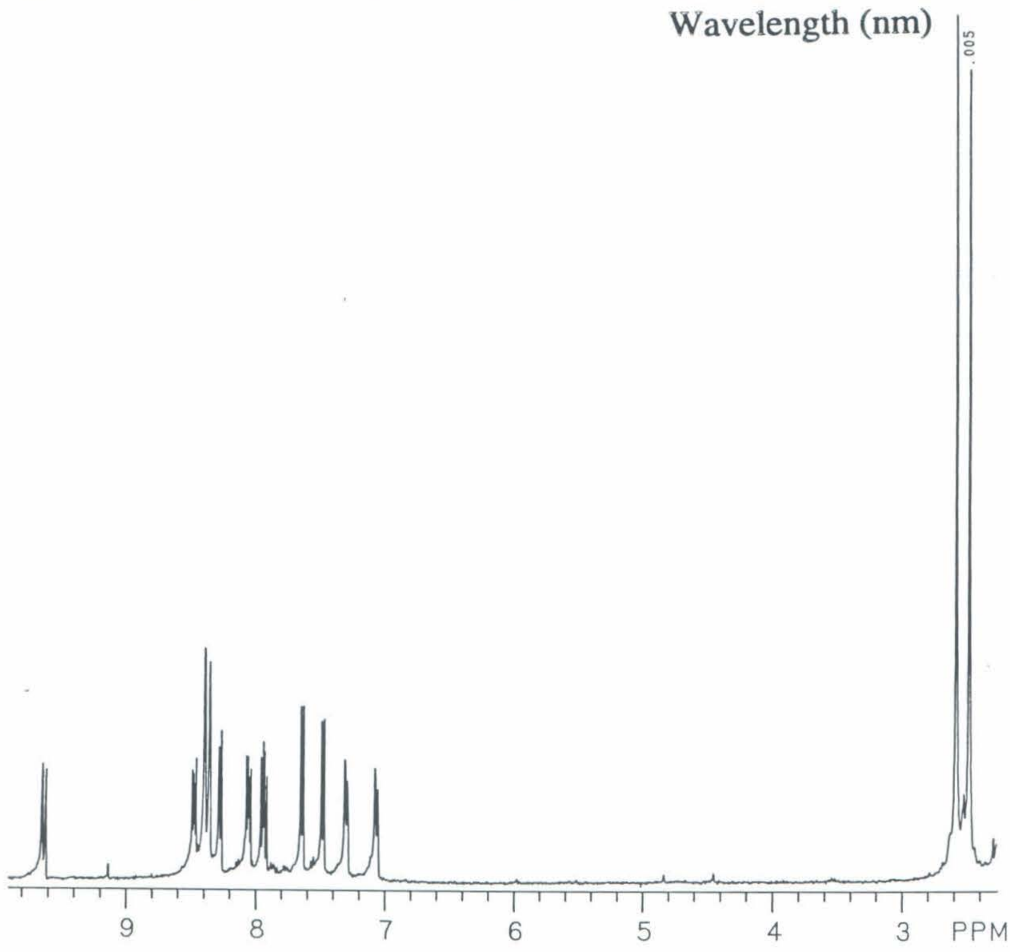
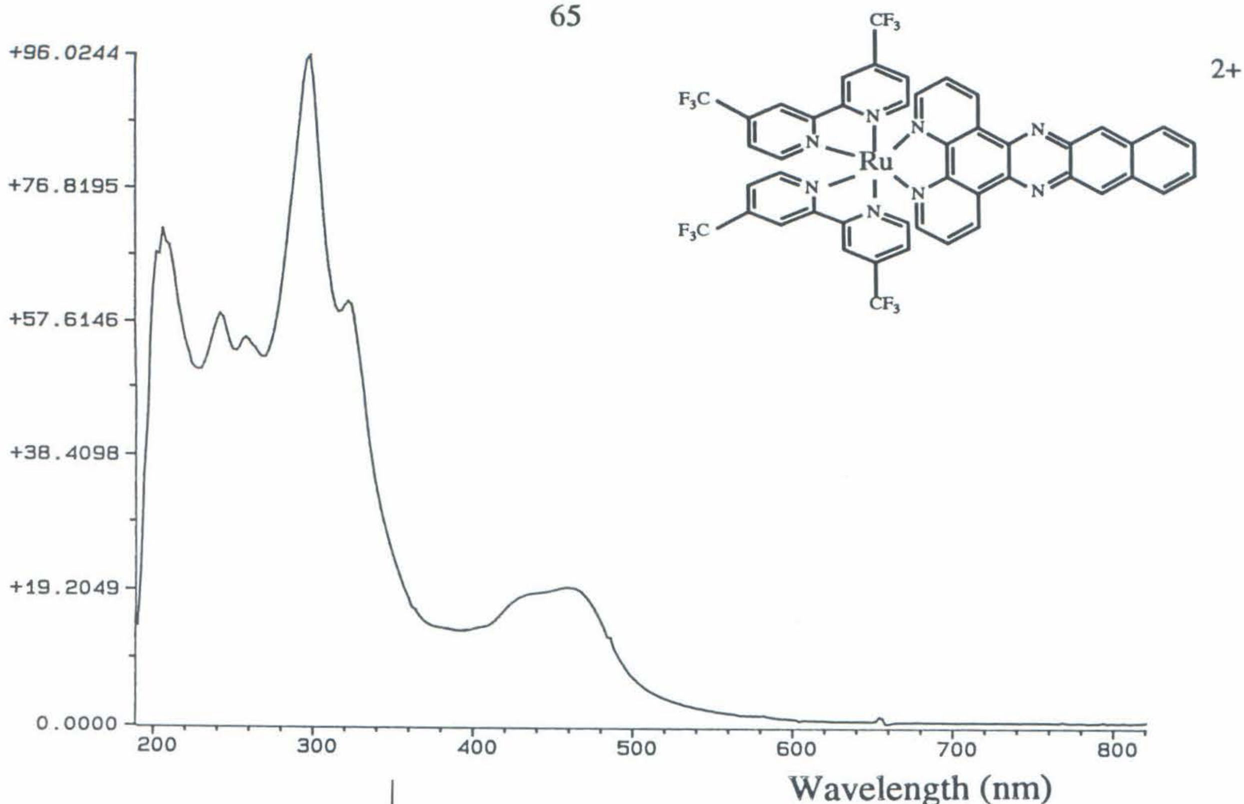

.005
9
8
7
6
5
4
3
PPM

Figure 2.18. UV-Vis(CH_3CN),[1]H NMR (CD_3CN) spectra of Ru(CF_3-bpy)$_2$(bdppz)(PF_6)$_2$.

65


CF3
F3C
Ru
N
F3C
CF3
2+
+96.0244
+76.8195
+57.6146
+38.4098
+19.2049
0.0000
200
300
400
500
600
700
800
Wavelength (nm)

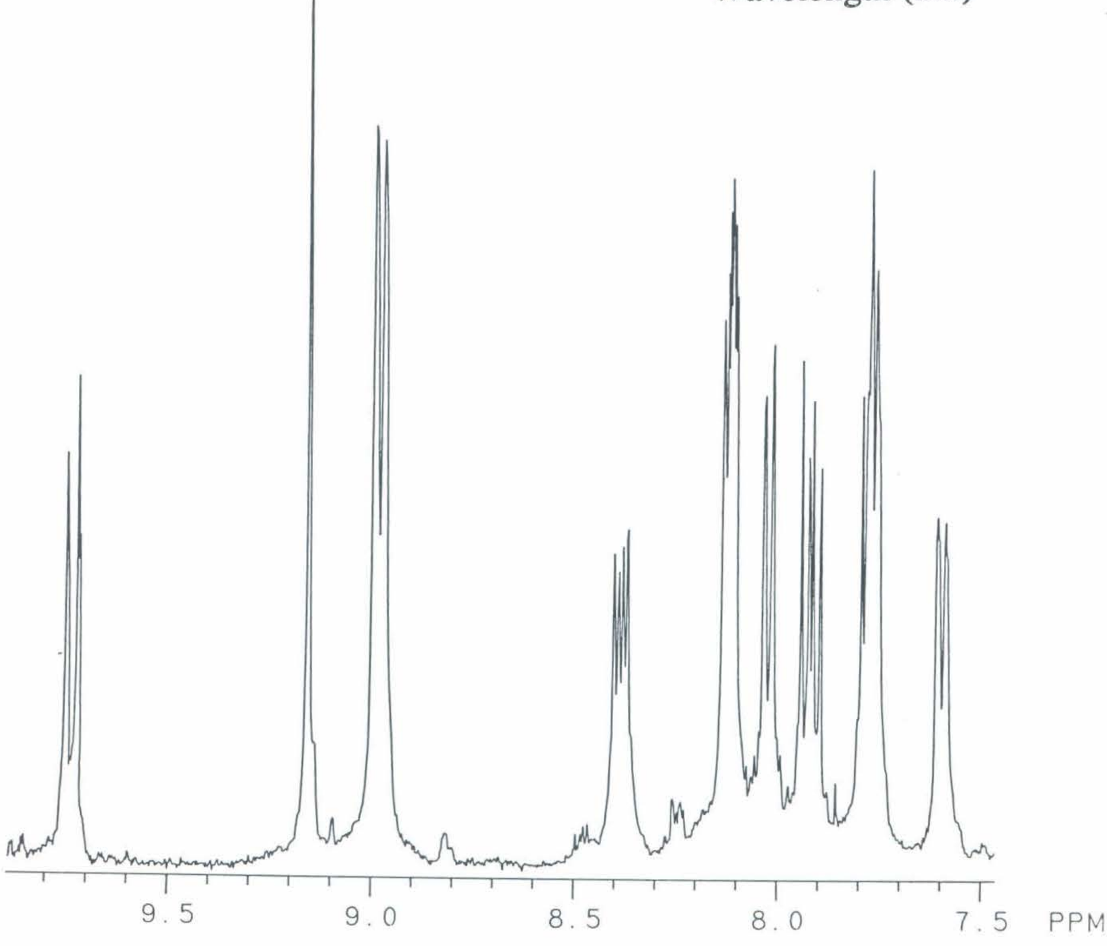
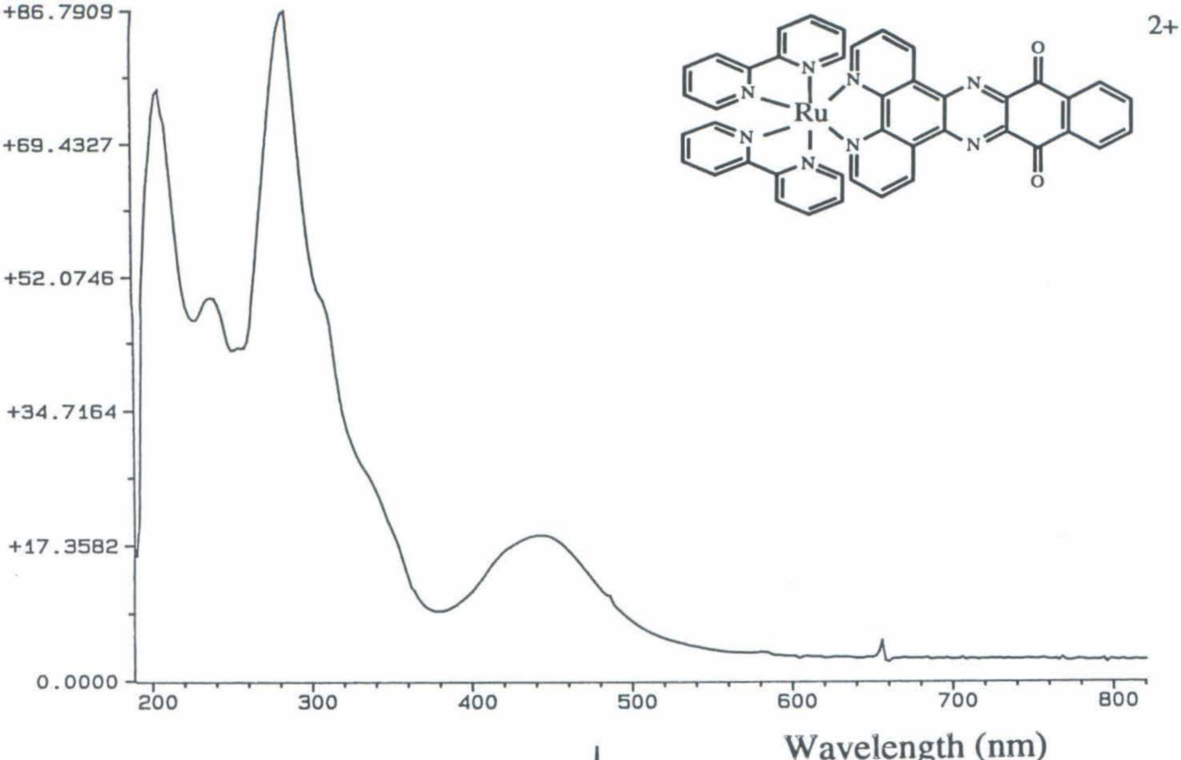

9.5
9.0
8.5
8.0
7.5
PPM

Figure 2.19. UV-Vis(CH_3CN),[1]H NMR (CD_3CN) spectra of $Ru(bpy)_2(bdppzd)(PF_6)_2$.


+86.7909
+69.4327
+52.0746
+34.7164
+17.3582
0.0000
200
300
400
500
600
700
800
Wavelength (nm)
2+
Ru
N
O

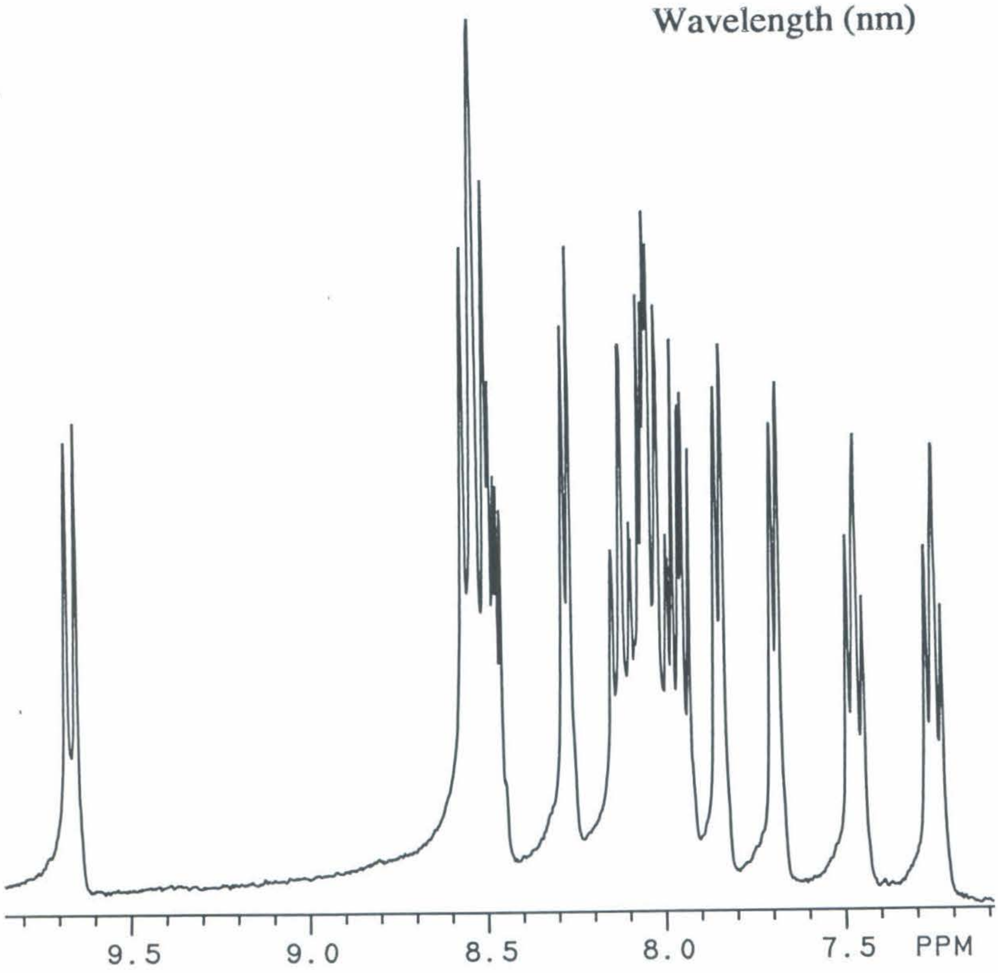

9.5
9.0
8.5
8.0
7.5
PPM

Figure 2.20. UV-Vis(CH_3CN), ^1H NMR (DMSO-d_6) spectra of $Re(CO)_3(dppz)Cl$.

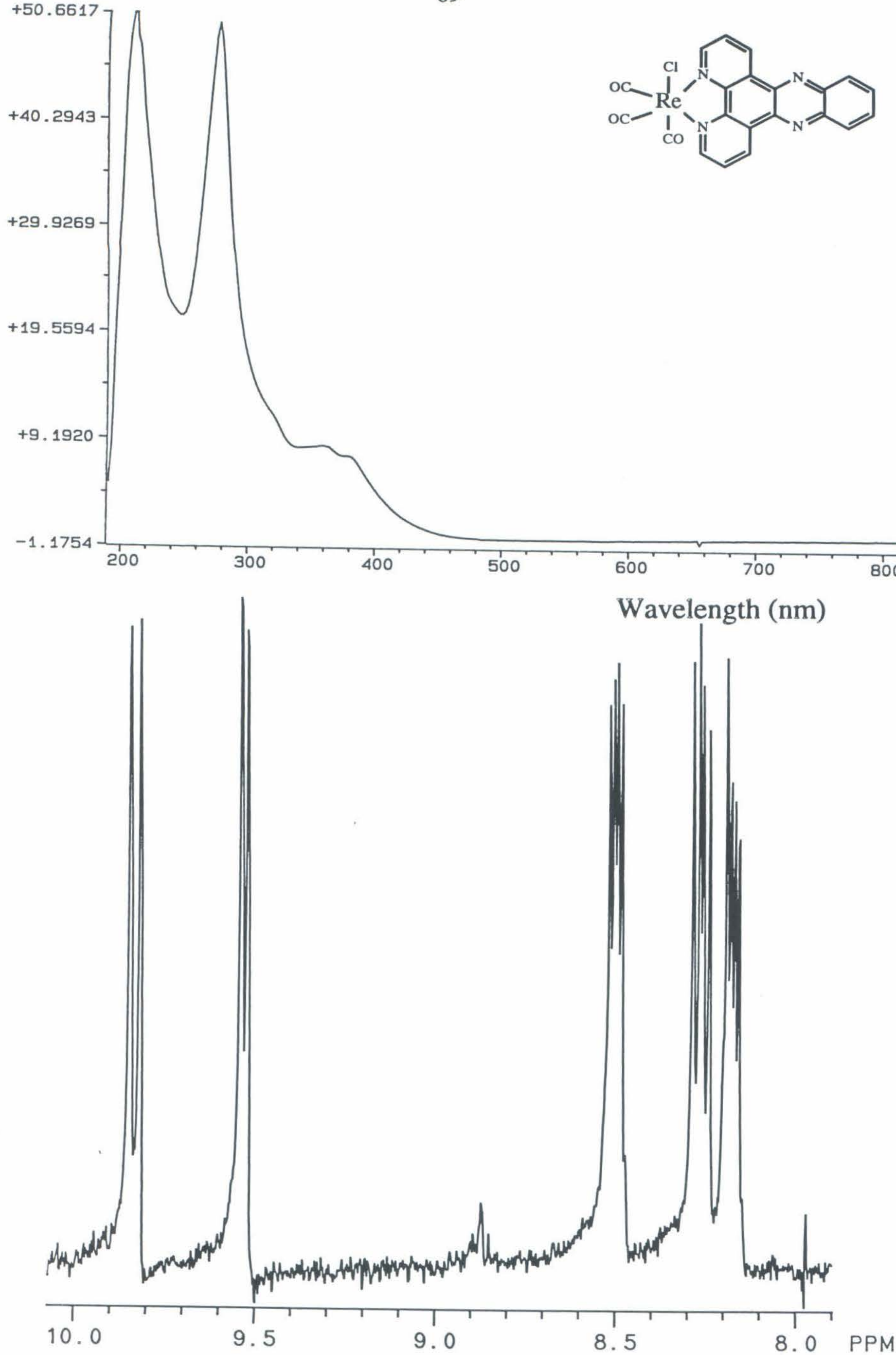
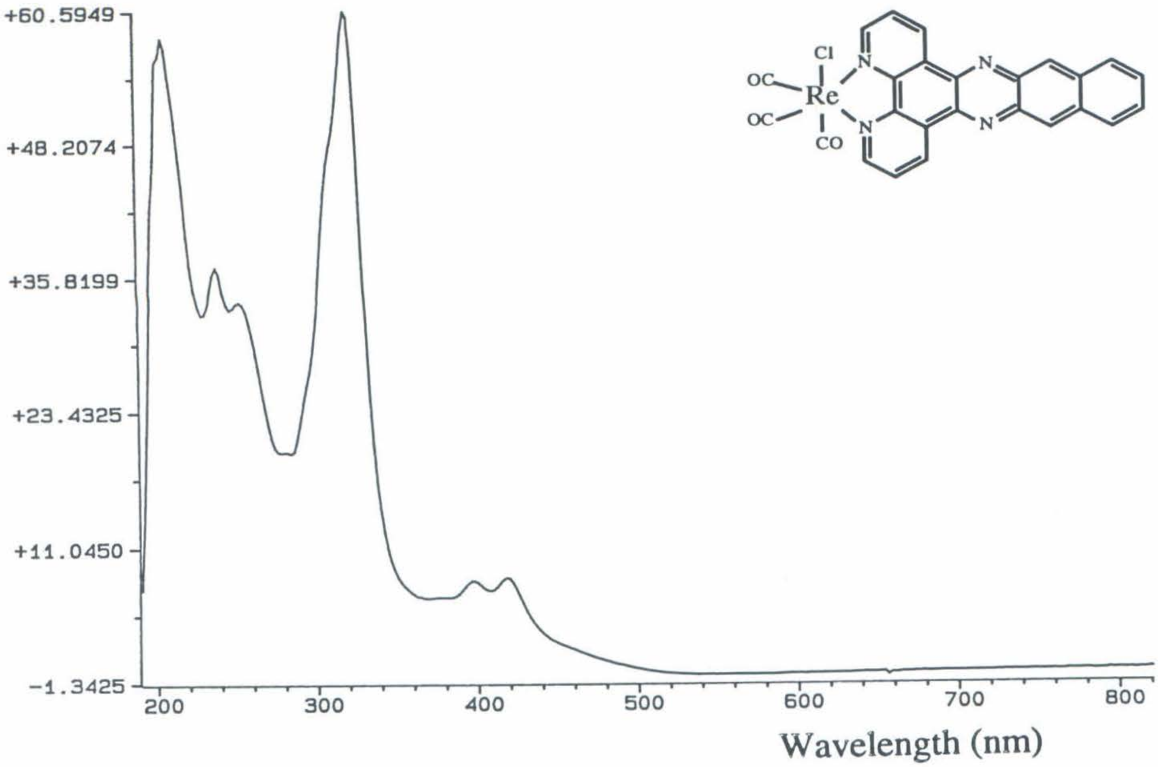

+50.6617
+40.2943
+29.9269
+19.5594
+9.1920
-1.1754
200
300
400
500
600
700
800
Wavelength (nm)
Cl
OC
Re
OC
CO
N
N
N
N
10.0
9.5
9.0
8.5
8.0
PPM

Figure 2.21. UV-Vis(CH_3CN), [1]H NMR (CD_3CN) spectra of $Re(CO)_3$(bdppz)Cl.


+60.5949
+48.2074
+35.8199
+23.4325
+11.0450
-1.3425
200
300
400
500
600
700
800
Wavelength (nm)
Cl
OC
Re
OC
CO
N
N
N
N

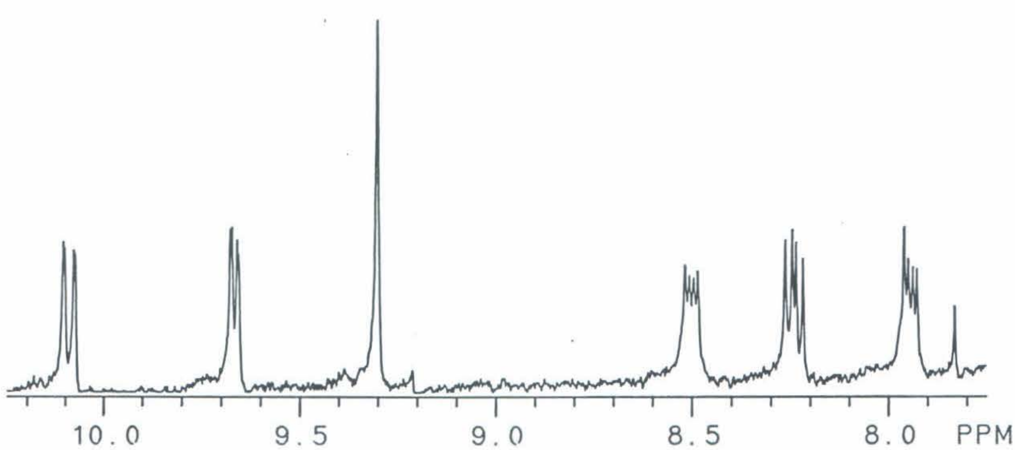
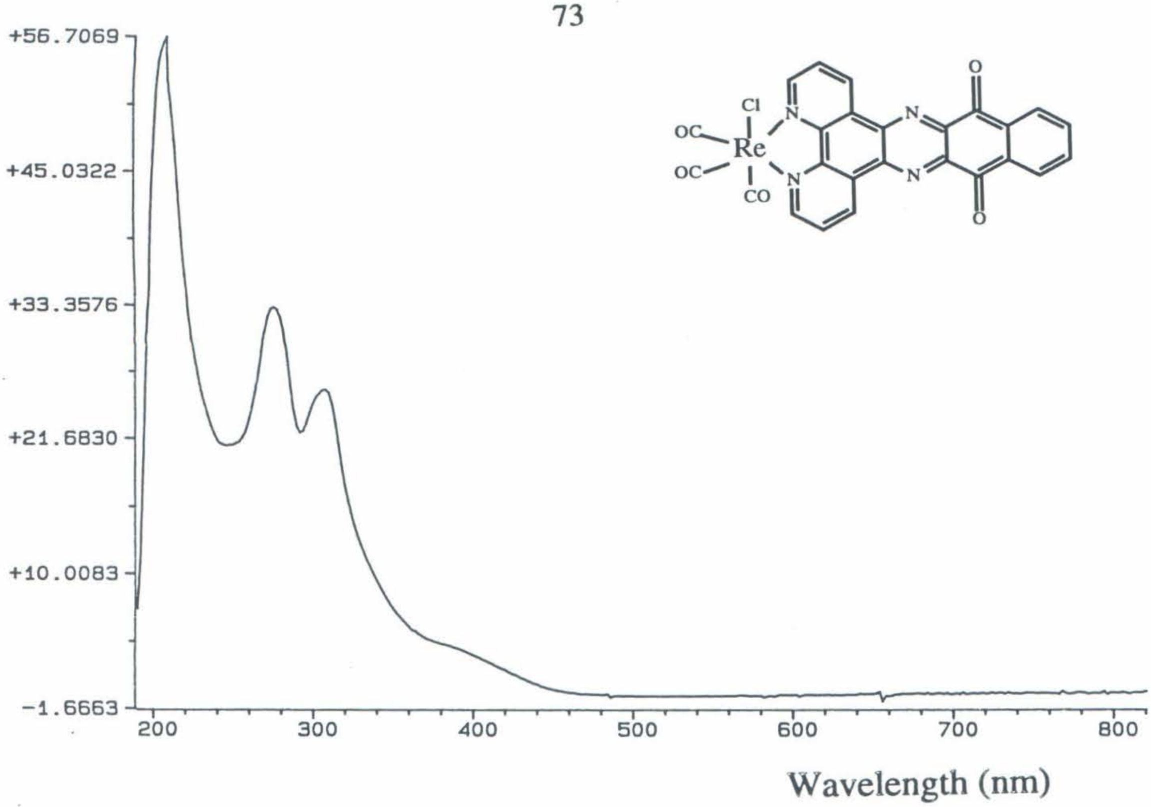

10.0
9.5
9.0
8.5
8.0
PPM

Figure 2.22. UV-Vis(CH_3CN),[1]H NMR (CD_3CN) spectra of $Re(CO)_3$(bdppzd)Cl.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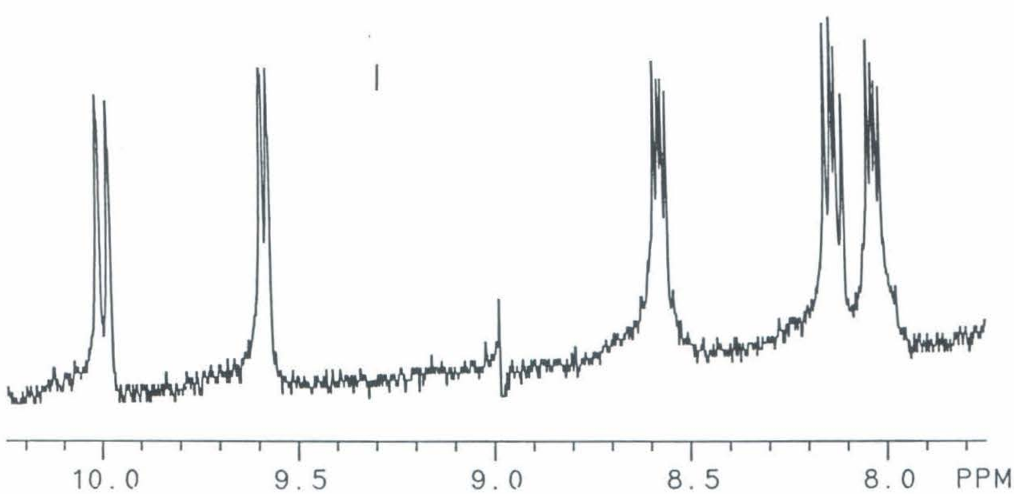
+45.0322
+33.3576
+21.6830
+10.0083
-1.6663
200
300
400
500
600
700
800
Wavelength (nm)
Cl
OC
OC
Re
CO
N
N
N
N
O
O


10.0
9.5
9.0
8.5
8.0
PPM

Physical Measurements.

300 MHz ^1H NMR spectra were recorded on a General Electric QE-300 NMR spectrometer. Chemical shifts were referenced relative to the shift of residual solvent protons. Electronic Absorption measurements were collected with a Hewlett-Packard HP-8452A spectrophotometer. Infrared measurements were made with a Mattson Galaxy 6020 spectrometer. Emission spectra were recorded with an SLM 8000 fluorimeter and a locally-built instrument that has been described previously.[18]

X-band EPR spectra were recorded on an IBM-Bruker ESP 300 equipped with a Bruker ER-411-VT temperature controller. The magnetic field was calibrated with 2,2-diphenyl-1-picrylhydrazyl hydrate. Nanosecond time-resolved absorbance measurements were carried out with an instrument described elsewhere.[18] Laser power at 480 nm (Coumarin 102, 25 ns pulse) was 2 mJ. Steady-state photolysis was done with a 1000 Watt Hanovia 977B00100 lamp housed in an Orion C-60-50 enclosure. Samples used for emission and time-resolved absorption spectroscopy were purged with argon for 10 min in a cell fitted with a septum.

Electrochemical experiments were performed using a Princeton Applied Research (PAR) model 173 potentiostat controlled by a model 175 universal programmer. Cyclic voltammetry was done at ambient temperature with a normal three-electrode configuration consisting of a glassy carbon working electrode, a platinum wire auxiliary electrode, and a AgCl/Ag reference electrode containing 1.0 M KCl. The working compartment of the electrochemical cell was separated from the reference compartment by a modified Luggin capillary. All three compartments contained a 0.1 M solution of supporting electrolyte. Acetonitrile (Burdick and Jackson) was distilled from P_2O_5 prior to use. Tetrabutylammonium hexafluorophosphate ($TBAPF_6$) (Southwestern Analytical) was used as received.

Potentials (vs. aqueous AgCl/Ag) were not corrected for the junction potential. Under conditions identical with those employed here, the ferrocenium/ferrocene couple has an $E^{o\prime}$ of 0.45 V.

The cells used for visible and infrared spectroelectrochemistry are modifications of cells that have been described elsewhere.[19]

X-ray Data Collection. Orange plates of $Ru(bpy)_2(bdppzd)(PF_6)_2$ were obtained by slow diffusion of diethyl ether through a 2 mm layer of methanol into an acetonitrile solution of the complex. A single crystal was mounted on a glass fiber with silicone grease and placed in the 130 K nitrogen stream of a Siemens R3m/V diffractometer with a modified Enraf-Nonius low-temperature apparatus. Two check reflections showed only random fluctuations (<2%) in intensity throughout the data collection. The data were corrected for Lorentz and polarization effects. Crystal data are given in Table 2.1.

Structure Solution and Refinement. Calculations were performed using SHELXTL PLUS (VMS version) software. Scattering factors and corrections for anomalous dispersion were taken from a standard source.[20] An absorption correction was applied.[21] The structure was solved in the monoclinic space group $P2_1/n$ by direct methods. Hydrogen atoms were added geometrically and refined using a riding model with isotropic thermal parameters equal to 0.04Å^2. The largest feature in the final difference map (0.073 e^-Å^{-3}) is located 0.947Å from C(47).

Table 2.1. Crystal Data for $Ru(bpy)_2(bdppz)(PF_6)_2$.

Table 2.1

Crystallographic Data

$Ru(bpy)_2(bdppzd)(PF_6)_2$

$C_{44.5}H_{26}F_{12}N_8O_{2.75}P_2Ru$	FW = 1107.7
a = 14.211(5) Å	$P2_1/n$, monoclinic
b = 12.417(4) Å	T = 130K
c = 26.608(7) Å	λ(MoKα) = 0.71073 Å
β = 101.84(2) °	μ(MoKα) = 0.509 mm^{-1}
V = 4595(3) $Å^3$	d_{calc} = 1.601 Mg/m^3
Z = 4	transm. factors = 0.86 - 0.90
$R(F_o)$ = 0.067	
$R_w(F_o)$ = 0.085	

$R = \Sigma \| F_o | - | F_c \| / \Sigma \|F_o|$; $R_w = \Sigma \| F_o | - | F_c | | w^{1/2} / \Sigma | F_o | w^{1/2}$

Results and Discussion

Synthesis

The versatile scheme employed here allows the synthesis of a large series of related compounds. The nature of the ET acceptor can be varied by condensing different ortho-diamines with phendione; the energetics of the system can be modulated by employing bpy ligands with electron donating- or withdrawing groups, shifting the potential of the $Ru^{3+/2+}$ couple. The synthesis of the Ru compounds is greatly facilitated by reaction of $Ru(diimine)_2Cl_2$ with the desired dipyridophenazine in ethylene glycol at high temperature. Using this method, one can make the desired compound from $Ru(diimine)_2Cl_2$, phendione and diamine in less than two hours, as opposed to the twelve hours required to synthesize $Ru(diimine)_2(phendione)^{2+}$ and condense it with a diamine. $Re(CO)_3(diimine)Cl$ complexes exhibit MLCT-excited-state behavior analogous to that of $Ru(bpy)_3^{2+}$.[16] The Re compounds were synthesized to allow the examination of an isolated dipyridophenazine ligand. IR spectroscopy of the CO ligands in these compounds provides insight into the electronic structure of the charge-separated state.

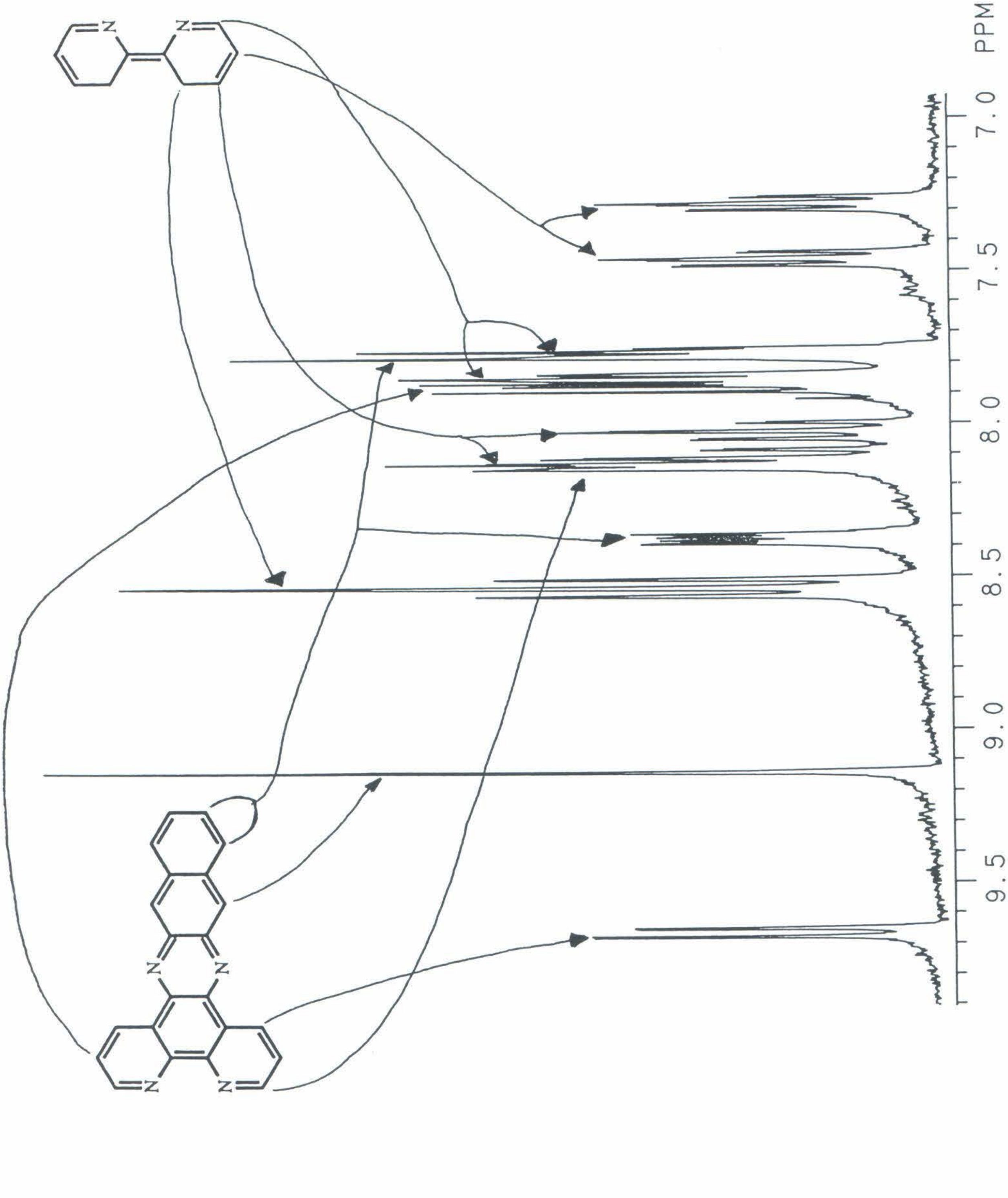
Characterization

Synthesis of a series of compounds allows comparisons which make assignment of their complicated ^1H NMR spectra possible. The spectrum of $Ru(bdppz)_3^{2+}$ (Figure 2.16) shows the resonances of the ligand when coordinated to Ru. The doublets at 8.35 and 9.75 ppm arise, respectively, from the 3,6 and 1,8 positions of the bpy portion of the ligand; the doublet of doublets at 7.9 ppm corresponds to the 2,7 positions. The singlet at 9.2 ppm is due to the 10,15 positions of the bpz of the ligand; the protons on the benzo ring give the multiplets at 7.7 and 8.45 ppm. The Re-complex spectra can be assigned in a similar manner. Assigning the bdppz resonances in the absence of bpy makes their identification in $Ru(bpy)_2(bdppz)^{2+}$ easier. The bpy positions corresponding to the remaining resonances can be deduced by comparing the spectra of $Ru(bpy)_2(bdppz)^{2+}$ (Figure 2.13) and $Ru(CH_3\text{-}bpy)_2(bdppz)^{2+}$ (Figure 2.18). The two doublets of overlapping doublets at 8.15 and 8.25 ppm (the signal at 8.25 ppm is superimposed upon the 3,6 protons of bdppz) disappear in the methyl compound; they are the 4,4' positions. The two doublets of overlapping doublets at 7.3 and 7.45 ppm become two doublets in the CH_3-bpy compound; they correspond to the 5,5' positions. The overlapping doublet of doublets at 8.55 ppm in the bpy compound becomes a pair of singlets in the methyl compound; they thus belong to the 3,3' positions. The 6,6' positions are not affected by methyl substitution, remaining doublets. In $Ru(bpy)_2(bdppz)^{2+}$, these resonances overlap with those of the 2,7 and benzo protons of bdppz. The completely assigned spectrum of $Ru(bpy)_2(bdppz)^{2+}$ is presented in Figure 2.23. The spectra of the other $Ru(diimine)_2(bdppz)^{2+}$ complexes can be assigned based on this spectrum; all NMR spectra are consistent with the structures proposed for the compounds.

An ORTEP drawing of the x-ray crystal structure of $Ru(bpy)_2(bdppz)^{2+}$ is presented in Figure 2.24. Thermal ellipsoids are drawn at 50% probability. Atomic coordinates and equivalent displacement coefficients are presented in Table 2.2, selected bond lengths and angles in Table 2.3. The structure is that expected based on that of $Ru(bpy)_3^{2+}$. [22] The slight bowing of the bdppz ligand is likely due to crystal packing. The distance of presumed ET from Ru to a quinone oxygen is 9.26 Å.

UV-Vis spectroscopy shows that dppz-type ligands have strong bpy and bpz character. Free bpy has 3 intense $\pi \rightarrow \pi^*$ transitions at 208, 236, and 278 nm. The visible absorption spectrum of bdppz consists of 3 $\pi \rightarrow \pi^*$ transitions at 202, 244, and 312 nm and a progression of 3 weaker peaks spaced 20 nm apart beginning at 370 nm. This progression is identical to that found in bpz[23] and is redshifted compared to that of pz[24] and dppz, as is expected when the aromatic system is extended. The absorption spectra of $Ru(bpy)_2(X\text{-}dppz)^{2+}$ compounds closely resemble that of $Ru(bpy)_3^{2+}$, whose chief features are an intense bpy-centered $\pi \rightarrow \pi^*$ transition at 286 nm and the Ru $\rightarrow$ bpy

Figure 2.23. 300 MHz ^1H NMR spectrum with assignments for $Ru(bpy)_2(bdppz)^{2+}$ in CD_3CN.



PPM
7.0
7.5
8.0
8.5
9.0
9.5

Figure 2.24. ORTEP drawing of the x-ray crystal structure of $Ru(bpy)_2(bdppz)^{2+}$.
Thermal ellipsoids are drawn at 50% probability.

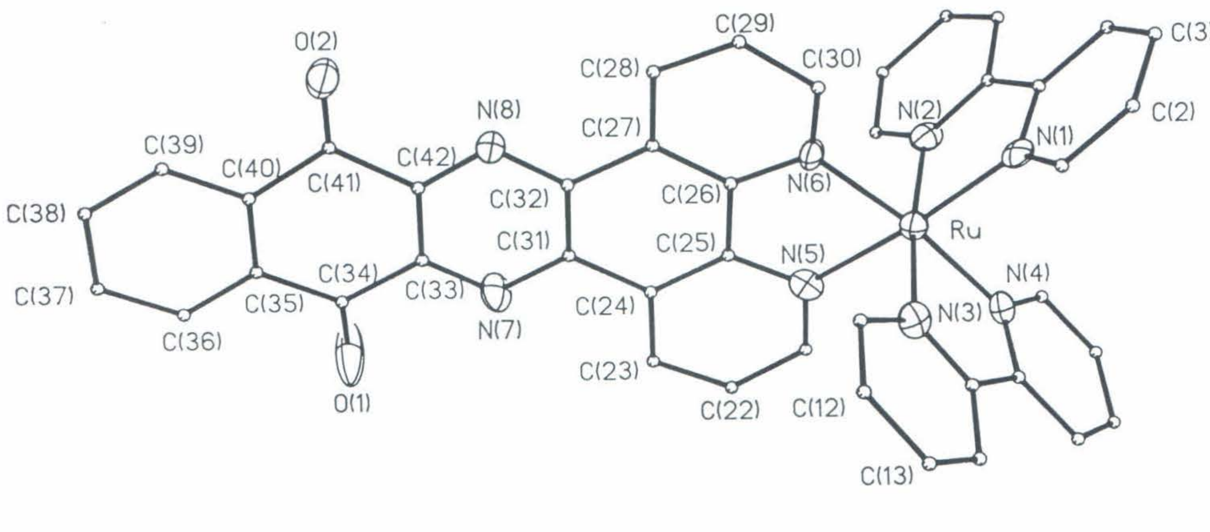

O(2)
C(39)
C(40)
C(41)
C(42)
N(8)
C(32)
C(27)
C(28)
C(29)
C(30)
C(26)
N(6)
N(2)
N(1)
C(3)
C(2)
C(38)
Ru
C(31)
C(25)
N(5)
N(4)
C(37)
C(35)
C(34)
C(33)
N(7)
C(24)
N(3)
C(36)
O(1)
C(23)
C(22)
C(12)
C(13)

Table 2.2. Atomic coordinates and displacement coefficients for $Ru(bpy)_2(bdppz)^{2+}$.

Table 2.2.

Atomic Coordinates (x 10^4) and Equivalent Displacement Coefficients ($Å^2$ x 10^3) for $Ru(bpy)_2(bdppz)^{2+}$.

	x	y	z	U(eq)*
Ru	2463(1)	1203(1)	1183(1)	22(1)
N(1)	1241(6)	1754(7)	1397(3)	24(3)
N(2)	1973(6)	2326(7)	613(3)	26(3)
N(3)	2898(6)	179(7)	1801(3)	27(3)
N(4)	3289(6)	2232(7)	1701(3)	25(3)
N(5)	3611(6)	598(7)	901(3)	25(3)
N(6)	1773(6)	9(7)	698(3)	21(3)
N(7)	4424(6)	-2370(7)	-108(4)	34(4)
N(8)	2449(6)	-2875(7)	-384(3)	28(3)
O(1)	5683(6)	-3592(9)	-493(5)	98(5)
O(2)	1941(5)	-4596(6)	-1028(3)	44(3)
C(1)	874(8)	1380(9)	1793(4)	34(3)
C(2)	9(8)	1737(10)	1892(5)	41(3)
C(3)	-503(9)	2509(9)	1571(4)	39(3)
C(4)	-142(8)	2909(9)	1175(4)	32(3)
C(5)	729(7)	2521(8)	1082(4)	23(3)
C(6)	1143(8)	2838(9)	652(4)	29(3)
C(7)	731(8)	3582(9)	273(4)	36(3)
C(8)	1150(8)	3769(10)	-138(4)	38(3)
C(9)	1981(8)	3233(9)	-170(5)	39(3)
C(10)	2379(8)	2522(9)	213(4)	31(3)
C(11)	2679(8)	-863(9)	1814(4)	31(3)
C(12)	2991(8)	-1490(10)	2238(5)	40(3)
C(13)	3527(8)	-1026(10)	2672(5)	45(3)
C(14)	3783(8)	43(9)	2652(5)	39(3)
C(15)	3458(7)	645(9)	2217(4)	26(3)
C(16)	3682(8)	1778(9)	2163(4)	31(3)
C(17)	4257(8)	2400(10)	2544(5)	40(3)
C(18)	4418(9)	3461(10)	2452(5)	43(3)
C(19)	4015(8)	3908(10)	1992(4)	42(3)
C(20)	3450(8)	3283(9)	1631(4)	31(3)
C(21)	4544(8)	875(9)	1028(4)	34(3)
C(22)	5287(8)	324(9)	864(4)	30(3)
C(23)	5048(8)	-577(9)	554(4)	29(3)
C(24)	4079(8)	-873(8)	397(4)	27(3)
C(25)	3383(7)	-266(8)	581(4)	25(3)
C(26)	2377(7)	-549(8)	463(4)	21(2)
C(27)	2056(7)	-1409(8)	135(4)	21(2)
C(28)	1082(7)	-1704(9)	45(4)	27(3)
C(29)	488(8)	-1128(9)	300(4)	31(3)
C(30)	862(7)	-288(8)	616(4)	22(3)
C(31)	3756(7)	-1767(8)	60(4)	24(3)
C(32)	2770(7)	-2037(8)	-74(4)	25(3)
C(33)	4105(8)	-3221(9)	-395(4)	32(3)
C(34)	4868(9)	-3887(10)	-573(5)	40(3)
C(35)	4531(9)	-4917(10)	-834(5)	41(3)
C(36)	5203(9)	-5617(10)	-947(5)	41(3)

Table 2.2 continued.

C(37)	4911(9)	-6580(10)	-1203(5)	41(3)
C(38)	3949(9)	-6823(10)	-1357(5)	41(3)
C(39)	3267(8)	-6121(10)	-1245(4)	39(3)
C(40)	3546(8)	-5155(9)	-986(4)	29(3)
C(41)	2790(9)	-4430(9)	-872(5)	35(3)
C(42)	3127(8)	-3467(8)	-534(4)	28(3)

*Equivalent isotropic U defined as one third of the orthogonalized trace of the orthogonalized U_{ij} tensor.

Table 2.3. Selected bond lengths and angles for $Ru(bpy)_2(bdppz)^{2+}$.

Table 2.3

Selected Bond Lengths (Å) and Angles (deg) for $Ru(bpy)_2(bdppz)^{2+}$

Bond Lengths

Ru-N(1)	2.053 (9)	Ru-N(2)	2.073 (8)
Ru-N(3)	2.071 (8)	Ru-N(4)	2.060 (8)
Ru-N(5)	2.071 (9)	Ru-N(6)	2.074 (8)
N(1)-C(1)	1.350 (15)	N(1)-C(5)	1.374 (12)
N(2)-C(6)	1.362 (14)	N(2)-C(10)	1.332 (15)
N(3)-C(11)	1.333 (14)	N(3)-C(15)	1.354 (13)
N(4)-C(16)	1.365 (13)	N(4)-C(20)	1.344 (14)
N(5)-C(21)	1.343 (14)	N(5)-C(25)	1.367 (13)
N(6)-C(26)	1.353 (14)	N(6)-C(30)	1.321 (13)
N(7)-C(31)	1.355 (14)	N(7)-C(33)	1.329 (14)
N(8)-C(32)	1.349 (13)	N(8)-C(42)	1.336 (15)
O(1)-C(34)	1.192 (15)	O(2)-C(41)	1.211 (14)

Bond Angles

N(1)-Ru-N(2)	78.6(3)	N(1)-Ru-N(3)	96.6(4)
N(2)-Ru-N(3)	174.3(4)	N(1)-Ru-N(4)	90.3(3)
N(2)-Ru-N(4)	97.6(3)	N(3)-Ru-N(4)	79.2(3)
N(1)-Ru-N(5)	174.5(3)	N(2)-Ru-N(5)	98.7(3)
N(3)-Ru-N(5)	86.3(3)	N(4)-Ru-N(5)	94.8(3)
N(1)-Ru-N(6)	95.3(3)	N(2)-Ru-N(6)	88.9(3)
N(3)-Ru-N(6)	94.7(3)	N(4)-Ru-N(6)	172.2(3)
N(5)-Ru-N(6)	79.8(3)	O(1)-C(34)-C(33)	120.5(11)
O(1)-C(34)-C(35)	123.8(12)	O(2)-C(41)-C(40)	122.7(10)
O(2)-C(41)-C(42)	120.7(11)		

MLCT transition at 450 nm; Ru(diimine)$_2$(X-dppz)$^{2+}$ compounds have the corresponding transitions at very similar wavelengths. These data are collected in Table 2.4. Examination of the Ru(bpy)$_{3-x}$(bdppz)$_x$$^{2+}$ series shows that the $\pi \rightarrow \pi^*$ transition at 324 nm increases at the expense of the transition at 286 nm as x increases, allowing assignment of the absorbance at 286 nm as bpy-centered and that at 324 as bdppz-centered. The energy of the MLCT band stays constant as x increases, showing that bdppz has orbitals which are electronically similar to bpy.

The same bpy character is present in Re(CO)$_3$(X-dppz)Cl compounds, whose absorbance data are also collected in Table 2.4. The maxima of the MLCT bands in Re(CO)$_3$(dppz)Cl and Re(CO)$_3$(bdppz)Cl are difficult to determine because low-energy ligand-centered transitions dominate in the 400 nm region. The MLCT band in these compounds does not tail any further than that of Re(CO)$_3$(bpy)Cl , however, so their maxima cannot differ greatly from the bpy compound.

This bpy character is further borne out by the spectra of the MLCT-based emission of these complexes; emission maxima are the same as those for the parent bpy complexes. Ru(bpy)$_3$$^{2+}$ has an emission maximum at 630 nm; Ru(bpy)bdppz^{2+}, whose emission spectrum is shown in Figure 2.25, has a maximum of 622 nm. Re(CO)$_3$(bdppz)Cl, Figure 2.26, has an emission maximum of 594 nm, nearly identical to that of Re(CO)$_3$(bpy)Cl, thus, the MLCT energies must be the nearly the same in the two compounds. In the Ru(bpy)$_{3-x}$(bdppz)$_x$$^{2+}$ series, the quantum yield of emission decreases with increasing x, as shown in Figure 2.27. These data in relation ET efficiency will be discussed later. Emission data are tabulated in Table 2.5. Emission quantum yields of Ru(bpy)$_{3-x}$ (bdppz)$_x$$^{2+}$ compounds are reported relative to the 0.04 quantum yield of Ru(bpy)$_3$$^{2+}$ in acetonitrile at 298 K.[25]

The ability of dppz and its derivatives to act as bpy and pz units is apparent in the electrochemistry of their complexes with Re(CO)$_3$Cl. Re(CO)$_3$(bpy)Cl exhibits one bpy-centered reduction at -1.25 V; Re(CO)$_3$(bdppz)Cl and Re(CO)$_3$(bdppzd)Cl, whose CVs

Table 2.4. UV-Visible electronic absorption spectral data for compounds in acetonitrile solution.

Table 2.4.

Absorption in Acetonitrile Solution. λ, nm; ε, $\underline{M}^{-1}$ cm^{1} x10^{-3}.

Compound	bpy $\pi \rightarrow \pi^*$	MLCT
bpy	236, 10.5 282,12.9	
bdppz	244, 46.6 312,64.2	
$Ru(bpy)_3^{2+}$	286, 102.4	450, 14.0
$Ru(bpy)_2(dppz)^{2+}$	284, 112.3	448, 19.4
$Ru(bpy)_2(Cl_2\text{-}dppz)^{2+}$	282, 116.5	438, 16.6
$Ru(bpy)_2(bdppz)^{2+}$	286, 72.3 322, 77.2	440, 18.0
$Ru(bpy)(bdppz)_2^{2+}$	284, 70.0 324, 104.5	440, 22.4
$Ru(bdppz)_3^{2+}$	324, 133.3	438, 21.4
$Ru(CH_3\text{-}bpy)_2(bdppz)^{2+}$	284, 62.6 322, 63.3	444, 16.7
$Ru(CF_3\text{-}bpy)_2(bdppz)^{2+}$	298, 96.0 322, 60.5	436, 18.8 458, 19.7
$Ru(bpy)_2(bdppzd)^{2+}$	284, 86.8	440, 16.4
$Re(CO)_3(bpy)Cl$	304, 32.6	368, 2.7
$Re(CO)_3(dppz)Cl$	320, 60.6	obscured
$Re(CO)_3(bdppz)Cl$	276, 49.7	obscured
$Re(CO)_3(bdppzd)Cl$	276, 33.2	390, 3.5

Figure 2.25. 298 K emission spectrum of an acetonitrile solution of $Ru(bpy)_2bdppz^{2+}$. 480 nm excitation.

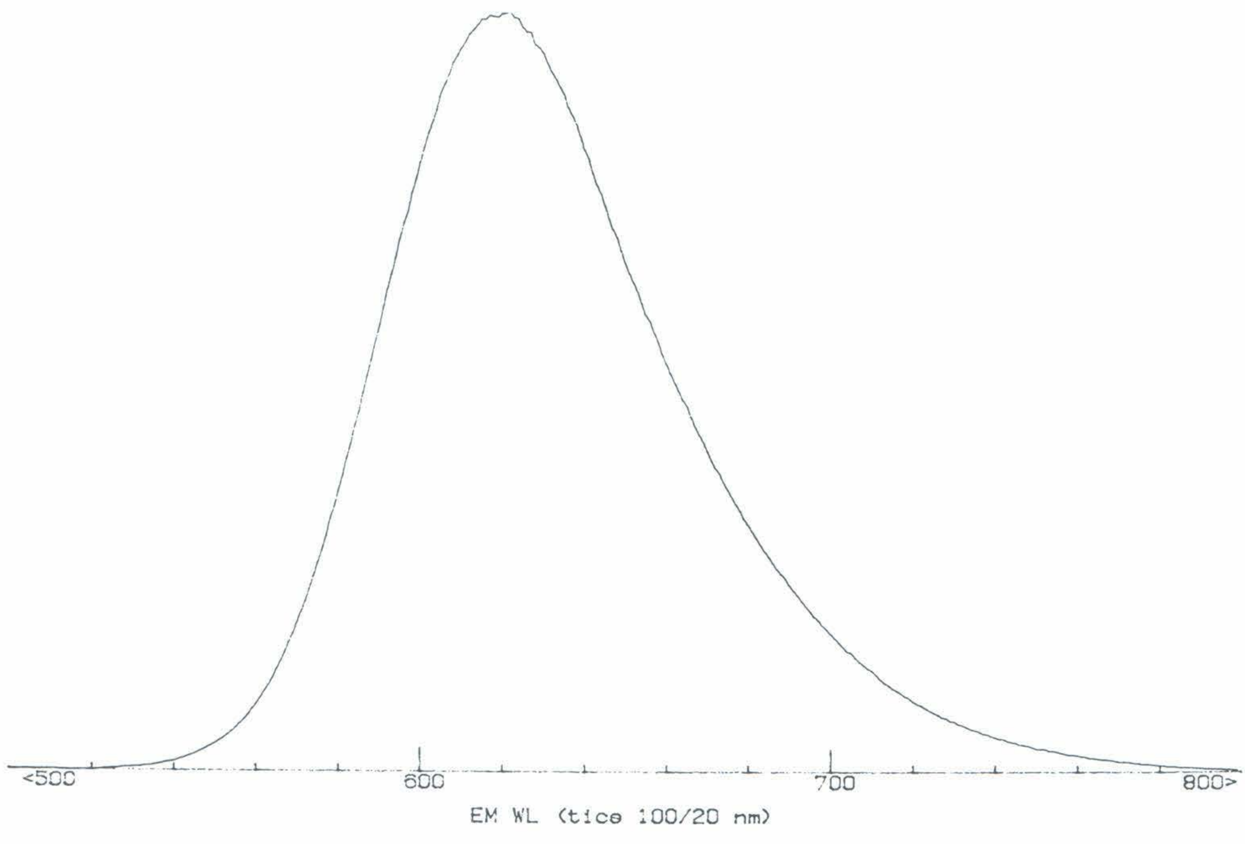
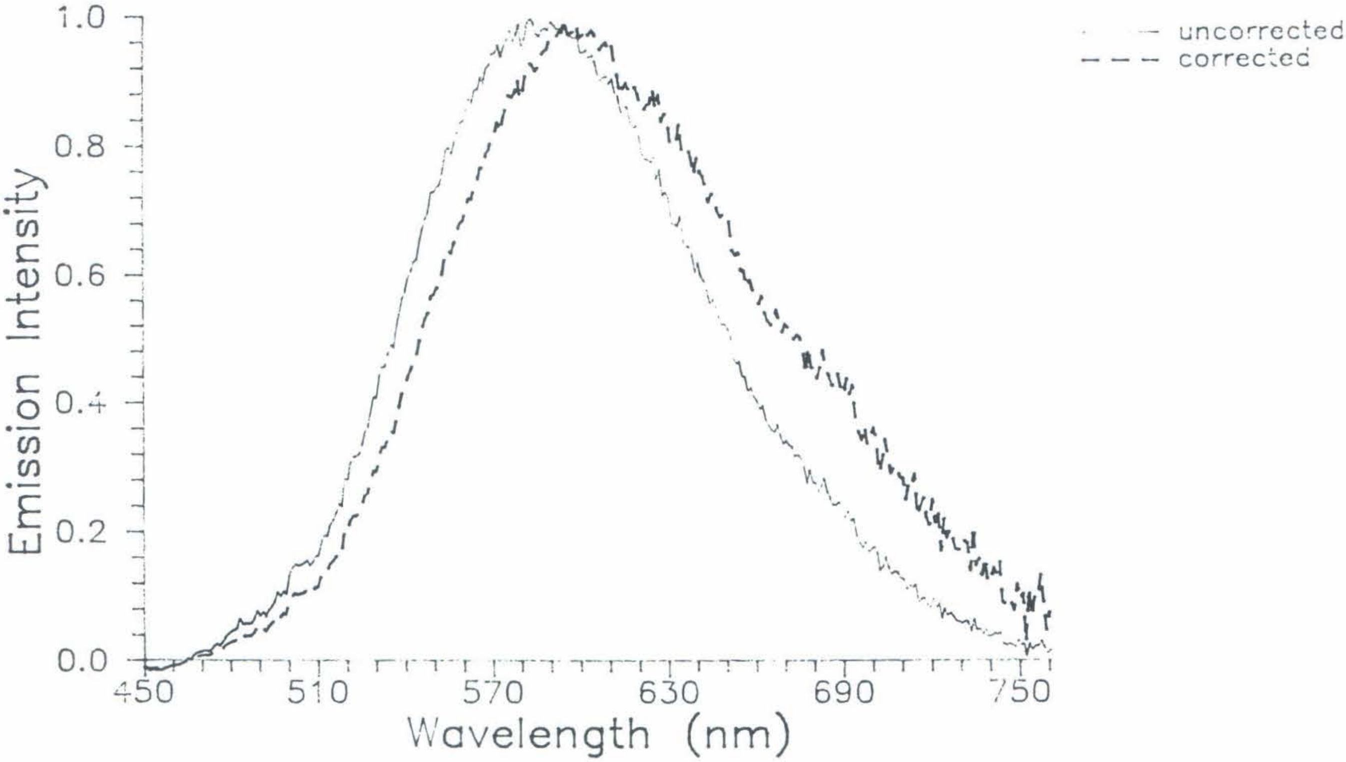

<500
600
700
800>
EM WL (tics 100/20 nm)

Figure 2.26. 298 K emission spectrum of a DMF solution of $Re(CO)_3(bdppz)Cl$. 436 nm excitation.



1.0
0.8
0.6
0.4
0.2
0.0
Emission Intensity
450
510
570
630
690
750
Wavelength (nm)
uncorrected
corrected

Figure 2.27. 298 K emission spectra of isoabsorptive acetonitrile solutions of $Ru(bpy)_{3-x}$ $bdppz_x^{2+}$. 442 nm excitation.

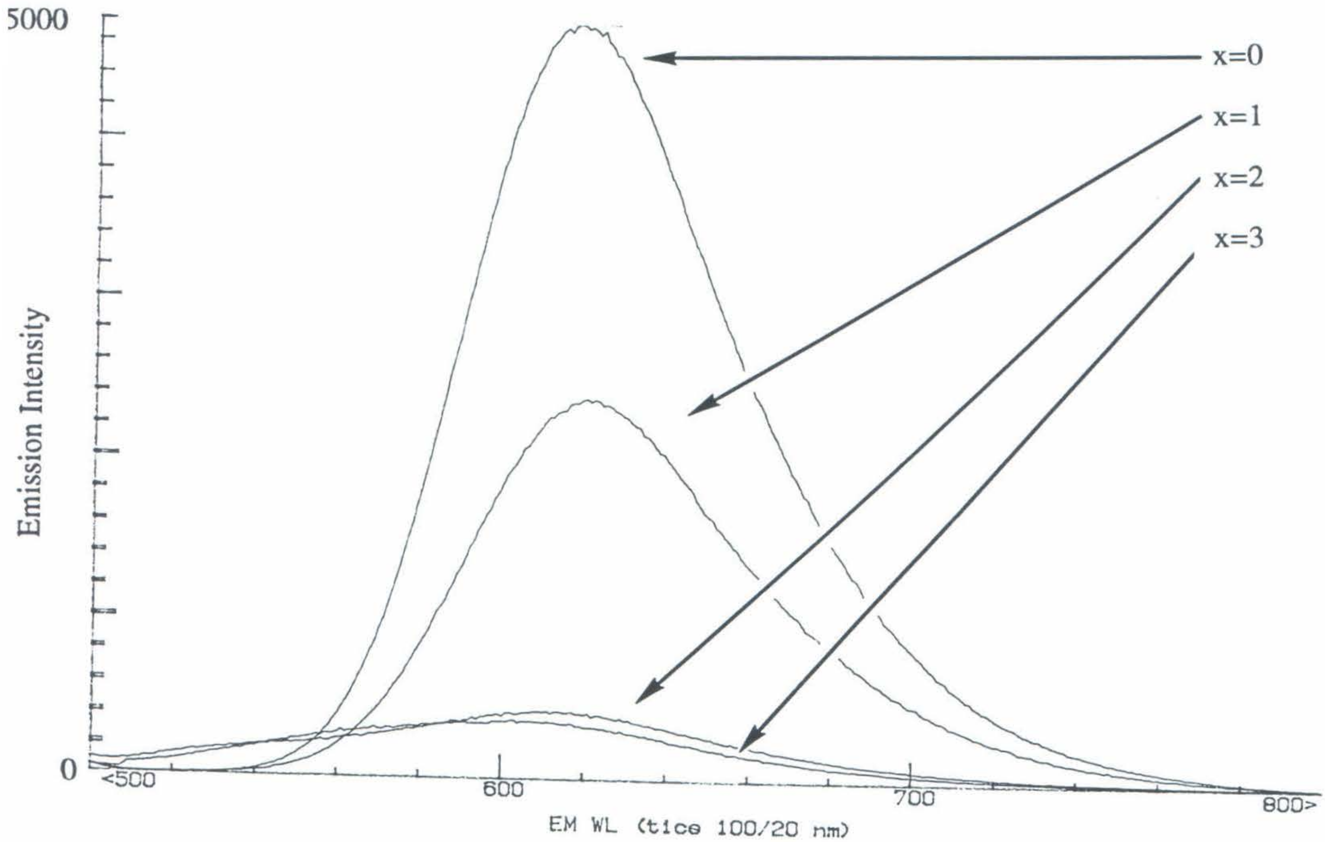

5000
0
Emission Intensity
x=0
x=1
x=2
x=3
<500
600
700
800>
EM WL (tice 100/20 nm)

Table 2.5. 298 K emission data for Ru and Re complexes. Emission maxima are not corrected for instrument response.

Complex	Emission Maximum (nm)	Relative Intensity
$Ru(bpy)_3^{2+}$	618	1
$Ru(bpy)_2(dppz)^{2+}$	630	
$Ru(bpy)_2(Cl_2\text{-}dppz)^{2+}$	634	
$Ru(bpy)_2(bdppz)^{2+}$	622	0.518
$Ru(bpy)(dppz)_2^{2+}$	610	0.139
$Ru(bdppz)_3^{2+}$	600	0.120
$Ru(CH_3\text{-}bpy)_2(bdppz)^{2+}$	637	0.237
$Ru(CF_3\text{-}bpy)_2(bdppz)^{2+}$	641	0.092
$Ru(bpy)_2(bdppzd)^{2+}$	630	
$Re(CO)_3(bpy)Cl$	590	
$Re(CO)_3(dppz)Cl$	598	
$Re(CO)_3(bdppz)Cl$	594	
$Re(CO)_3(bdppzd)Cl$	no emission observed	

Ru compounds in acetonitrile. Re compounds in DMF.

are shown in Figures 2.28 and 2.29, each possess two ligand-centered reductions. One reduction occurs near the potential of that in the bpy compound. The other reduction occurs at a more positive potential. The irreversible Re oxidation was not measured. Similar behavior is seen in the Ru complexes- in fact, the CVs of the Ru compounds are almost identical to those of the Re complexes, with two additional reduction waves present for the two bpy ligands. In $Ru(bpy)_2(bdppz)^{2+}$, Figure 2.30, the fourth reduction was beyond the solvent limit; the fifth reduction of $Ru(bpy)_2(bdppzd)^{2+}$, Figure 2.31, is the second reduction of a bpy ligand. The potential of the reversible Ru^{3+}/Ru^{2+} couple can also be measured. Electrochemical data for the compounds examined in this chapter can be found in Table 2.6.

The absorption and emission spectra presented earlier showed that dppz and its derivatives have orbitals that are bpy in character; MLCT absorption and emission maxima are the same in dppz-type compounds as they are in bpy compounds. It is reasonable to assign the reductions at more negative voltage in $Re(CO)_3(bdppz)Cl$ and $Re(CO)_3(bdppzd)Cl$, -1.30 and -1.05 V, respectively, to reduction of the bpy-character orbitals. $Re(CO)_3(bpy)Cl$ is reduced at -1.30 V, so one sees that, in $Re(CO)_3(bdppz)Cl$, the bpy portion of the molecule is not perturbed by the attached fused ring system. The same assignments for the bpy-character orbitals of the Ru compounds can also be made. As with $Re(CO)_3(bdppz)Cl$, the bpy orbitals of the ligand in $Ru(bpy)_2(bdppz)^{2+}$ are unaffected by its bpz part; reduction occurs at -1.35 V, the same potential as the first reduction of $Ru(bpy)_3^{2+}$.

Visible spectroelectrochemistry shows that the new reductions present at more positive potentials are due to the pz-character orbitals of the ligands. The spectral changes accompanying reduction of the quinone compounds $Re(CO)_3(bdppzd)Cl$ and $Ru(bpy)_2(bdppzd)^{2+}$ at the indicated potentials are shown in Figures 2.32 and 2.33, respectively. The changes seen do not offer much insight into the nature of the orbital which receives the electron. The spectroelectrochemistry of the bdppz complexes is

Figure 2.28. Cyclic voltammagram of $Re(CO)_3$(bdppz)Cl in 0.1 M TBAH/ CH_2Cl_2.

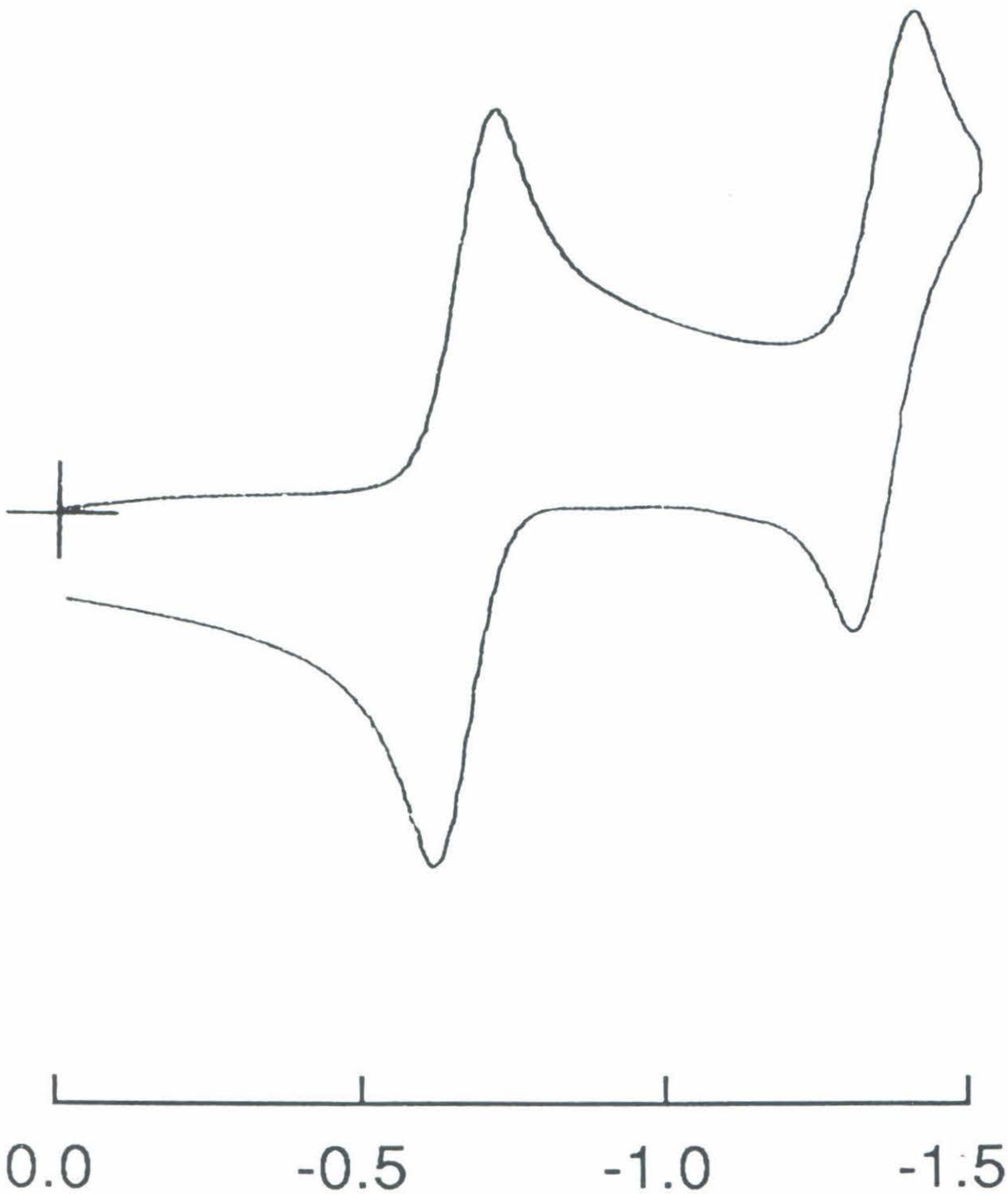

0.0
-0.5
-1.0
-1.5

Figure 2.31. Cyclic voltammagram of $Re(CO)_3$(bdppzd)Cl in 0.1 M TBAH/ CH_2Cl_2.

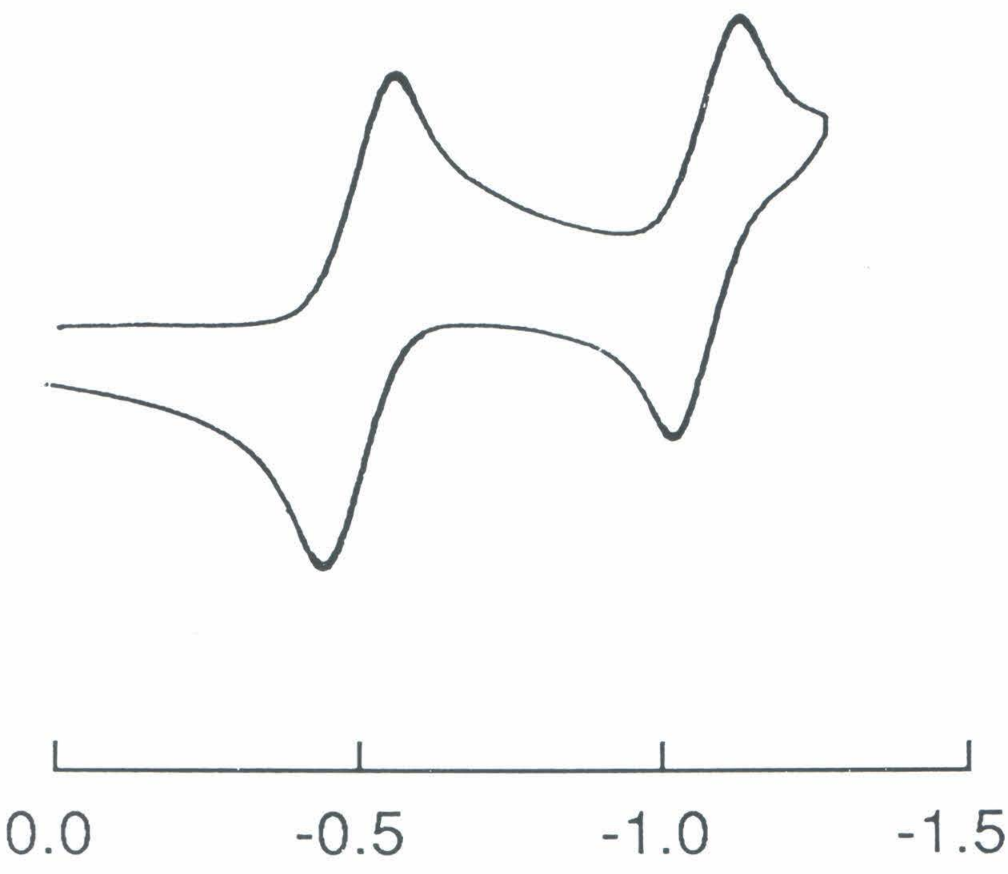

0.0
-0.5
-1.0
-1.5

Figure 2.30. Cyclic voltammagram of $Ru(bpy)_2(bdppz)^{2+}$ in 0.1 M TBAH/ acetonitrile.

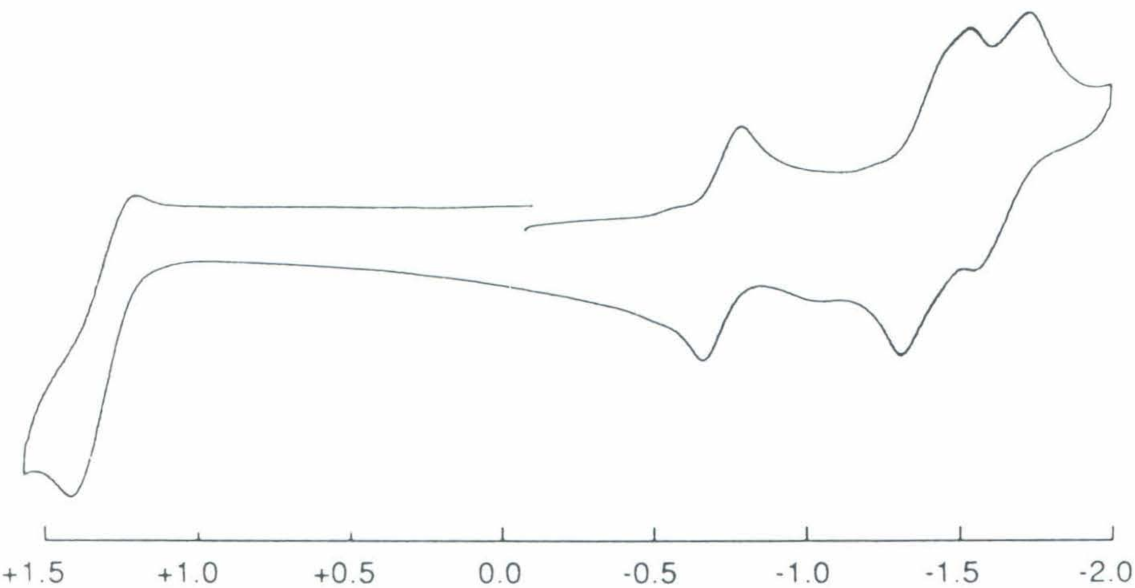
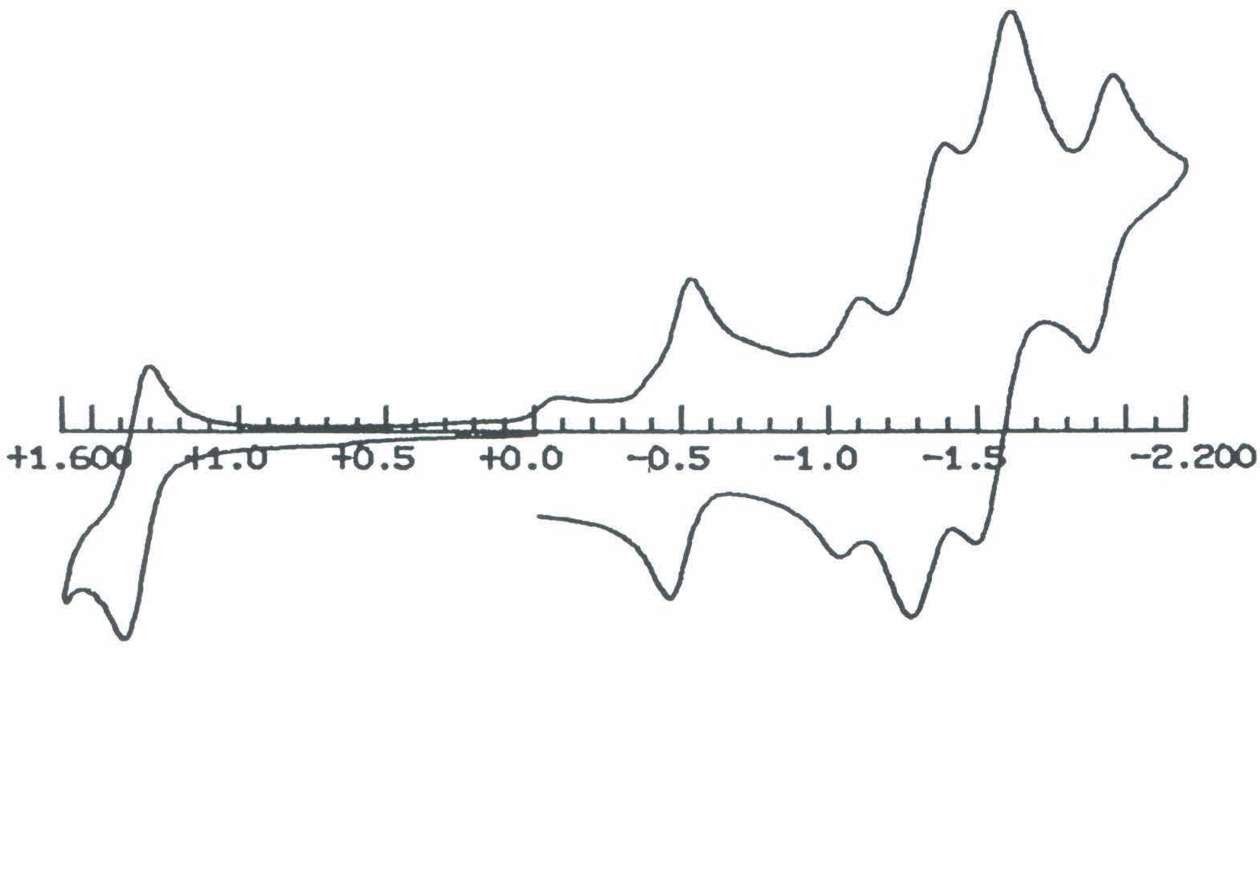

+1.5
+1.0
+0.5
0.0
-0.5
-1.0
-1.5
-2.0

Figure 2.31. Cyclic voltammagram of $Ru(bpy)_2(bdppzd)^{2+}$ in 0.1 M TBAH/ acetonitrile.



+1.600
+1.0
+0.5
+0.0
-0.5
-1.0
-1.5
-2.200

Table 2.6. Electrochemical data for complexes.

Table 2.6. Electrochemical data for complexes.

Compound	$\mathbf{Ru^{3+/2+}}$	$\mathbf{X\text{-}pz^{0/-}}$	$\mathbf{bpy^{0/-}}$
$Ru(bpy)_3{}^{2+}$	+1.35		-1.32
$Ru(bpy)_2(dppz)^{2+}$	+1.35	-0.95	-1.39
$Ru(bpy)_2(Cl_2\text{-}dppz)^{2+}$	+1.35	-0.77	-1.37
$Ru(bpy)_2(bdppz)^{2+}$	+1.35	-0.73	-1.35
$Ru(bpy)(bdppz)_2{}^{2+}$		-0.45, -0.74	-1.40
$Ru(CH_3\text{-}bpy)_2(bdppz)^{2+}$	+1.22	-0.60	
$Ru(CF_3\text{-}bpy)_2(bdppz)^{2+}$	+1.72	-0.49	-0.79
$Ru(bpy)_2(bdppzd)^{2+}$	+1.32	-0.50	-1.07
$Re(CO)_3(bpy)Cl$			-1.30
$Re(CO)_3(bdppz)Cl$		-0.73	-1.32
$Re(CO)_3(bdppzd)Cl$		-0.51	-1.12

Ru potentials in 0.1M TBAH/ acetonitrile. Re potentials in 0.1M TBAH/ dichloromethane. Potentials vs. Ag/AgCl.

Figure 2.32. Spectral changes accompanying electrochemical reduction of $Re(CO)_3$(bdppzd) in 0.1 M TBAH/ CH_2Cl_2 at the potential indicated.

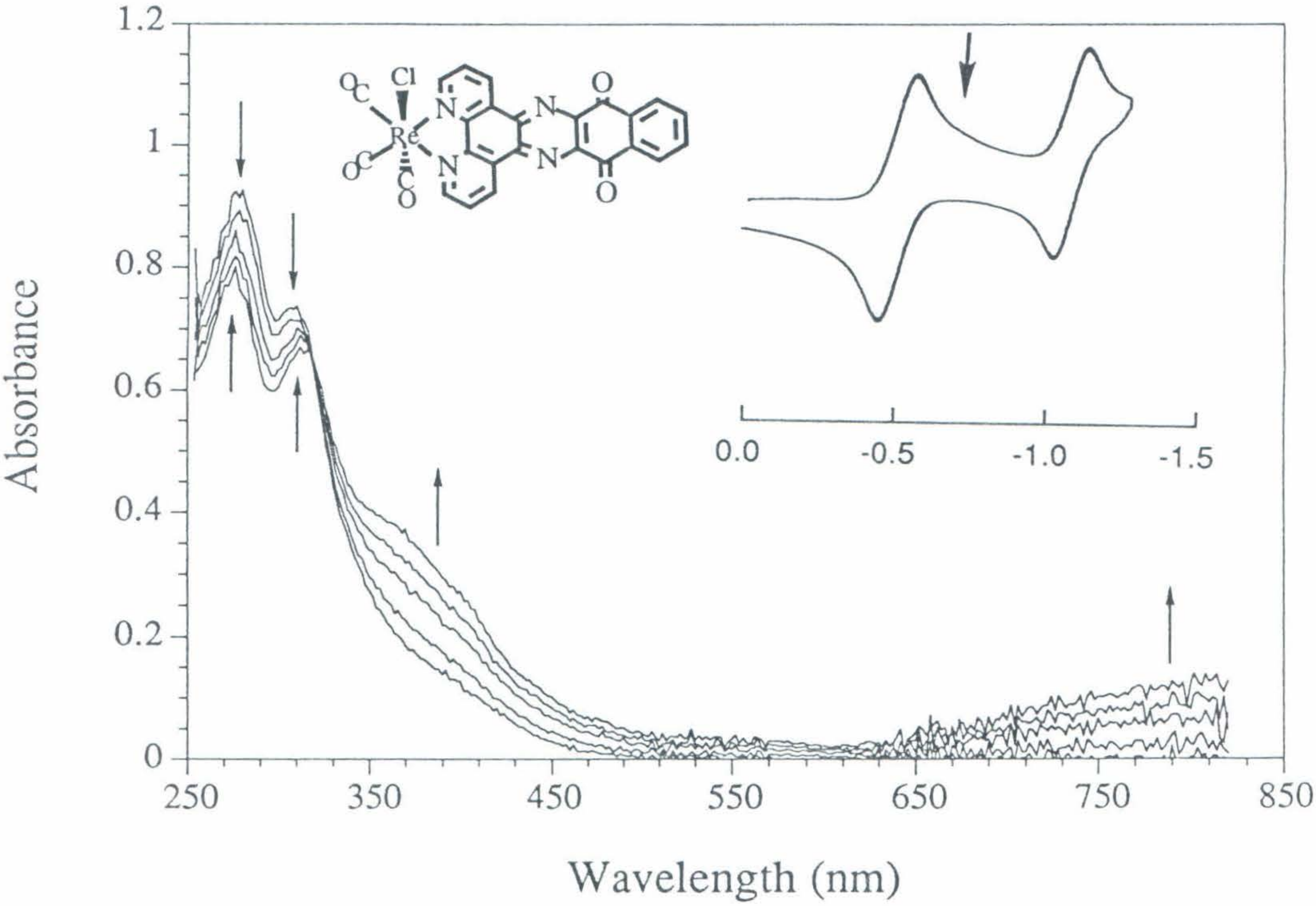
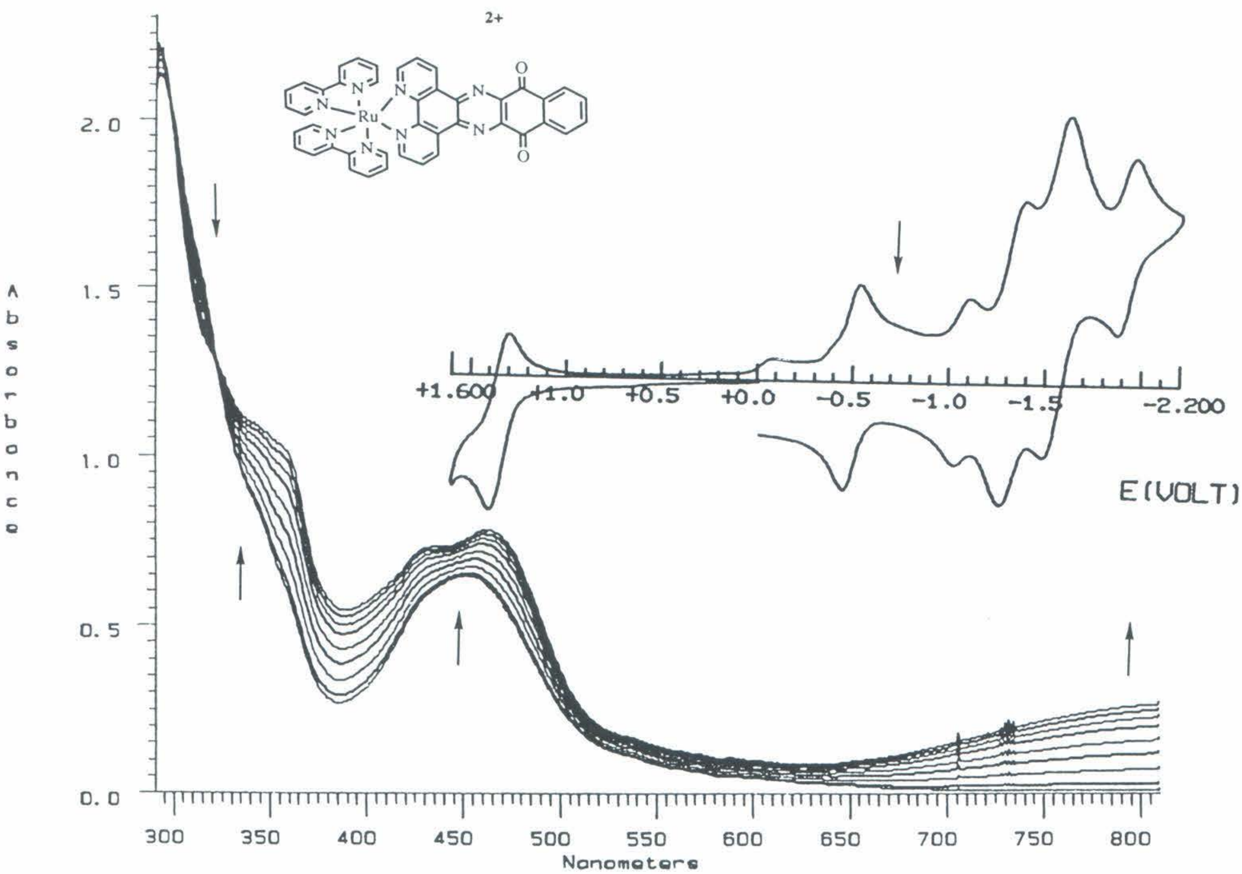

1.2
1
0.8
0.6
0.4
0.2
0
Absorbance
250
350
450
550
650
750
850
Wavelength (nm)
0.0
-0.5
-1.0
-1.5
Cl
Re
N
O

Figure 2.33. Spectral changes accompanying electrochemical reduction of $Ru(bpy)_2(bdppzd)^{2+}$ in 0.1 M TBAH/ acetonitrile at the potential indicated.


2+
Ru
N
O
2.0
1.5
1.0
0.5
0.0
Absorbance
300
350
400
450
500
550
600
650
700
750
800
Nanometers
+1.600
+1.0
+0.5
+0.0
-0.5
-1.0
-1.5
-2.200
E(VOLT)

much more instructive. The spectral changes resulting from incremental reduction of $Re(CO)_3(bdppz)Cl$ and $Ru(bpy)_2(bdppz)^{2+}$ at the indicated potentials are shown in Figures 2.34 and 2.35, respectively. The same changes are seen in both compounds: absorbance increases with maxima at 375, 570, and 650 nm and the maximum at 335 nm decreases upon reduction. The radical anion of pz produced by γ-irradiation in 3-methyltetrahydrofuran at 77 K exhibits absorption maxima at 512 and 550 nm.[26] In $dppz^{\bullet-}$, these absorbances shift to 540 and 572 nm and a large absorbance is also seen at 375 nm. Given the redshifts seen in the absorption spectra of bpz and bdppz relative to pz and dppz, the absorbances at 570 and 650 nm in $Ru(bpy)_2(bdppz)^{\bullet+}$ can be assigned to reduction of the bpz-character orbital of bdppz. There is no optical transition which populates this orbital- no absorbance is seen at lower energy than the MLCT in any compound- thus it cannot be strongly coupled to the metal center.

Time-resolved absorbance can be used to determine if intramolecular ET from the MLCT excited state to the bpz and bpzd orbitals of bdppz and bdppzd takes place; if it does, the charge-separated state formed upon laser excitation will exhibit the same spectral features as those seen spectroelectrochemically. Following the time course of these absorbance changes allows determination of the rate of both formation and recombination of the charge-separated state. In this way, an inorganic chromophore can be used to probe the electronic structure of the medium separating an electron donor and acceptor.

Neither $Re(CO)_3(bdppzd)Cl$ nor $Ru(bpy)_2(bdppzd)^{2+}$ displays a transient absorption signal in the 650-800 nm region where spectroelectrochemistry shows the growth of a very broad, unstructured band upon reduction. Thus it appears that the hoped-for long-lived Ru^{3+}-semiquinone state is not produced. $Re(CO)_3(bdppz)Cl$ and $Ru(bpy)_2(bdppz)^{2+}$, whose original purpose was to serve as model compounds lacking excited-state charge separation, display unexpected behavior. As shown in Figures 2.36 and 2.37, when monitoring absorbance at 580 nm, the first of the two low-energy maxima

Figure 2.34. Spectral changes accompanying electrochemical reduction of $Re(CO)_3$(bdppz) in 0.1 M TBAH/ CH_2Cl_2 at the potential indicated.

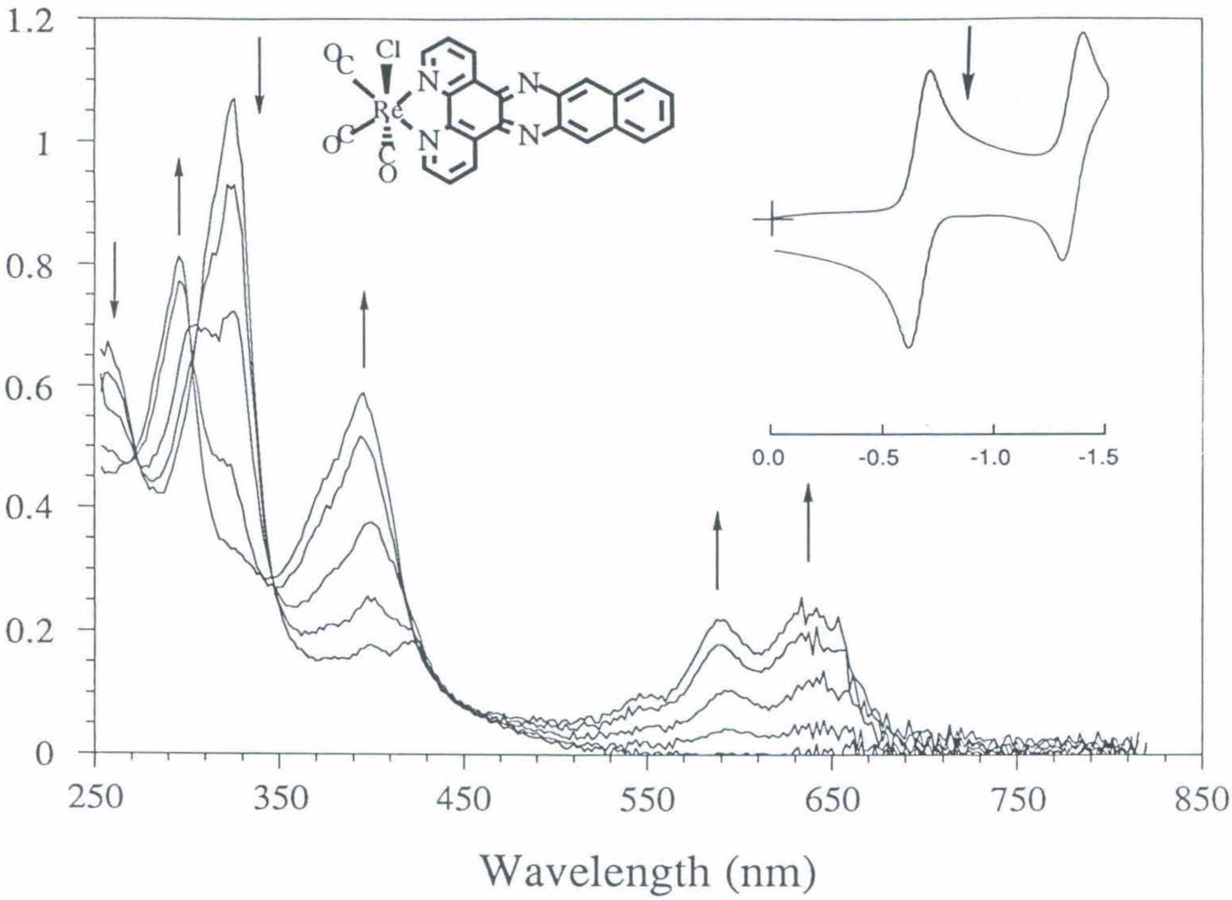
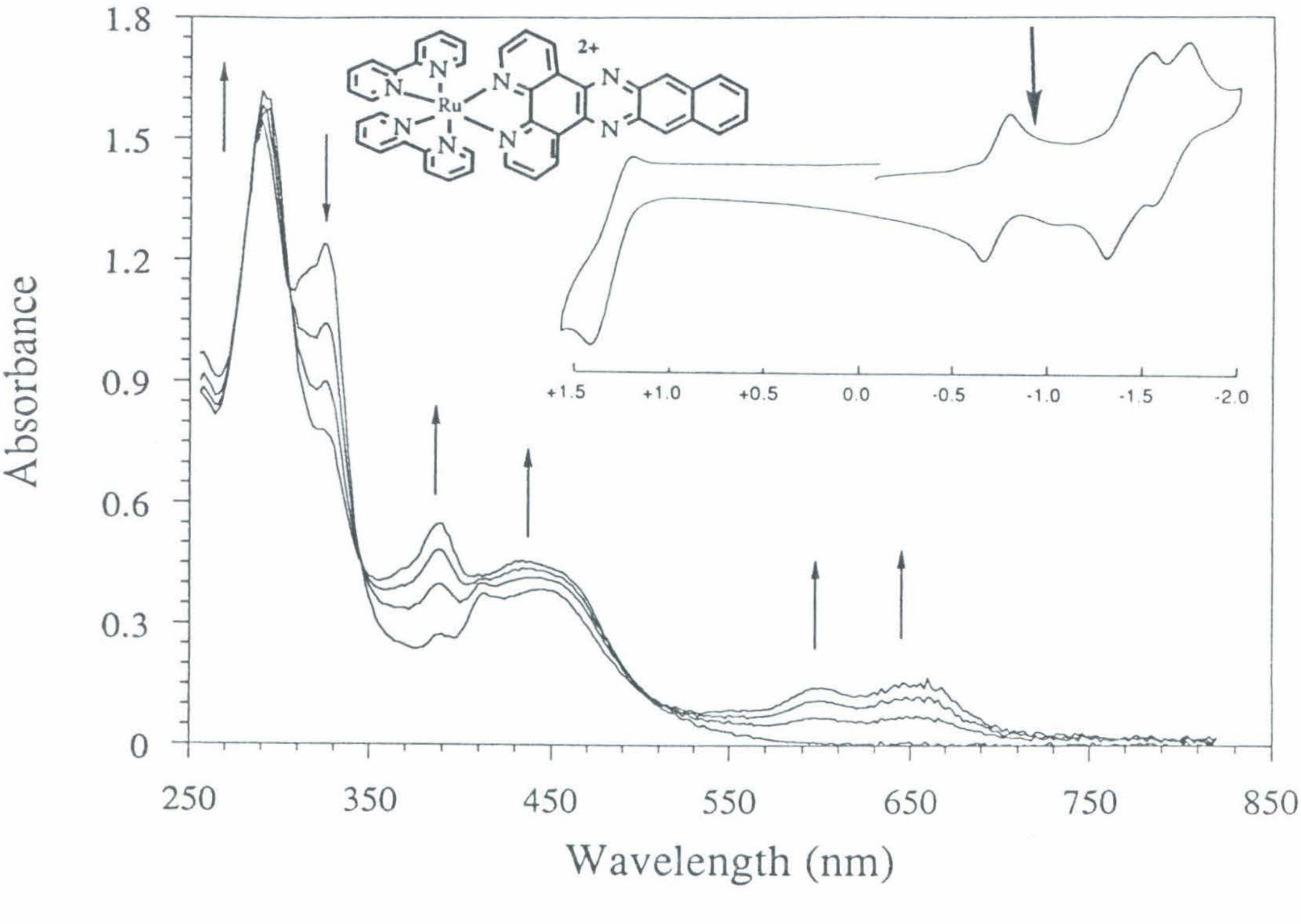

1.2
1
0.8
0.6
0.4
0.2
0
250
350
450
550
650
750
850
Wavelength (nm)
Cl
Re
N
N
N
N
0.0
-0.5
-1.0
-1.5

Figure 2.35. Spectral changes accompanying electrochemical reduction of $Ru(bpy)_2(bdppz)^{2+}$ in 0.1 M TBAH/ acetonitrile at the potential indicated.



1.8
1.5
1.2
0.9
0.6
0.3
0
Absorbance
250
350
450
550
650
750
850
Wavelength (nm)
2+
Ru
N
+1.5
+1.0
+0.5
0.0
-0.5
-1.0
-1.5
-2.0

Figure 2.36. 580 nm transient absorption observed upon 480 nm laser irradiation of a nitrogen-purged 4 x 10^{-5} M acetonitrile solution of $Re(CO)_3$(bdppz).

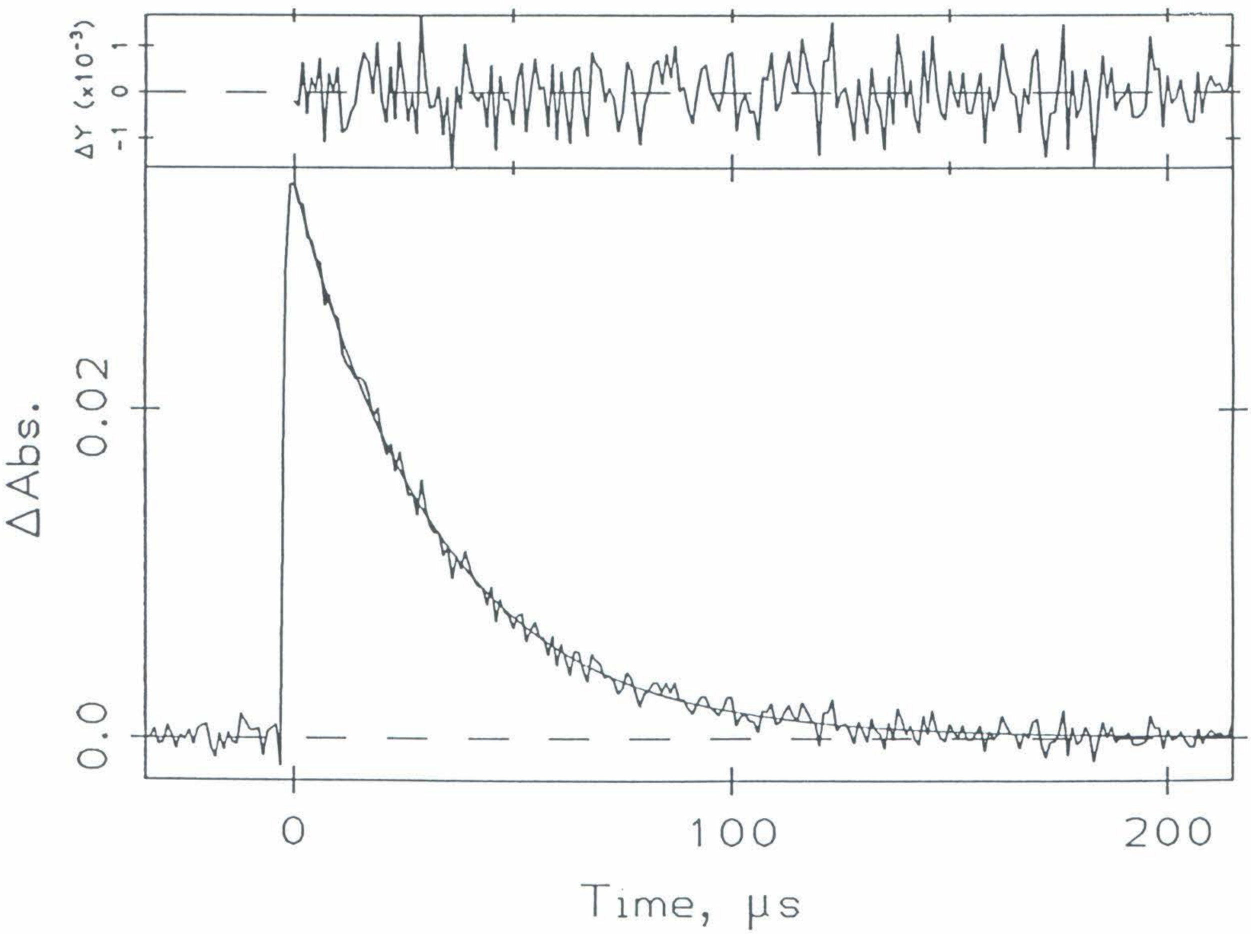
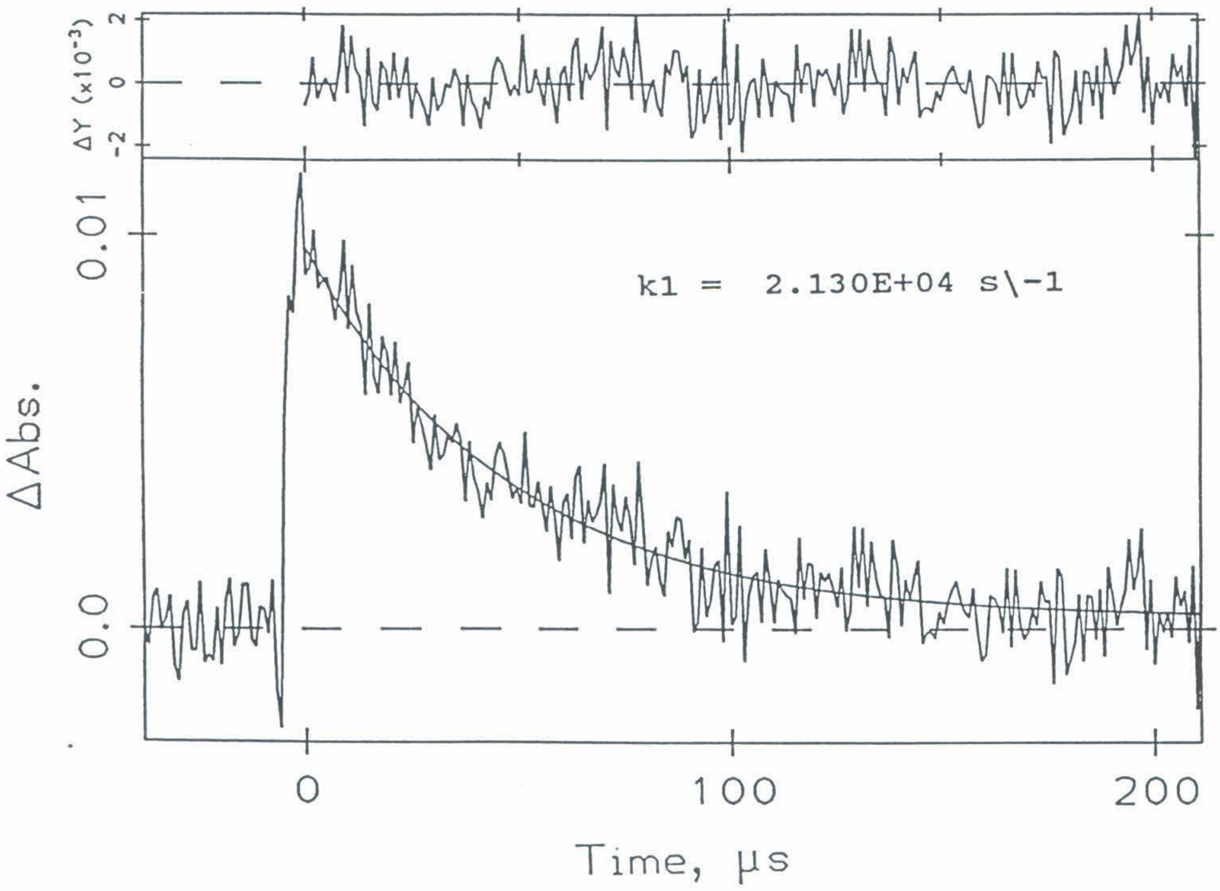

ΔY (x10⁻³)
1
0
-1
ΔAbs.
0.02
0.0
0
100
200
Time, μs

Figure 2.37. 580 nm transient absorption observed upon 480 nm laser irradiation of a nitrogen-purged 2 x 10^{-5} M solution of $Ru(bpy)_2(bdppz)^{2+}$ in 0.1 M TBAH/ acetonitrile.

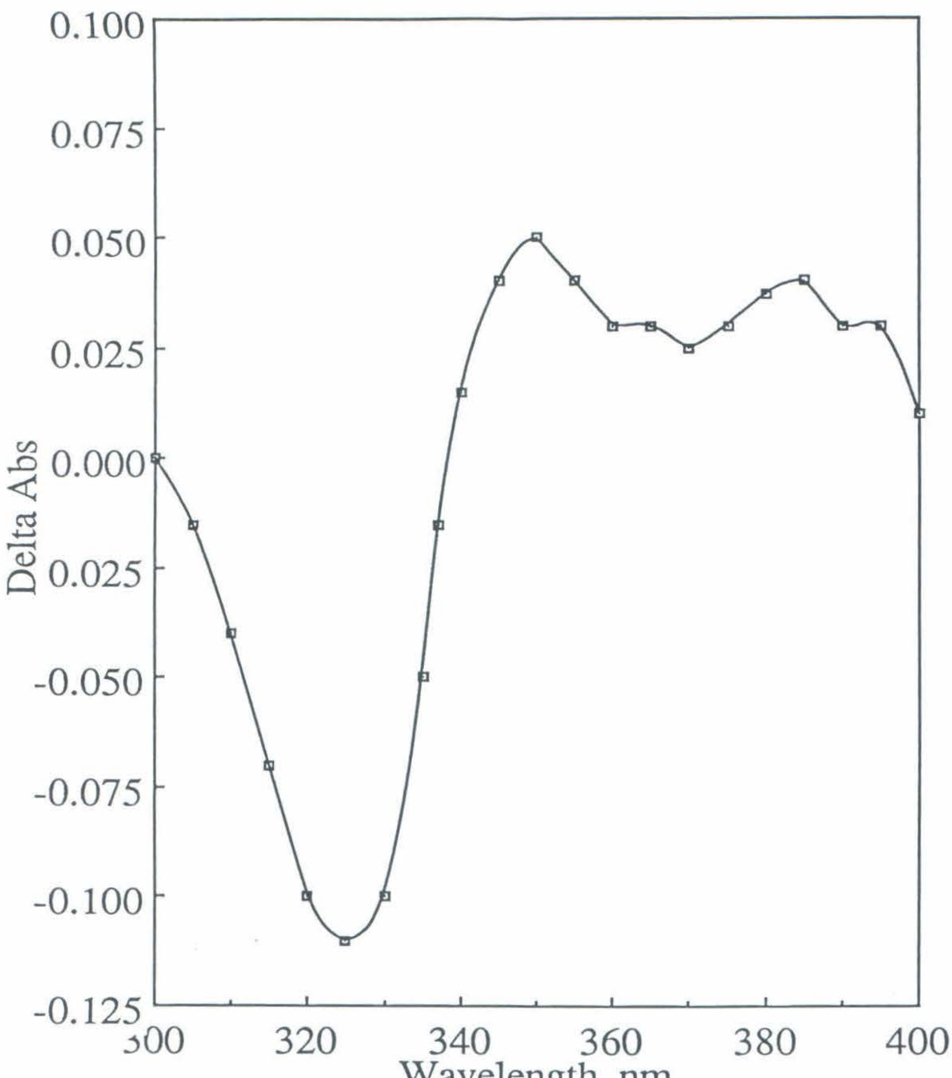

ΔY (x10⁻³)
2
0
-2
0.01
0.0
ΔAbs.
k1 = 2.130E+04 s\-1
0
100
200
Time, μs

seen spectroelectrochemically, a large positive absorbance change takes place upon 480 nm laser irradiation of the MLCT bands of these compounds. This transient decays with a first-order rate constant of 3.79 x 10^4 s^{-1} in $Re(CO)_3(bdppz)Cl$; the rate constant for $Ru(bpy)_2(bdppz)^{2+}$ is 2.07 x 10^4 s^{-1}. If these transients are due to Ru → bpz ET, the lifetimes of the charge-separated states, 26.38 and 48.31 μs, respectively, are without precedent in molecules as simple as these. Molecules in which microsecond-lifetime separation has been achieved are much more complex, as the pentad discussed earlier and shown in Figure 2.9.

There is much evidence supporting the view that the long-lived transient observed is the Ru^{3+} / $bpz^{\bullet-}$ state. Pz fluoresces in aerated solution with an appreciable lifetime and quantum yield;[27] in the presence of oxygen, which efficiently quenches the luminescence of Ru chromophores, $Ru(bpy)_2(bdppz)^{2+}$ gives no transient signal, showing that the phenomenon is not due to direct excitation of the ligand. Energy transfer from the MLCT excited state of the Ru center state generating a long-lived bpz triplet state could give rise to the transient seen, but the transient positive change in optical density is observed out to 750 nm. The lowest-energy absorbance in the triplet spectrum of pz is at 504 nm[28]; even with the red shift which accompanies extending the aromatic system, one would not expect the triplet state of bdppz to be shifted so far.

Direct spectroscopic evidence for intramolecular ET comes from the transient difference spectrum of $Ru(bpy)_2(bdppz)^{2+}$ presented in Figure 2.38. The spectrum was generated by plotting the absorbance change measured 1 μs after the laser pulse as a function of observation wavelength. The 300-400 nm region spectrum shown in the figure exhibits the same optical density decrease centered at approximately 330 nm that is seen spectroelectrochemically. Thus the spectral changes generated by electrochemical reduction are duplicated photochemically. The transient is due to ET from the Ru center to the bpz portion of the ligand.

Figure 2.38. Transient difference spectrum measured 1 μs after 480 nm laser irradiation of a nitrogen-purged 2 x 10^{-5} M solution of $Ru(bpy)_2(bdppz)^{2+}$ in 0.1 M TBAH/ acetonitrile.

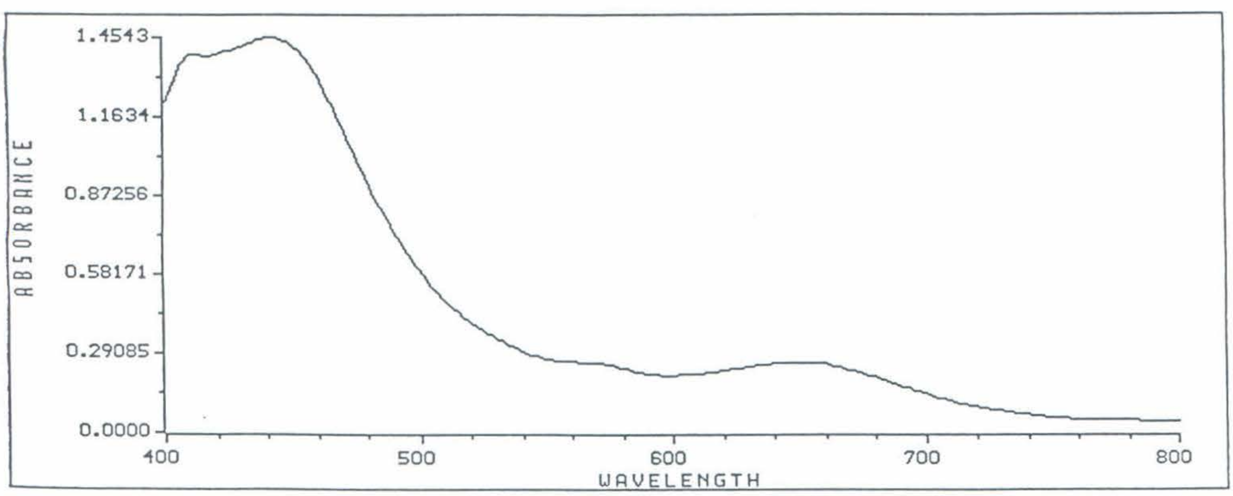

0.100
0.075
0.050
0.025
0.000
0.025
-0.050
-0.075
-0.100
-0.125
Delta Abs
300
320
340
360
380
400
Wavelength, nm

The electron which is transferred from Ru to bpz can be trapped there by employing a molecule which reduces transient Ru^{3+} more rapidly than does charge recombination. Aniline has been used as a sacrificial electron donor in other systems;[28] steady-state photolysis of an acetonitrile solution of $Ru(bpy)_2(bdppz)^{2+}$ and aniline at λ>400 nm leads to the spectrum shown in Figure 2.39. The features which grow in are the same as those seen spectroelectrochemically. The electron is trapped as $bpz^{\bullet-}$.

These experiments show that a long-lived charge-separated state is produced via ET in Re and Ru compounds of bdppz. The extraordinarily long lifetime of this state is governed by the factors set forth in the Marcus equation for ET. The driving force for charge recombination, 2.0 eV for $Ru(bpy)_2(bdppz)^{2+}$, puts it in the energy regime in which inverted behavior has been observed in several other systems.[5] Electrochemical irreversibility of the $Re2^{+/+}$ couple of $Re(CO)_3(bdppz)Cl$ makes exact determination of its recombination driving force impossible; it is likely the same as that of $Ru(bpy)_2(bdppz)^{2+}$. Inverted behavior is likely present, but it alone can not explain the slow kinetics. In systems where inverted behavior has been seen, recombination over a similar distance (9 Å) and with a similar driving force is at least three orders of magnitude faster than that seen here. Clearly, donor-acceptor coupling also plays a role in producing long-lived charge separation in these compounds.

It is not surprising that weak coupling retards back ET in complexes with bdppz. The data presented thus far have shown that the ligand behaves as separate bpy and bpz units. Charge-recombination ET from bpz to Ru must take place through the bpy portion of the ligand; if it is not well-coupled to the bpz portion, it should act as an "insulator" between donor and acceptor. There are several ways of gauging how uncoupled the components of bdppz are. Chemical reduction of $Re(CO)_3(bdppz)Cl$ with cobaltacene gives $Re(CO)_3(bdppz)Cl^{\bullet-}$. The electron goes into the LUMO of the molecule, the bpz-character orbital of the ligand. The bpy-character orbital is vacant; if there is no communication between these two orbitals, the Re$\rightarrow$bpy MLCT will be unaffected. This

Figure 2.39. Spectrum of 2 x 10^{-5} M $Ru(bpy)_2(bdppz)^{2+}$ after continuous irradiation in a solution of 1 x 10^{-3} M aniline/acetonitrile. A 400 nm cutoff filter was used on the 1000 W Hg/Xe light source.


1.4543
1.1634
0.87256
0.58171
0.29085
0.0000
ABSORBANCE
400
500
600
700
800
WAVELENGTH

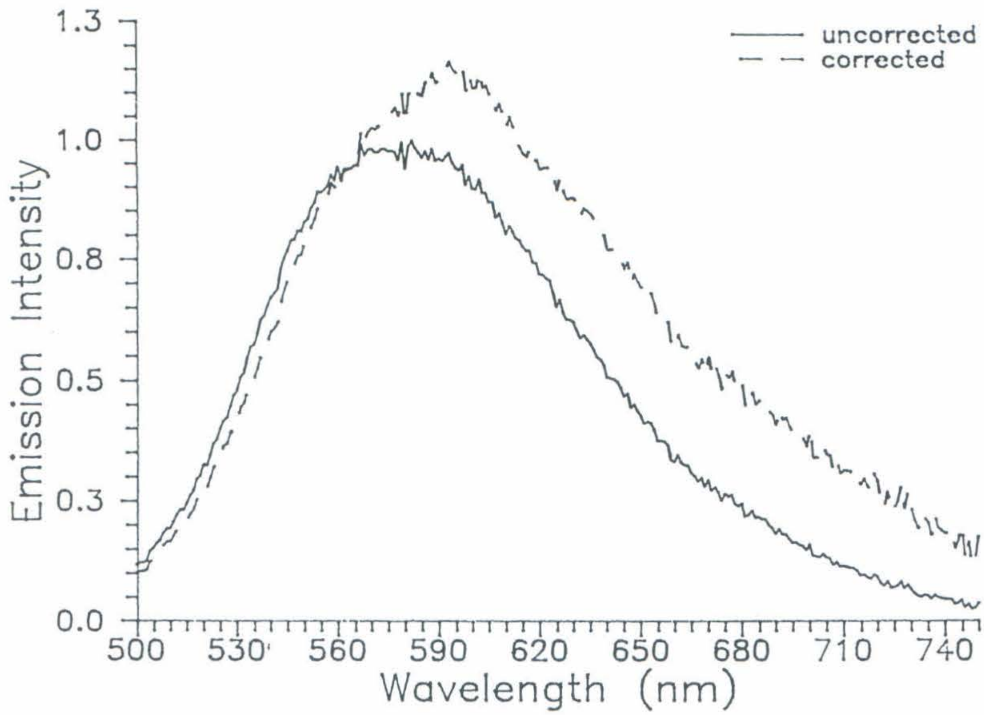
is borne out experimentally. Shown in Figure 2.40 are emission spectra of $Re(CO)_3(bdppz)Cl$ and cobaltacene-generated $Re(CO)_3(bdppz)Cl^{\bullet-}$. Neither the energy nor the intensity of emission is affected greatly by filling the bpz orbital, showing that the electron does not interact with the bpy orbital and block MLCT-based emission.

X-band EPR of $Re(CO)_3(bdppz)Cl^{\bullet-}$ also shows that the electron resides in the bpz part of the ligand. The measured spectrum is shown in the top of Figure 2.41, a simulated spectrum at the bottom. The observed spectrum is simulated using N(9,16)=5.0 G, H(10,15)=4.8 G, H(11,14)=1.5 G, and H(12,13)=1.25 G. No protons on the bpy portion of bdppz are needed in the simulation; very little electron density resides at these positions.

A measure of the degree of communication between the metal center and the electron residing on bdppz in $Re(CO)_3(bdppz)Cl^{\bullet-}$ can be made by employing IR spectroelectrochemistry. Just as the visible spectral changes which accompany reduction can be followed, so can changes in IR stretching frequencies be observed by electrochemically reducing a compound *in situ* in an IR cell. CO stretching frequencies are sensitive to the amount of density on the metal to which they are attached; if an electron is put into an orbital of $Re(CO)_3(diimine)Cl$ which is coupled to the metal, a shift to lower energy proportional to the amount of electron density the orbital shares with Re will be seen. Reduction of $Re(CO)_3(phen)Cl$, Figure 2.42, leads to a 30 cm^{-1} shift to lower energy of the three CO stretching modes. This large shift is expected; the high degree of coupling between Re and phen is responsible for the intense MLCT band exhibited by the complex.

In $Re(CO)_3(dppz)Cl$, Figure 2.43, a much smaller 3 cm^{-1} shift is seen, in accordance with the bpy/pz character of the ligand. The electron goes into the pz-character LUMO which is poorly coupled to Re. Surprisingly, the Re complexes of bdppz and bdppzd, as shown in Figures 2.44 and 2.45, respectively, have CO-stretching frequency shifts that are the same as those of $Re(CO)_3(dppz)Cl$, 3 cm^{-1}.

Figure 2.40. Emission spectra of unreduced (top) and cobaltacene-reduced $Re(CO)_3$(bdppz)Cl. 436 nm excitation.


uncorrected
corrected
1.3
1.0
0.8
0.5
0.3
0.0
Emission Intensity
500
530
560
590
620
650
680
710
740
Wavelength (nm)

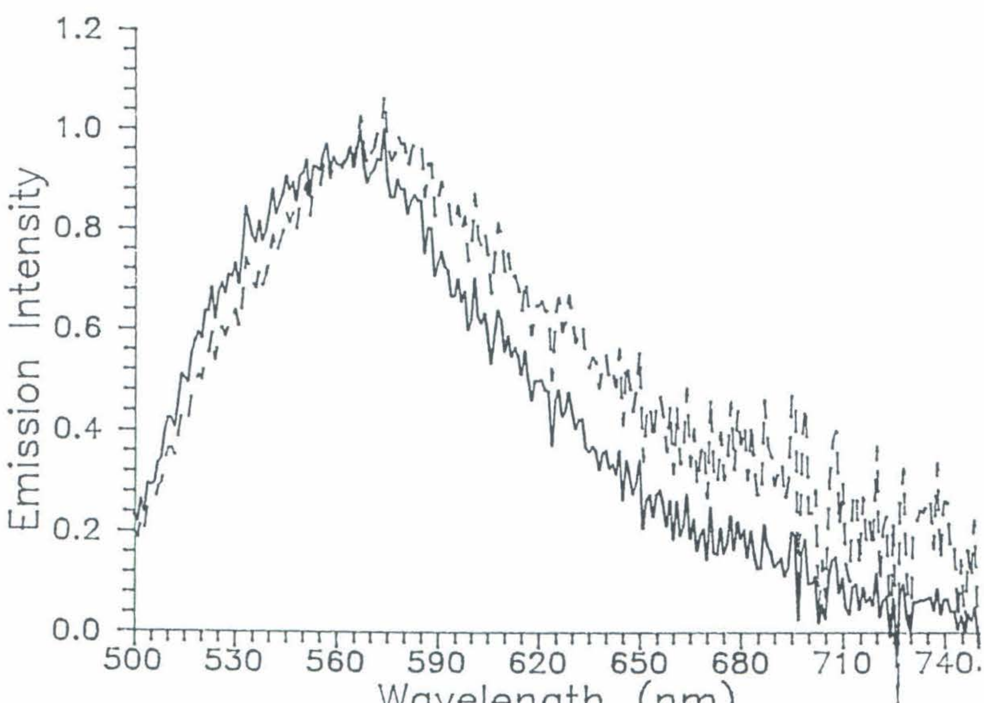
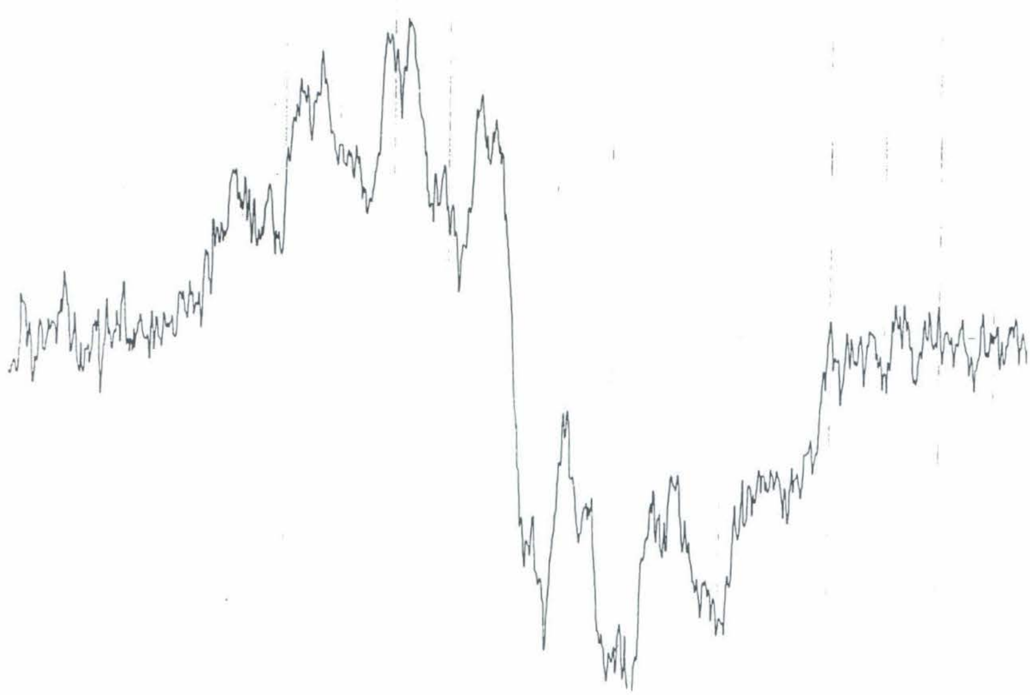

1.2
1.0
0.8
0.6
0.4
0.2
0.0
Emission Intensity
500
530
560
590
620
650
680
710
740
Wavelength (nm)

Figure 2.41. Experimental (top) and simulated EPR of $Re(CO)_3(bdppz)Cl^{\bullet -}$. The spectrum is simulated using N(9,16)=5.0 G, H(10,15)=4.8 G, H(11,14)=1.5 G, and H(12,13)=1.25 G.



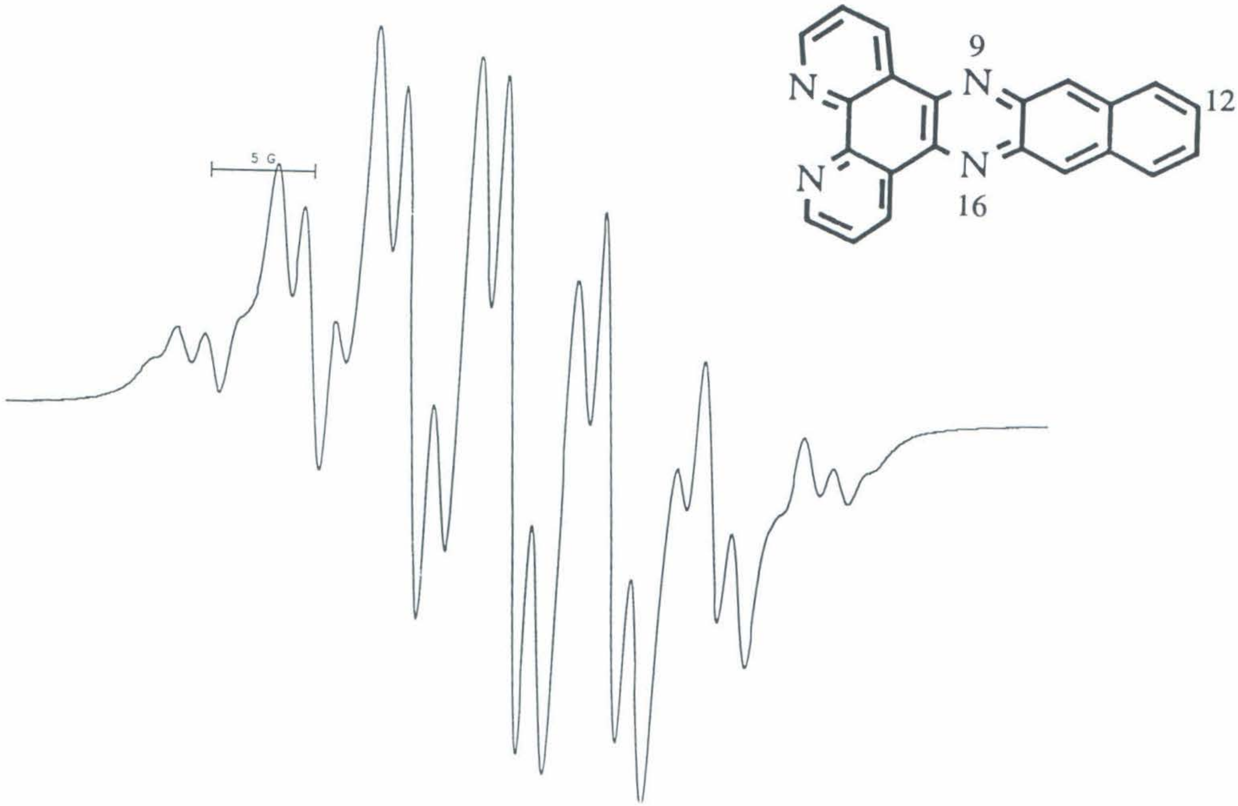

5 G
9
N
N
12
N
N
16

Figure 2.42. IR spectroelectrochemical reduction of $Re(CO)_3(phen)Cl$ in 0.1 M TBAH/ CH_2Cl_2.

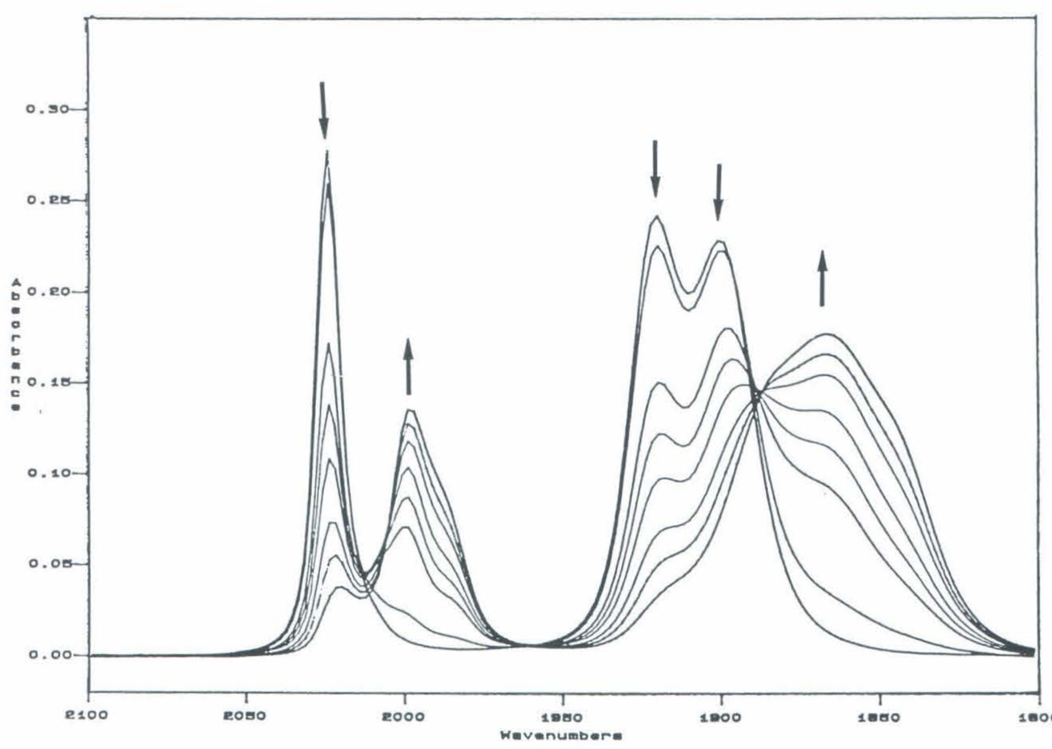

Absorbance
0.30
0.25
0.20
0.15
0.10
0.05
0.00
2100
2050
2000
1950
1900
1850
1800
Wavenumbers

Figure 2.43. IR spectroelectrochemical reduction of $Re(CO)_3(dppz)Cl$ in 0.1 M TBAH/ CH_2Cl_2.

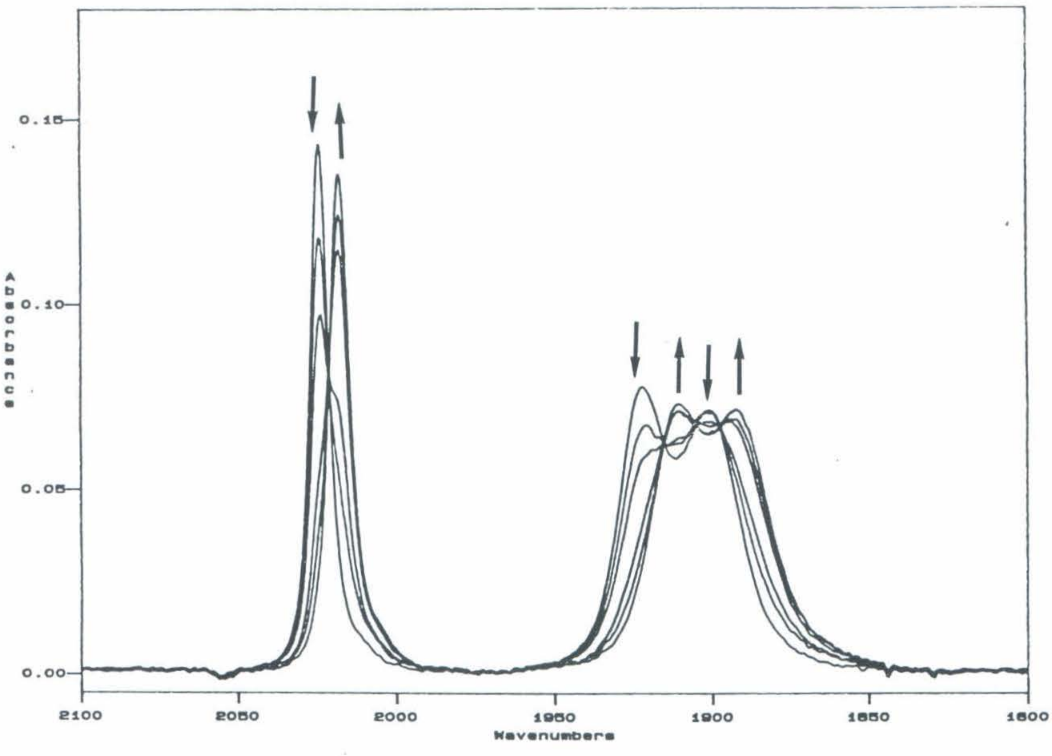

0.15
0.10
0.05
0.00
Absorbance
2100
2050
2000
1950
1900
1850
1800
Wavenumbers

Figure 2.44. IR spectroelectrochemical reduction of $Re(CO)_3$(bdppz)Cl in 0.1 M TBAH/ CH_2Cl_2.

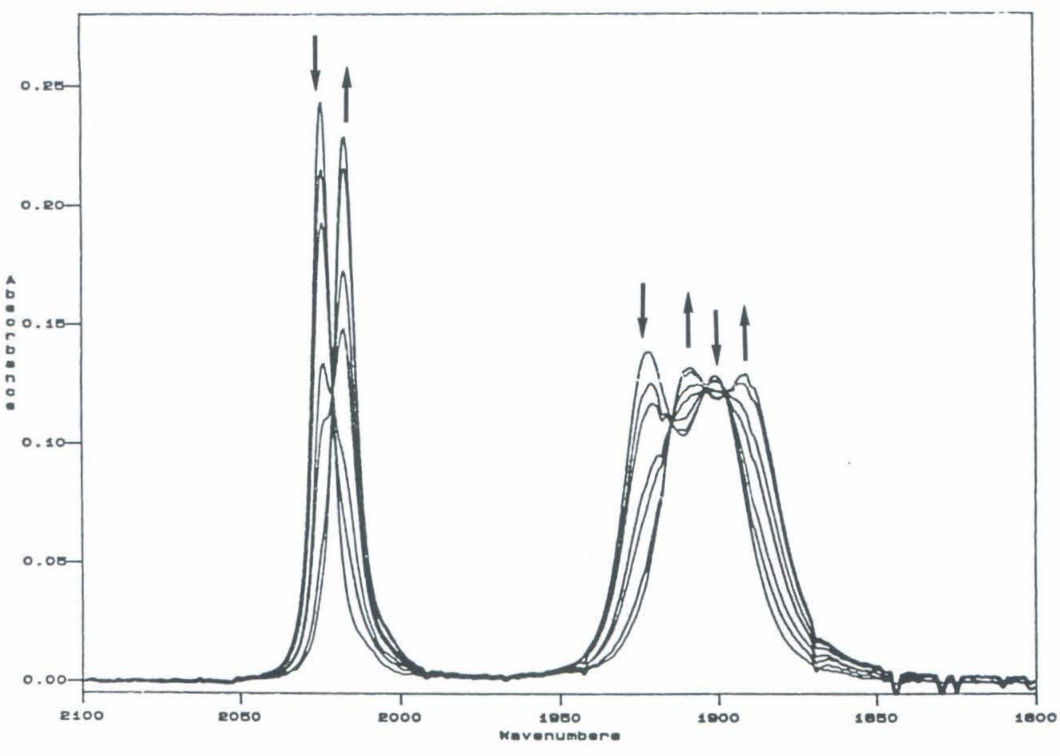
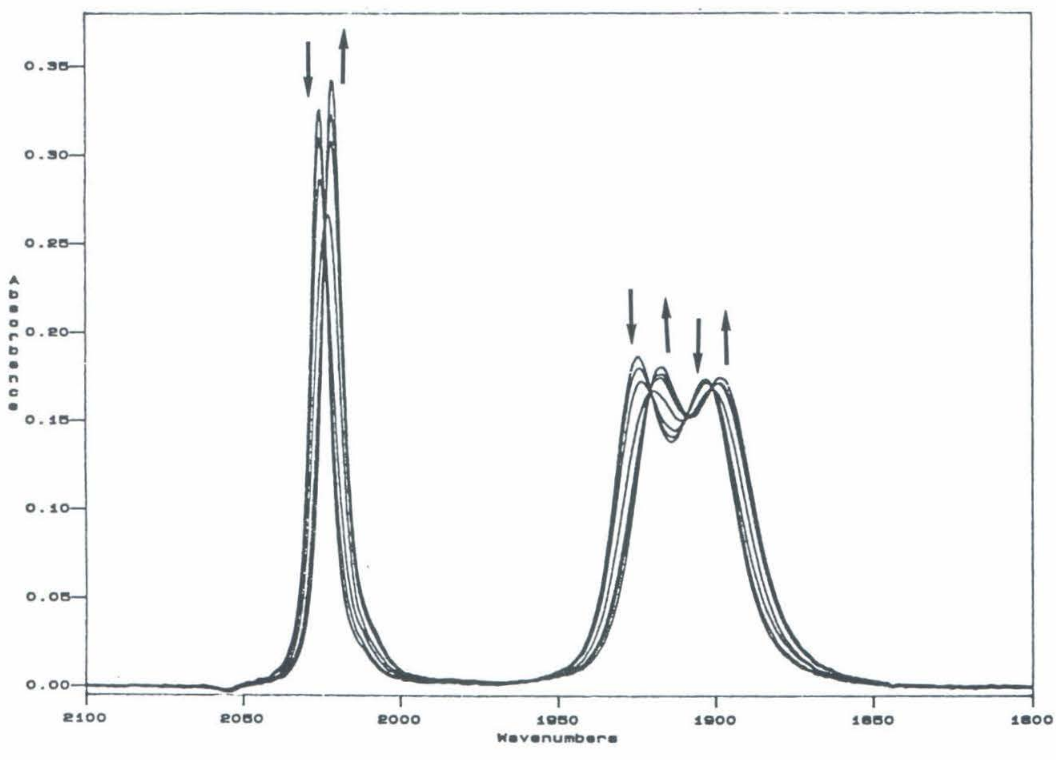

0.25
0.20
0.15
0.10
0.05
0.00
Absorbance
2100
2050
2000
1950
1900
1850
1800
Wavenumbers

Figure 2.45. IR spectroelectrochemical reduction of $Re(CO)_3$(bdppzd)Cl in 0.1 M TBAH/ CH_2Cl_2.


0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Absorbance
2100
2050
2000
1950
1900
1850
1800
Wavenumbers

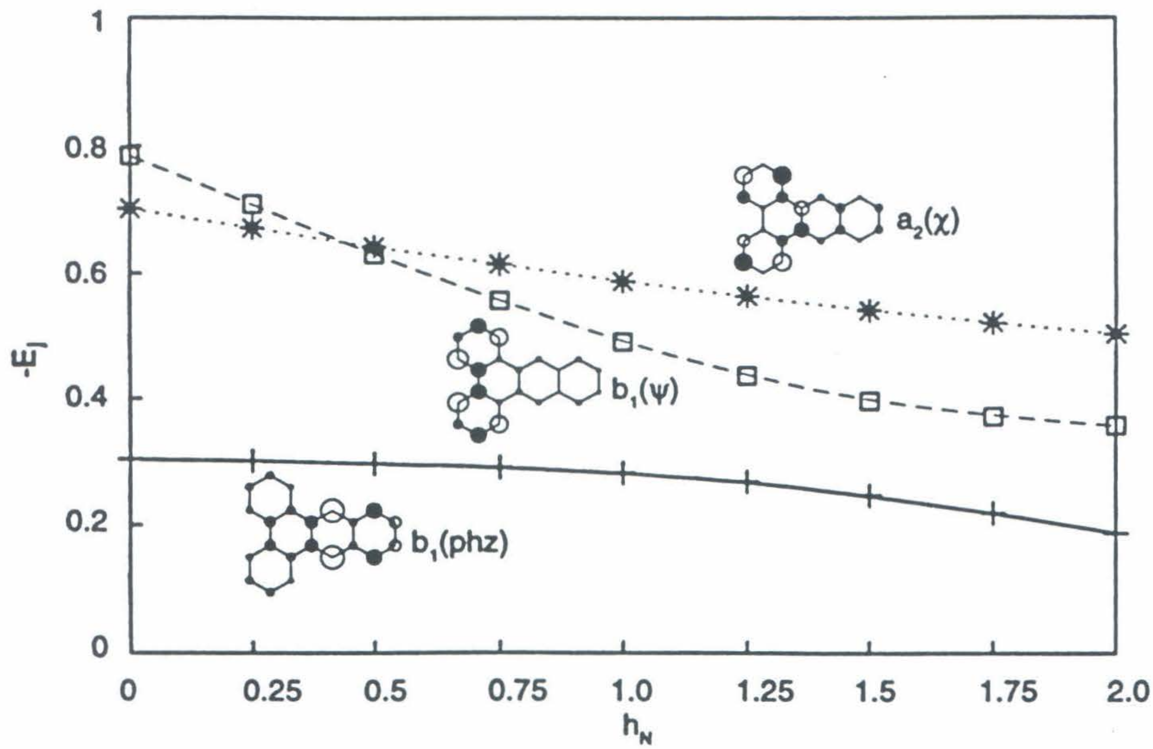
The results are surprising for two reasons: first, if the bpz part of bdppz and the pz part of dppz are coupled to the metal center to the same degree, why are the back transfer rates so different? The recombination rate in $Ru(bpy)_2(dppz)^{2+}$ is 3.7 x 10^6 s^{-1} [11], over two orders of magnitude larger than that of $Ru(bpy)_2(bdppz)^{2+}$, even though the back-transfer driving force for $Ru(bpy)_2(dppz)^{2+}$ is 0.3 eV larger, putting it deeper into the inverted region. Secondly, why is no charge-separated transient seen for bdppzd complexes if the quinone part of the ligand is as poorly-coupled to the metal center as pz is in dppz complexes?

A discussion of the second question will be presented later. Turning to the first, a possible answer is offered in an excellent study of the electronic nature of $Ru(bpy)_2(dppz)^{2+}$ by Fees et al.[29] Hückel MO treatment of dppz agrees with the data presented thus far: the ligand has a b_1(pz) LUMO whose electron density is concentrated on the pz part of the ligand; the second-lowest unoccupied $b_1(\psi)$ orbital is essentially bpy in character and is well-coupled to the metal center. The relative energies of these orbitals as a function of the Coulomb integral h_N is reproduced in Figure 2.46. The Coulomb integral is varied to simulate the coordination of a Ru atom.

If the electron resides in theb_1(pz) orbital and charge recombination takes place via the much better-coupled $b_1(\psi)$ orbital, the difference in energy between the two orbitals may be the barrier to back ET. The first bpy-based reductions of $Ru(bpy)_2(dppz)^{2+}$ and $Ru(bpy)_2(bdppz)^{2+}$ are the same; it is reasonable to assume that the energy of the $b_1(\psi)$ orbital is the same in both. The bpz reduction of $Ru(bpy)_2(bdppz)^{2+}$ is 0.2 V more positive than the pz reduction of $Ru(bpy)_2(dppz)^{2+}$. This difference in LUMO energy should give $Ru(bpy)_2(bdppz)^{2+}$ a larger barrier to recombination. The energy scheme is depicted in Figure 2.47.

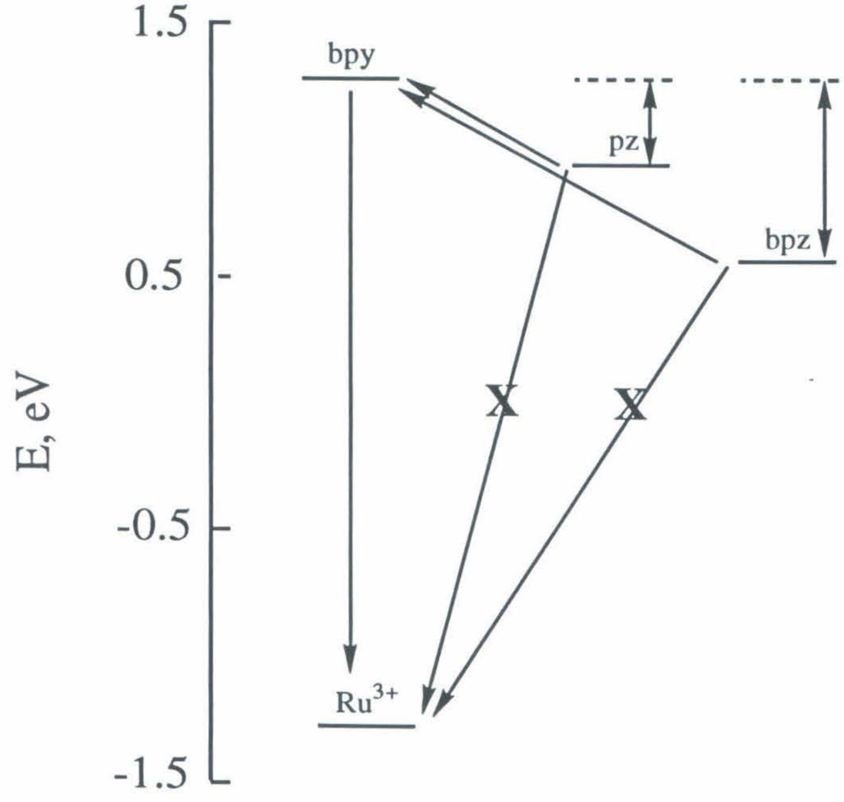
In order to determine if such a barrier is responsible for the marked difference in rates, one can examine $Ru(bpy)_2(11,12\text{-dichloro-dppz})^{2+}$, whose electrochemistry is identical to that of $Ru(bpy)_2(bdppz)^{2+}$ and whose singly-reduced absorption spectrum is

Figure 2.46. The relative energies of the unoccupied orbitals of dppz as a function of the Coulomb integral h_N. Figure reproduced from Reference 29.



1
0.8
0.6
0.4
0.2
0
-E_j
a_2(χ)
b_1(ψ)
b_1(phz)
0
0.25
0.5
0.75
1.0
1.25
1.5
1.75
2.0
h_N

Figure 2.47. Energy scheme showing barrier to recombination in $Ru(bpy)_2(dppz)^{2+}$ and $Ru(bpy)_2(bdppz)^{2+}$. Energies taken from electrochemical measurements.

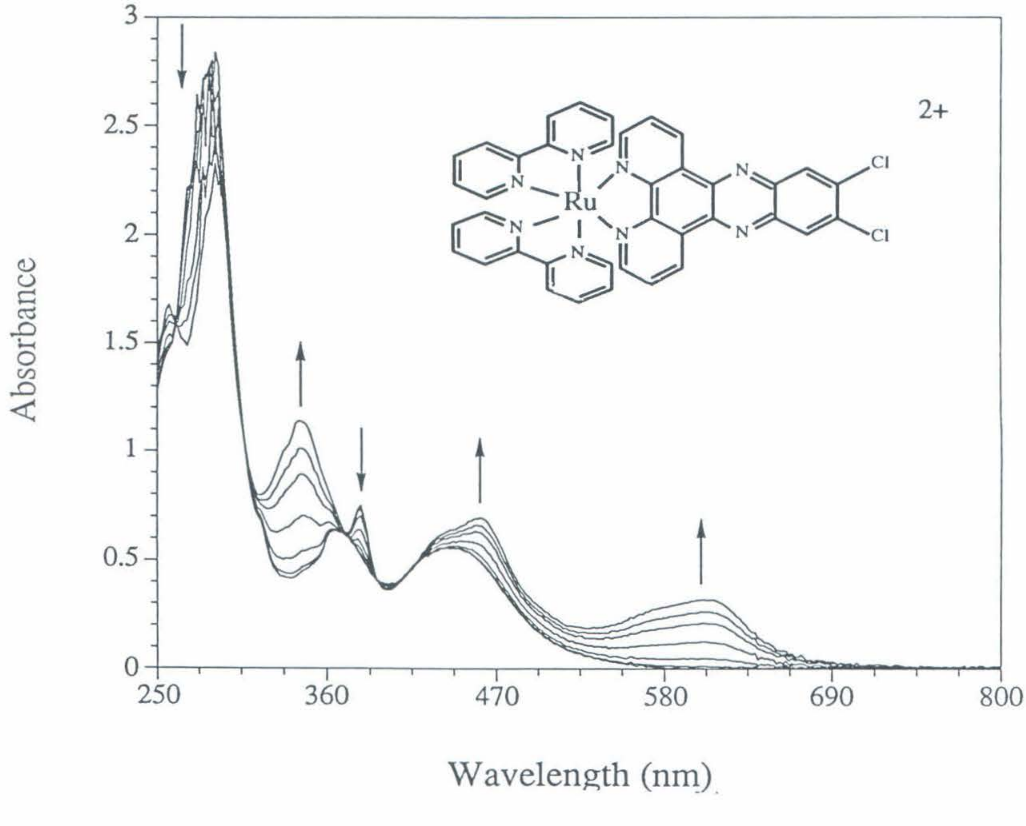

1.5
0.5
-0.5
-1.5
E, eV
bpy
pz
bpz
Ru^{3+}
X
X

the same as $Ru(bpy)_2(dppz)^{+\bullet}$. These data are presented in Figure 2.48. $Ru(bpy)_2$(11,12-dichloro-dppz)$^{2+}$ should have the same Ru-pz coupling as $Ru(bpy)_2(dppz)^{2+}$; substituting ^1H with Cl alters MO energies without affecting overall electron distribution. If operative, its barrier to recombination should be the same as that of $Ru(bpy)_2(bdppz)^{2+}$. $Ru(bpy)_2$(11,12-dichloro-dppz)$^{2+}$ exhibits no long-lived charge separation; thus it appears that no such barrier exists. Back ET takes place through the LUMO.

Close examination of the electron density distribution in the Hückel-calculated LUMOs for dppz and bdppz,[30] shown in Figure 2.49, reveals what is likely the reason for the very long charge-separated lifetimes seen in $Ru(bpy)_2(bdppz)^{2+}$ and $Re(CO)_3$(bdppz)Cl: extending the aromatic system outward pulls electron density away from the bpy portion of bdppz, reducing electronic coupling to the metal center relative to dppz. Squaring the MO coefficient gives the electron density on a specific atom; these data are collected in Tables 2.7 and 2.8, respectively, for dppz and bdppz. Positions 1-12 are the bpy-portion atoms. In dppz, 29.5% of the LUMO electron density lies at these positions. In bdppz, only 2.9% of the total LUMO electron density lies on the bpy portion of the ligand. The bpy part functions essentially as an insulator between the electron localized on the bpz part of the ligand and the metal center, leading to an extraordinarily long charge-separated lifetime. K_{ET} is proportional to the square of the coupling matrix element; if H_{ab} is proportional to the amount of electron density on the bpy portion of the ligand, the 10-fold difference in electron density translates well to the 100-fold difference seen in the charge recombination rates of $Ru(bpy)_2(bdppz)^{2+}$ and $Ru(bpy)_2(dppz)^{2+}$.

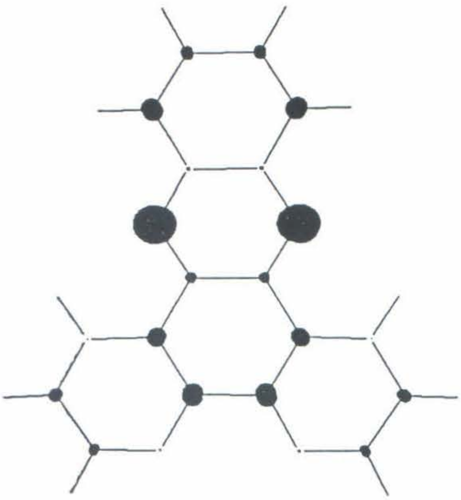
MO calculations also show why no long-lived transient is formed in bdppzd complexes. The Hückel-calculated LUMO for bdppz has appreciable electron density very close to the metal center at positions 13 and 28 in addition to the density on the bpy atoms. This leads to metal-quinone coupling large enough to prevent trapping of an electron by the quinone.

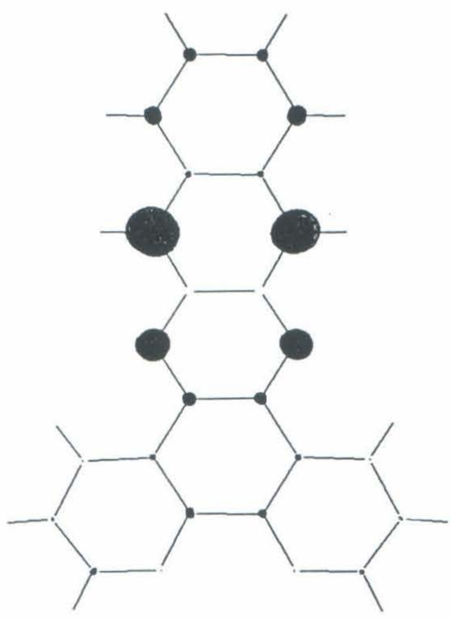
Figure 2.48. UV-visible spectroelectrochemical reduction of $Ru(bpy)_2$(11,12-dichloro-dppz)$^{2+}$ in 0.1 M TBAH/ acetonitrile, top. Electrochemical data for relevant complexes, bottom.



Complex	$Ru^{3+/2+}$	$Ru^{2+/+}$	$Ru^{+/0}$
$Ru(bpy)_2(dppz)^{2+}$	+1.35	-0.95	-1.35
$Ru(bpy)_2(bdppz)^{2+}$	+1.35	-0.73	-1.39
$Ru(bpy)_2(Cl_2\text{-}dppz)^{2+}$	+1.35	-0.77	-1.37

Figure 2.49. Hückel-calculated LUMOs of (top to bottom) dppz, bdppz and bdppzd.





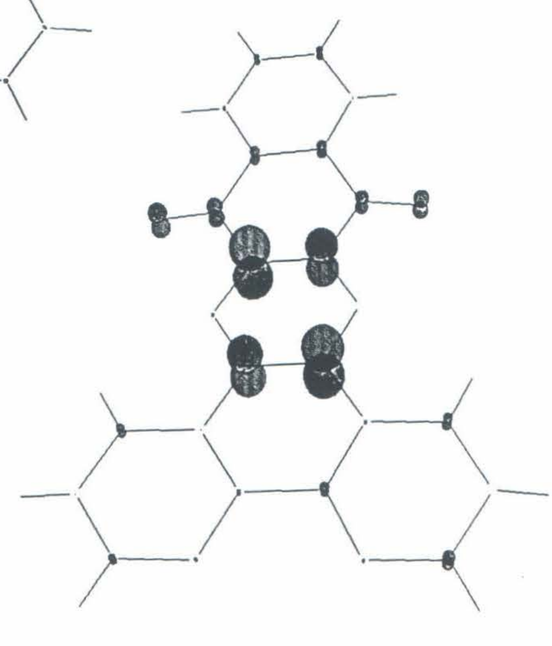


Table 2.7. MO coefficients, electron densities, and electron density distribution for dppz.

Table 2.7. MO calculations for dppz.

Atom	Orbital Coefficient x10^{-2}	Electron Density x10^{-3}	Percentage of Total
1	-6.076	3.692	4.964
2	0.237	0.00563	0.008
3	3.921	1.538	2.067
4	3.192	1.019	1.370
5	-0.646	0.0417	0.056
6	6.853	4.670	6.314
7	6.830	4.665	6.271
8	-0.636	0.0404	0.054
9	-3.218	1.036	1.392
10	3.904	1.524	2.049
11	0.247	0.00608	0.008
12	-6.089	3.707	4.934
13	-3.516	1.236	1.662
14	13.69	18.74	25.19
15	-1.120	0.125	0.169
16	-6.709	4.501	6.051
17	3.966	1.572	2.114
18	4.034	1.627	2.187
19	-6.702	4.491	6.038
20	-1.160	0.134	0.181
21	13.70	18.78	25.24
22	-3.478	1.201	1.626

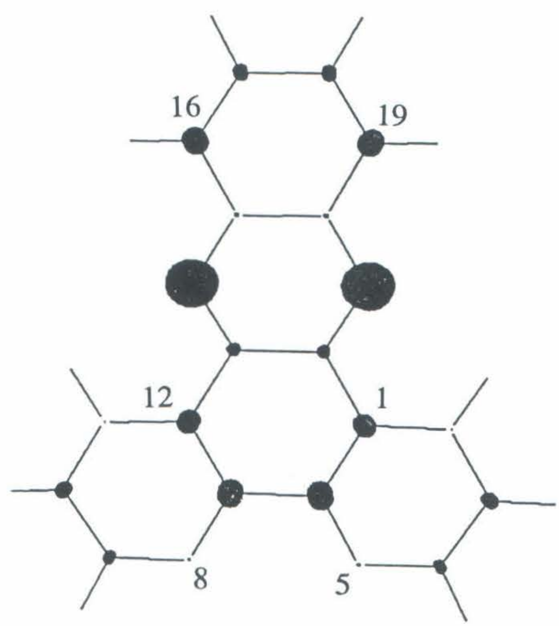
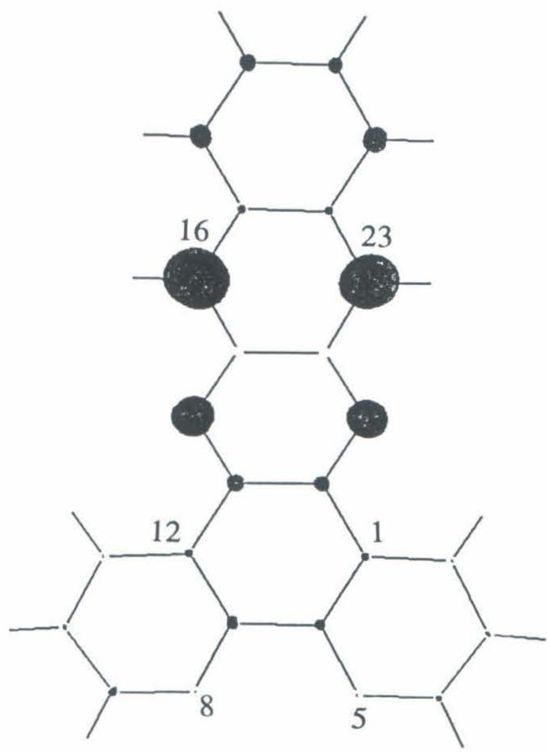


Table 2.8. MO coefficients, electron densities, and electron density distribution for bdppz.

Table 2.8. MO Calculations for bdppz.

Atom	Orbital Coefficient x10^{-2}	Electron Density x10^{-3}	Percentage of Total
1	1.782	0.317	0.359
2	-0.306	0.0093	0.106
3	-1.018	0.104	0.117
4	1.117	0.125	0.141
5	0.218	0.0048	0.005
6	-2.216	0.491	0.556
7	-2.757	0.760	0.861
8	0.159	0.0025	0.003
9	1.610	0.259	0.294
10	-1.038	0.108	0.122
11	-0.524	0.027	0.031
12	1.951	0.381	0.431
13	4.556	2.076	2.351
14	-1.035	10.89	12.33
15	0.0006	0	0
16	16.53	27.32	30.93
17	-1.802	0.325	0.368
18	-5.464	2.986	3.381
19	3.716	1.381	1.563
20	3.379	1.412	1.292
21	-5.672	3.217	3.642
22	-1.746	0.305	0.345
23	14.93	22.30	25.25
24	0.0015	0	0
25	-1.112	12.37	14.00
26	3.780	1.429	1.618



The intensity of the visible absorbance band arising from the metal→LUMO transition is a direct measure of the coupling between the metal and the LUMO; in dppz, bdppz, and bdppzd, this transition should be approximately 70 nm to the red of the MLCT maximum based on the measured potentials for the first and second reductions of the metal complexes. There is still considerable MLCT absorption at this wavelength. Work has shown that the extinction coefficient of the metal→LUMO band depends on the LUMO coefficients for the coordinating nitrogens of the diimine ligand.[31] The coefficients are all so small for all three ligands that the transition is very weak and is not seen above the MLCT. If it were possible to see this band, it is likely that its extinction coefficient would be the same for complexes of all three ligands since its intensity is dependent only on the amount of electron density at the coordinating nitrogens, very small for dppz, bdppz, and bdppzd. If not merely because it is more qualitative than quantitative, this may be the reason why IR spectroelectrochemistry gives the same result for the their Re complexes. If seen, the metal→LUMO band would not show how the electron density is distributed beyond the chelating nitrogens, providing no indication of what charge-recombination kinetics could be expected.

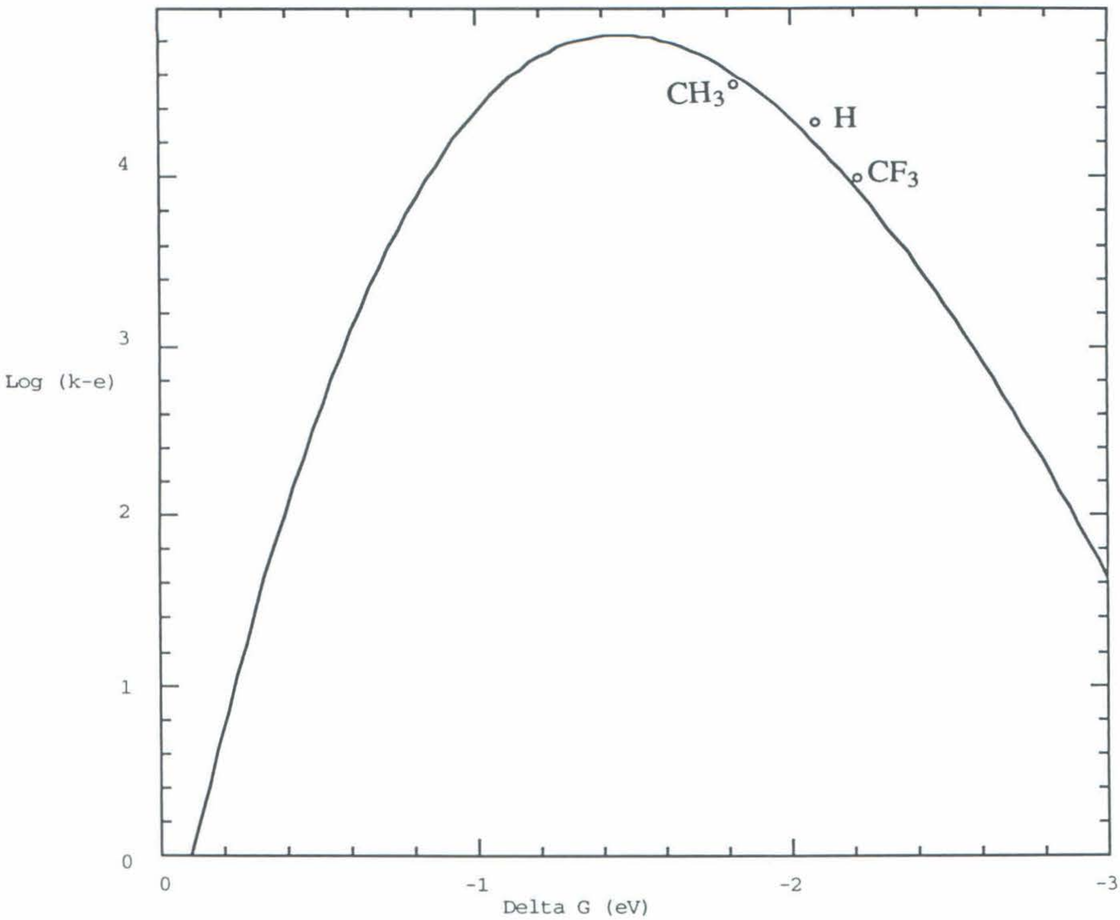
Weak donor-acceptor coupling and inverted behavior likely combine to produce the long-lived charge-shifted states seen in Ru and Re complexes of bdppz. Conclusive proof that these factors work in tandem requires that a series of compounds of varying driving force be studied. From the rate versus driving force data, one can then construct a Marcus plot. It will be obvious from inspection if rates lie in the inverted region; H_{ab} and λ can be extracted from the fit of the Marcus equation to the data. Altering the substituents on the bpy ligands of $Ru(bpy)_2(bdppz)^{2+}$ provides such a series. Substitution with electron-donating methyl groups moves the $Ru^{3+/2+}$ couple to a more negative potential relative to $Ru(bpy)_2(bdppz)^{2+}$, increasing the excited-state driving force for ET and decreasing the driving force for thermal back ET; electron-withdrawing trifluoromethyl groups have the opposite effect. Driving forces for the series of three compounds and a plot of the charge recombination rate versus driving force are given in Figure 2.50. The rates do lie in the inverted region ; the fit yields H_{ab}=0.02 cm^{-1} and λ=1.5 eV. The rate of ET from the Ru MLCT excited state to bpz can also be measured. The transient absorbance trace for formation of the charge-separated state of $Ru(bpy)_2(bdppz)^{2+}$ is shown in 2.51. Even at the low driving force for the forward reaction, a high ET rate is observed. Driving force data and a Marcus fit for forward ET in $Ru(bpy)_2(bdppz)^{2+}$ and $Ru(CH_3\text{-}bpy)_2(bdppz)^{2+}$ are presented in Figure 2.52. The parameters used for the fit are H_{ab}=20 cm^{-1} and λ=1.5 eV.

Marcus curves for the forward and reverse ET reactions are shown together in Figure 2.53. This behavior is remarkable. A four-order-of-magnitude difference exists between the donor-acceptor coupling for the forward and reverse reactions. In effect, bdppz acts as a molecular diode, allowing free electron motion only in the forward photoinduced direction. Excited-state ET takes place through bdppz via an orbital lying above the LUMO which is well-coupled to the metal center. Once on the bpz part of the ligand, the electron falls into the poorly-coupled LUMO and is trapped.

The extremely small donor-acceptor coupling in $Ru(bpy)_2(bdppz)^{2+}$, 0.02 cm^{-1}, has no precedence in a molecule so simple. Model systems with comparable donor-acceptor separations have H_{ab} several orders of magnitude higher, as evidenced by ET rates six orders of magnitude larger than those presented here.[32] In order to find couplings this low, one must look to biological systems. Studies of ruthenium-modified cytochrome *c* yield couplings that are similar,[6] but ET in these systems takes place via pathways containing 14 to 20 sigma bonds. ET in bdppz complexes most likely takes place through the π system of the ligand, so no direct comparison of effective ET pathway length can be made. Obviously, though, much less intervening medium is needed by bdppz to produce a coupling comparable to that in proteins.

This comparison points to the possibility that current models of the distance dependence of ET do not apply to $Ru(bpy)_2(bdppz)^{2+}$. While there has been

Figure 2.50. Driving force data and Marcus plot for charge recombination in $Ru(X_2$-bpy$)_2$(bdppz$)^{2+}$ (X=H, CH_3, CF_3). Curve fit using H_{ab}=0.02 cm^{-1}, λ=1.5 eV.



Recombination Driving Forces for $Ru(X_2\text{-bpy})_2(bdppz)^{2+}$

X	**$Ru^{2+/3+}$**	**$bdpz^{0/-}$**	**$-\Delta G^0$ (eV)**	**k_{ET}**
CH_3	+1.22	-0.60	1.82	3.47×10^4
H	+1.35	-0.73	2.08	2.09×10^4
CF_3	+1.72	-0.49	2.21	9.75×10^3

Figure 2.51. Transient absorbance of formation of the charge-separated state. 355 nm laser excitation.

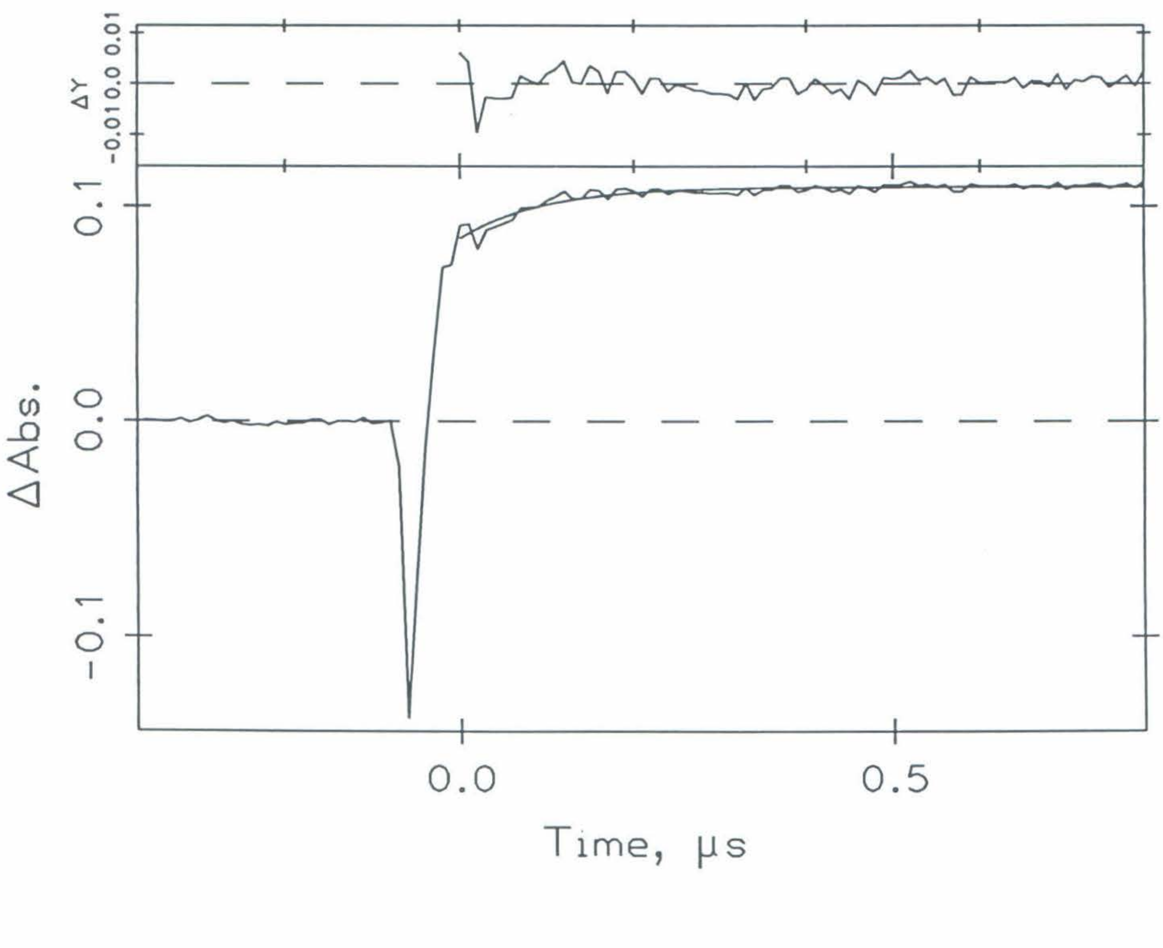
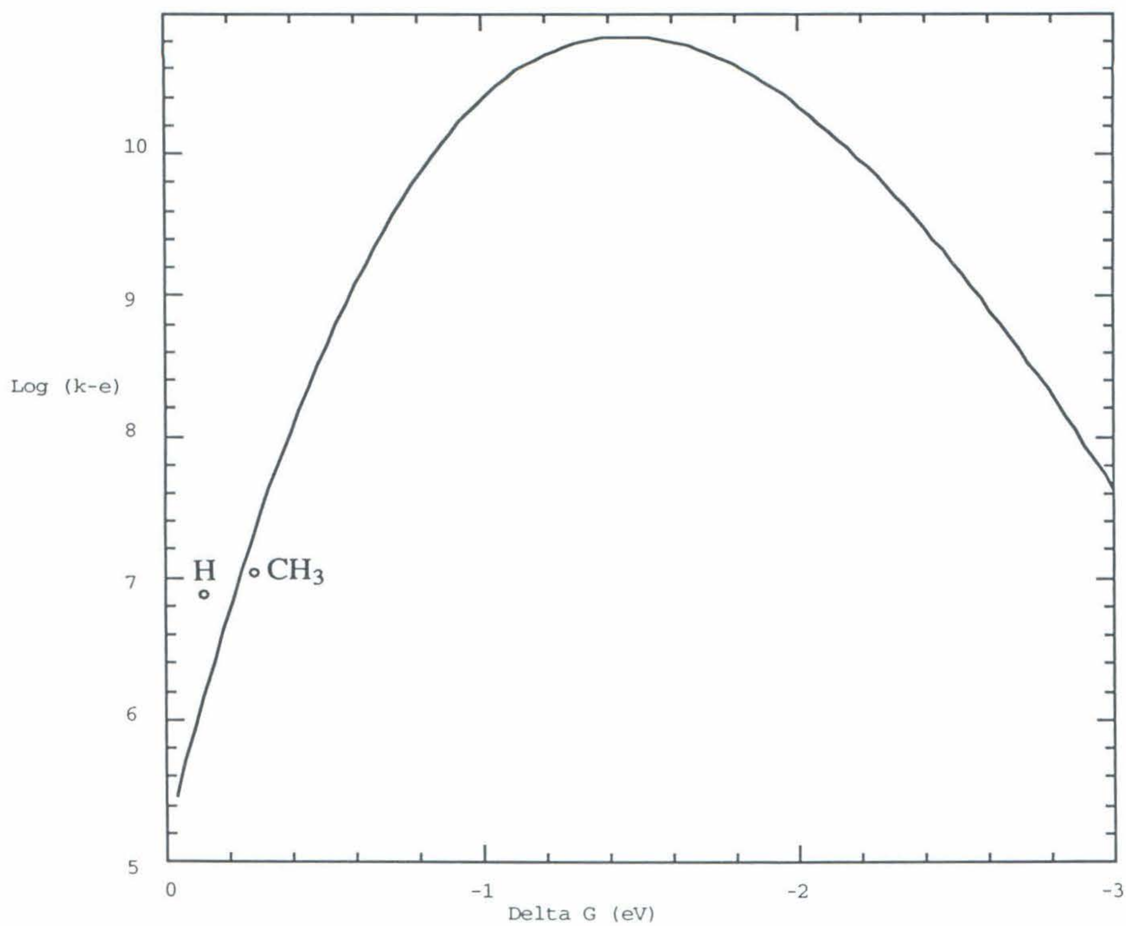

ΔY
-0.010.0 0.01
ΔAbs.
0.1
0.0
-0.1
0.0
0.5
Time, μs

Figure 2.52. Driving force data and Marcus plot for charge separation in $Ru(X_2$-bpy$)_2$(bdppz$)^{2+}$ (X=H, CH_3). Curve fit using H_{ab}=20 cm^{-1}, λ=1.5 eV.

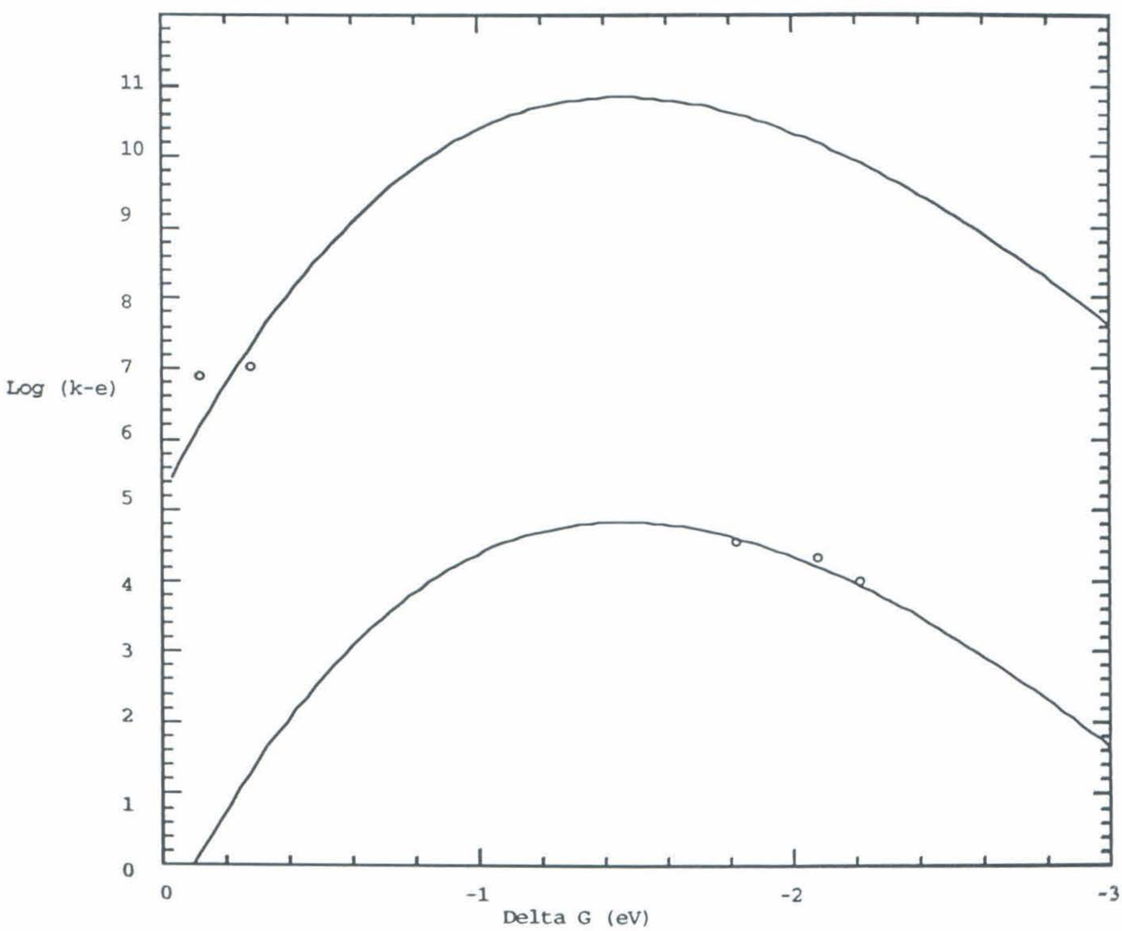


Forward Driving Forces for $Ru(X_2\text{-bpy})_2(bdppz)^{2+}$

X	$Ru^{3+/2+}$	$Ru^{3+/2+*}$	$bdpz^{0/-}$	$-\Delta G^0$ (eV)	k_{ET}
CH_3	+1.22	-0.98	-0.60	0.38	1.08×10^7
H	+1.35	-0.85	-0.73	0.12	7.56×10^6

$E^0(Ru^{3+/2+*}) = E^0(Ru^{3+/2+}) - E_{0\text{-}0}$. $E_{0\text{-}0} = 2.2$ eV (565 nm).

Figure 2.53. Marcus curves for charge separation (top) and charge recombination in $Ru(X_2\text{-bpy})_2(bdppz)^{2+}$ (X=H, CH_3, CF_3).


11
10
9
8
7
Log (k-e)
6
5
4
3
2
1
0
0
-1
-2
-3
Delta G (eV)

disagreement on how to measure donor-acceptor distance,[32] it is agreed that H_{ab} drops off exponentially with distance. This arises from the fact that the overlap between electronic wavefunctions across the space separating donor and acceptor falls off exponentially with the distance separating the ET pair. It is assumed that electron density is distributed uniformly among all of the wavefunctions; in bdppz, there is no such homogenous distribution, so the overlap between adjacent wavefunctions can vary, leading to an overall coupling that is not distance-dependent. Any calculation of donor-acceptor coupling will have to take this unequal density distribution into account.

It was stated earlier that no direct Ru→bpz transition was seen in $Ru(bpy)_2(bdppz)^{2+}$ because the transition was likely weak due to the nearly-total lack of electron density on the coordinating nitrogens of bdppz; such a weak transition would be obscured by the nearby, intense MLCT transition. Taking the experimentally-determined H_{ab} of 0.02 cm^{-1}, the extinction coefficient of the Ru→bpz transition can be estimated using Hush theory.[33] The relationship between band intensity and H_{ab} is given in equation 2.

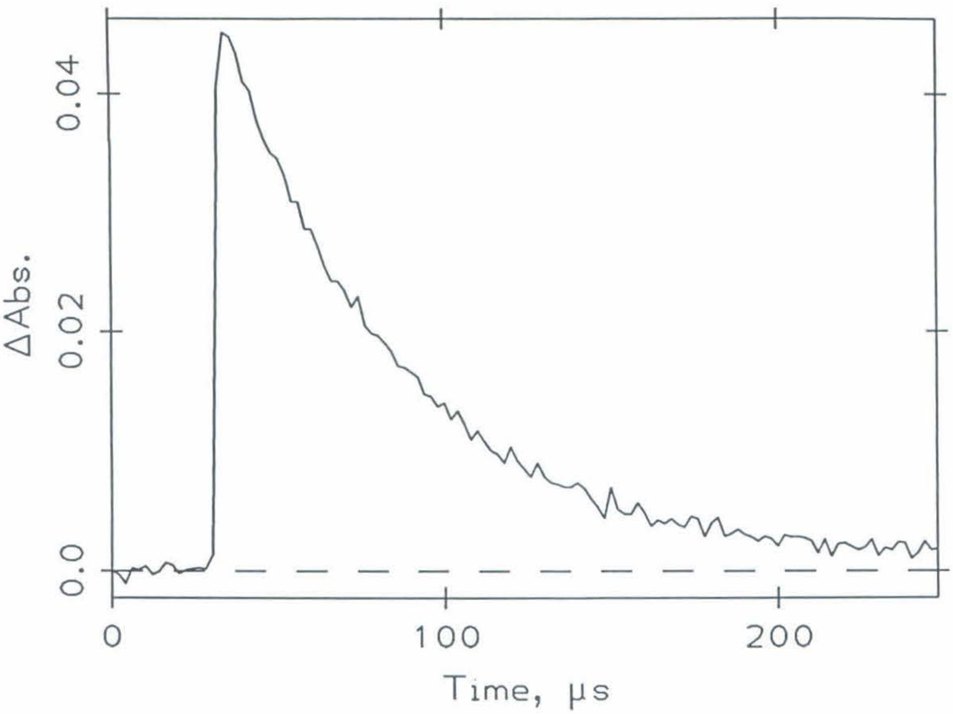
$$\varepsilon = \left(\frac{r\,H_{ab}}{2.05 \times 10^{-2}\,\nu}\right)^2 \times \frac{\nu}{\nu_{1/2}} \qquad 2$$

R is the donor-acceptor separation, taken to be 9Å; $\nu_{1/2}$ is the half-height width of the absorbance band whose maximum is at energy ν. Assuming respective values of 3300 and 18000 cm^{-1} (100 and 550 nm), the calculated extinction coefficient is 1.3×10^{-6} $\underline{M}^{-1}$ cm^{-1}. The only way to measure ground-state Ru-bpz coupling is by extracting the parameter from a Marcus curve.

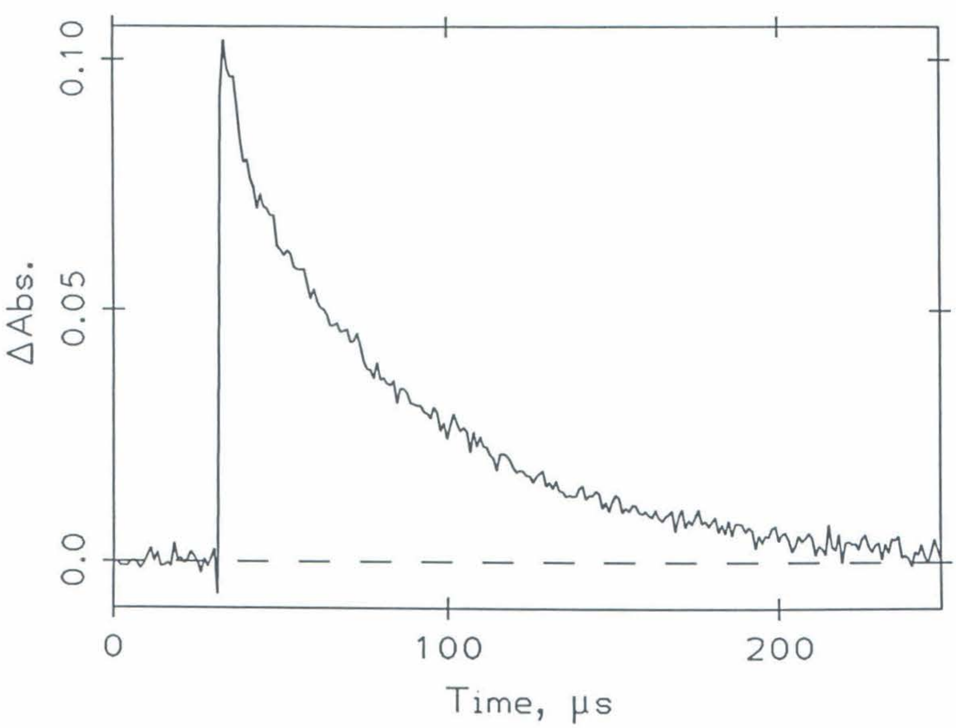
One wants to store photon energy as efficiently as possible. Since emission is observed from $Ru(bpy)_2(bdppz)^{2+}$, photon energy that could be producing charge separation is being wasted. For this reason, the $Ru(bpy)_{3-x}(bdppz)_x{}^{2+}$ series of compounds was synthesized. It was hoped that having more bpz units surrounding the metal center would lead to a higher probability of charge separation. As shown in Figure

2.27, emission quantum yield decreases with increasing x. This suggests that the loss of emission intensity may be due to increased quenching of the excited state by ET. Transient absorbance traces are shown for iso absorptive solutions of $Ru(bpy)_2(bdppz)^{2+}$ and $Ru(bdppz)_3{}^{2+}$ in Figure 2.54. A larger initial increase in optical density is seen in $Ru(bdppz)_3{}^{2+}$, showing that the loss of emission is indicative of increased formation of the charge-separated state.

Figure 2.54. Transient absorbance traces for $Ru(bpy)_2(bdppz)^{2+}$ (top) and $Ru(bdppz)_3{}^{2+}$. 355 nm laser excitation.



0.04
0.02
0.0
ΔAbs.
0
100
200
Time, μs



0.10
0.05
0.0
ΔAbs.
0
100
200
Time, μs

Conclusion

A combination of inverted behavior and weak donor-acceptor coupling serve to produce the extremely long-lived charge separation seen in Ru and Re complexes of bdppz. Donor-acceptor coupling for forward photoinduced ET is four orders of magnitude higher than it is for recombination, allowing rapid intramolecular ET from the MLCT excited state to the bpz portion of the ligand. Once on bpz, the electron is trapped by the near-total lack of electron density between it and the metal center.

Long-lived charge separation is achieved in these systems differently than in the photosynthetic reaction center. In biological systems, a low reorganization gives a narrow Marcus curve which falls precipitously in the inverted region, leading to slow recombination at relatively low driving force. Taking advantage of a small λ is not possible in a system which operates in fluid solution; extensive solvent reorganization leads to λ in excess of 1 eV. With this reorganization energy, the ET does not drop off as quickly in the inverted region. While this does allow charge recombination that is slowed relative to forward ET, it is difficult to achieve the differential present in the reaction center when donor-acceptor coupling is the same for forward and reverse ET. Differential ground- and excited-state donor-acceptor coupling has not been exploited in previous work in model systems; the use of ligands with electronic properties like those of bdppz may bring the ET performance of artificial systems closer to that of organisms.

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Chapter 3

Energy and Electron Transfer in Bimetallic Tetrapyridophenazine Complexes

Introduction

ET between metal atoms is essential for life. Photosynthesis in plants and respiration in animals both use metalloproteins to couple the transport of electrons to physiological processes. Inorganic photochemistry has played a major role in elucidating the means by which this transport takes place. Surface modification of metalloproteins with chromophores which posses excited-state redox properties allows direct probing of the ET-mediating properties of the intervening peptide medium.[1] Just as metal chromophore/ organic quencher model systems like that discussed in Chapter 2 give greater insight into the operation of the metalloporphyrin chromophore/ quinone quencher photosynthetic reaction center, so too can synthetic metal chromophore/ metal acceptor systems be used for models of biological metal-to-metal ET. Model systems may also have practical use as molecular electronic devices.[2]

The primary question to be addressed in studies of metal-to-metal ET is the nature of H_{ab}, the donor-acceptor coupling matrix element in the Marcus equation. Opinions differ on the relationship between H_{ab} and the structure of the medium separating donor and acceptor. One school of thought holds that organic material acts as an average medium, k_{ET} exhibiting a simple exponential relationship to the distance between donor and acceptor regardless of the chemical identity of the spacer that separates them.[3] Another theory posits that k_{ET} has a complex distance dependence in proteins. At the same donor-acceptor separation, a wide variation in k_{ET} is seen between different proteins or between different sites of modification in the same protein; this is explained by ET through specific pathways in the protein.[4] The complexity of the systems used in these studies makes distinguishing between the two opposing viewpoints difficult; distances can be measured in many different ways, many possible pathways exist. Understanding ET in simpler systems will aid in understanding those more complex.

What is needed is a system in which two metal atoms can be held at a known distance. It must be possible to modulate this distance, and thus H_{ab}, by incrementally varying the length of the spacer separating the two metals. It must also be possible to measure the electronic coupling which allows ET between the two metals. A number of systems have been devised which possess these properties.[5] Condensation of phendione with polyamines allows the synthesis of a series of binucleating ligands whose metal complexes meet these criteria. The ligands, tetrapyrido[3,2-*a*:2',3'-*c*:3",2"-*f*:2"',3"'-*h*] phenazine (tppz); 5,7,12,14-tetraaza-tetrapyrido[3,2-*a*:2',3'-*c*:3",2"-*h*:2"',3"'-*j*]pentacence (tatpp); and tetrapyrido[3,2-*d*:2',3'-*f*:3",2"-*d'*:2"',3"'-*f'*]biphenazine (tpbpz); are shown in Figure 3.1. Coordination of two metal centers gives homo- or heterobimetallic complexes in which H_{ab} can be measured in a variety of ways.

The prototype for studying coupling between coordinated metals is the Creutz-Taube ion, shown in Figure 3.2.[6] The molecule is most stable as a +6 ion. If the metals do not interact with each other, one observes a single two-electron wave in a cyclic voltammagram as both metals are simultaneously reduced. Such an ion acts as two independent Ru^{3+} centers. If the metals do interact, electron density is delocalized and the molecule acts as one +6 entity. Separate one-electron reduction waves are observed as the ion is reduced first to a +5 then a +4 state. Electrochemical behavior for systems without and with metal-metal interaction is shown in Figure 3.3.

While no direct relationship exists, the difference between the potentials of these successive reductions is an indication of the degree of coupling between the two metals. Even when the difference between the $E_{1/2}$ values for the successive reductions is small, appreciable interaction exists; a sensitive method for measuring $\Delta E_{1/2}$ is needed. For large $\Delta E_{1/2}$, where two discernible reduction waves are present, conventional cyclic voltammetry suffices. When $\Delta E_{1/2}$ is small (<120 mV), however, no peak separation is seen and a single distorted reduction wave is seen, making accurate measurement difficult. Differential-pulse voltammetry has been shown to be a very sensitive technique for determining $\Delta E_{1/2}$, allowing resolution of $\Delta E_{1/2}$ as small as 70 mV. Current-potential curves for a range of $\Delta E_{1/2}$ are shown in Figure 3.4.[7]

Figure 3.1. (Top to bottom): Tetrapyrido[3,2-*a*:2',3'-*c*:3",2"-*f*:2"',3"'-*h*] phenazine (tppz); 5,7,12,14-tetraaza-tetrapyrido[3,2-*a*:2',3'-*c*:3",2"-*h*:2"',3"'-*j*]pentacence (tatpp); and Tetrapyrido[3,2-*d*:2',3'-*f*:3",2"-*d'*:2"',3"'-*f*]biphenazine (tpbpz).

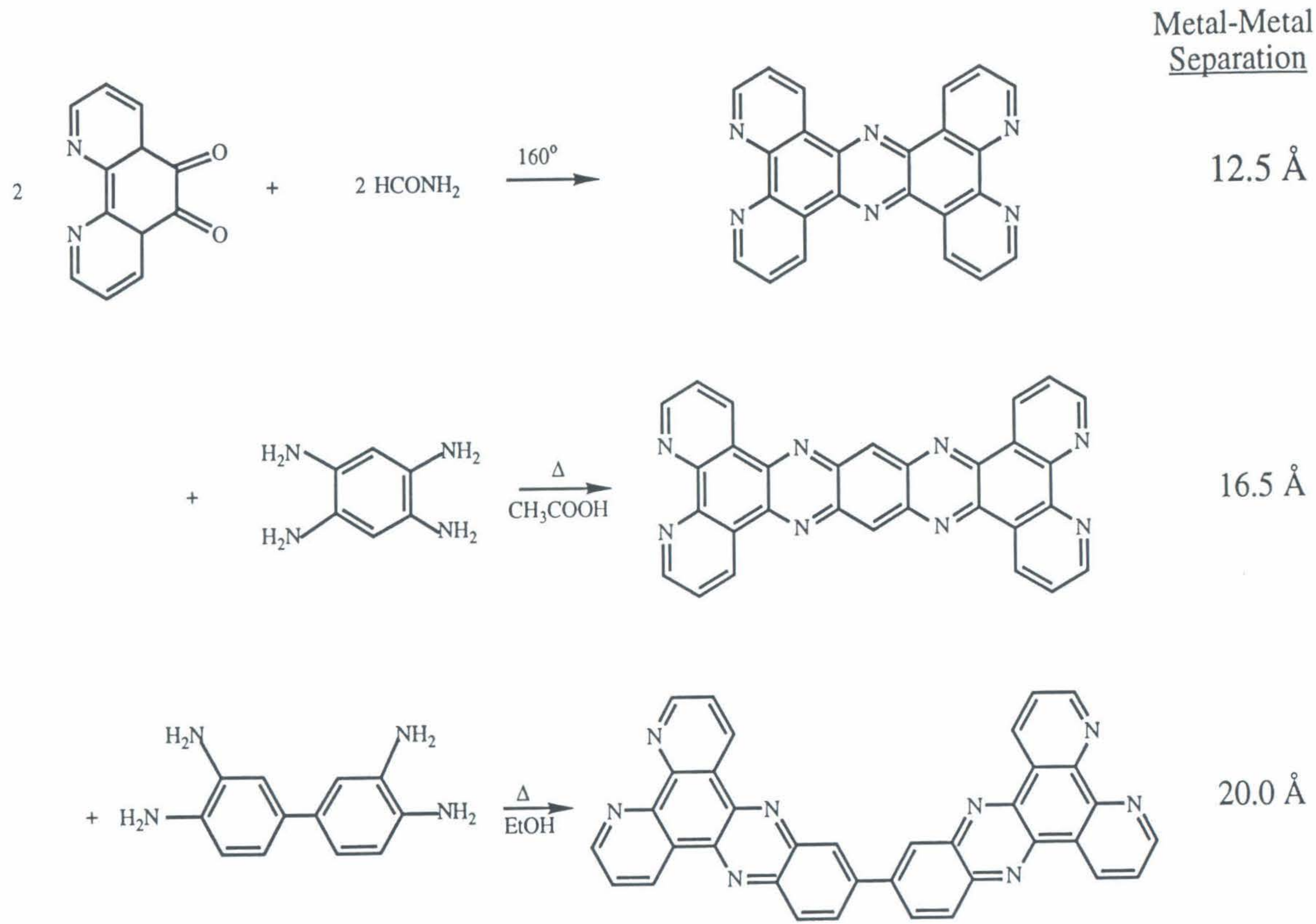

Metal-Metal
Separation
12.5 Å
16.5 Å
20.0 Å
2
2 HCONH2
160°
Δ
CH3COOH
Δ
EtOH
H2N
NH2
O
N

Figure 3.2. The Creutz-Taube ion, bis(Ruthenium pentamine)pyrazine.

6+

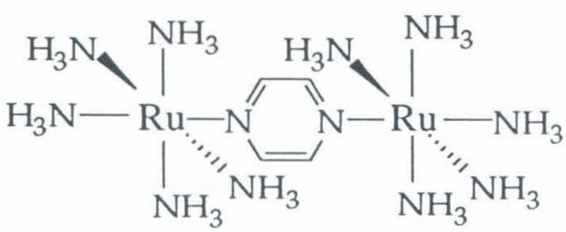
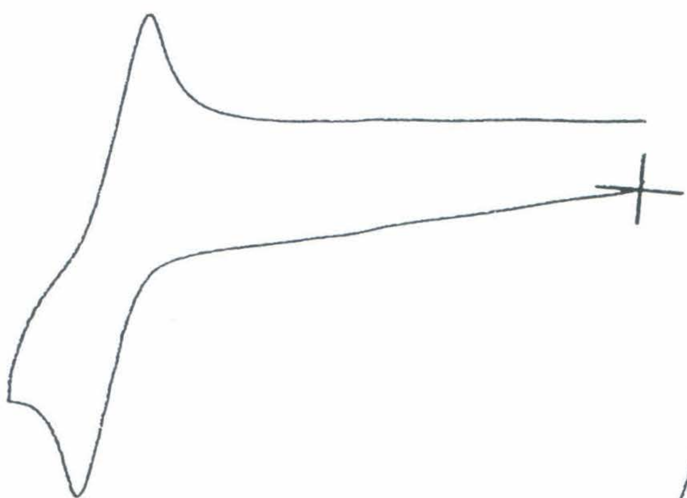


Figure 3.3. Cyclic voltammagrams of noninteracting (left) and interacting homobimetallic complexes.



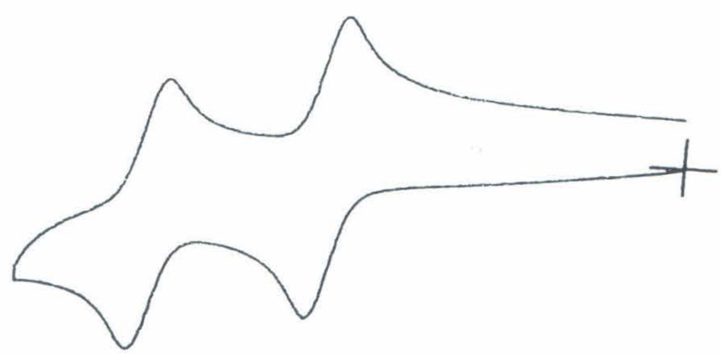
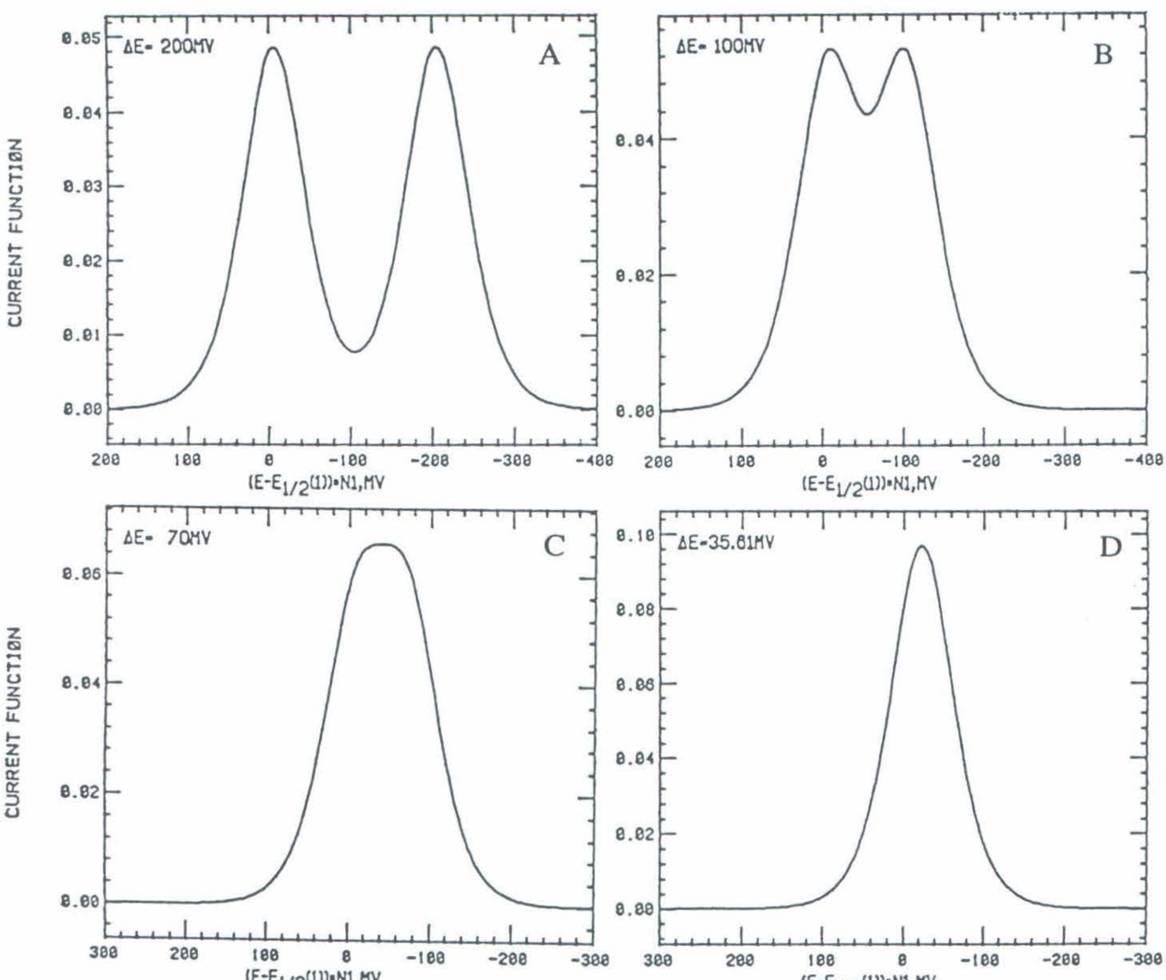


Figure 3.4. Differential pulse voltammagrams for varying $\Delta E_{1/2}$. The $\Delta E_{1/2}$ values are (A) 200, (B) 100, (C) 70, and (D) 35.61 mV. Figure reproduced from Reference 7.



ΔE= 200MV
A
ΔE= 100MV
B
ΔE= 70MV
C
ΔE=35.61MV
D
CURRENT FUNCTION
CURRENT FUNCTION
(E-E1/2(1))•N1,MV
(E-E1/2(1))•N1,MV
(E-E1/2(1))•N1,MV
(E-E1/2(1))•N1,MV

Electrochemistry can be used to determine if two metals in a homobimetallic system interact; it can also be used to produce a mixed-valence species in which the magnitude of coupling can be directly measured. When a molecule is selectively oxidized or reduced at one of the coupled metal centers, the optical transition corresponding to the transfer of an electron from one metal to the other can be observed. Since this is a low-energy transition- the energy required to move the electron is $\Delta E_{1/2}$- the absorption band for the transition is often observed in the near IR. The properties of this band are related to H_{ab} through Equation 1, formulated by Hush,[8] where ε is the

$$H_{ab} = 2.05 \times 10^{-2} \left(\frac{\varepsilon \Delta \nu_{1/2}}{\nu}\right)^{1/2} \frac{\nu}{r} \qquad 1$$

extinction coefficient of the band of energy ν whose bandwidth at half-intensity is $\Delta\nu_{1/2}$ and r is the metal-metal separation in Å. The intervalence charge-transfer band in a well-coupled system is shown in Figure 3.5.[9] Application of the Hush equation to the compound, a Ruthenium dimer based on tetrapyridylbiphenyl, yields H_{ab}= 1200 cm^{-1}.

Magnetochemistry can also be used to characterize metal-metal interactions. In a compound with two coordinated paramagnetic metal atoms, the magnitude of the exchange interaction, J, can be determined by measuring the magnetic susceptibility, χ, of the compound as a function of temperature and applying the Bleaney-Bowers equation.[10] The effect of increasing exchange interaction in a binuclear molecule with two unpaired spins is shown in Figure 3.6.[11] J is related to H_{ab} by Equation 2.[12]

$$2J = -(2H_{ab})^2/J_{aa}-J_{ab} \qquad 2.$$

J_{aa}-J_{ab} is the difference in energy between the ground state in which the unpaired electrons are on separate atoms and the excited state in which both electrons are on one metal atom; the quantity is readily obtained from photoelectron spectra. Magnetochemistry has been used to study Ru^{3+}/Ru^{3+} molecules related to the Creutz-Taube ion; metal-metal coupling measured in the Ru^{3+}/Ru^{3+} form by magnetic

Figure 3.5. Near-IR spectrum of a compound exhibiting a mixed-valence intervalence charge-transfer band. Figure reproduced from Reference 9.

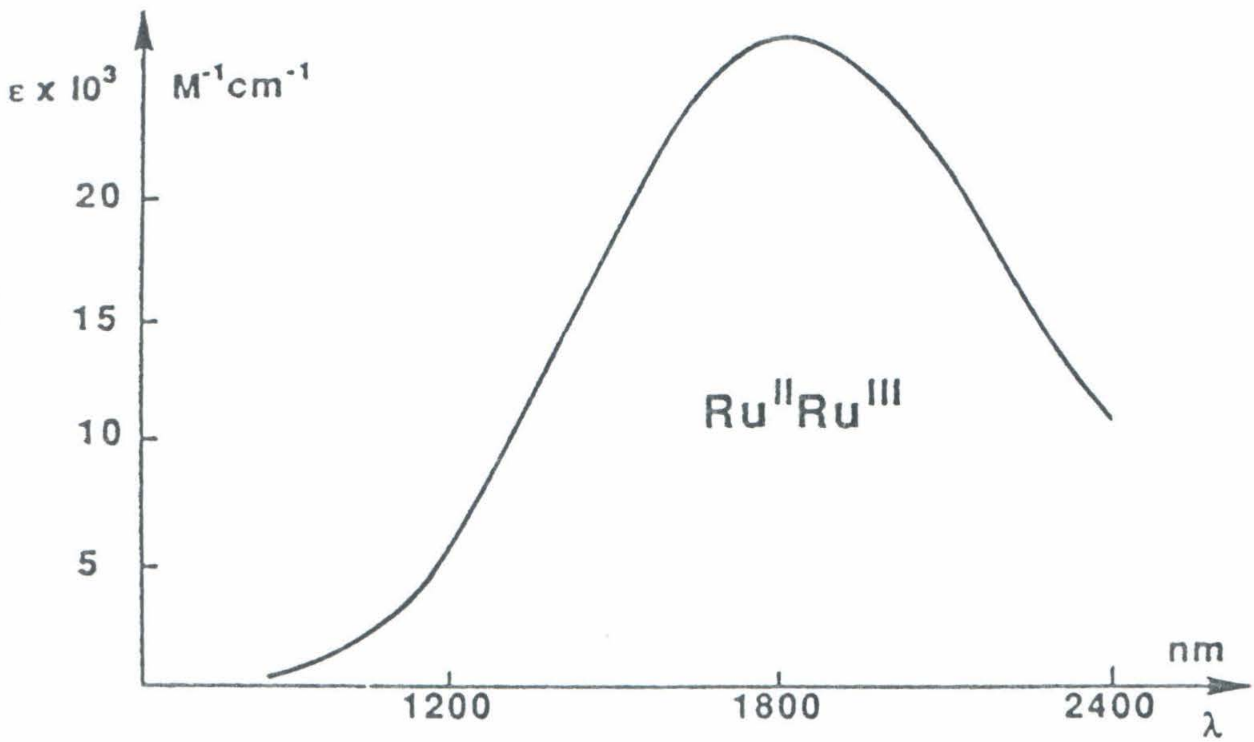
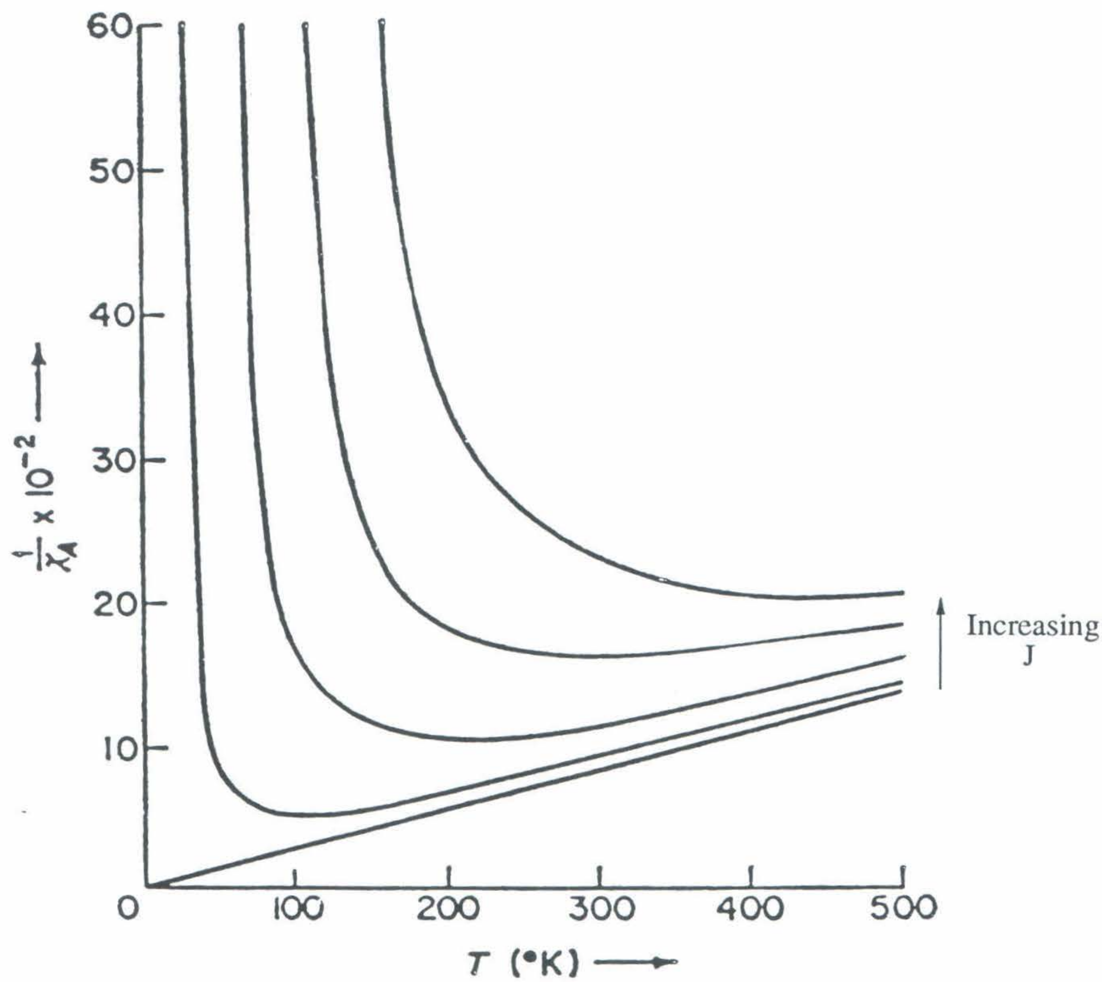

ε x 10^3 M^-1cm^-1
20
15
10
5
Ru^II Ru^III
nm
1200
1800
2400
λ

Figure 3.6. Variation of susceptibility with temperature for increasing exchange interaction, J. Figure reproduced from Reference 11.


60
50
40
30
20
10
0
100
200
300
400
500
T (°K)
Increasing
J

susceptibility agrees with H_{ab} measured from the intervalence charge transfer band of the mixed-valence Ru^{3+}/Ru^{2+} state.[11]

As shown in Chapter 2, ground- and excited-state donor acceptor coupling can be measured using time-resolved spectroscopy on a series of compounds with different thermodynamic driving forces. The use of transition metals in high oxidation states as electron acceptors allows very large driving forces for forward photoinduced ET to be generated compared to those possible with organic acceptors. Unlike organic acceptors, one can say with certainty where the transferred electron resides; it resides in a d orbital on the metal acceptor. The well-defined spectra of the different oxidation states of metal complexes makes assignment of transient spectra possible.

The use of transition metal complexes also allows the study of energy transfer, possible only when the emission spectrum of the energy donor overlaps with the absorption spectrum of the energy acceptor. Since most organic acceptors do not absorb at the low energies at which complexes such as $Ru(bpy)_3^{2+}$ emit, energy transfer is most often studied between metals. Exploring energy transfer over the range of distances provided by the tetrapyridophenazine ligands presented earlier allows the assignment of the operative transfer mechanism. If energy transfer takes place via a dipole-dipole interaction between the excited state of the energy donor and the ground state of the acceptor, i.e., the Förster mechanism,[13] the rate of energy transfer will have an inverse sixth-power dependence on the donor-acceptor distance. The Dexter electron-exchange mechanism, like Marcus theory, predicts an energy transfer rate that is proportional to the electronic coupling between donor and acceptor.[14] In its simplest formulation, the coupling drops off exponentially with distance; the energy transfer rate should do the same.

If energy transfer occurs via the Dexter mechanism, it brings to four the number of independent ways which metal-metal coupling can be measured in a bimetallic system. Surprisingly, no one appears to have employed more than two of these techniques to any one compound, and no one has compared the coupling matrix element backed out of a Marcus fit to one measured by other means. Given the intense interest in the way on which H_{ab} is dependent on the medium separating donor and acceptor, one would like to gain as thorough an understanding as possible of the factors affecting coupling. Bimetallic compounds based on tetrapyridophenazine ligands are an attractive system to carry out a study of donor-acceptor coupling. Attaching two $Ru(bpy)_2^{2+}$ units gives a system which can be oxidized to a mixed-valence species for treatment with the Hush model. Coordination of two paramagnetic $CuCl_2$ centers allows investigation of metal coupling with magnetic susceptibility measurements. Synthesis of heterodimers containing a $Ru(bpy)_2^{2+}$ unit as an excited-state electron donor and a $CuCl_2$ or $Os(bpy)_2^{3+}$ unit as an electron acceptor provides compounds in which intramolecular ET can be studied. When Os is in its +2 oxidation state, its absorbance spectrum overlaps with the emission spectra of Ru chromophores; intramolecular energy transfer can be studied. The incremental change in donor-acceptor separation provided by the series of three ligands allows coupling to be measured as a function of distance, providing valuable information on how the bridge between donor and acceptor works to promote ET.

The study of ET in these dimers will also provide insight into the remarkable behavior displayed by the compounds discussed in Chapter 2. If these ligands exhibit a large differential in ground- and excited-state coupling ability, the large driving force and strong coupling for forward photoinduced electron transfer should give rapid formation of the charge-separated state. Behavior like bdppz should then give very long-lived charge separation as weak coupling and low driving force combine to retard back ET. Chapter 3 presents the study of complexes of tetrapyridophenazine ligands.

Experimental Section

Preparation of Compounds.

Chemicals were used as received from Aldrich. Phendione was prepared according to the method of Yamada.[15] Heating the reaction mixture at 120° for 4 h gave a higher yield than the procedure given in the paper. The free base of 1,2,4,5-tetraminobenzene was prepared from the tetrahydrochloride using the method of Vogel and used promptly thereafter.[16] 2,2'-bipyridine-d_8 was kindly provided by Dr. Cynthia Dupreur; Ru(bpy-d_8)$_2$Cl$_2$ was synthesized according to the procedure developed by Sullivan.[17] Os(bpy)$_2$Cl$_2$ was synthesized according to Lay.[18]

Tetrapyrido[3,2-*a*:2',3'-*c*:3'',2''-*f*:2''',3'''-*h*] phenazine, tppz. The synthesis of this compound was adapted from Scheidt's preparation of tetrabenzophenazine.[19] 500 mg of phendione in a solution of 7.5 ml of formamide and 0.5 ml acetic acid was refluxed for 2 h. The lustrous gold product which precipitated was collected and washed with acetone and ether. Yield: 240 mg. M.P.>350°. λ_{max}(tetralin) 354, 374, 384, 394 nm. DEIMS, M^+ 384.

5,7,12,14-tetraaza-tetrapyrido[3,2-*a*:2',3'-*c*:3'',2''-*h*:2''',3'''-*j*]pentacence, tatpp. 500 mg of phendione and 150 mg of 1,2,4,5-tetraminobenzene were refluxed under nitrogen in 25 ml of degassed acetic acid. The orange precipitate was collected and washed with acetone and ether. Yield: 300 mg. M.P.>350°. λ_{max}(tetralin) 412, 436, 462 nm. DEIMS, M^+ 486.

Tetrapyrido[3,2-*d*:2',3'-*f*:3'',2''-*d'*:2''',3'''-*f'*]biphenazine, tpbpz. 275 mg of phendione and 125 mg of 3,3'-diaminobenzidne were heated at reflux for 1 h in 25 ml of 100% ethanol. The yellow-brown product was collected and washed with acetone and ether. Yield: 260 mg. M.P.>350°. The Uv-Vis spectrum of a tetralin solution of the compound had no sharp features. DEIMS, M^+ 562.

Synthesis of $[(M(bpy)_2)_2$tetrapyridophenazine$]^{4+}$.

A magnetically-stirred suspension of 50 mg of the appropriate ligand in 25 ml of ethylene glycol was heated to 150°. 2.2 equivalents of $M(bpy)_2Cl_2$ were added and heating continued until all of the ligand had gone into solution, indicating completion of the reaction. Reactions involving tatpp were conducted while a vigorous stream of nitrogen was bubbled through the reaction mixture. After cooling, the solution was diluted with 25 ml of water. The complex was precipitated with saturated aqueous NH_4PF_6, collected, and washed with ethanol and ether. Purification was achieved by chromatography on neutral alumina using acetonitrile as the eluent; the product was the first band to come off the column. The yield was typically 70%.

$[(Ru(bpy)_2)_2$tppz$](PF_6)_4$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.7.

$[(Os(bpy)_2)_2$tppz$](PF_6)_4$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.8. FABMS $[M^{4+} + 3\ PF_6^-]^+$ 1824.

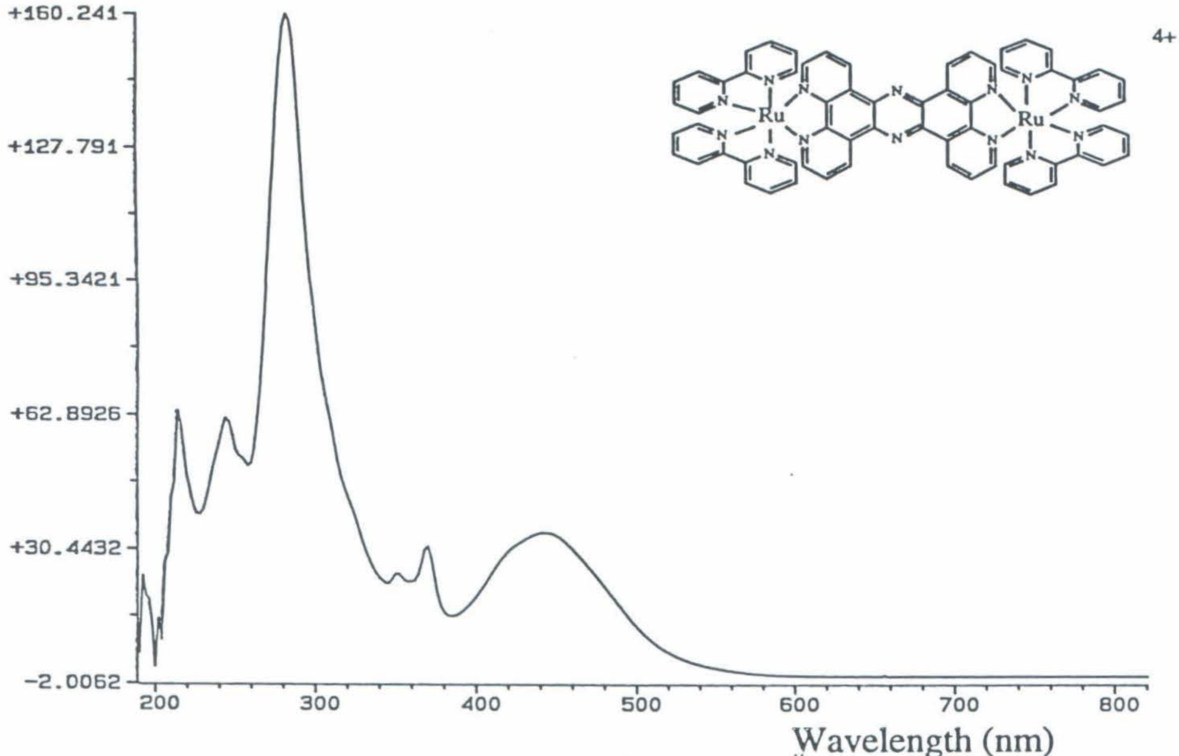
$[(Ru(bpy)_2)_2$tatpp$](PF_6)_4$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.9. FABMS $[M^{4+} + 3\ PF_6^-]^+$ 1749. Calculated for $C_{70}H_{46}N_{16}Ru_2P_4F_{24}{\bullet}5H_20$: C, 42.46; H, 2.83; N, 11.32. Found: C, 42.47; H, 2.83; N, 11.32.

$[(Ru(bpy)_2)_2$tpbpz$](PF_6)_4$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.10. FABMS $[M^{4+} + 3\ PF_6^-]^+$ 1824. Calculated for $C_{76}H_{50}N_{16}Ru_2P_4F_{24}{\bullet}7H_20$: C, 43.54 ;H, 2.97; N, 10.70. Found: C, 43.54; H, 3.05; N, 10.38.

$[(Os(bpy)_2)_2$tpbpz$](PF_6)_4$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.11.

$[(CuCl_2)_2$tppz$]$ was synthesized by adding a large excess of $CuCl_2$ to a suspension of 25 mg of tppz in 25 ml of ethylene glycol at 160°; heating was continued for 15 min. The cooled mixture was diluted with 25 ml of water and the green product collected and washed with acetone and ether. Its lack of solubility prevented its characterization in solution.

Figure 3.7. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[(Ru(bpy)_2)_2tppz](PF_6)_4$.


+160.241
+127.791
+95.3421
+62.8926
+30.4432
-2.0062
200
300
400
500
600
700
800
Wavelength (nm)
4+
Ru
Ru
N

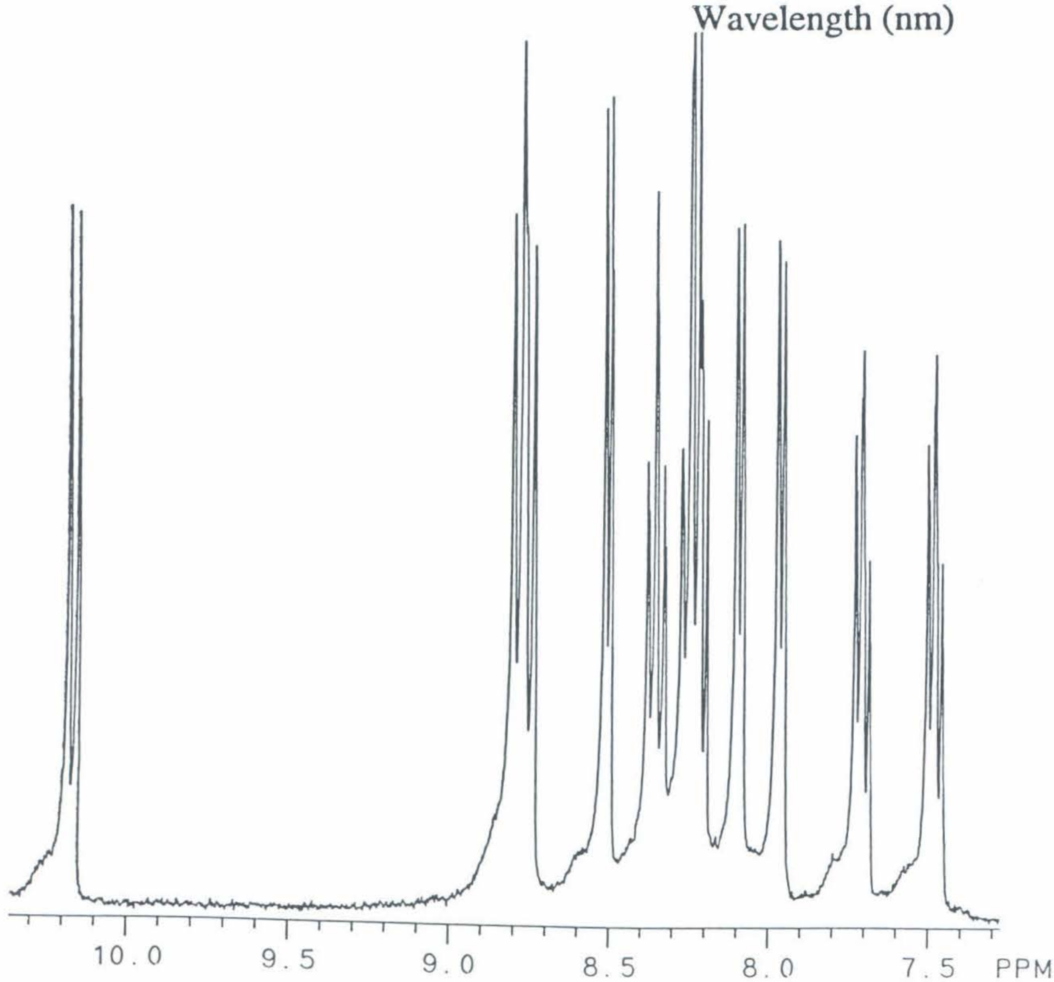
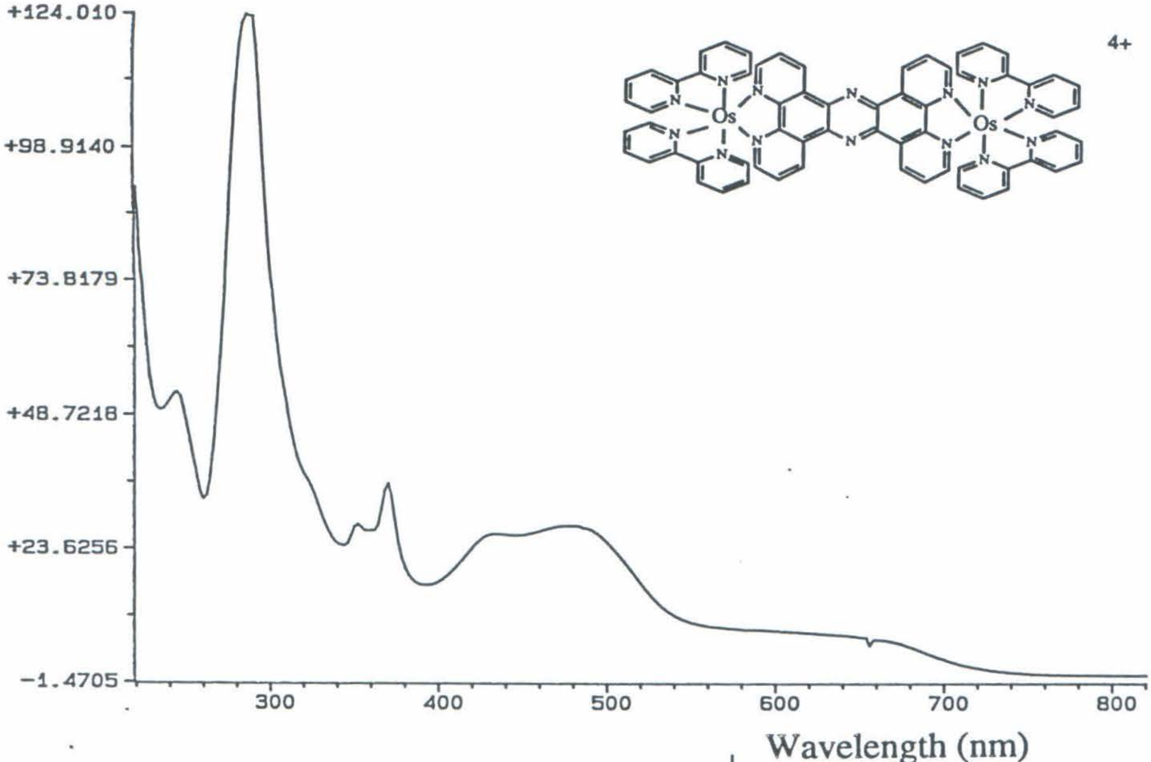

10.0
9.5
9.0
8.5
8.0
7.5
PPM

Figure 3.8. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[(Os(bpy)_2)_2tppz](PF_6)_4$.


+124.010
+98.9140
+73.8179
+48.7218
+23.6256
-1.4705
300
400
500
600
700
800
Wavelength (nm)
4+
Os
Os

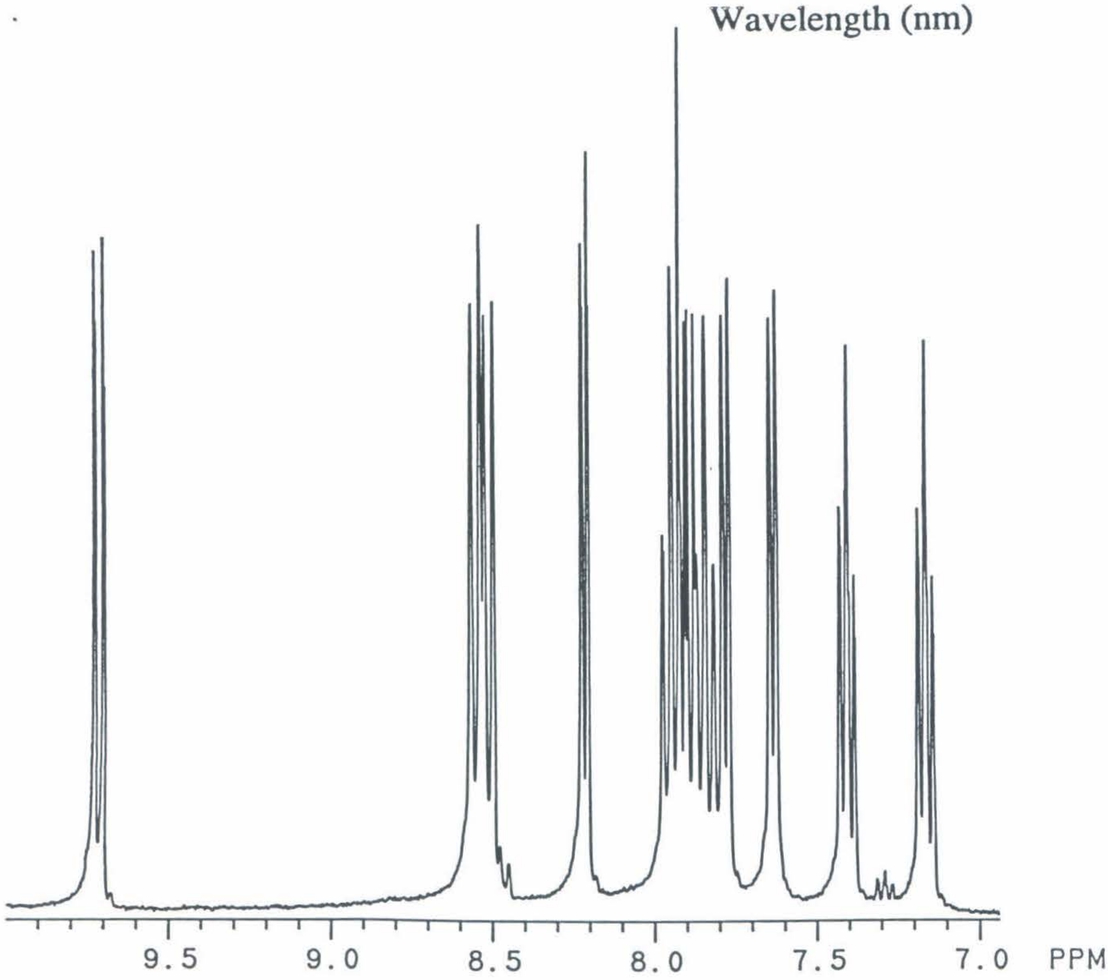
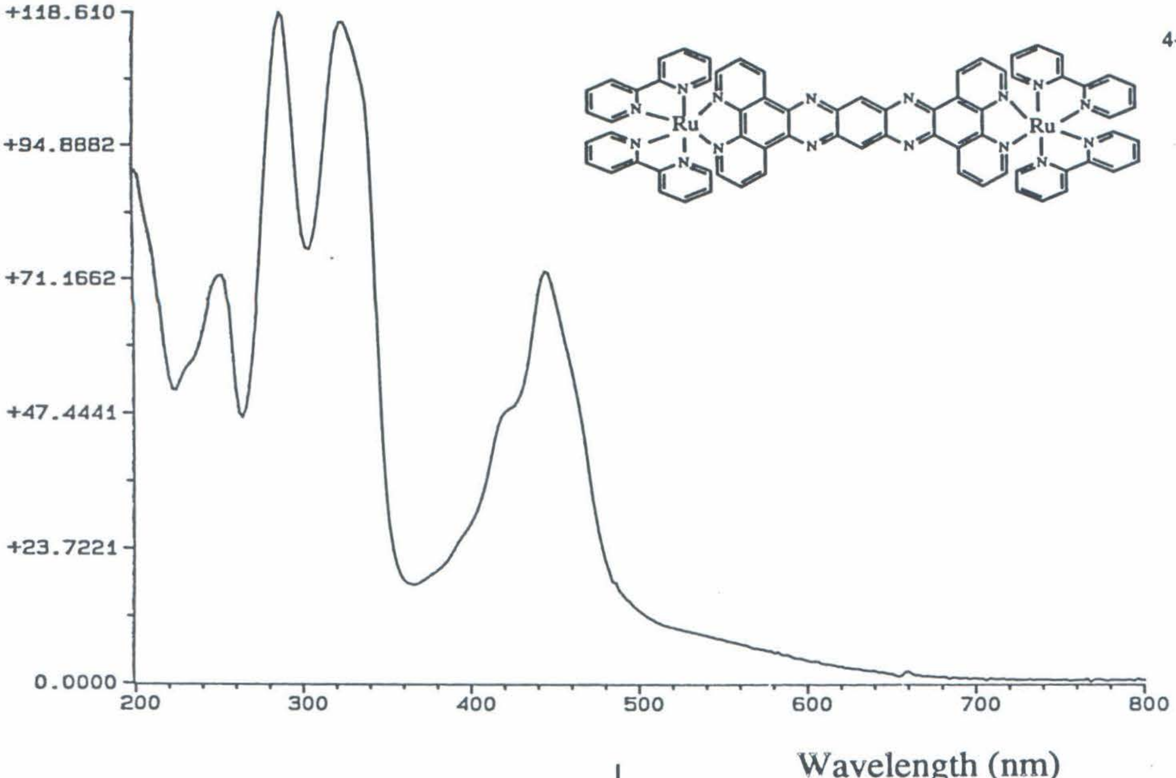

9.5
9.0
8.5
8.0
7.5
7.0
PPM

Figure 3.9. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[(Ru(bpy)_2)_2tatpp](PF_6)_4$.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+94.8882
+71.1662
+47.4441
+23.7221
0.0000
200
300
400
500
600
700
800
Wavelength (nm)
4+
Ru
Ru

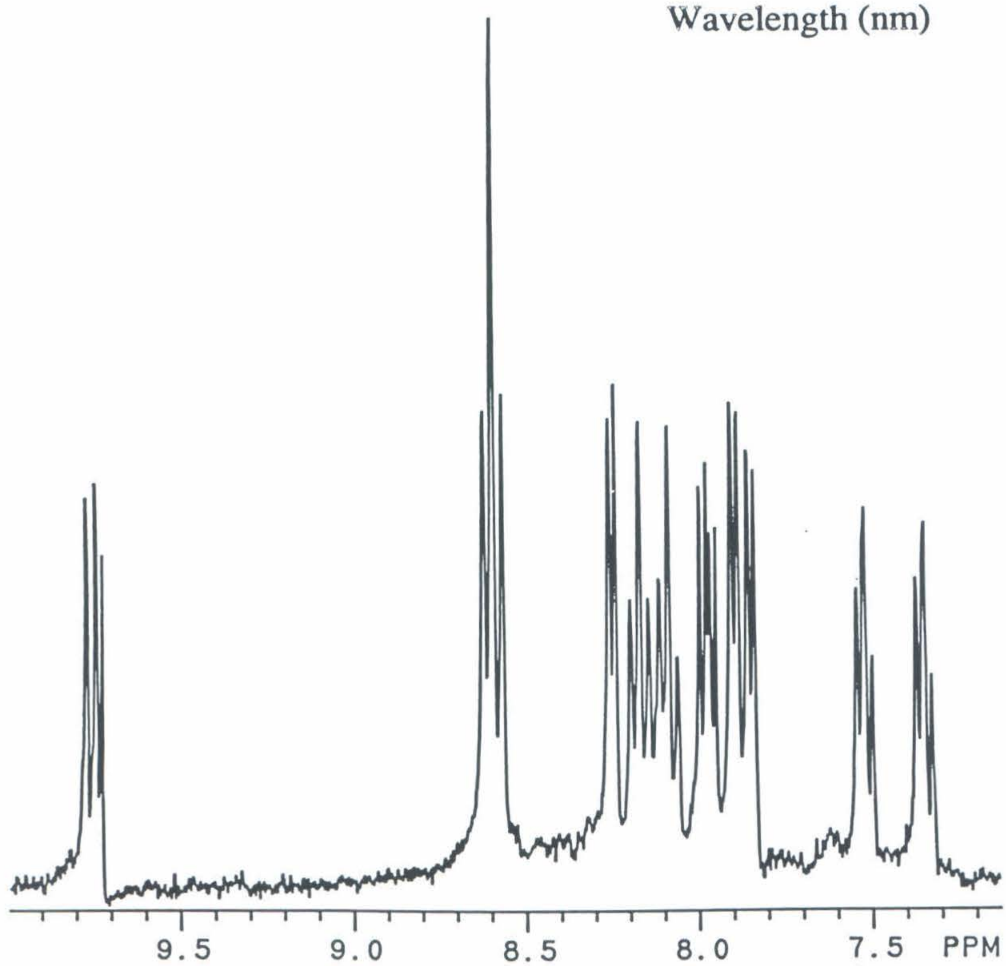
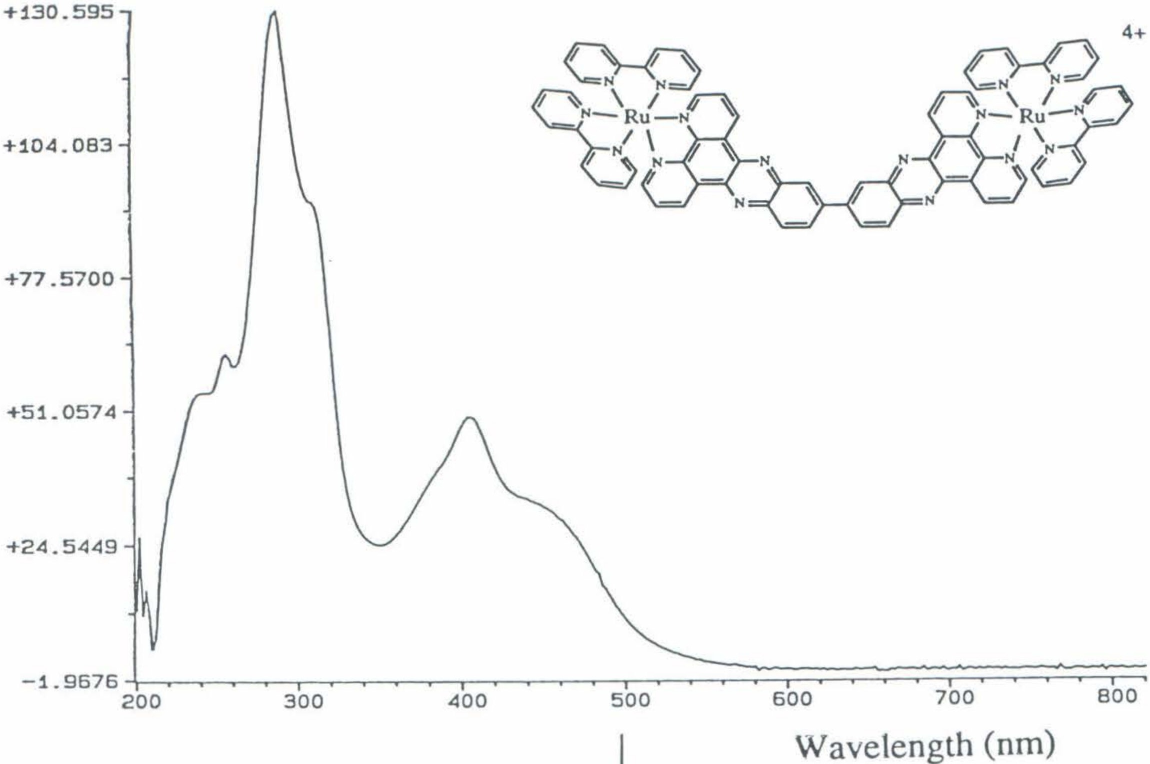
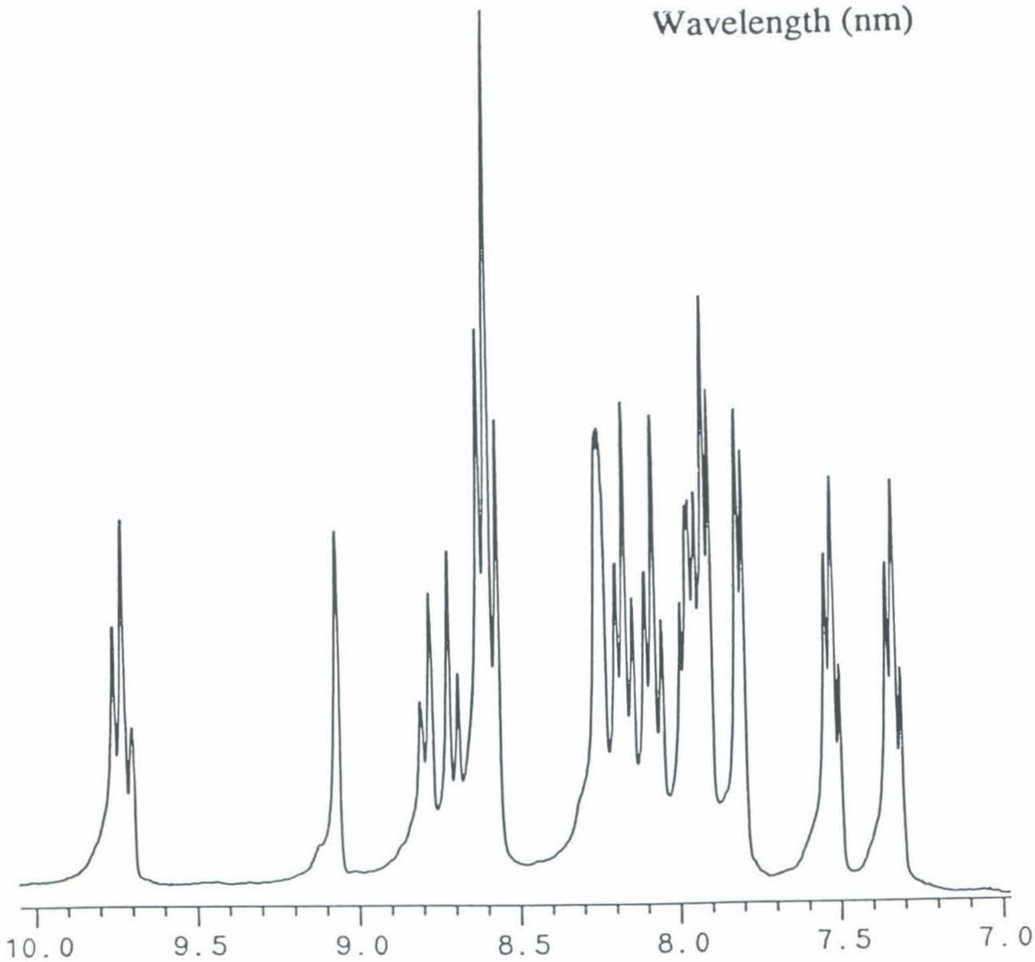

9.5
9.0
8.5
8.0
7.5
PPM

Figure 3.10. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[(Ru(bpy)_2)_2tpbpz](PF_6)_4$.

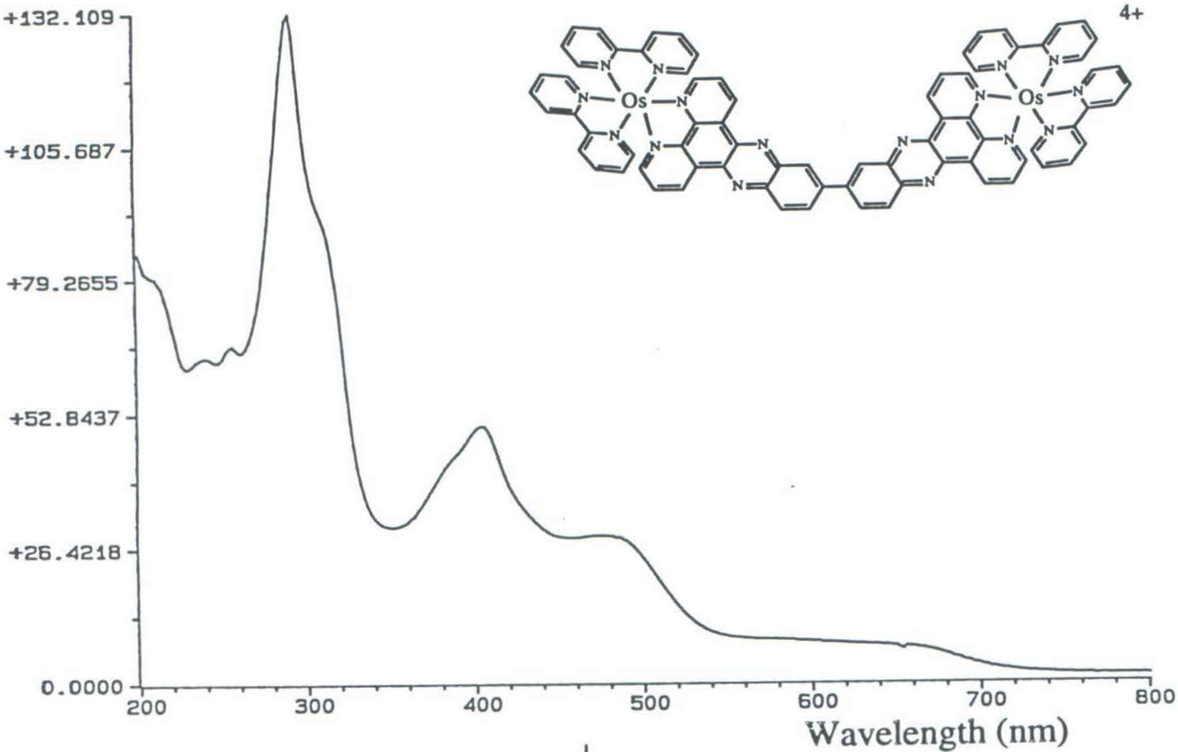


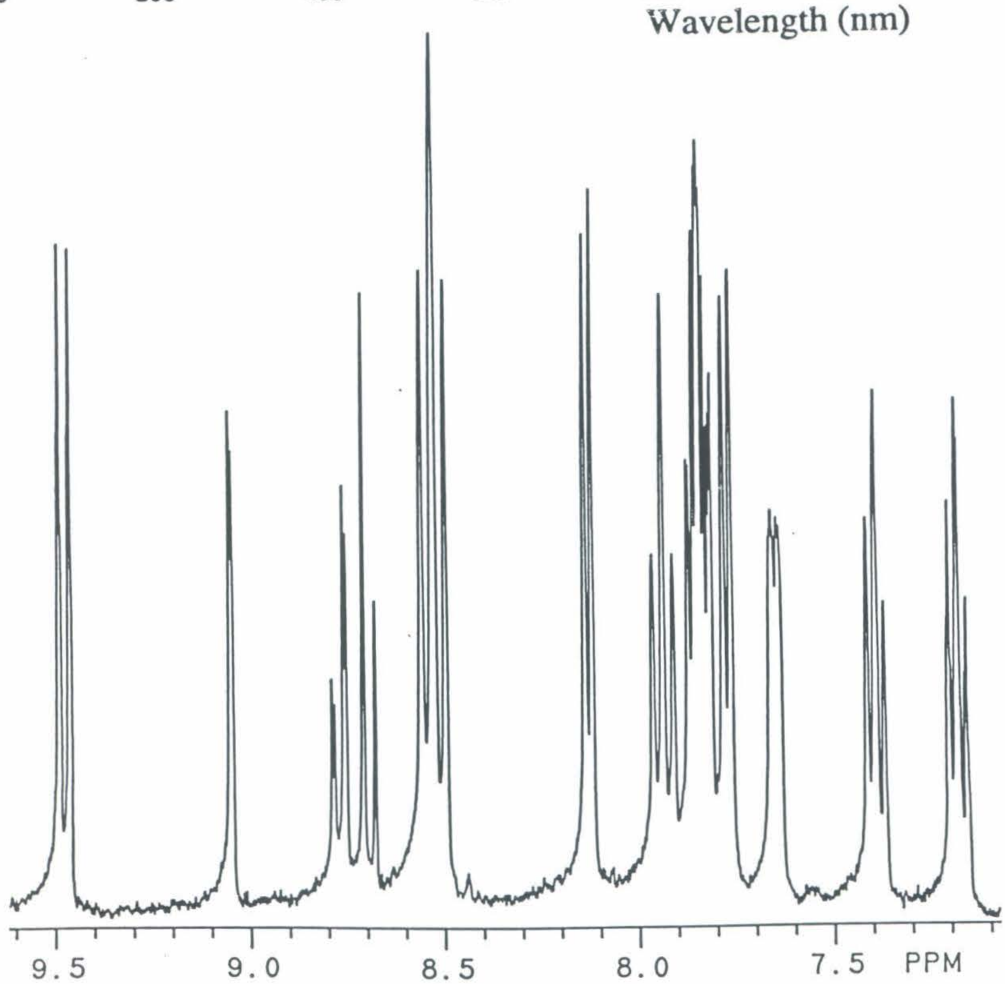
+130.595
+104.083
+77.5700
+51.0574
+24.5449
-1.9676
200
300
400
500
600
700
800
Wavelength (nm)
4+
Ru
N



10.0
9.5
9.0
8.5
8.0
7.5
7.0

Figure 3.11. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[(Os(bpy)_2)_2tpbpz](PF_6)_4$.


+132.109
+105.687
+79.2655
+52.8437
+26.4218
0.0000
200
300
400
500
600
700
800
Wavelength (nm)
4+
Os
N


9.5
9.0
8.5
8.0
7.5
PPM

Synthesis of $Ru(bpy)_2L^{2+}$, L=tppz, tpbpz.

A vigorously-stirred suspension of 30 mg of the appropriate ligand in 50 ml of ethylene glycol was heated to 150°. 0.5 equivalents of $Ru(bpy)_2Cl_2$ were added; heating was stopped immediately. After cooling and dilution with 25 ml of water, the unreacted ligand was filtered off. The complex was precipitated by addition of saturated aqueous NH_4PF_6 to the filtrate. The solid was collected and washed with ethanol and ether. $Ru(bpy)_2tppz^{2+}$, which NMR showed to be contaminated with approximately 10% $[(Ru(bpy)_2)_2tppz]^{4+}$, was purified by dissolving in 10 ml of acetone, adding 5 ml of isopropanol, and recrystallization by slow evaporation of the acetone. Yield: 12 mg. $Ru(bpy)_2tpbpz^{2+}$, which contained an appreciable amount of $[(Ru(bpy)_2)_2tpbpz]^{4+}$, was purified by chromatography on neutral alumina using acetonitrile as the eluent. The monomer came off the column first; an increase in absorbance at 450 nm relative to that at 406 nm in successive fractions indicated that the dimer had begun to come off. Yield: 3 mg. $[Os(bpy)_2tppz](PF_6)_2$ was prepared on a NMR-sample scale by reacting $Os(bpy)_2Cl_2$ an excess of tppz in 3 ml of ethylene glycol. Precipitation with NH_4PF_6 gave a product that required no further purification.

$[Ru(bpy)_2tppz](PF_6)_2$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.12. FABMS $[M^{2+} + PF_6^-]^+$ 943.

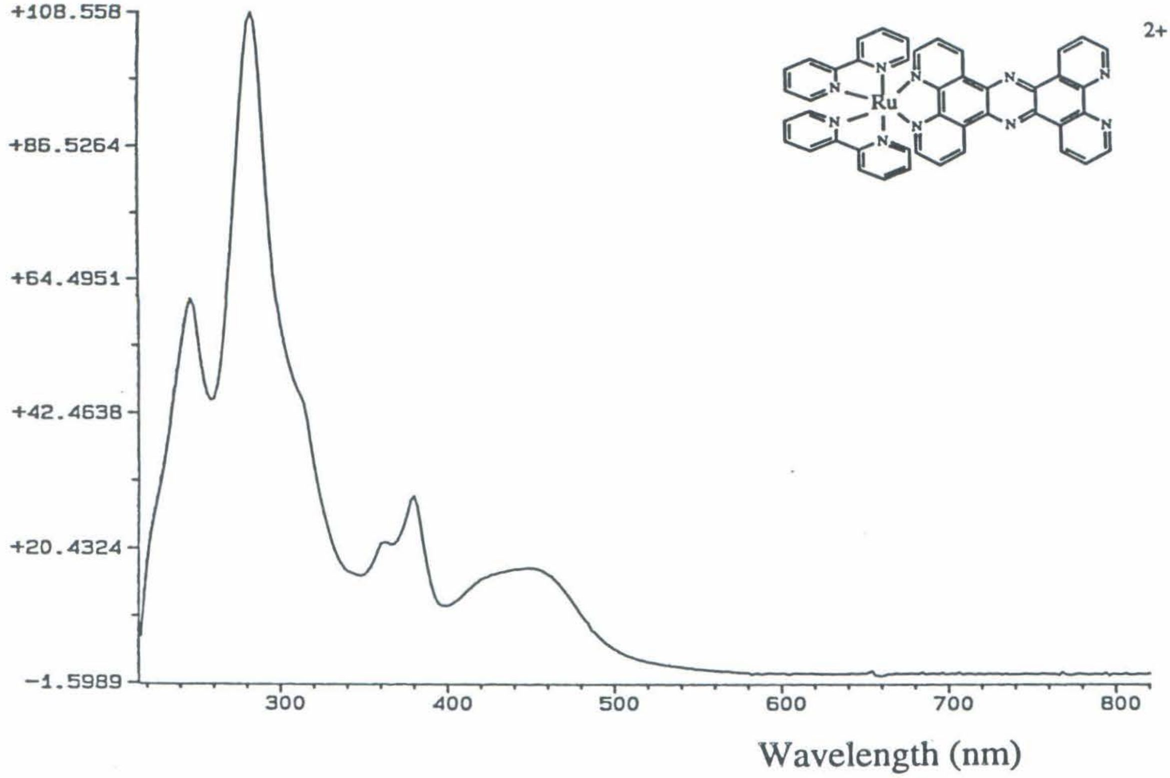
$[Os(bpy)_2tppz](PF_6)_2$. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) Figure 3.13.

$[Ru(bpy)_2tpbpz](PF_6)_2$. Uv-Vis(CH_3CN), FABMS $[M^{2+} + PF_6^-]^+$ 1121 Figure 3.14.

Synthesis of $[(Ru(bpy)_2)L(Os(bpy)_2)]^{4+}$, L=tppz, tpbpz.

A suspension of 5 mg of $[Ru(bpy)_2L](PF_6)_2$ in 15 ml of ethylene glycol was heated to 150°. 1.2 equivalents of $Os(bpy)_2Cl_2$ were added; heating was continued for 30 min. After cooling, the mixture was diluted with an equal volume of water. The complex was precipitated with saturated aqueous NH_4PF_6, collected, and washed with ethanol and

Figure 3.12. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[Ru(bpy)_2tppz](PF_6)_2$.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+86.5264
+64.4951
+42.4638
+20.4324
-1.5989
300
400
500
600
700
800
Wavelength (nm)
2+
Ru

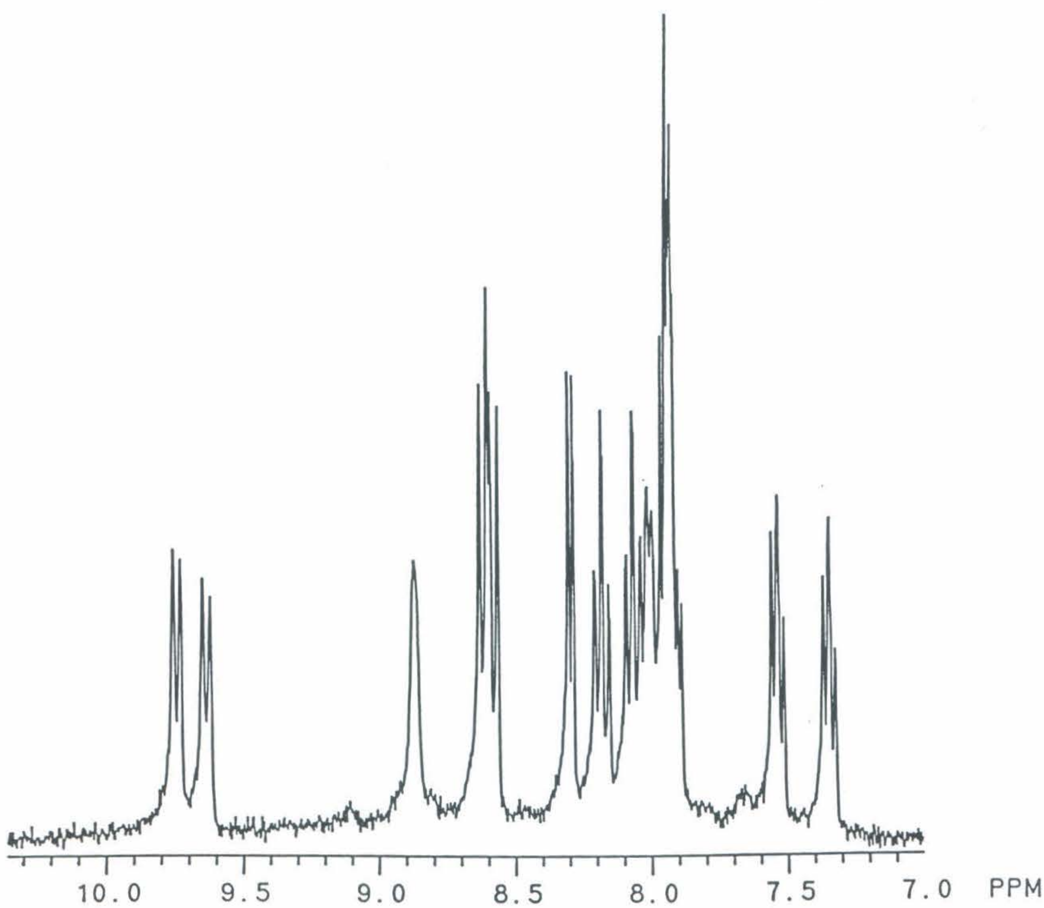
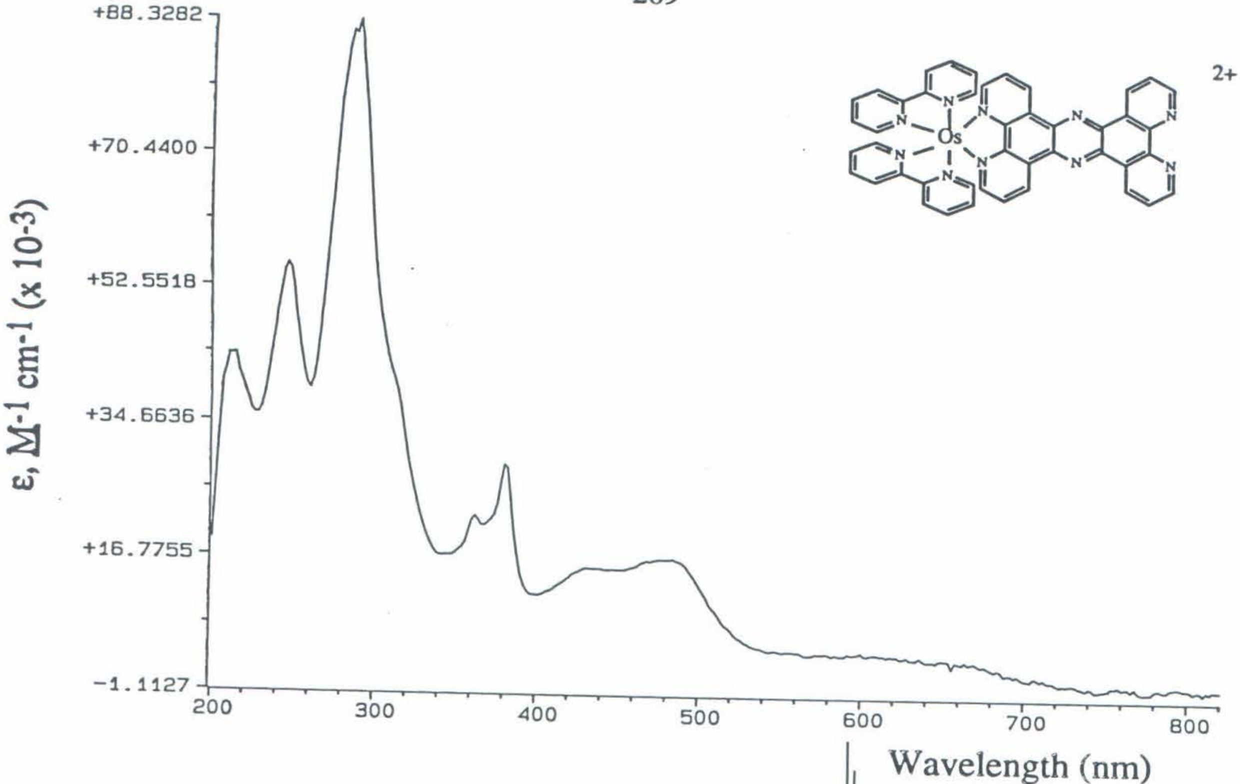

10.0
9.5
9.0
8.5
8.0
7.5
7.0
PPM

Figure 3.13. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[Os(bpy)_2tppz](PF_6)_2$.


+88.3282
+70.4400
+52.5518
+34.6636
+16.7755
-1.1127
ε, M-1 cm-1 (x 10-3)
200
300
400
500
600
700
800
Wavelength (nm)
Os
2+

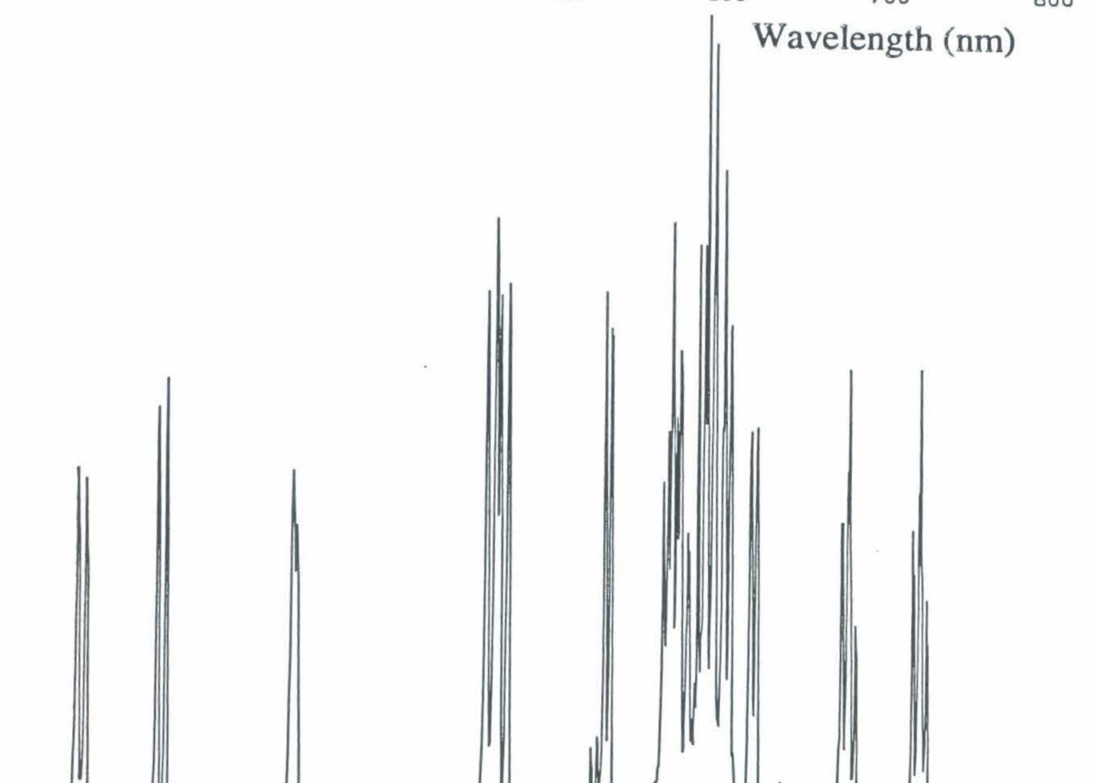
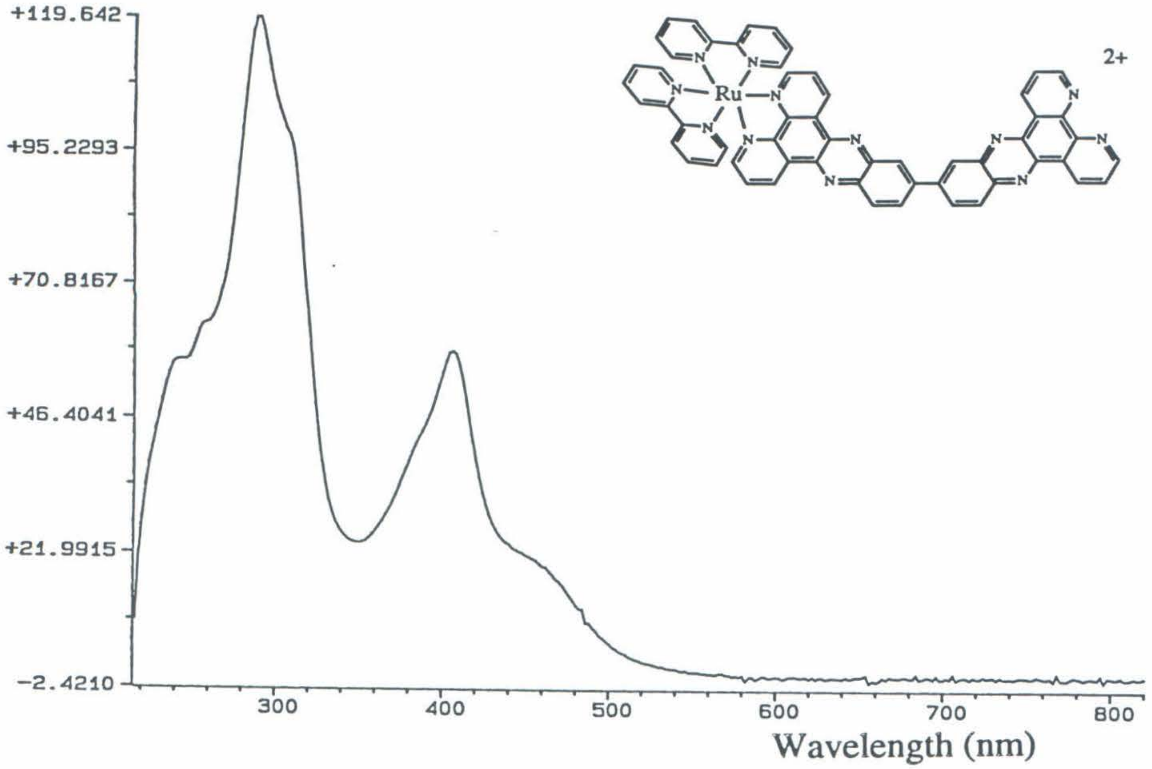
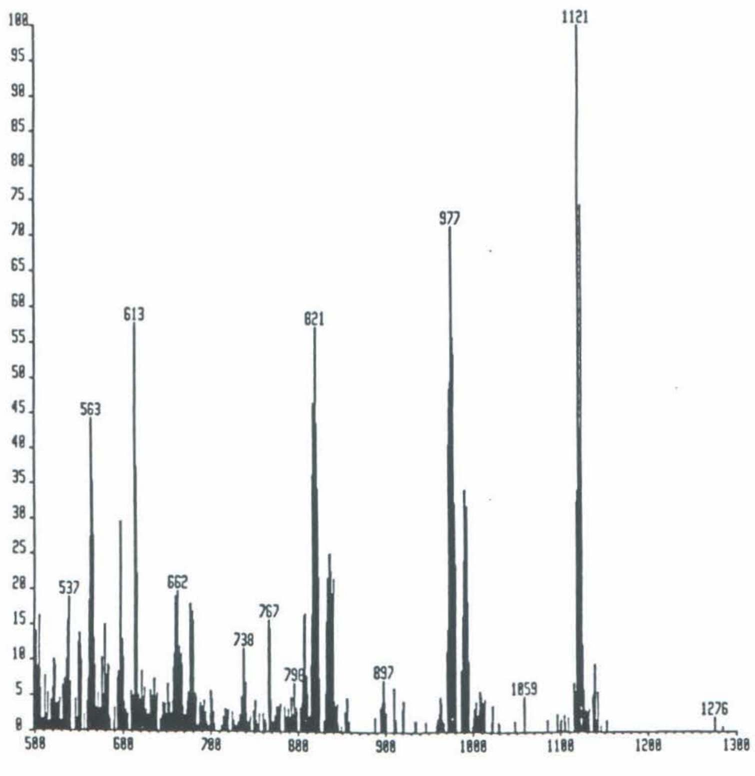

10.0
9.5
9.0
8.5
8.0
7.5
7.0
PPM

Figure 3.14. Uv-Vis(CH_3CN), FABMS of $[Ru(bpy)_2tpbpz](PF_6)_2$.


+119.642
+95.2293
+70.8167
+46.4041
+21.9915
-2.4210
300
400
500
600
700
800
Wavelength (nm)
Ru
2+


1121
977
613
821
563
537
662
767
738
796
897
1059
1276

ether. Purification was achieved by chromatography with neutral alumina/ acetonitrile. Yield: 90%.

$[(Ru(bpy)_2)tppz(Os(bpy)_2)](PF_6)_4$. Uv-Vis($CH_3CN$), ^1H NMR (CD_3CN) Figure 3.15. FABMS $[M^{4+} + 3\ PF_6^-]^+$ 1736.

$[(Ru(bpy)_2)tpbpz(Os(bpy)_2)](PF_6)_4$. Uv-Vis($CH_3CN$), ^1H NMR (CD_3CN) Figure 3.16.

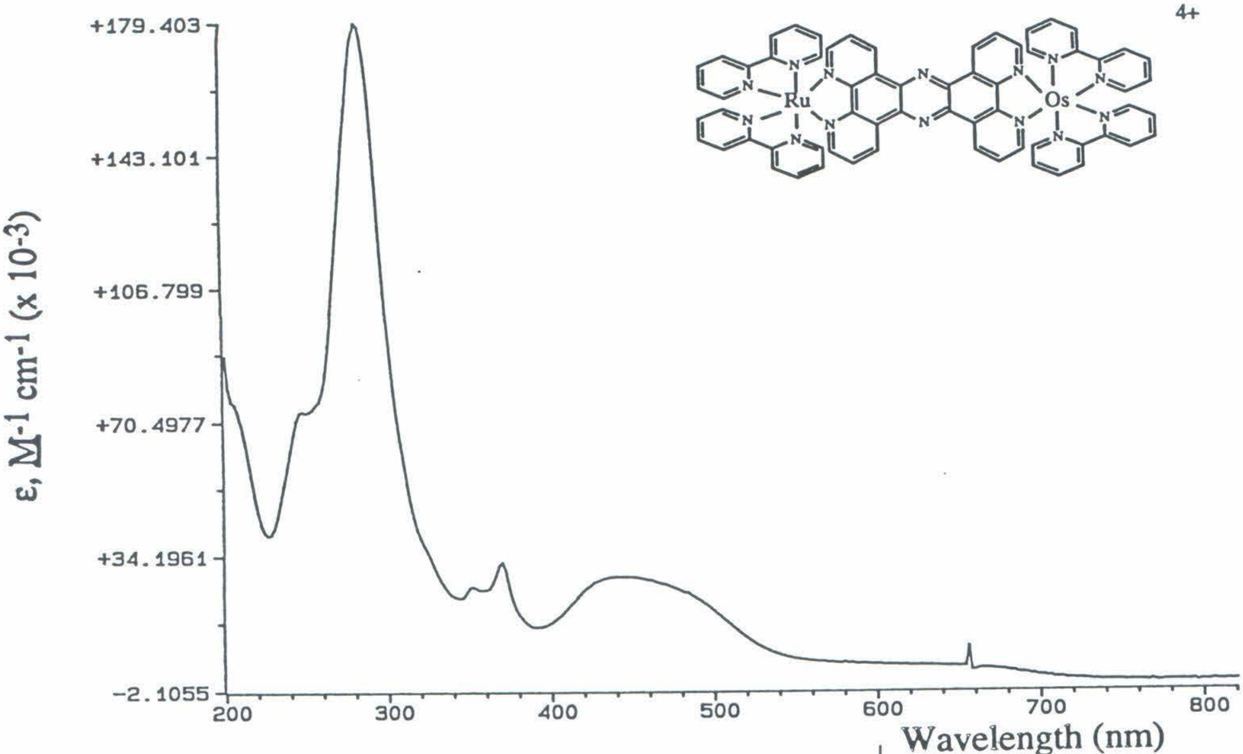
Synthesis of $[(Ru(bpy)_2)L(CuCl_2)]^{2+}$, L=tppz, tpbpz.

5 mg of the PF_6^- salt of $Ru(bpy)_2L^{2+}$ was metathesized to the Cl^- salt by addition of a saturated acetonitrile solution of tetrabutylammonium chloride to a concentrated acetonitrile solution of the Ru complex. The precipitated Cl^- salt was collected and washed with acetonitrile and ether. $[Ru(bpy)_2L](Cl)_2$ was dissolved in 5 ml of ethanol and 1 ml of a saturated ethanol solution of $CuCl_2$. The Ru-Cu complex which precipitated was collected and washed with ethanol and ether. Yield: 90%.

$[(Ru(bpy)_2)tppz(CuCl_2)](Cl)_2$. Uv-Vis (dmso), FABMS $[M^{2+} + Cl^-]$ 933 Figure 3.17.

$[(Ru(bpy)_2)tpbpz(CuCl_2)](Cl)_2$. Uv-Vis (dmso), FABMS $[M^{2+} + Cl^-]$ 1113 Figure 3.18.

Figure 3.15. Uv-Vis(CH_3CN), [1]H NMR (CD_3CN) of $[(Ru(bpy)_2)tppz(Os(bpy)_2)](PF_6)_4$.


4+
Ru
Os
N
+179.403
+143.101
+106.799
+70.4977
+34.1961
-2.1055
ε, M-1 cm-1 (x 10-3)
200
300
400
500
600
700
800
Wavelength (nm)

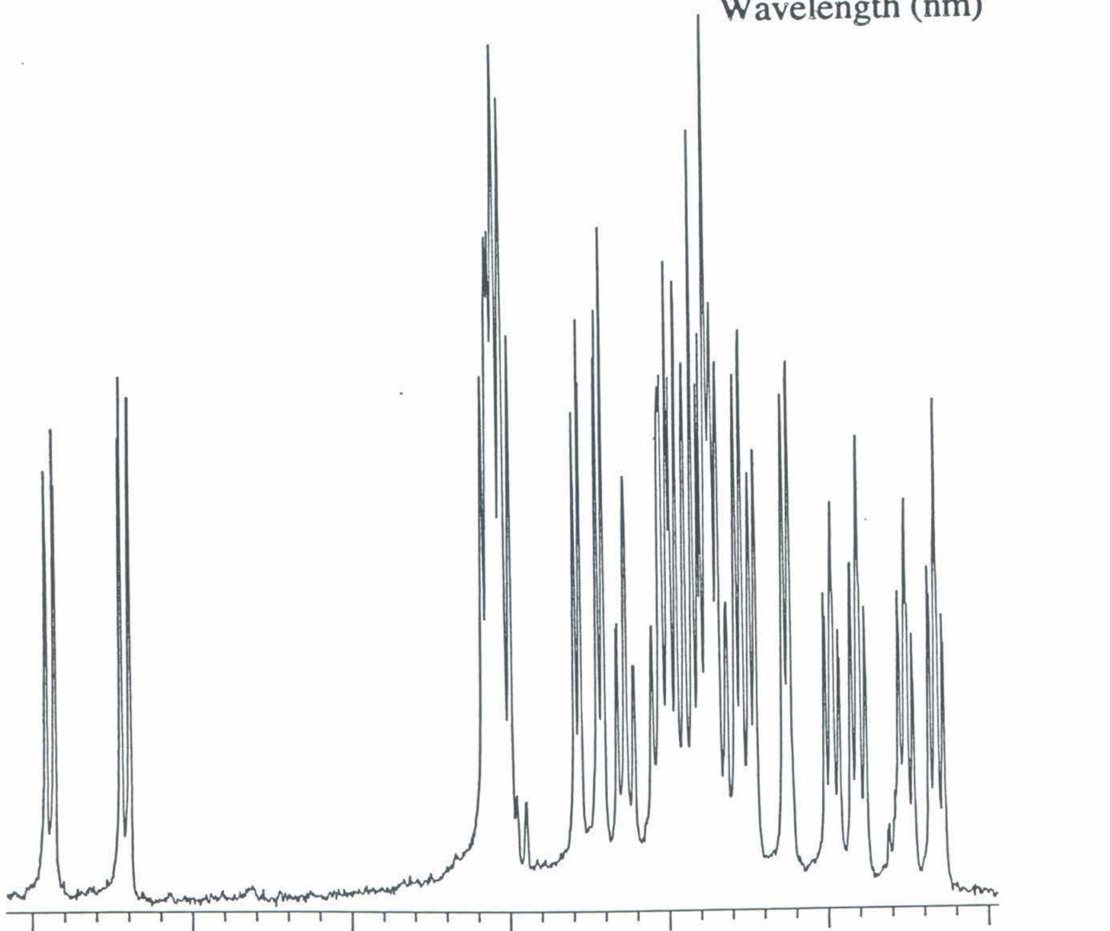
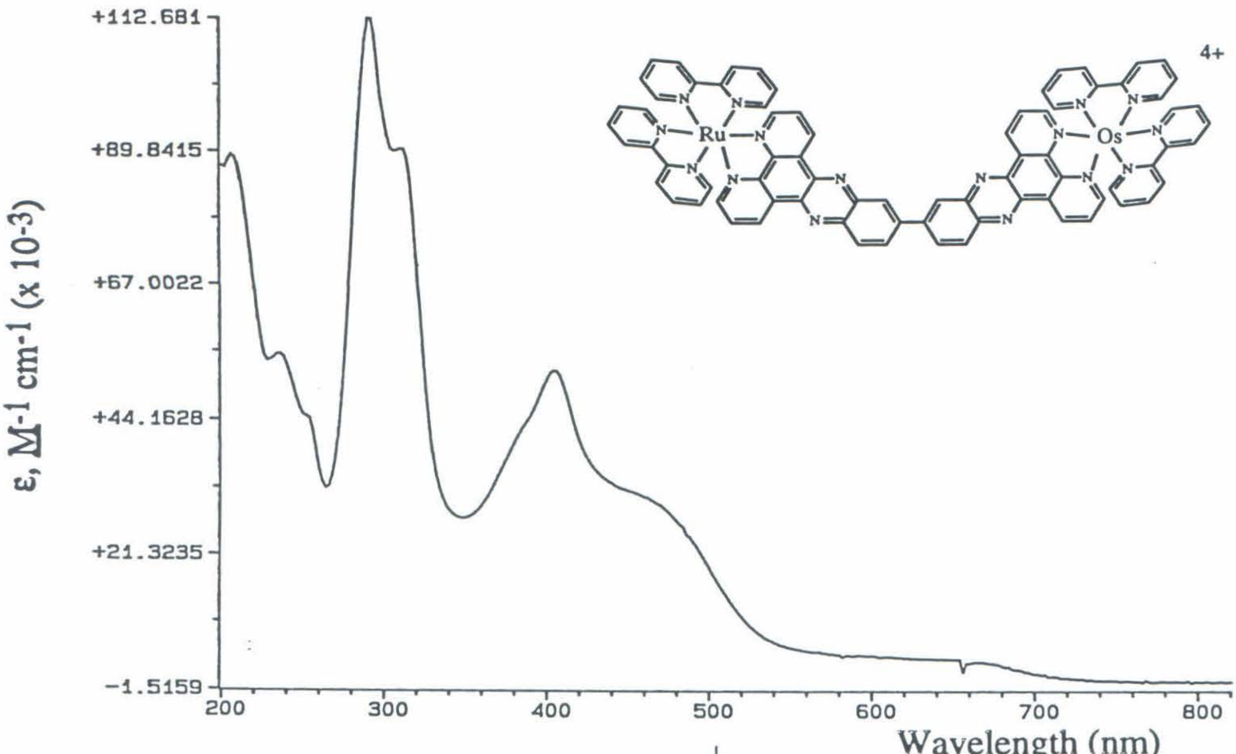

10.0
9.5
9.0
8.5
8.0
7.5
7.0
PPM

Figure 3.16. Uv-Vis(CH_3CN), ^1H NMR (CD_3CN) of $[(Ru(bpy)_2)tpbpz(Os(bpy)_2)](PF_6)_4$.


ε, M-1 cm-1 (x 10-3)
+112.681
+89.8415
+67.0022
+44.1628
+21.3235
-1.5159
200
300
400
500
600
700
800
Wavelength (nm)
4+
Ru
Os
N

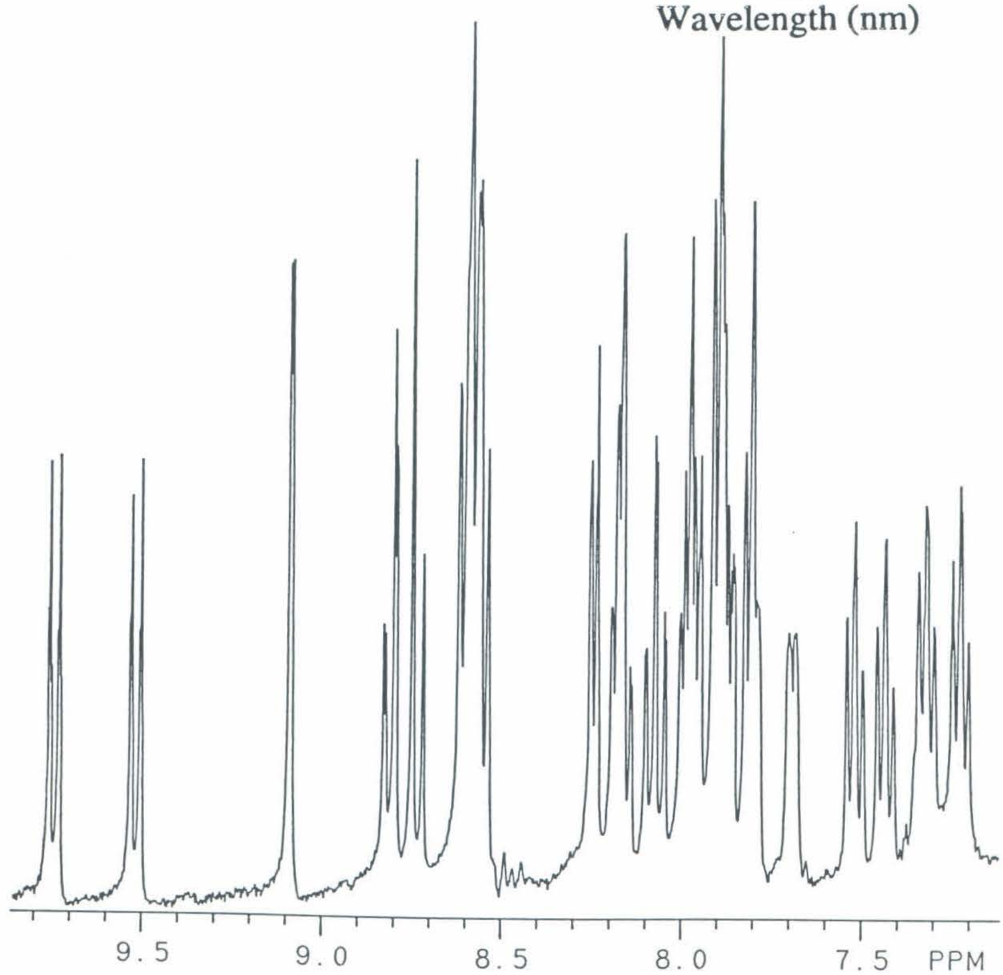
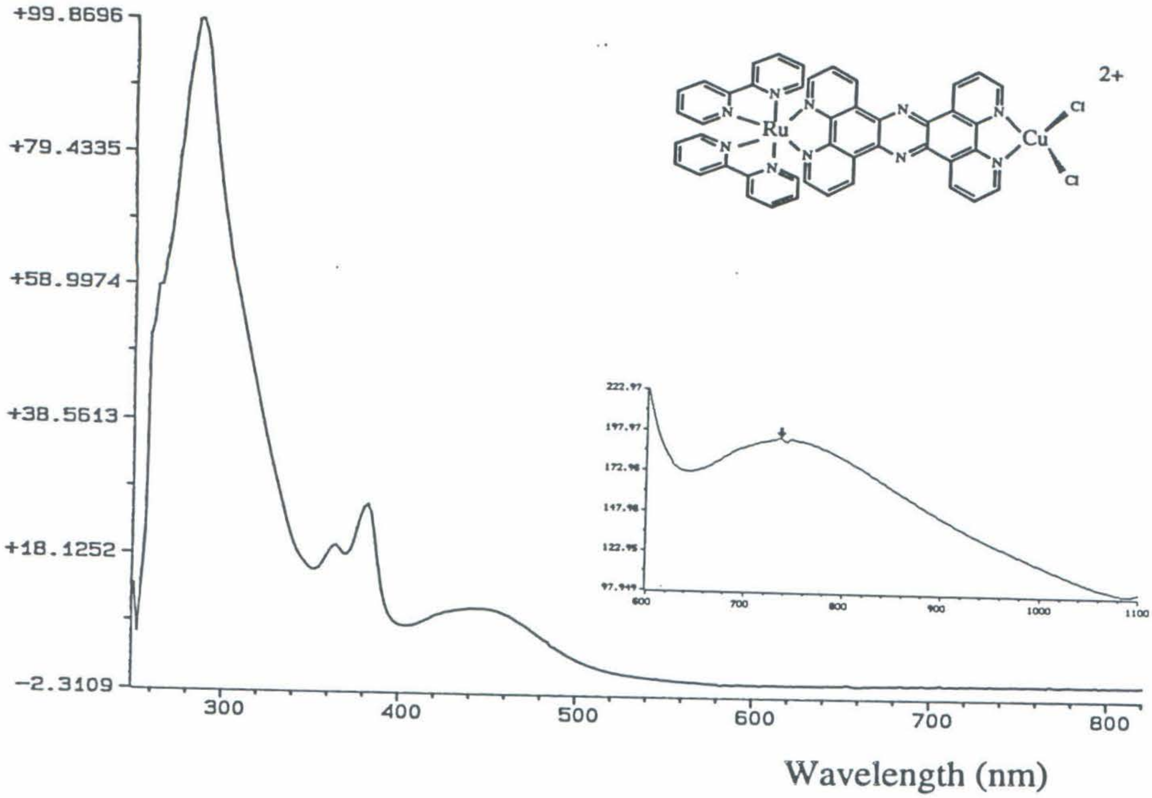

9.5
9.0
8.5
8.0
7.5
PPM

Figure 3.17. Uv-Vis (dmso), FABMS of $[(Ru(bpy)_2)tppz(CuCl_2)](Cl)_2$.


+99.8696
+79.4335
+58.9974
+38.5613
+18.1252
-2.3109
300
400
500
600
700
800
Wavelength (nm)
Ru
Cu
Cl
Cl
N
2+

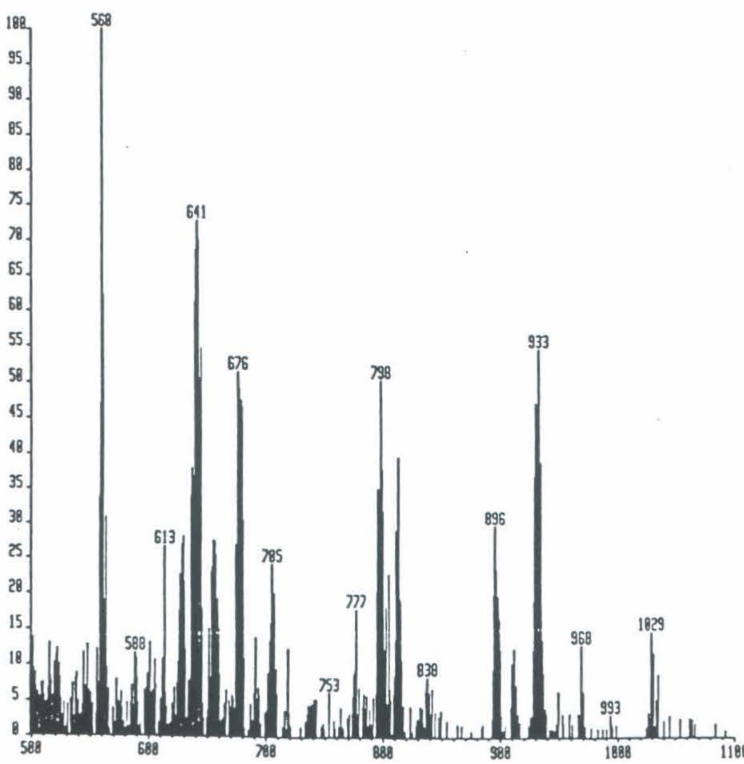
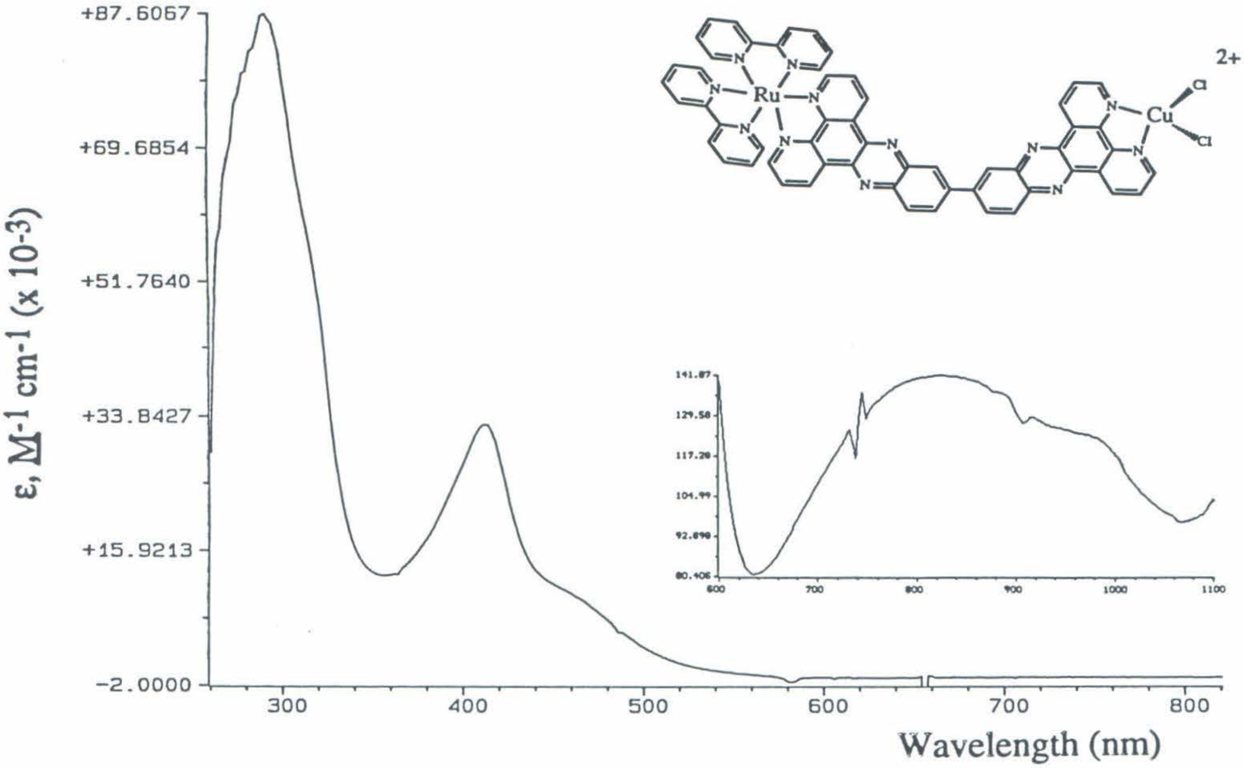
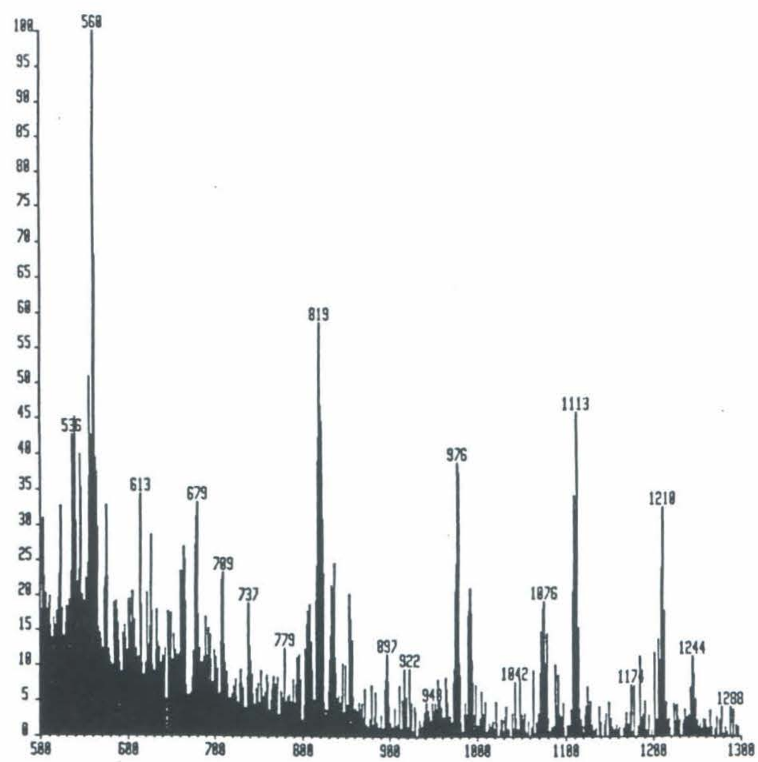

568
641
676
798
933
613
705
896
777
588
968
1029
838
753
993
500
600
700
800
900
1000
1100

Figure 3.18. Uv-Vis (dmso), FABMS of $[(Ru(bpy)_2)tpbpz(CuCl_2)](Cl)_2$.


+87.6067
+69.6854
+51.7640
+33.8427
+15.9213
-2.0000
ε, M-1 cm-1 (x 10-3)
300
400
500
600
700
800
Wavelength (nm)
2+
Ru
Cu
N
Cl
141.87
129.58
117.28
104.99
92.698
80.406
600
700
800
900
1000
1100


560
536
613
679
709
737
779
819
897
922
940
976
1042
1076
1113
1174
1210
1244
1288
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
500
600
700
800
900
1000
1100
1200
1300

Physical Measurements.

300 MHz ^{1}H NMR spectra were recorded on a General Electric QE-300 NMR spectrometer. Chemical shifts were referenced relative to the shift of residual solvent protons. Mass spectrometry was performed at the University of California, Riverside Mass Spectrometry facility. Magnetic susceptibility measurements were carried out on a Quantum Design MPMS machine. Electronic Absorption measurements were collected with a Hewlett-Packard HP-8452A spectrophotometer. Emission spectra were recorded with an SLM 8000 fluorimeter. Nanosecond time-resolved absorbance measurements were carried out with an instrument described elsewhere.[18] The third harmonic (355 nm) of a Quanta-Ray Nd-YAG laser (pulse width 20 ns) was used for excitation. Samples used for emission and nanosecond time-resolved absorption spectroscopy were purged with argon for 10 min in a cell fitted with a septum.

Electrochemical experiments were performed using a Princeton Applied Research (PAR) model 173 potentiostat controlled by a model 175 universal programmer. Cyclic voltammetry was done at ambient temperature with a normal three-electrode configuration consisting of a glassy carbon working electrode, a platinum wire auxiliary electrode, and a AgCl/Ag reference electrode containing 1.0 M KCl. The working compartment of the electrochemical cell was separated from the reference compartment by a modified Luggin capillary. All three compartments contained a 0.1 M solution of supporting electrolyte. Acetonitrile (Burdick and Jackson) was distilled from P_2O_5 prior to use. Tetrabutylammonium hexafluorophosphate ($TBAPF_6$) (Southwestern Analytical) was used as received.

Potentials (vs. aqueous AgCl/Ag) were not corrected for the junction potential. Under conditions identical with those employed here, the ferrocenium/ferrocene couple has an $E^{o\prime}$ of 0.45 V.

Picosecond Transient Absorption. The transient absorption experiments performed on the picosecond time scale were done with a Nd:YAG-based system. In all cases, the samples were excited with one mJ of 355 nm light, and probed with continuum light generated from the 532 nm laser light. $[(Ru(bpy)_2)tppz(CuCl_2)](Cl)_2$, dissolved in dmso, was flowed through a cell with a 2 mm path length. Time points were collected randomly, and UV/VIS spectra of the compounds were acquired before and after the experiment to ensure that sample degradation is not reflected by the kinetics.

A Coherent Antares Nd:YAG provides the 76 MHz train of 100 picosecond (ps) pulses used seed a Continuum RGA60 regenerative amplifier running at 10 Hz. Three watts of the Antares' fundamental output are first focused into 100 meters of 1064 nm single mode optical fiber, and the resulting one watt of spectrally-broadened pulses are fed into the oscillator stage of the regenerative amplifier. The narrow gain profile of Nd:YAG causes spectral clipping -- and hence temporal shortening -- of the seed pulses while they are being amplified: The first stage generates 10 mJ pulses with autocorrelation widths averaging 45 ps. The pulses are then further compressed using a Milton Roy gold grating (1200 grooves/mm). After compression, pulse power has been attenuated to three mJ, but the autocorrelation width has decreased to 14 ps (close to the Nd:YAG transform limit). The regenerative amplifier's second stage then provides a ten-fold increase in pulse power, but induces no measurable pulse broadening. An Inrad 5-14B autocorrelator was used for the pulse-width measurements.

Harmonic generation of 532 nm and 355 nm light is done in KD*P crystals, and the colors are separated with a pellin-broca prism. The green light is sent down a delay stage eight feet long, where a retroreflector forces it to travel the stage's length four times before the light is used to generate the continuum probe light. The 355 nm light passes through a half-wave plate before going through a polarizer set at 54∞ from vertical and being focused onto the sample. After the polarizer, some of the pump beam is directed onto a photodiode, the output of which is fed into a home-built discriminator. The half-wave plate is used to offset long-term pump power fluctuations occurring during the course of the experiment. The discriminator window was set at 15%.

After traveling through the delay stage, the 532 nm light is focused with a 1.5 m focal-length lens into a 5 cm cell containing a 50:50 (v:v) mixture of H2SO4 and D2O. The resulting continuum passes through a 532 nm mirror to remove residual laser light before being collected and focused onto a 400 mm pinhole. A polarizer after the pinhole ensures vertical polarization, and a fused-silica plate then divides the probe light into two parts, one which travels through the sample, the other which is used as a reference.

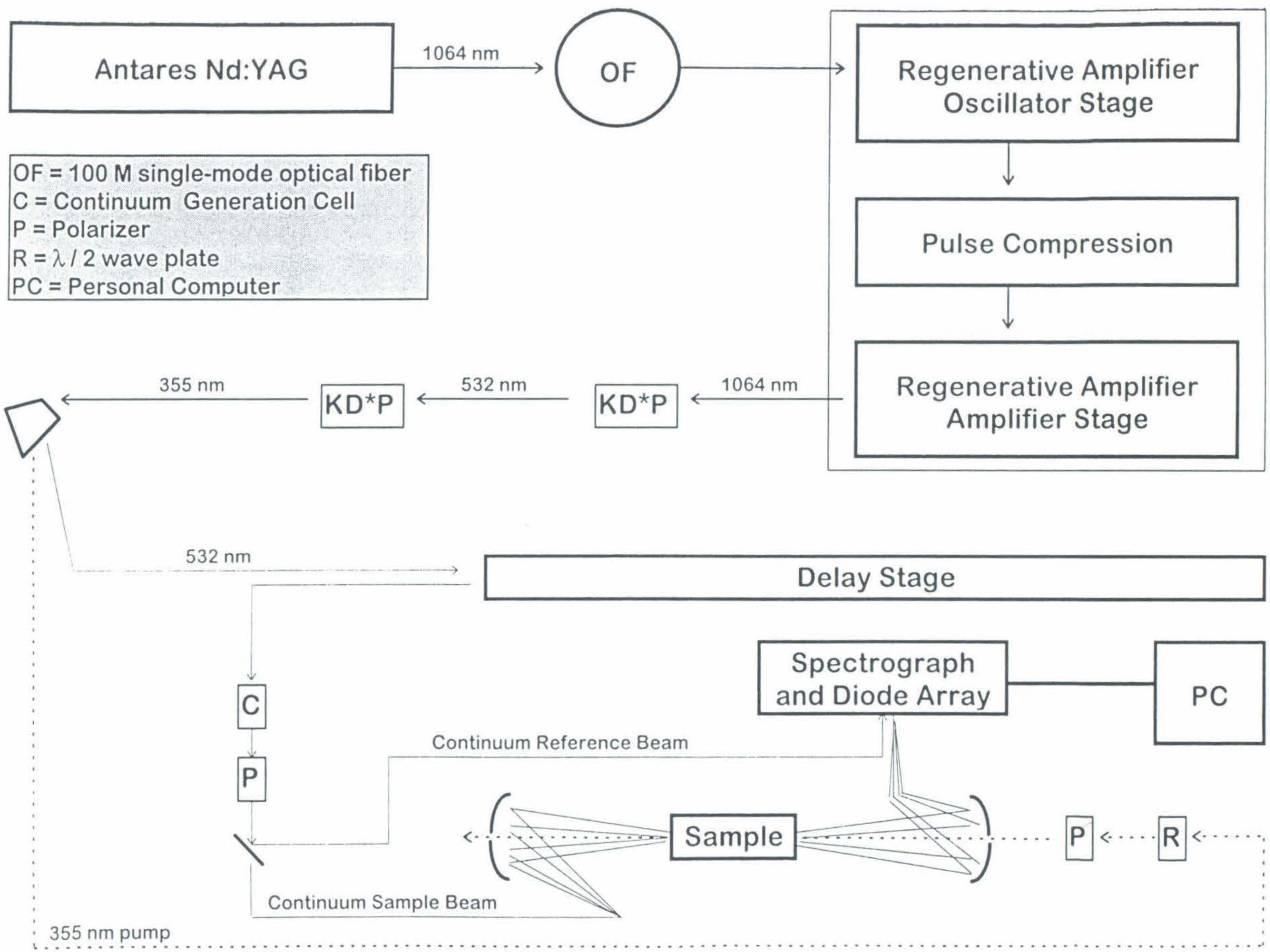
The mirrors used to focus the probe light onto the sample have holes drilled in their centers, though which the 355 nm pump light enters and exits. This ensures a perfectly collinear pump-probe geometry, but also demands sample path lengths of no more than two mm for the best system response given the pulse widths, since the pump and probe pulses interact over the entire length. The 355 nm light travels away from the spectrograph, while the probe travels towards it, hence reducing the amount of scattered pump light entering the slits. Filters placed before the spectrograph further ensure that only the probe light is collected. For these experiments, a combination of a 385 nm bandpass filter (to remove stray pump light) and BG3 filters (to remove any green light which may have passed through the 532 nm mirror before the pinhole) was used.

Sample and reference beams are collected at f15 and focused into an Acton Research (SpectraPro 275) spectrograph. A Princeton Instruments dual diode array (DPDA -1024) is used for detection; one array is used for the sample beam, and the other for the reference. The data is transferred to a PC, where it is filtered to remove sets containing overflows or negligible probe light before the sample/reference ratios are used to calculate optical density changes. A laser system is digrammed in Figure 3.19.

X-ray Data Collection. Orange blocks of $[(Ru(bpy)_2)_2tppz](PF_6)_4$ were obtained by slow diffusion of diethyl ether through a 2 mm layer of methanol into an acetonitrile solution of the complex. A single crystal was mounted on a glass fiber with silicone grease and placed in the 128 K nitrogen stream of a Siemens P4 diffractometer with an LT-2 low-temperature apparatus. A 4.5% decay in the intensities of two standard

Figure 3.19. Picosecond transient absorption apparatus.

Picosecond Transient Absorption Experiment



reflections was observed during data collection, and the data were scaled to account for this decay. The data were corrected for Lorentz and polarization effects. Crystal data are given in Table 3.1.

Structure Solution and Refinement. Calculations were performed using SHELXTL PLUS (VMS version) software. Scattering factors and corrections for anomalous dispersion were taken from a standard source.[20] An absorption correction was applied.[21] The structure was solved in the monoclinic space group C2/c by direct methods. Hydrogen atoms were added geometrically and refined using a riding model with isotropic thermal parameters equal to 0.035Å^2. The largest feature in the final difference map (0.77 e$^-$Å^{-3}) is located 1.8Å from F(6).

Table 3.1. Crystal Data for $[(Ru(bpy)_2)_2tppz](PF_6)_4 \bullet 5CH_3CN$.

Table 3.1
Crystallographic Data
$[(Ru(bpy)_2)_2tppz](PF_6)_4 \cdot 5CH_3CN$.

$C_{74}H_{59}F_{24}N_{19}P_4Ru_2$	FW = 1996.4
a = 40.903(12) Å	C2/c, monoclinic
b = 12.800(3) Å	T = 130K
c = 14.688(3) Å	$\lambda(CuK\alpha)$ = 1.54178 Å
β = 91.35(2) °	d_{calc} = 1.725 Mg/m^3
V = 7688(3) $Å^3$	transm. factors = 0.52 - 0.56
Z = 4	
$R(F_o)$ = 0.0457	
$R_w(F_o)$ = 0.0479	

$R = \Sigma \| F_o | - | F_c \| / \Sigma |F_o|$; $R_w = \Sigma \| F_o | - | F_c \| w^{1/2} / \Sigma | F_o | w^{1/2}$

Results and Discussion

Synthesis

As shown by the synthesis of the ligands in Chapter 2, condensation of phendione with polyamines is a simple, versatile method for obtaining novel metal-coordinating ligands. Binucleating ligands can be constructed by condensing two equivalents of phendione to a tetramine spacer, as with tatpp and tpbpz, or by directly coupling two molecules of phendione to each other in the presence of the ammonia formed by the thermal decomposition of formamide. The series of ligands so formed allows the study of ground- and excited-state electronic interaction of coordinated transition metal centers as a function of metal-metal separation.

Due to their large planar structures, the ligands are soluble only at elevated temperatures in ethylene glycol, and even then only slightly so. While this is not a problem when making homodinuclear compounds, it presents a difficulty when coordination at only one site is desired; the incoming $M(bpy)_2Cl_2$ fragment, which is freely soluble, is present in excess of the number of coordination sites, leading to unwanted formation of the dimetallic compound. Using an excess of ligand in a large reaction volume reduces the amount of dimer formed; chromatography and recrystallization can be used to separate mono- and bi-metallic species. The overall yield is unavoidably low, however. The extremely low solubility of tatpp prevented synthesis of monomeric, and thus heterodimetallic, derivatives.

Once the monomeric species has been obtained, any metal capable of coordinating a diimine can be attached at the vacant site. $CuCl_2$ is especially attractive because the heterodinuclear complex precipitates from ethanol solution, requiring no further purification. $M(bpy)_2Cl_2$, as shown by the synthesis of homodimers, can also be easily placed at the second coordination site. The variety and versatility of tetrapyrido-phenazines allows the synthesis of an extensive series of compounds.

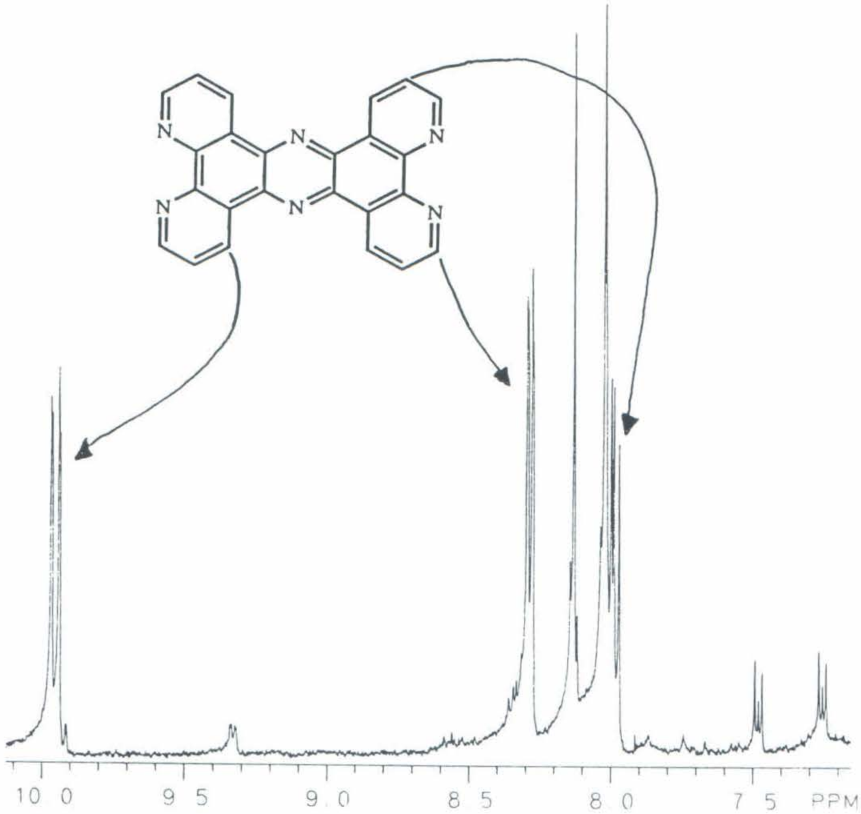
Characterization

Interpretation of the complicated [1]H NMR of these compounds is simplified by synthesizing bpy-d_8 derivatives of the Ru homodimers. One then sees only the resonances due to the bridging ligand, which can be picked out in the spectrum of the corresponding undeuterated compound; the remaining resonances, due to bpy, can then be assigned. The assigned [1]H NMR of the bpy-d_8 and bpy forms of Ru_2tppz, Ru_2tatpp, and Ru_2tpbpz are shown, respectively, in Figures 3.20-22. In asymmetric compounds, two sets of bridging ligand resonances are observed, reflecting the two different coordination environments; RuOs compounds also exhibit two complete sets of bpy resonances. These differences are shown comparatively by the spectra of Ru_2tppz, Ru•tppz, and Ru•tppz•Os in Figure 3.23. The [1]H NMR spectra of all compounds for which data could be obtained agree with their proposed structures.

An ORTEP drawing of the x-ray crystal structure of $(Ru_2tppz)(PF_6)_4 \cdot 5CH_3CN$ is presented in Figure 3.24. Thermal ellipsoids are drawn at 50% probability. Atomic coordinates and equivalent displacement coefficients are presented in Table 3.2, selected bond lengths and angles in Table 3.3. The asymmetric unit contains one-half molecule of the dimer, 2 PF_6^- ions, and 2.5 molecules of acetonitrile. The half-molecule of acetonitrile is disordered across a 2-fold rotation axis. As seen in Figure 3.25, the tppz ligand is twisted; deviations of the tppz atoms from the mean plane of the complex are presented in Figure 3.26. This distortion is not due to intermolecular interactions or other packing effects; it is the lowest-energy conformation of the complex. It is surprising that such an extended aromatic system is not planar. MOPAC geometric optimization of the dipyridophenazine ligands in Chapter 2 showed their lowest-energy conformations to deviate slightly from planarity; perhaps the effect is magnified here.

Uv-Vis spectroscopy shows that, like dipyridophenazines, tetrapyridophenazines contain orbitals of bpy character; MLCT bands of $M(bpy)_2$-containing derivatives are not

Figure 3.20. 300 MHz ^{1}H NMR spectra of bpy-d_8 Ru_2tppz (top) and Ru_2tppz. Assignments are indicated by arrows.


N
N
N
N
N
N
10.0
9.5
9.0
8.5
8.0
7.5
PPM

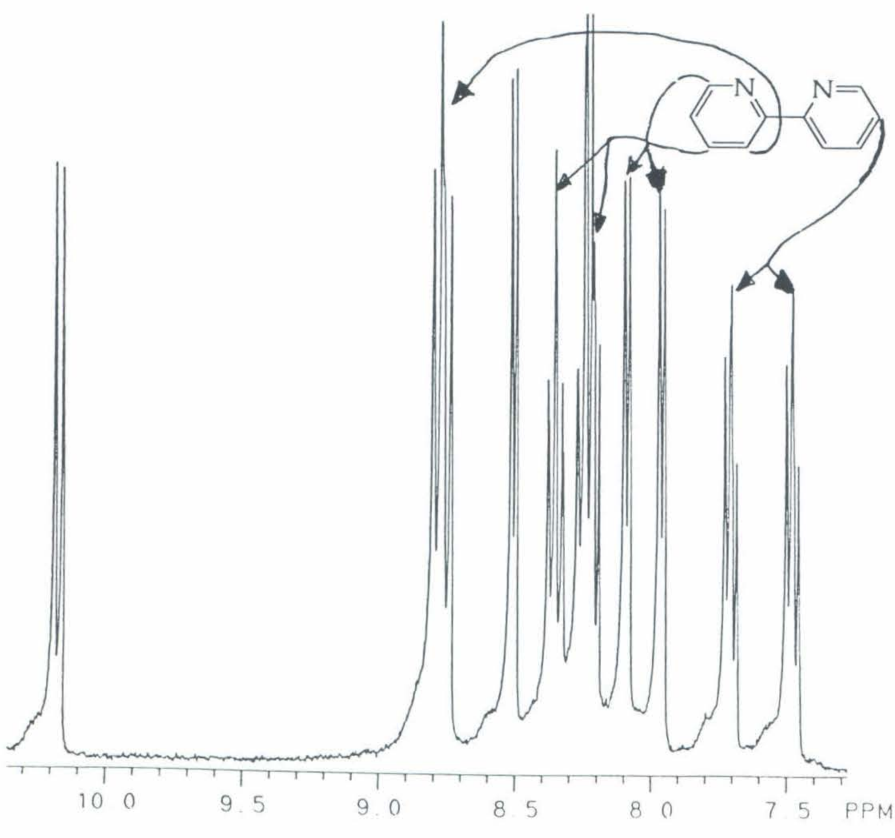
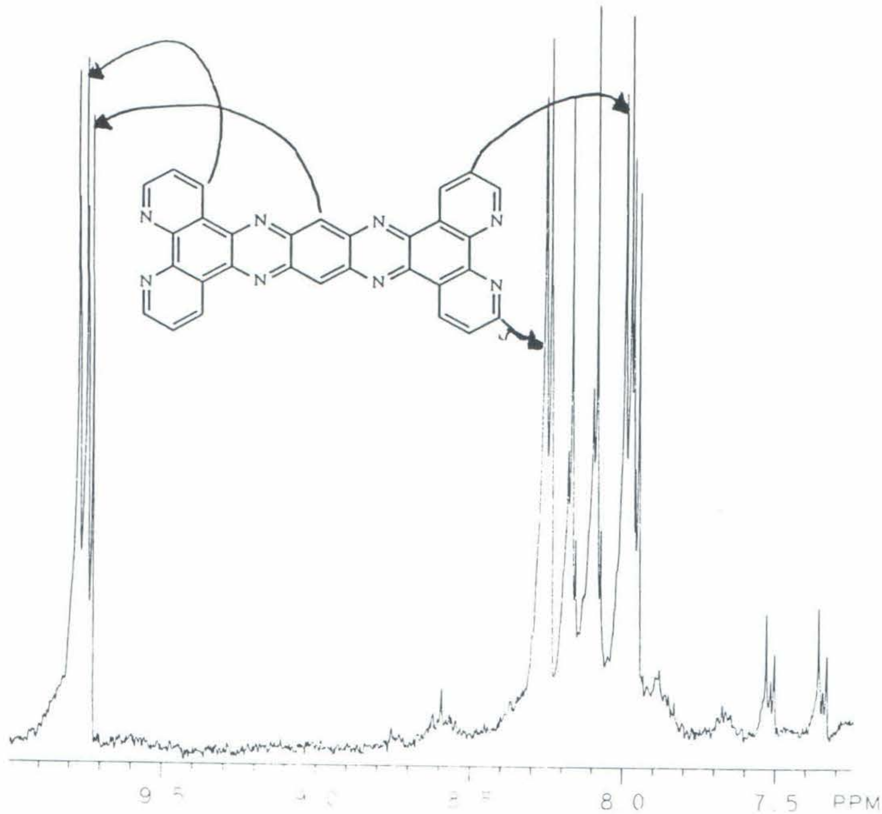

N
N
10.0
9.5
9.0
8.5
8.0
7.5
PPM

Figure 3.21. 300 MHz ^{1}H NMR spectra of bpy-d_8 Ru_2tatpp (top) and Ru_2tatpp. Assignments are indicated by arrows.


N
9.5
8.0
7.5
PPM

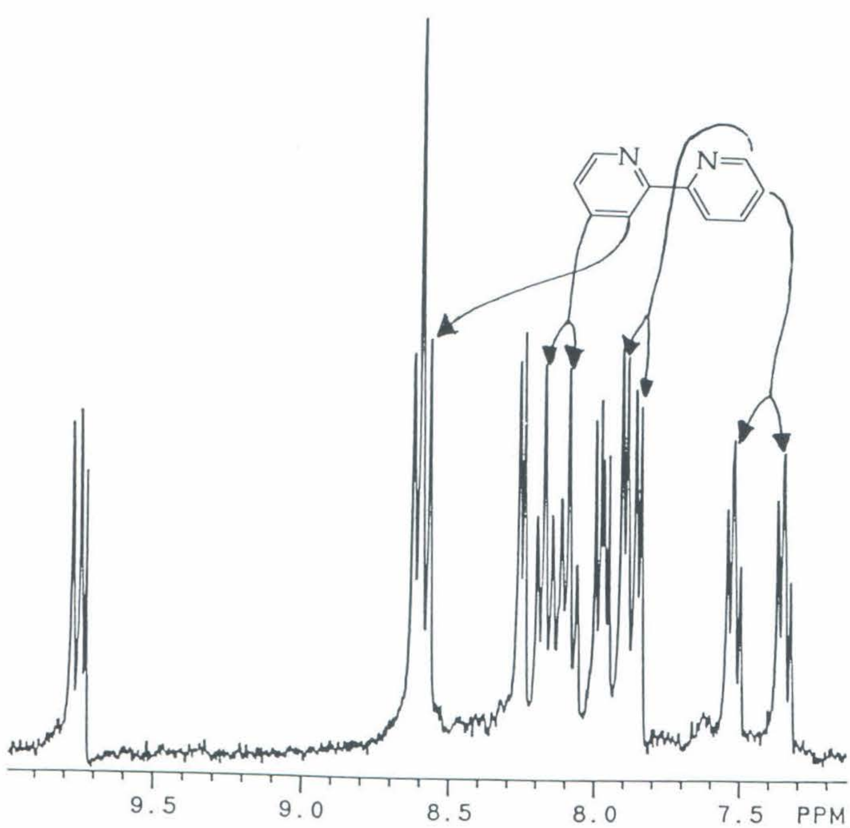
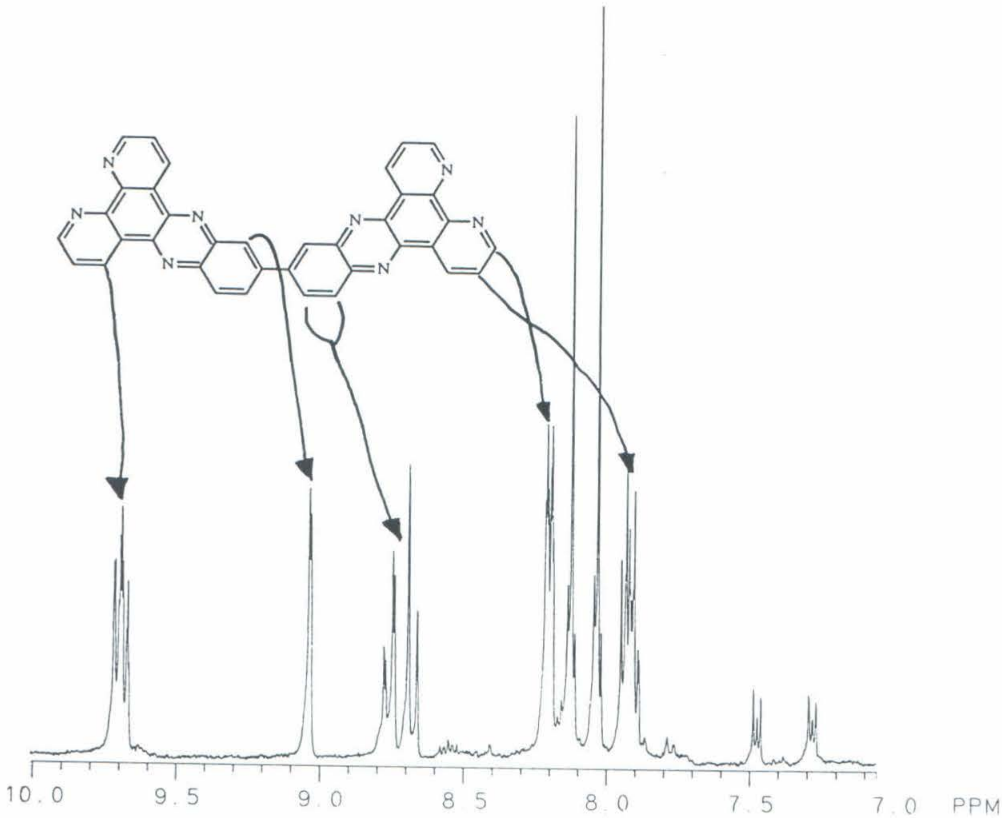

N
9.5
9.0
8.5
8.0
7.5
PPM

Figure 3.22. 300 MHz ^{1}H NMR spectra of bpy-d_8 Ru_2tpbpz (top) and Ru_2tpbpz. Assignments are indicated by arrows.


N
N
N
N
N
N
N
N
N
N
N
N
10.0
9.5
9.0
8.5
8.0
7.5
7.0
PPM

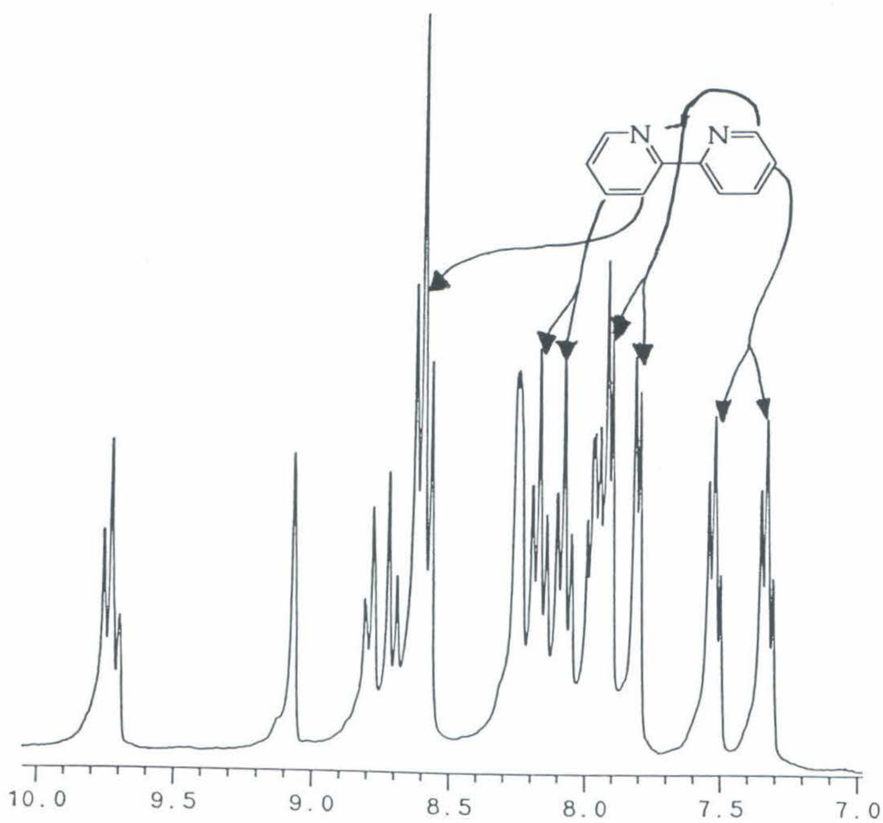
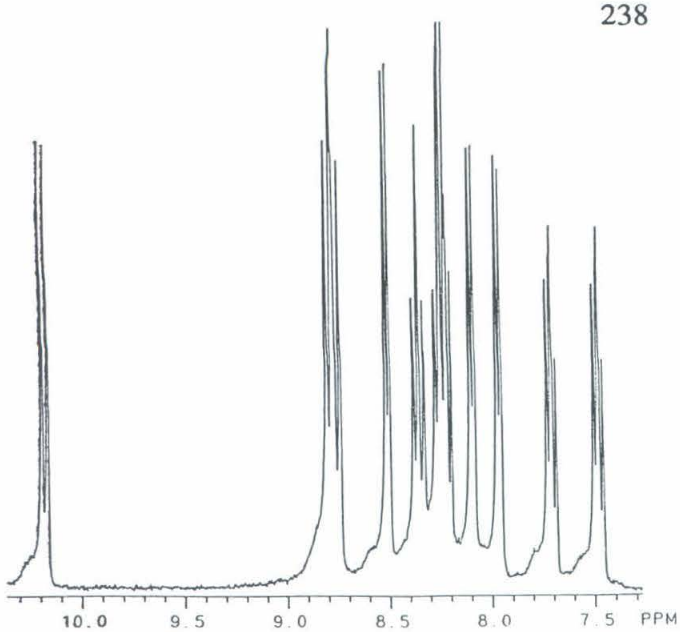
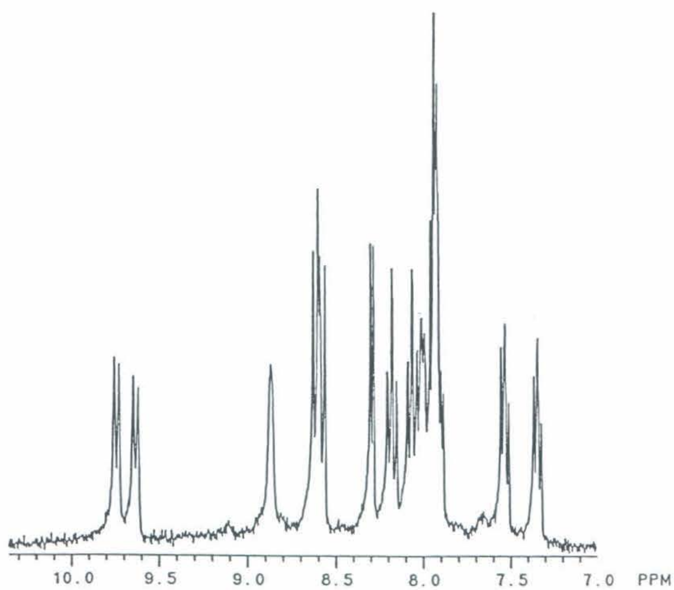

N
N
10.0
9.5
9.0
8.5
8.0
7.5
7.0

Figure 3.23. 300 MHz ^{1}H NMR spectra of (top to bottom) Ru_2tppz, Ru•tppz and Ru•tppz•Os.


10.0
9.5
9.0
8.5
8.0
7.5
PPM


10.0
9.5
9.0
8.5
8.0
7.5
7.0
PPM

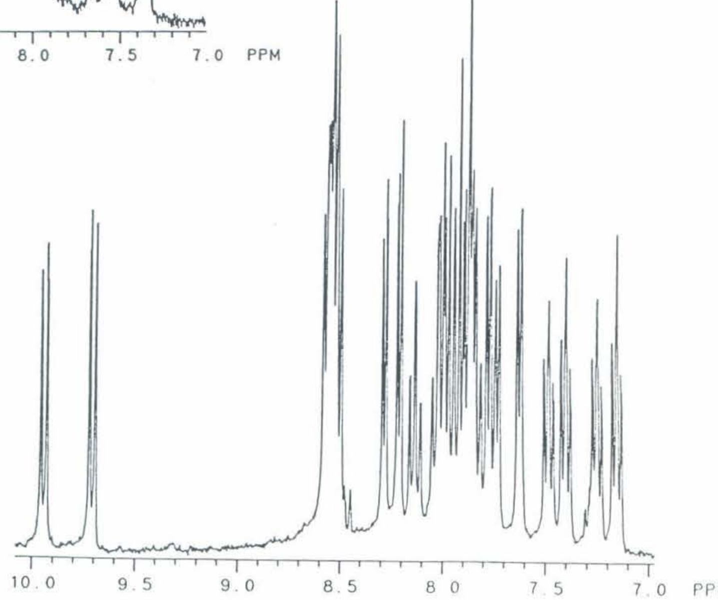

10.0
9.5
9.0
8.5
8.0
7.5
7.0
PPM

Figure 3.24. ORTEP drawing of $(Ru_2tppz)(PF_6)_4{\bullet}5CH_3CN$. Thermal ellipsoids are drawn at 50% probability.

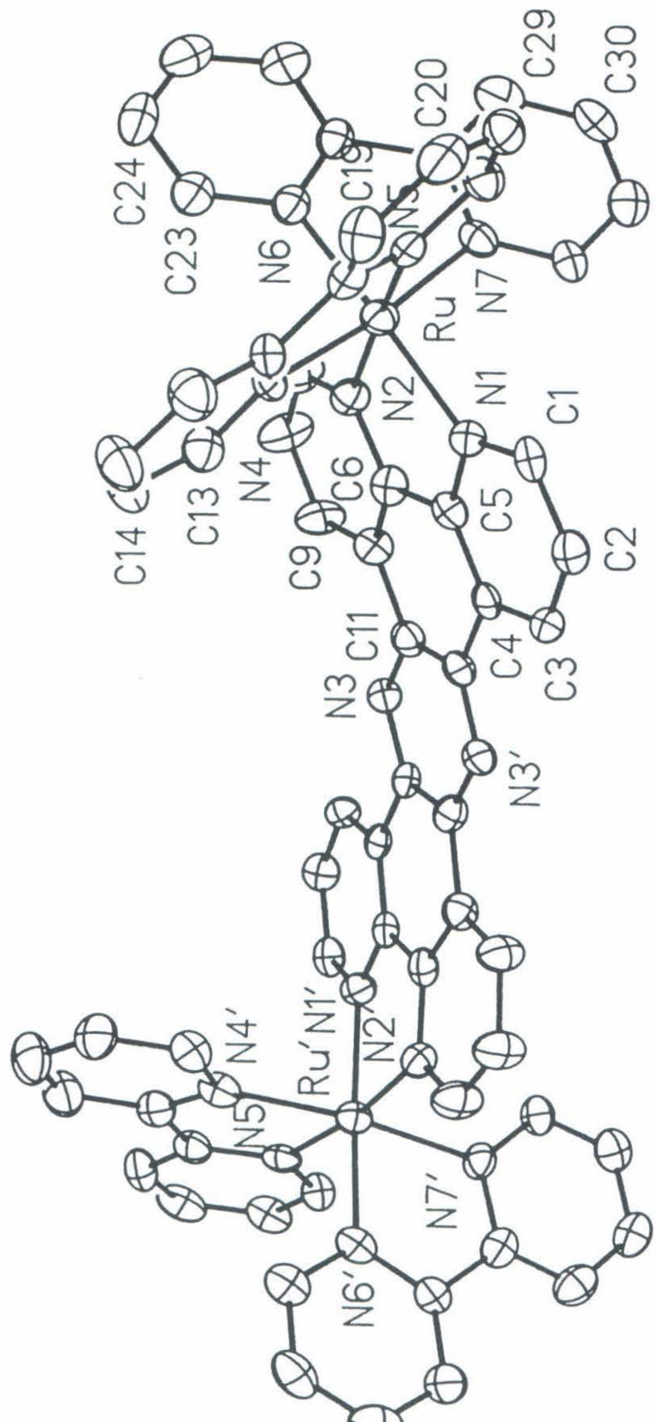

C29
C30
C20
C24
C23
N6
N7
Ru
N1
N2
C1
C14
C13
N4
C6
C5
C2
C9
C11
C4
C3
N3
N3′
N4′
Ru′
N1′
N2′
N5
N7′
N6′

Figure 3.25. Another view of the structure of $(Ru_2tppz)(PF_6)_4{\bullet}5CH_3CN$ emphasizing the twisting of the tppz ligand.

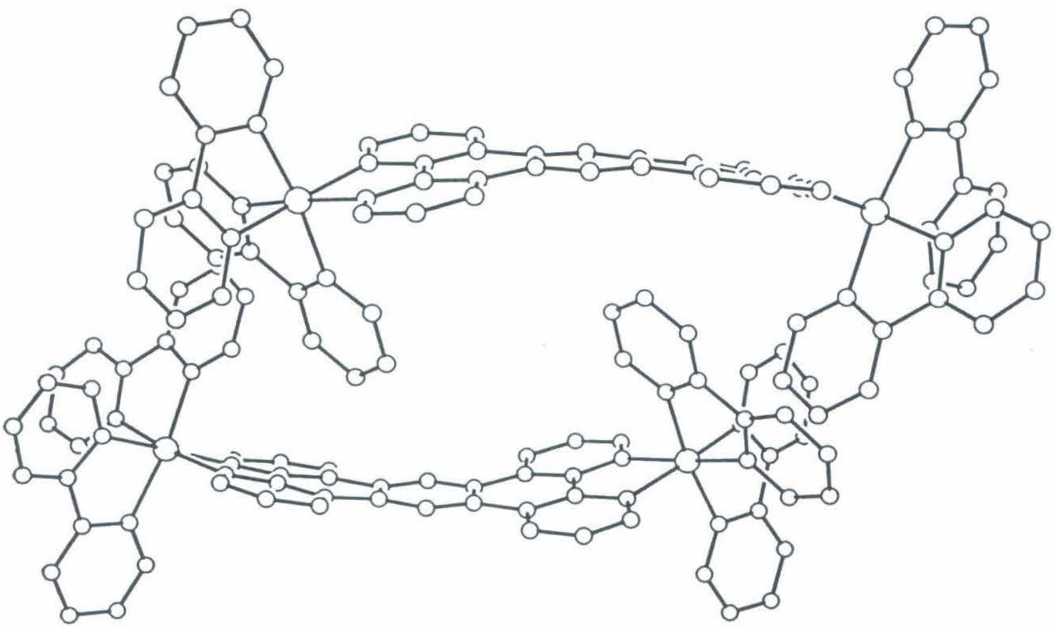


Figure 3.26. Deviations from planarity (Å x 10^2) of the tppz atoms of $(Ru_2tppz)(PF_6)_4$•
$5CH_3CN$.

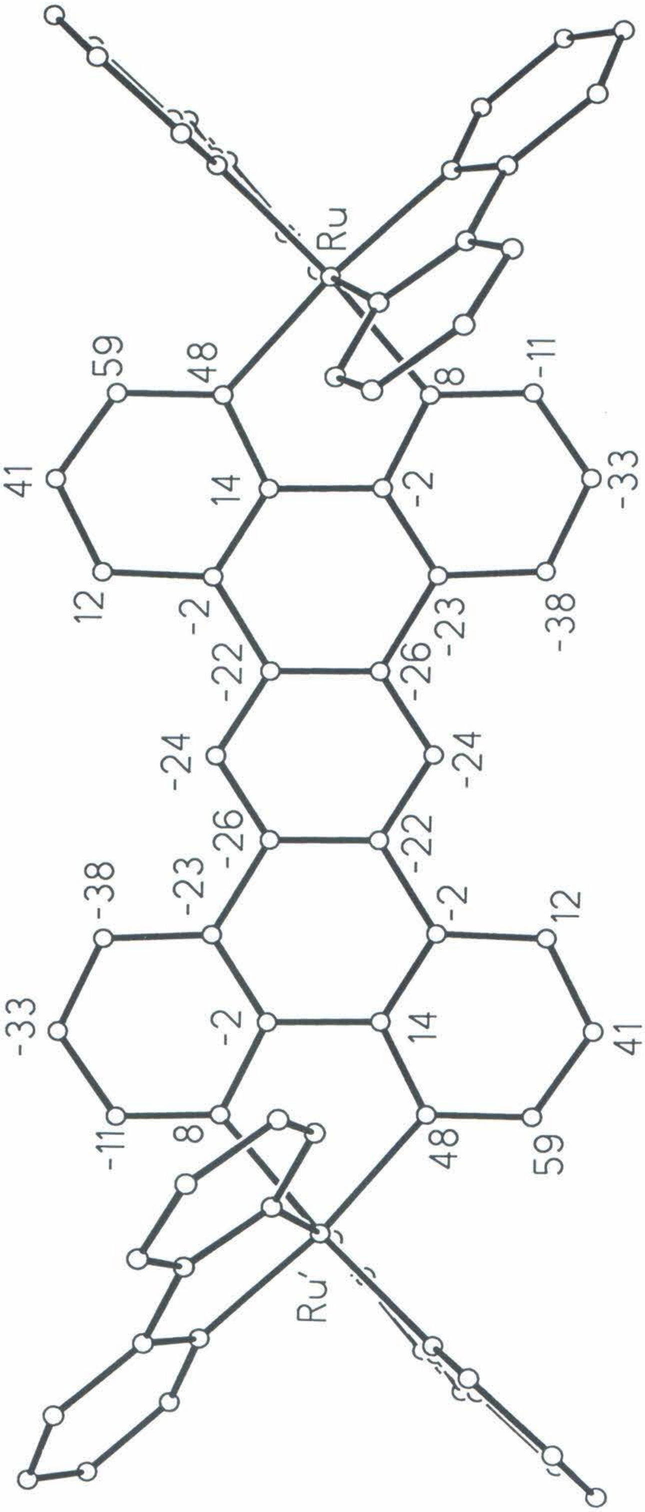

Ru
Ru'
59
48
-11
8
41
14
-2
-33
12
-2
-23
-38
-22
-26
-24
-24
-26
-22
-38
-23
-2
12
-33
-2
14
41
-11
8
48
59

Table 3.2. Atomic coordinates and displacement coefficients for $(Ru_2tppz)(PF_6)_4$• 5 CH_3CN.

Table 3.2.

Atomic Coordinates (x 10^4) and Equivalent Displacement Coefficients ($Å^2$ x 10^3) for $(Ru_2tppz)(PF_6)_4$• $5CH_3CN$.

	x	y	z	U(eq)*
Ru	1337(1)	2070(1)	9696(1)	27(1)
N(1)	869(1)	1530(4)	9935(3)	27(2)
N(2)	1170(1)	1840(4)	8380(3)	30(2)
N(3)	164(1)	1276(4)	6676(3)	25(2)
N(4)	1142(1)	3550(4)	9832(3)	30(2)
N(5)	1446(1)	2390(5)	11039(3)	28(2)
N(6)	1794(1)	2572(5)	9347(3)	30(2)
N(7)	1588(1)	670(4)	9641(3)	29(2)
C(1)	722(2)	1380(5)	10733(4)	28(2)
C(2)	390(2)	1206(5)	10794(4)	32(2)
C(3)	193(2)	1173(5)	10022(4)	26(2)
C(4)	345(2)	1283(5)	9181(4)	23(2)
C(5)	676(2)	1452(5)	9159(4)	24(2)
C(6)	844(2)	1574(5)	8302(4)	27(2)
C(7)	1331(2)	1927(6)	7606(4)	41(3)
C(8)	1185(2)	1786(6)	6759(4)	43(3)
C(9)	857(2)	1558(6)	6679(4)	36(3)
C(10)	679(2)	1451(5)	7481(4)	28(2)
C(11)	326(2)	1297(5)	7481(4)	28(2)
C(12)	159(2)	1259(5)	8306(4)	24(2)
C(13)	986(2)	4105(6)	9177(4)	36(3)
C(14)	872(2)	5102(6)	9317(5)	43(3)
C(15)	903(2)	5545(6)	10167(5)	49(3)
C(16)	1049(2)	4968(6)	10856(5)	46(3)
C(17)	1168(2)	3973(6)	10675(4)	31(2)
C(18)	1340(2)	3313(6)	11362(4)	33(2)
C(19)	1394(2)	3602(6)	12275(4)	38(3)
C(20)	1561(2)	2929(7)	12843(5)	43(3)
C(21)	1670(2)	1985(6)	12515(5)	38(3)
C(22)	1607(2)	1738(6)	11617(4)	32(2)
C(23)	1878(2)	3574(6)	9181(4)	37(3)
C(24)	2188(2)	3847(7)	8916(4)	45(3)
C(25)	2416(2)	3085(7)	8824(4)	45(3)
C(26)	2343(2)	2056(7)	9013(5)	40(3)
C(27)	2030(2)	1832(5)	9269(4)	29(2)
C(28)	1917(2)	773(6)	9463(4)	32(2)
C(29)	2115(2)	-93(6)	9487(4)	41(3)
C(30)	1984(2)	-1082(6)	9656(4)	37(3)
C(31)	1656(2)	-1159(6)	9785(4)	37(3)
C(32)	1466(2)	-275(6)	9772(4)	31(2)

*Equivalent isotropic U defined as one third of the orthogonalized trace of the orthogonalized U_{ij} tensor.

Table 3.3. Selected bond lengths and angles for $(Ru_2tppz)(PF_6)_4 \cdot 5CH_3CN$.

Table 3.3

Selected Bond Lengths (Å) and Angles (deg) for $(Ru_2tppz)(PF_6)_4\bullet 5CH_3CN$.

Bond Lengths

Ru-N(1)	2.076 (5)	Ru-N(2)	2.057 (5)
Ru-N(4)	2.067 (6)	Ru-N(5)	2.053 (5)
Ru-N(6)	2.051 (5)	Ru-N(7)	2.067 (6)
N(1)-C(1)	1.343 (8)	N(1)-C(5)	1.373 (7)
N(2)-C(6)	1.381 (8)	N(2)-C(7)	1.332 (8)
N(3)-C(11)	1.340 (7)	C(12)-N(3')	1.324 (8)
C(1)-C(2)	1.379 (9)	C(2)-C(3)	1.376 (8)
C(3)-C(4)	1.403 (8)	C(4)-C(5)	1.374 (8)
C(4)-C(12)	1.477 (8)	C(5)-C(6)	1.456 (8)
C(6)-C(10)	1.376 (8)	C(7)-C(8)	1.380 (9)
C(8)-C(9)	1.374 (9)	C(9)-C(10)	1.406 (9)
C(10)-C(11)	1.459 (9)	C(11)-C(12)	1.406 (8)

Bond Angles

N(1)-Ru-N(2)	79.8(2)	N(1)-Ru-N(4)	85.9(2)
N(2)-Ru-N(4)	95.8(2)	N(1)-Ru-N(5)	94.7(2)
N(2)-Ru-N(5)	172.5(2)	N(4)-Ru-N(5)	78.5(2)
N(1)-Ru-N(6)	175.2(2)	N(2)-Ru-N(6)	95.4(2)
N(4)-Ru-N(6)	95.4(2)	N(5)-Ru-N(6)	90.0(2)
N(1)-Ru-N(7)	100.3(2)	N(2)-Ru-N(7)	89.6(2)
N(4)-Ru-N(7)	172.4(2)	N(5)-Ru-N(7)	96.5(2)
N(6)-Ru-N(7)	78.8(2)	Ru-N(1)-C(1)	129.0(4)
Ru-N(1)-C(5)	113.4(4)	C(1)-N(1)-C(5)	117.0(5)
Ru-N(2)-C(6)	114.3(4)	Ru-N(2)-C(7)	129.1(4)
C(6)-N(2)-C(7)	116.5(5)	N(3)-C(11)-C(10)	118.0(5)
N(3)-C(11)-C(12)	121.4(5)	C(10)-C(11)-C(12)	120.3(5)
C(4)-C(12)-C(11)	120.0(5)	C(4)-C(12)-N(3')	118.4(5)
C(11)-C(12)-N(3')	121.4(5)		

shifted relative to $M(bpy)_3^{2+}$. MLCT extinction coefficients for monomers are roughly half that of the corresponding homometallic dimers. The spectra of heteronuclear dimers are more or less the sum of the spectra of their component monomers, as shown for Ru•tppz•Os in Figure 3.27. RuCu dimers exhibit the same weak absorbance at low energy as $Cu(phen)Cl_2$. In all cases, Uv-Vis spectroscopy shows that coordination of a second metal does not perturb the electronic structure of the first, providing an initial indication that interaction between the two metal centers is very small if not nonexistent. In the presence of electron delocalization, absorbances shift to longer wavelengths. In a $Ru(bpy)_2$ - based trimer with strongly-communicating metal centers, the MLCT maximum shifts to 600 nm.[22]

Once again, the bpy character of the tetrapyridophenazine ligands is shown in the emission properties of their Ru-containing derivatives; emission maxima are the same as $Ru(bpy)_3^{2+}$. Ru•tppz is an intensely emissive compound, having an emission quantum yield 1.5 times that of the 4% yield of $Ru(bpy)_3^{2+}$. Interestingly, Ru homodimers are less emissive than their mononuclear counterparts; heterometallic compounds also have less-intense emission than their parent Ru monomers. In contrast to $Os(bpy)_3^{2+}$, mono- and heterodinuclear Os complexes of these ligands show no emission. Emission properties will be discussed in the treatment of energy- and electron transfer in these compounds. Absorption and emission data for the complexes discussed in this chapter are given in Table 3.4.

While UV-visible spectroscopy gives an indication of the degree of interaction between coordinated metals in dinuclear derivatives, electrochemistry provides a direct measure of intermetal communication. The CVs of Os_2- and Ru_2tppz are shown in Figure 3.28. In both, a single 2-electron wave is seen for the $M^{3+/2+}$ couple. Recalling the electrochemical behavior of coupled systems, it is clear that there is very little, if any, metal-metal interaction in these dimers. The more-sensitive differential-pulse method shows that the metals are essentially uncoupled. Figure 3.29 shows the differential-pulse

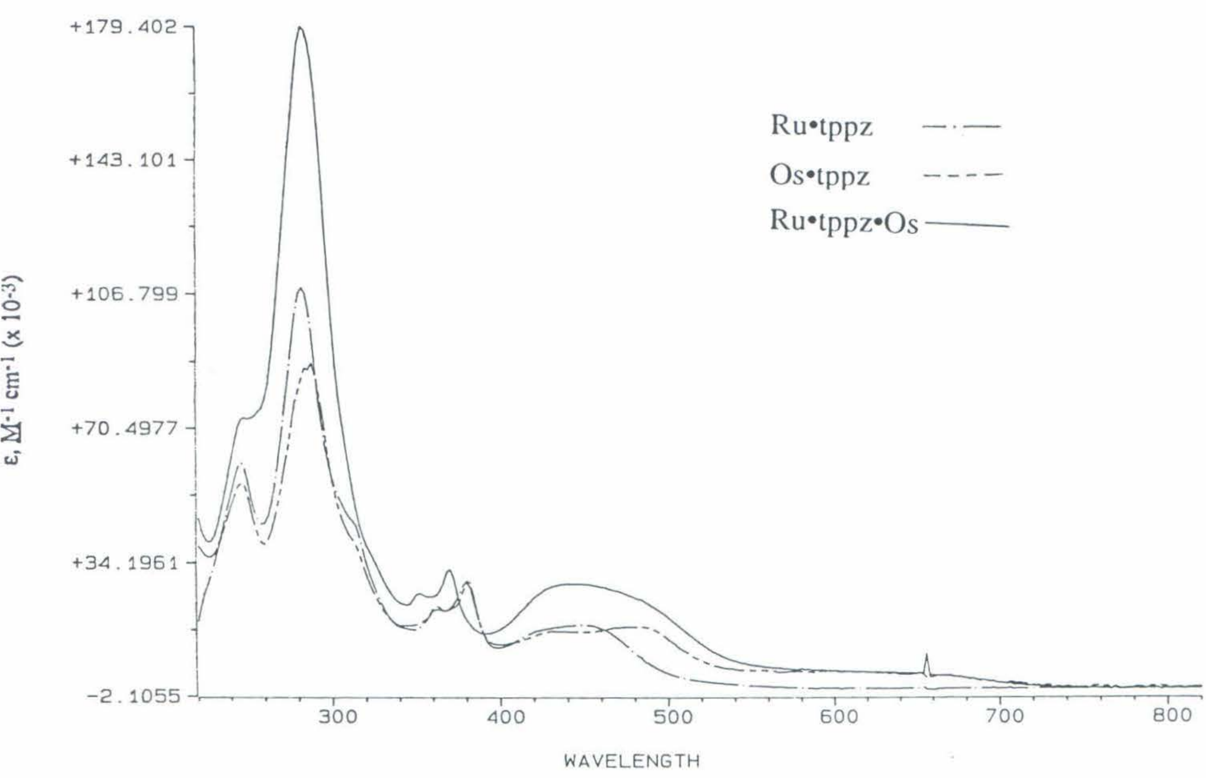


Figure 3.27. Uv-Vis spectrum of equimolar solutions of Ru•tppz, Os•tppz, and Ru•tppz•Os.

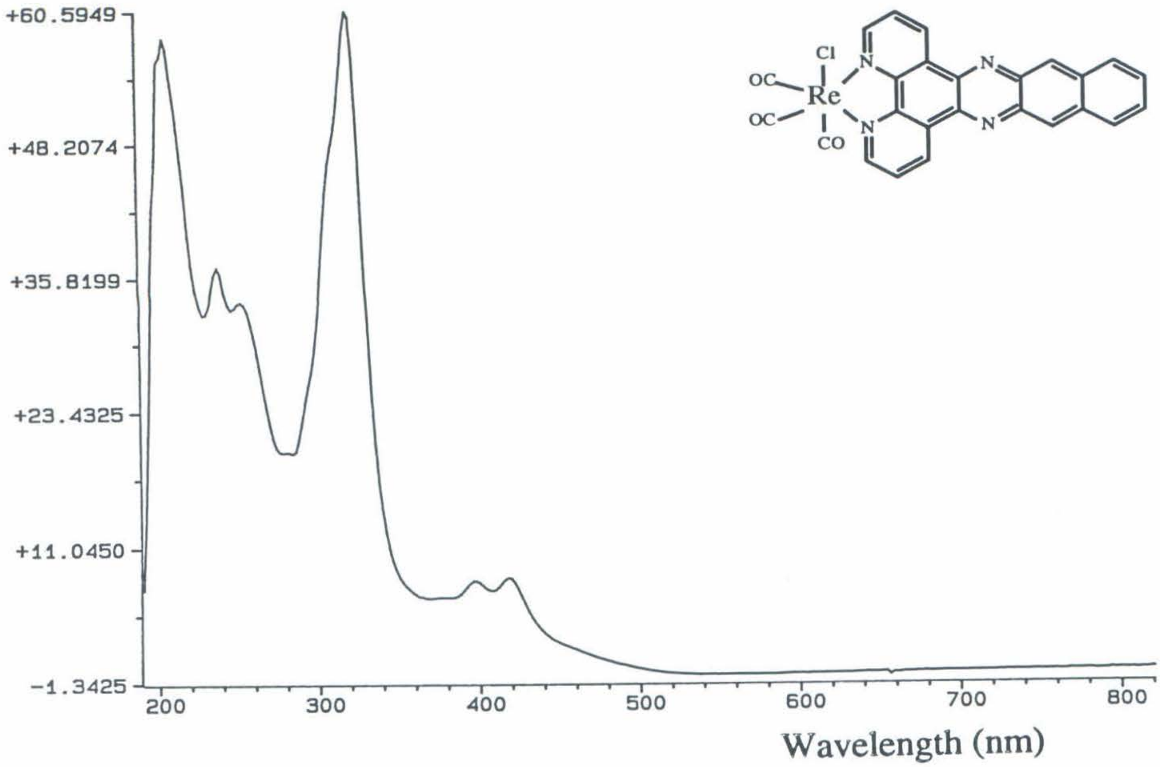
Table 3.4. Absorption and emission data for acetonitrile solutions of compounds.

Table 3.4

Absorption and Emisson in acetonitrile solution. λ, nm; ε, M^{-1} cm^{-1} x 10^{-3}.

Compound	**bpy π–π***	**"pz"**	**MLCT**	**λ_{em}**	**I_{rel}**	**Other**
$Ru(bpy)_3^{2+}$	286, 102.4		450, 14.0	618	100	
$Os(bpy)_3^{2+}$	290, 78.0		579, 3.27	743	2.2	
$Cu(phen)Cl_2$						ε_{746}=0.050
Ru•tppz	282, 108.6	362, 21.5	448, 17.3	609	154	I_{rel}=105
		380, 28.9				in dmso
Os•tppz	288, 88.3	362, 22.4	608, 4.63		0	
		380, 29.1				
Ru_2tppz	282, 160.2	352, 24.5	442, 34.4	624	17	
		370, 31.1				
Os_2tppz	286, 124.0	352, 28.3	600, 8.19		0	
		370, 35.9				
Ru•tppz•Os	282, 179.4	352, 25.8	440, 28.4	610	7.9	
		370, 32.4	600, 4.71			
Ru•tppz•Cu	286, 99.9	364, 19.8	440, 10.4	624	3.1	ε_{736}=0.194
in dmso		382, 26.0				
Ru_2tatpp	286, 118.6	424, 48.3	444, 72.4	620	1.9	MLCT and
	324, 116.9	444, 72.4				pz overlap
Ru•tpbpz	290, 119.6	406, 58.4	442, 23.0	624	84	I_{rel}=5.1
						in dmso
Ru_2tpbpz	288, 130.6	406, 49.6	442, 34.0	624	28	
Os_2tpbpz	292, 132.1	404, 50.4	600, 8.16		0	
RuOs tpbpz	290, 112.7	404, 52.3	442, 31.32	629	14	
	310, 90.2		592, 4.32			
Ru•tpbpz•Cu	290, 87.6	412, 32.7	448, 11.7	638	0.6	ε_{824}=0.142

Figure 3.28. Cyclic voltammagrams of Os_2tppz (top) and Ru_2tppz.


+60.5949
+48.2074
+35.8199
+23.4325
+11.0450
-1.3425
200
300
400
500
600
700
800
Wavelength (nm)
Cl
OC
Re
OC
CO
N
N
N
N

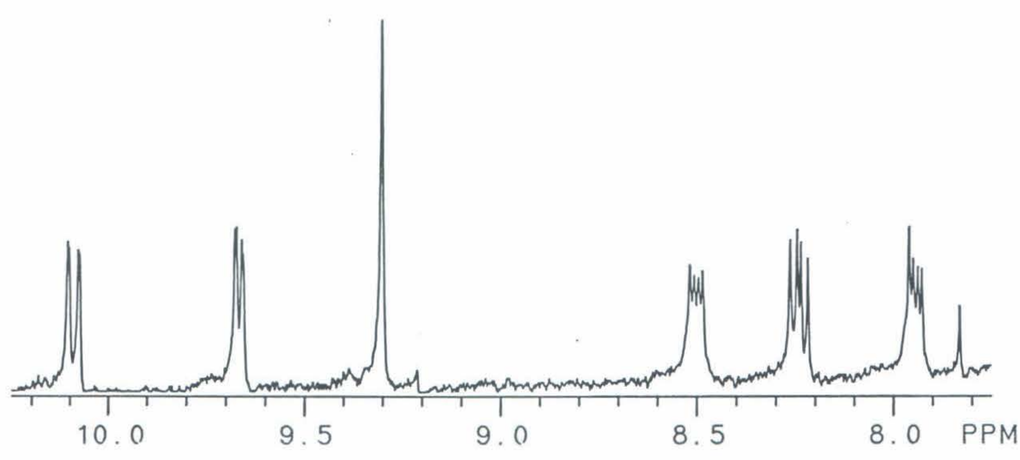
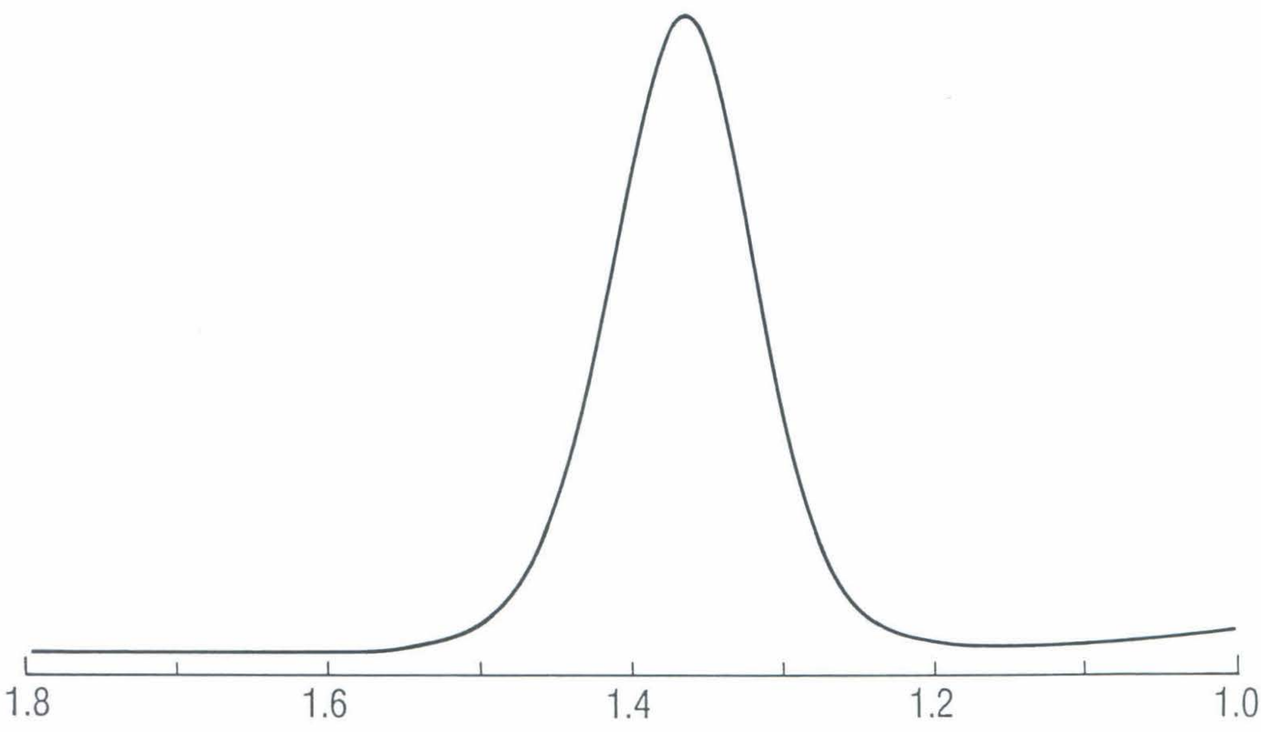

10.0
9.5
9.0
8.5
8.0
PPM

Figure 3.29. Differential-pulse voltammagram of Ru_2tppz.


1.8
1.6
1.4
1.2
1.0

voltammagram of Ru_2tppz; the sharp peak indicates that the metals are reduced independently of one another. The near-IR spectrum of electrochemically-generated mixed-valence $Ru^{II}Ru^{III}$tppz is featureless out to 2000 nm.

Given that no coupling is seen at the shortest metal-metal separation in the series of three ligands, it is not surprising that Ru_2tatpp and Ru_2tpbpz, whose CVs are presented in Figure 3.30, possess no metal-metal interaction. The first tpbpz-centered reductions of Ru_2tpbpz provide an interesting look into the nature of coupling through the ligand bridge. If the two linked dppz units were strongly coupled to each other, one would expect to see two reduction waves separated by approximately 0.5 V, as in a molecule like methyl viologen.[23] The separation in tpbpz is much less, indicating that the dppz units are not coupled very well. As with bdppz, electrons density is not evenly distributed throughout the ligand, underscoring the unique electronic properties of these systems.

As a consequence of the lack of metal-metal interaction, the CV of Ru•tppz•Os, Figure 3.31, is the superposition of the CVs of the two homodinuclear complexes. Also shown in the figure is the reversible $Cu^{2+/+}$ couple of Ru•tppz•Cu. The electrochemical data for the series of tppz derivatives, representative of the behavior of all tetrapyrido-phenazine complexes, are laid out in Table 3.5.

Temperature-dependent magnetic susceptibility measurements confirm that the metals in bimetallic complexes do not see each other. A plot of $1/\chi$ versus temperature over the range of 1.8 - 300 K is presented in Figure 3.32. Recalling Figure 3.6, a straight line in such a plot results from the complete lack of (anti)ferromagnetic coupling. Thus it is amply proven that there is no electron delocalization in dinuclear complexes of tppz. Since this was the ligand most likely to give rise to metal-metal coupling, investigations of coupling in tatpp and tpbpz were not pursued.

This work was carried out simultaneously with that presented in Chapter 2; it was conceived before investigation of Re and Ru complexes revealed the unusual ground-

Figure 3.30. Cyclic voltammagrams of Ru_2tatpp (top) and Ru_2tpbpz.

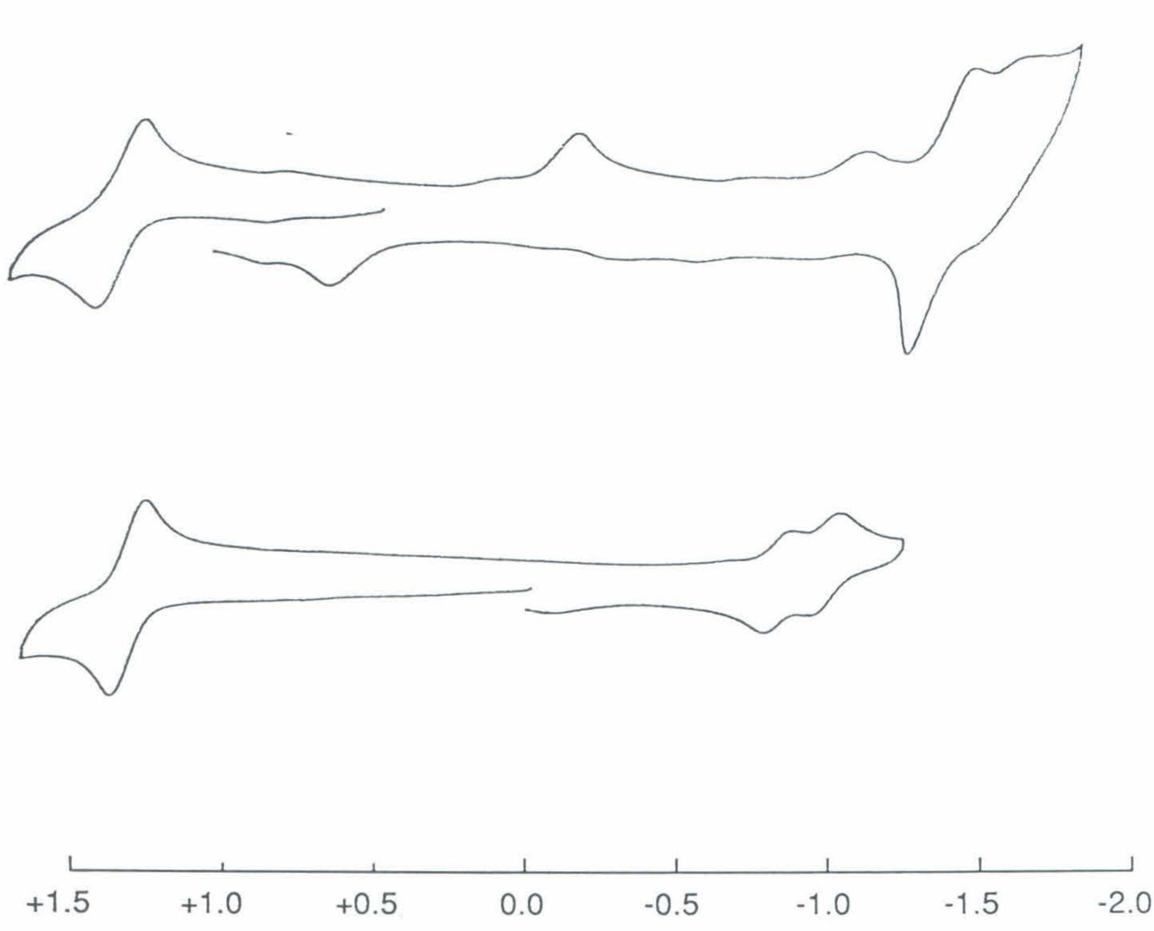

+1.5
+1.0
+0.5
0.0
-0.5
-1.0
-1.5
-2.0

Figure 3.31. Cyclic voltammagrams of Ru•tppz•Os (top) and the $Cu^{2+/+}$ couple of Ru•tppz•Cu. Cyclic voltammetry of Ru•tppz•Cu was performed in 0.1 M TBAH/ dmso.

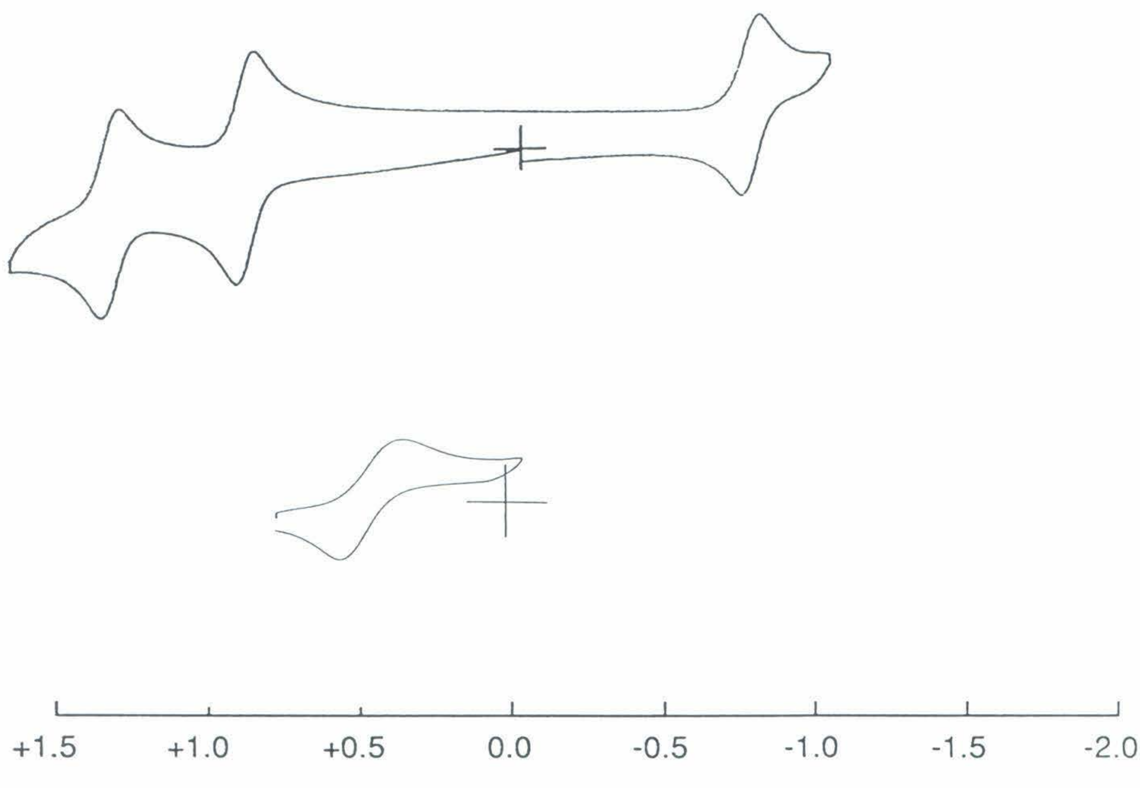
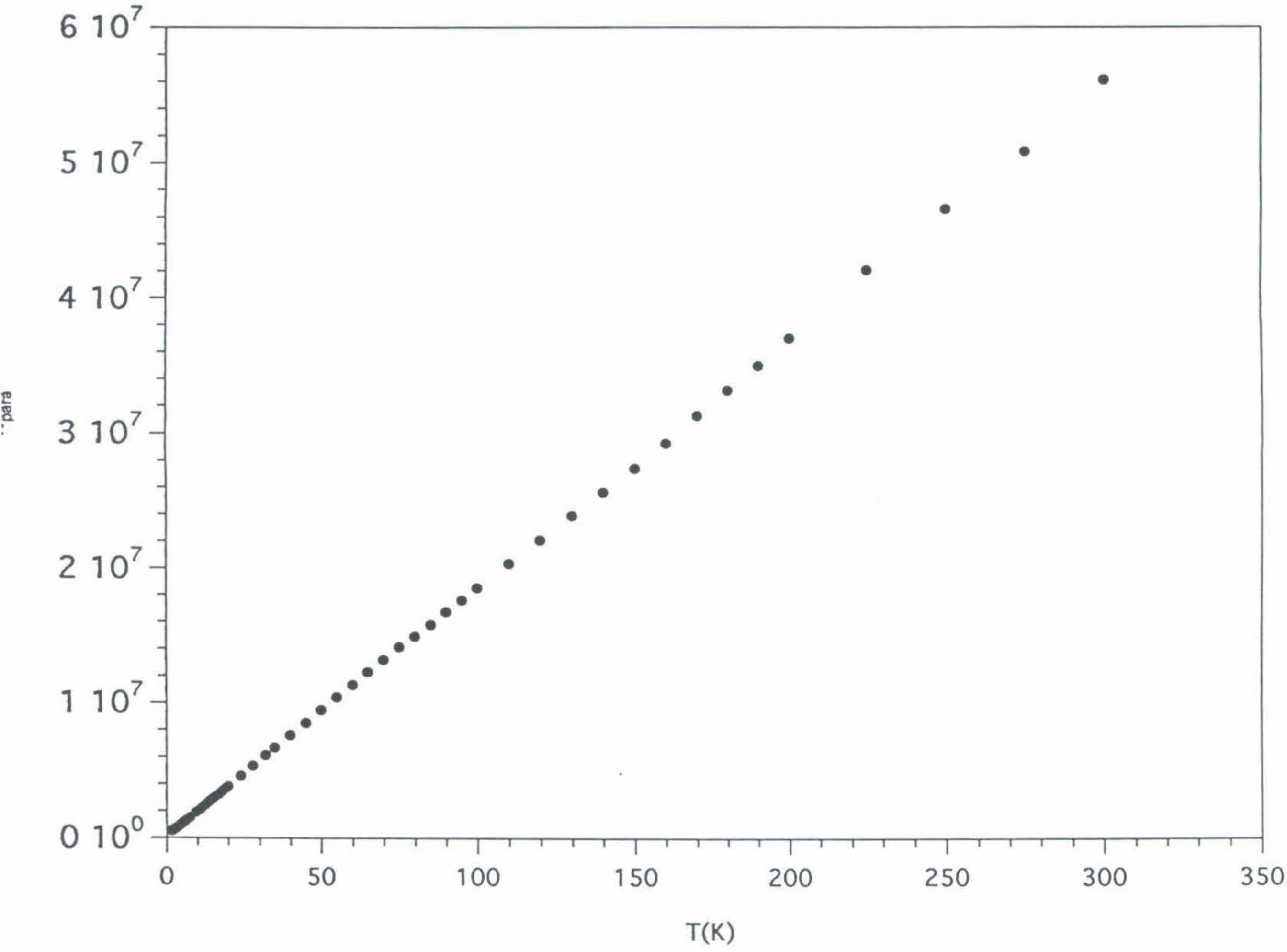

+1.5
+1.0
+0.5
0.0
-0.5
-1.0
-1.5
-2.0

Table 3.5. Electrochemical data for tppz complexes.

Table 3.5. Electrochemical Data for tppz Derivatives.

Compound	$M^{3+/2+}$	"pz"	"bpy"
Ru•tppz	+1.36	-0.76	-1.34
Ru_2tppz	+1.36	-0.77	-1.34
Os_2tppz	+0.90	-0.76	-1.31
Ru•tppz•Os	+1.36, +0.90	-0.76	-1.34
Ru•tppz•Cu	+0.30 ($Cu^{2+/+}$, dmso)		

Figure 3.32. Plot of $1/\chi$ versus T over the temperature range 1.8 - 300 K for Cu_2tppz.


6 10^7
5 10^7
4 10^7
3 10^7
2 10^7
1 10^7
0 10^0
0
50
100
150
200
250
300
350
T(K)
para

state electronic properties of polypyridophenazines. Work by McLendon[24] using polyphenylene spacers has suggested that ET in a totally coplanar π-system should exhibit no distance dependence; it was expected that extended aromatic systems like those of tppz, tatpp, and tpbpz would promote long-distance ground-state interaction of coordinated metals. In view of the results obtained from studies of bdppz, it is not surprising that no such interaction is seen; ground-state coupling in these systems is greatly affected by the fact that very little electron density lie on the bpy portions of polypyridophenazine LUMOs, preventing metals from coupling to the bridge.

The ability to study the distance-dependence of H_{ab} by a variety of independent methods is greatly circumscribed in a series of compounds in which no such ground-state coupling exists. In better-coupled systems, the strategy employed here, comparison of electro-, spectro-, and magnetochemical measurements, should provide greater understanding of the factors which affect metal-metal interactions in bridged systems. Studies of mixed-valence systems have relied almost exclusively on near-IR spectra; while the Hush theory has been shown to apply to some of these systems, it must be remembered that it is an empirical formulation based upon a manifestation of electron delocalization, the intervalence band. The theory is less accurate in describing heterodinuclear systems. Temperature-dependent magnetic susceptibility yields a direct measure of interaction regardless of the system's composition. Hopefully, magnetic measurements will play a greater role in future investigations; multiple techniques should mutually reinforce each other.

Coupling matrix elements extracted from rates of thermal and photoinduced electron transfer measured using time-resolved techniques, to the author's knowledge, have not been compared to those obtained using the methods described above. This, too, will aid in understanding the factors affecting ground-state metal-metal interaction. Such work lies in the future with systems displaying stronger ground-state coupling than that in tetrapyridophenazine-based complexes. The study of the excited-state kinetic properties of these compounds is still of great interest, however; as shown in Chapter 2, lack of ground-state coupling is no indication of the degree of coupling through the higher-lying orbitals used in excited-state donor-acceptor interactions. The $Ru^{II}Cu^{II}$ complexes allow direct measurement of the rate of Ru*-to-Cu ET; oxidation of $Ru^{II}M^{II}$ dimers (M=Ru, Os) to mixed-valence $Ru^{II}M^{III}$ species allows measurement of the rate of Ru^{II*}-to-M^{III} ET at very high driving force. Spectral overlap of Ru MLCT emission and Os MLCT absorption in $Ru^{II}Os^{II}$ dimers leads to excited-state energy transfer.

There are two methods of measuring rates of photoinduced energy and electron transfer. Both require measurement of the emission lifetime, τ_0, of a donor-only model complex in which no such transfer occurs. One can then either measure the emission lifetime, τ_{DA}, of the donor-acceptor compound or the steady-state emission intensities, I_0 and I_{DA} of the two compounds. Electron- and energy-transfer rates (k_{ET}, k_{EN}) can then be calculated using Equations 3 and 4.

$$k_{ET,\ EN} = 1/\tau_{DA} - 1/\tau_0 \qquad 3.$$

$$k_{ET,\ EN} = 1/\tau_0\ (I_0/I_{DA}) \qquad 4.$$

Lifetime measurements for Ru monomers and homodimers are laid out in Table 3.6. The difference in lifetimes between the monomers and dimers is unexpected; in systems as non-interacting as these, the two metal centers should behave independently of each other, yet the dimers have shorter lifetimes. It should also be recalled that they have lower quantum yields of emission. Intermolecular triplet-triplet annihilation occurs in concentrated solutions of $Ru(bpy)_3^{2+}$;[25] the high effective concentration in a dinuclear system could give rise to this phenomenon. Such behavior has not been seen in other Ru dimers, however; the Ru moieties act as separate entities, displaying the same luminescence properties of their component monomers.[26] The bridging ligands in such compounds are not themselves electron acceptors. The behavior of the Ru dimers presented here can be explained in terms of the non-innocence of the phenazine-derived bridging ligand. Photoreduction of the bridge by one of the metal centers produces a

Table 3.6. Emission lifetime data. 532 nm laser excitation of argon-purged samples.

Table 3.6. Emission Lifetimes

Compound	**Solvent**	**τ, ns**
Ru•tppz	acetonitrile	1219
	dmso	426
Ru•tpbpz	acetonitrile	682
	dmso	98.8
Ru_2tppz	acetonitrile	96.1
Ru_2tpbpz	acetonitrile	238

phenazine radical anion which exhibits strong absorption in the same region where the Ru chromophores emit. Transient absorption spectroscopy of Ru•tpbpz shows this absorption. The emission of the other chromophore is quenched by energy transfer to the phenazine anion, reducing both the quantum yield and lifetime of emission from the dimer. For this reason, Ru•tppz and Ru•tpbpz are used as model compounds for measurements of τ_0 and I_0. An ideal model compound would have a nonquenching +2 metal ion at the other coordination site, but, given the fact that there is no ground-state metal-metal interaction with these bridging ligands, the monomers suffice.

Picosecond time-resolved transient absorption provides τ_{DA} for Ru•tppz•Cu and electrochemically-generated mixed-valence Ru^{II}•tppz•Ru^{III}. Monitoring the decay of the bpy radical anion absorbance at 390 nm[27] allows measurement of the MLCT excited-state lifetime. The technique requires that an entire data set be collected for each time point; the compound under study must be stable for at least 15 min. The mixed-valence dimer is unstable, showing some decomposition over the course of the experiment. Optimization of both the laser system and oxidation conditions will make picosecond experiments more tractable in the future; preliminary results show that k_{ET} is very fast, on the order of 10^9 s^{-1}. The study of ET in mixed-valence systems is very attractive both for the extremely high forward driving force (2.1 eV) and for the use of easily-synthesized homonuclear complexes. Such experiments will be pursued.

Ru•tppz•Cu is a very stable compound. A transient absorption spectrum of the complex at 0 ps after laser excitation of a dmso solution of the complex is shown in Figure 3.33. The $bpy^{\bullet -}$ absorption is seen, as is the bleach of the MLCT band. A monoexponential fit of the decay of the 390 nm absorbance is given in Figure 3.34. The rate observed is 3.02 x 10^8 s^{-1}, corresponding to an excited state lifetime of 3.11 ns. The lifetime of Ru•tppz under the same conditions is 426 ns. Equation 3 yields k_{ET} = 3.00 x 10^8 s^{-1} at a driving force of 1.1 eV.

Figure 3.33. Transient absorption spectrum of Ru•tppz•Cu 0 ps after 355 nm laser pulse.

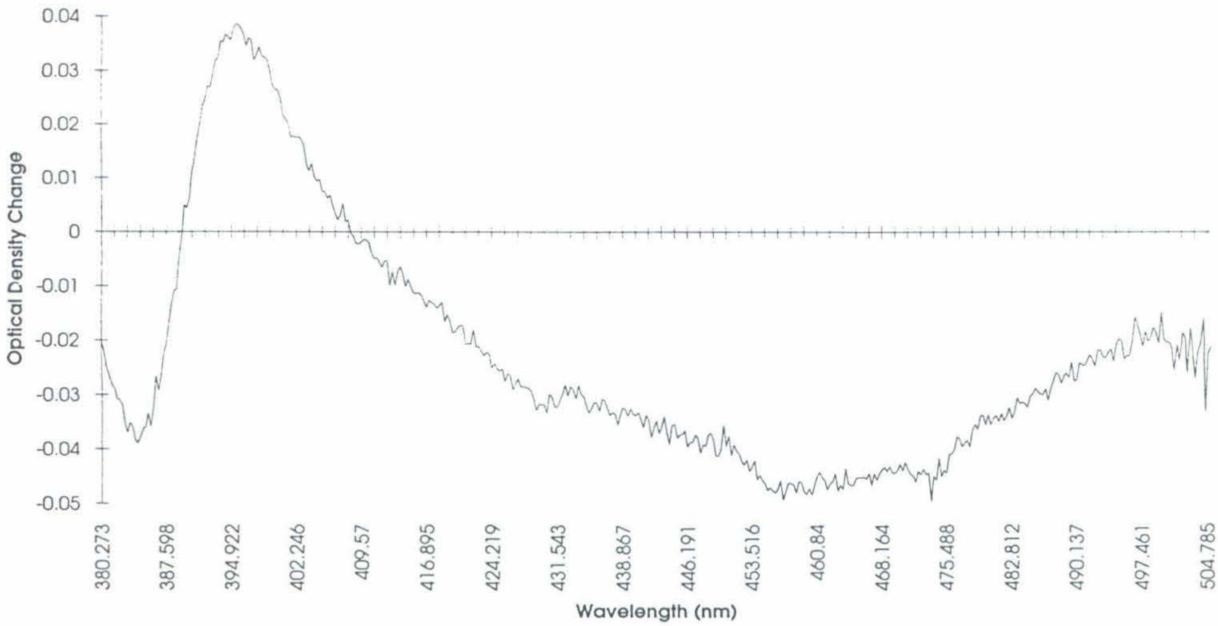
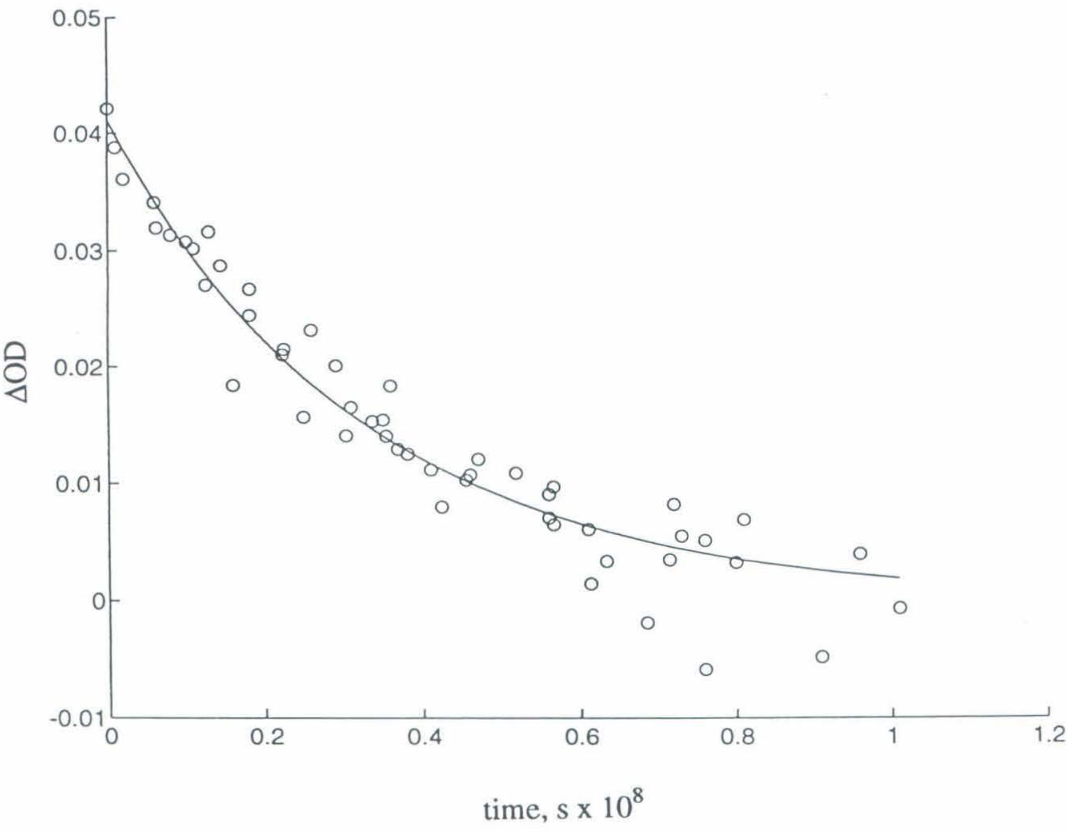

0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
Optical Density Change
380.273
387.598
394.922
402.246
409.57
416.895
424.219
431.543
438.867
446.191
453.516
460.84
468.164
475.488
482.812
490.137
497.461
504.785
Wavelength (nm)

Figure 3.34. Fit of transient absorbance observed at 390 nm for Ru•tppz•Cu. k = 3.02 x 10^8 s^{-1}.


0.05
0.04
0.03
0.02
0.01
0
-0.01
ΔOD
0
0.2
0.4
0.6
0.8
1
1.2
time, s x 10^8

All other rates were measured using the static emission technique. The emission spectra of solutions of Ru•tppz and Ru•tppz•Cu isoabsorptive at the excitation wavelength of 440 nm are presented together in Figure 3.35. The loss of emission intensity upon coordination of the Cu center is apparent. Ru•tppz has an intensity of 5807; the intensity of Ru•tppz•Cu is 172. Substitution of these values along with τ_0 = 426 ns into Equation 4 yields $k_{ET} = 7.91 \times 10^7$, in reasonable agreement with the value determined by transient absorption. While the absorbance due to the Cu center overlaps with the MLCT emission of the Ru center, the extreme weakness of the band (ε_{736} = 193 $\underline{M}^{-1}$ cm^{-1}) makes energy transfer an unlikely quenching mechanism.

ET in RuOs dimers can be studied by oxidizing the Os center with Ce^{4+}. The spectral changes effected by addition of successive 10 µl portions of 0.1 $\underline{M}$ $(NH_4)_2Ce(NO_3)_6$ in acetonitrile to a 10^{-3} $\underline{M}$ acetonitrile solution of Ru•tppz•Os ate shown in Figure 3.36. The Os-to-bpy MLCT transitions disappear, leaving a spectrum that looks exactly like that of Ru•tppz. Emission intensities of equimolar solutions of Ru•tppz and $Ru^{II}Os^{III}$tppz can be compared directly without need to correct for absorption due to Os. Emission spectra for equimolar Ru•tppz - Ru^{II}•tppz•Os^{III} and Ru•tpbpz - Ru^{II}•tpbpz•Os^{III} are shown in Figure 3.37. Emission is severely quenched by ET to the Os^{III} center. The driving force for the reaction is 1.6 eV.

Measure of energy transfer rates in $Ru^{II}Os^{II}$ complexes requires that correction be made for inner-filter absorption of Ru emission by Os MLCT bands. Experiments are carried out at an excitation wavelength at which the Ru and Os centers have the same extinction coefficient as indicated by the spectra of their monomers. Referring to Figure 3.27, this wavelength is 460 nm for Ru•tppz and Os•tppz. Since Os•tpbpz was not synthesized, this isosbestic point is taken from the spectra of Ru_2tpbpz and Os_2tpbpz for determination of the energy-transfer rate in Ru•tpbpz•Os. It, too, is 460 nm. This assures that the Ru center receives a constant photon input. The emission spectra of three solutions containing equal amounts of Ru are taken; these are shown in Figure 3.38 for

Figure 3.35. Emission spectra of equimolar dmso solutions of Ru•tppz and Ru•tppz•Cu. Excitation at 440 nm.

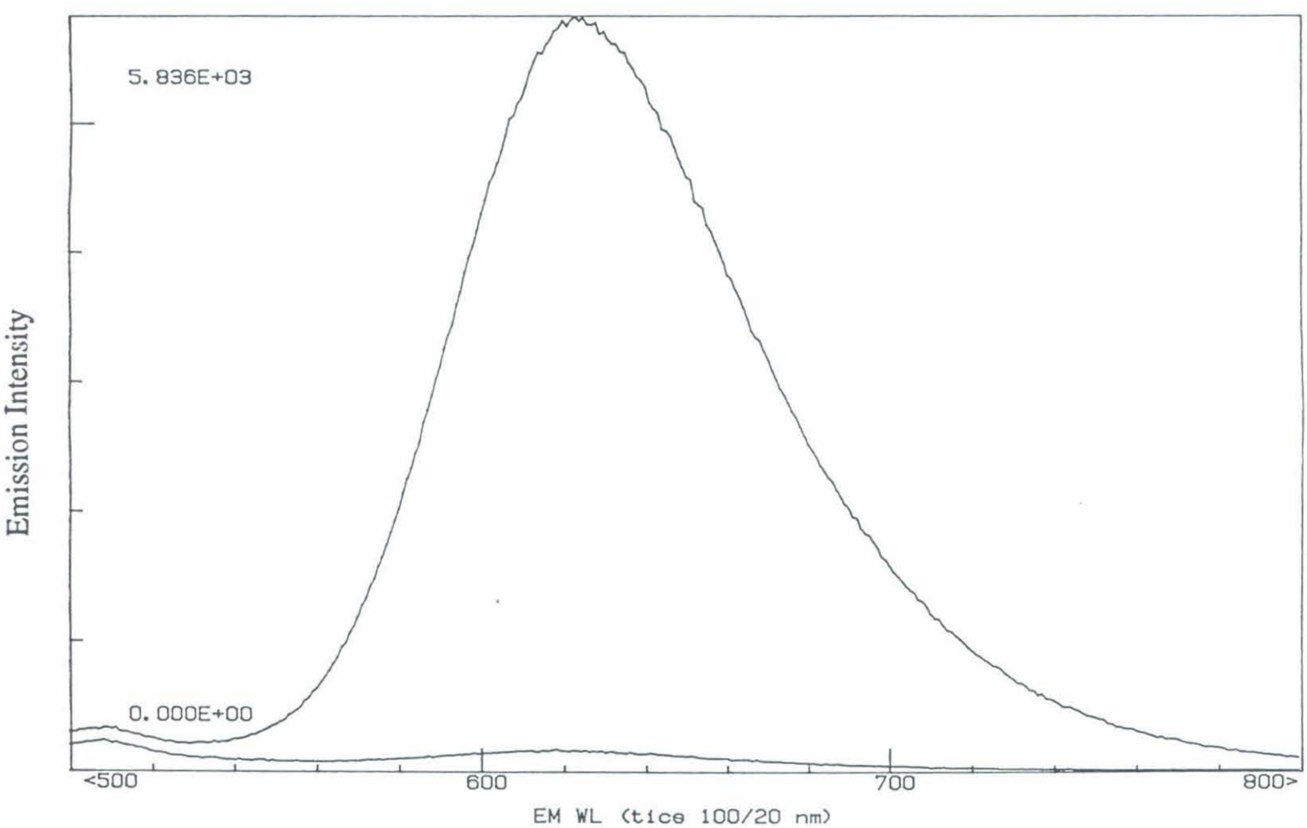

Emission Intensity
5. 836E+03
0. 000E+00
<500
600
700
800>
EM WL (tics 100/20 nm)

Figure 3.36. Spectral changes accompanying incremental oxidation of Ru•tppz•Os by Ce^{4+}.

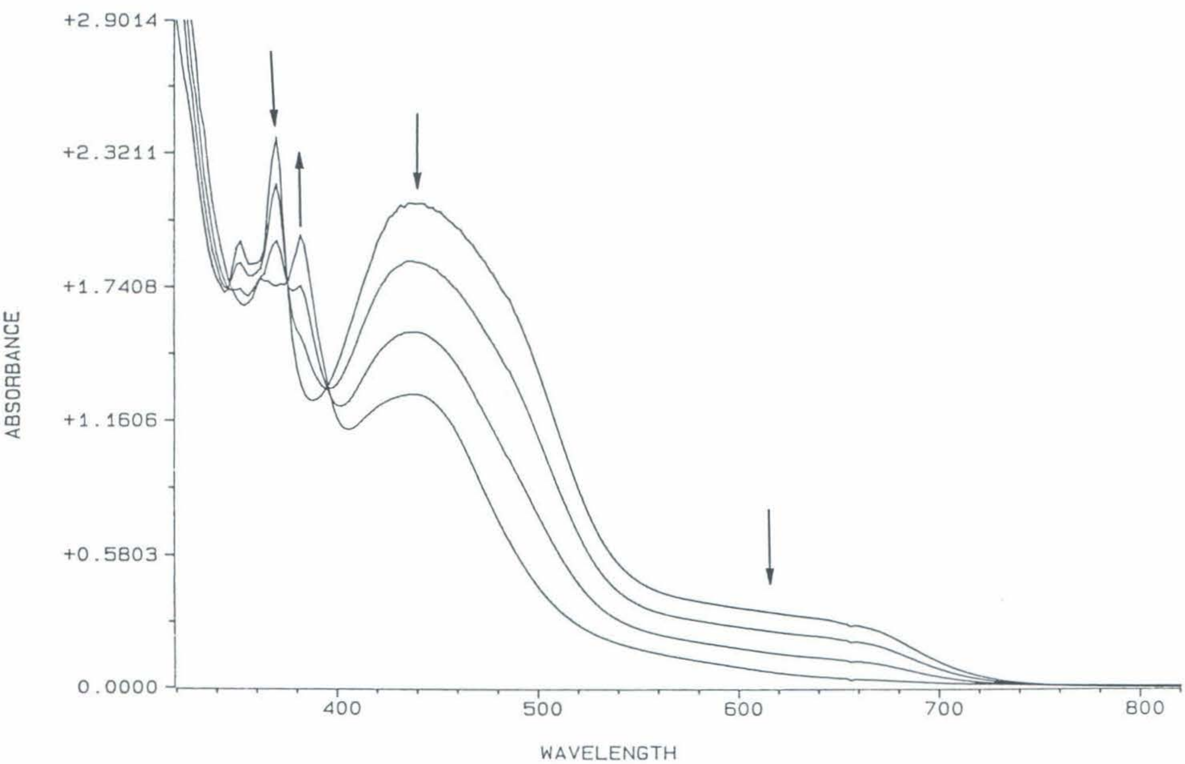
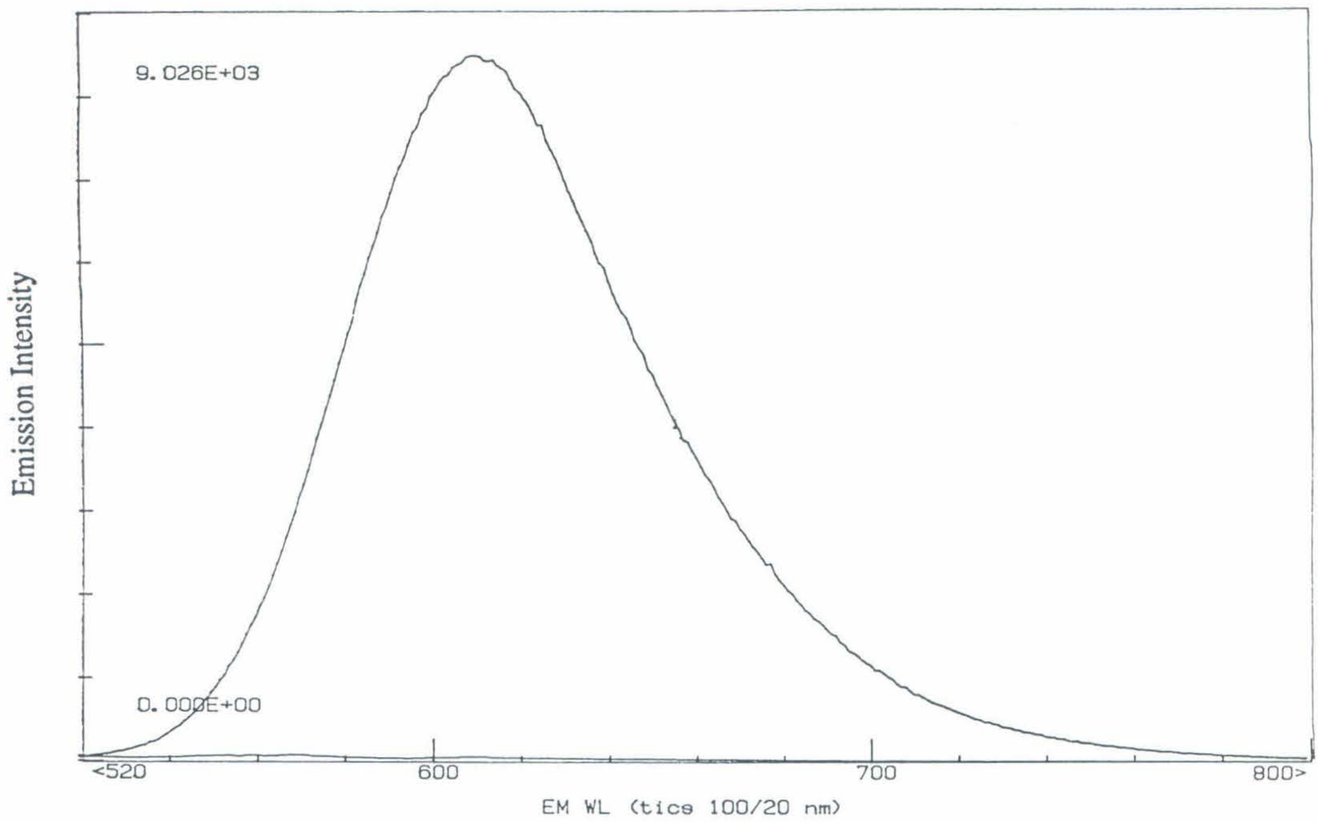
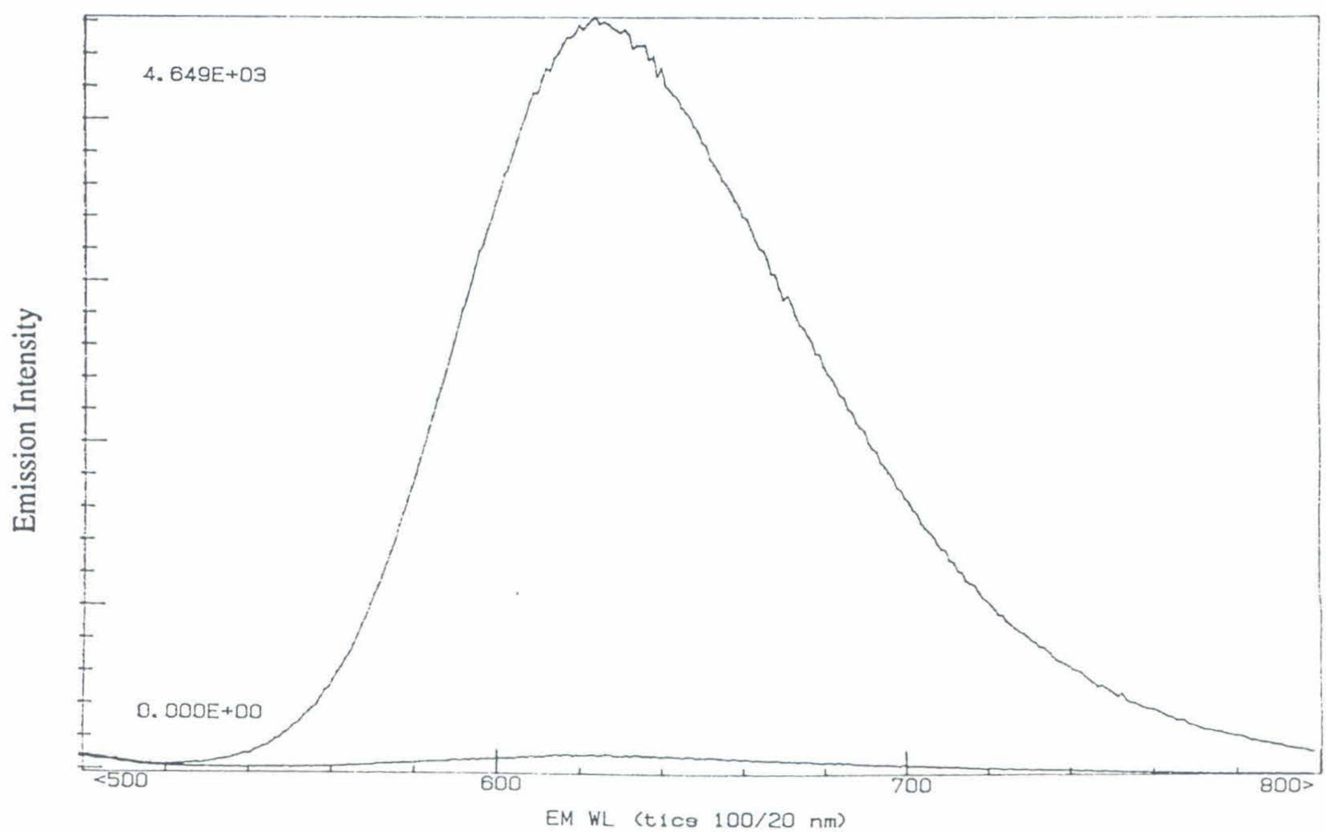

+2.9014
+2.3211
+1.7408
+1.1606
+0.5803
0.0000
ABSORBANCE
400
500
600
700
800
WAVELENGTH

Figure 3.37. Emission spectra of equimolar acetonitrile solutions of Ru•tppz/Ru^{II}•tppz•Os^{III} (top) and Ru•tpbpz/Ru^{II}•tpbpz•Os^{III}.


9.026E+03
0.000E+00
Emission Intensity
<520
600
700
800>
EM WL (tics 100/20 nm)


4.649E+03
0.000E+00
Emission Intensity
<500
600
700
800>
EM WL (tics 100/20 nm)

complexes of tppz. The most-intense emission comes from Ru•tppz. A 1:1 mixture of Ru•tppz and Os•tppz displays less-intense emission due to inner-filter absorption. One sees that an appreciable amount of emission is absorbed by Os MLCT bands; the micromolar concentrations used in the experiment preclude loss of intensity due to intermolecular energy transfer. Finally, the spectrum of Ru•tppz•Os is recorded. Emission is greatly quenched. I_0/I_{DA} is then the ratio of the emission intensity of equal amounts of noncovalently-linked Ru and Os to that of Ru•tppz•Os. In the study of Ru•tpbpz•Os, 1:0.5 Ru•tpbpz:Os_2tpbpz was used to correct for the inner filter effect.

Kinetic data are collected in Table 3.7. ET in these systems appears to take place at a rate independent of donor-acceptor separation. The rates for Ru•tppz•Cu and Ru•tpbpz•Cu are within experimental error of being equal; it should also be remembered that the ET rate in Ru•tppz•Cu as determined by picosecond time-resolved spectroscopy is higher. This result, frankly, is disconcerting. If it were one pair of compounds which displayed this behavior, one would be inclined to label the result a mistake; two pairs of compounds requires that one seriously consider the possibility that k_{ET}, and thus H_{ab}, is invariant with distance in tppz and tpbpz.

Weak distance dependence has been seen previously in several systems possessing extended π-systems. The decay of k_{ET} with distance is commonly expressed using Equation 5. The preexponential factor A_0 is the maximal ET rate possible (when donor

$$k_{ET} = A_0 \exp(-\beta r) \qquad 5.$$

and acceptor are in Van der Waals contact), r is the donor-acceptor separation, and β is the measure of the severity of the exponential decay of H_{ab}. In most systems, β has a value of at least 1 $Å^{-1}$. In systems employing polyene[28] and polyphenylene[24,29] bridges, weaker distance dependence is observed as evidenced by their β values of 0.4 $Å^{-1}$. ET through the π-stacked bases of DNA occurs over a distance of more than 20 Å in ps.[30]

Table 3.7. Kinetic Data

Table 3.7. Kinetic Data

Electron Transfer			
Complex	**$1/\tau_0$**	**I_o/I_{DA}**	**k_{ET}**
Ru•tppz•Cu	2.342×10^6	33.8	$7.91 \pm 1 \times 10^7$
Ru•tpbpz•Cu	1.012×10^7	9.37	$9.42 \pm 1 \times 10^7$
Ru^{II}•tppz•Os^{III}	8.201×10^5	135	$1.12 \pm 1 \times 10^8$
Ru^{II}•tpbpz•Os^{III}	1.871×10^6	40.4	$7.56 \pm 1 \times 10^7$
Energy Transfer			
Ru•tppz•Os	8.201×10^5	14.7	$1.30 \pm 1 \times 10^7$
Ru•tpbpz•Os	1.871×10^6	7.40	$1.38 \pm 1 \times 10^7$

Thus there is ample experimental evidence that extended conjugation leads to weak distance dependence. Distance-independent ET through optimally-conjugated (i.e., planar) π-systems has been predicted by Larsson[31] in polyene and by Onuchic and Beratan[32] in polyphenylene spacers. Onuchic and Beratan postulate that the coupling within a ring (β in their terminology) is greater than the coupling between rings (γ) because nonplanarity destroys the overlap between p orbitals on adjacent rings. The ratio ($\nu=\gamma/\beta$) determines the overall coupling for the system. Their model predicts that k_{ET} should drop off by less than a factor of ten with each additional ring when the angle θ formed by the planes of adjacent rings is 50°, the equilibrium geometry of biphenyl. Work done by McLendon and co-workers shows that k_{ET} falls by a factor of 7 when θ in a biphenyl spacer is varied from 0 to 50°.[33] They therefore deduce that ν is proportional to cos θ, the consequence being that no variation in k_{ET} will be observed in a coplanar aromatic system in which the distance is varied.

The extended planar aromatic system of tppz should provide optimal excited-state donor-acceptor coupling. One would expect that, if theory is correct, no change in k_{ET} should be seen in going from tppz to tatpp since the plane is merely extended without breaking conjugation. Effort directed at making donor-acceptor systems employing tatpp will be well-spent. It is interesting and also problematic that no difference is seen in k_{ET} between complexes employing tppz and tpbpz. On one hand, fusing donor and acceptor by condensation of phendione with 3, 3'-diaminobenzidene makes possible a system in which the metals are separated by over 20 Å with only one conjugation-breaking bond. On the other, the presence of this bond, if it forces θ to 50°, should decrease k_{ET} by a factor of 7 relative to that in tppz. While such a small variation alone would be impressive, it is not seen; no variation is seen. It must be that the equilibrium geometry of the ligand favors the optimal overlap across this bond. X-ray crystallographic structure determination would be interesting in this regard, as would the use of a substituted diaminobenzidene whose inter-ring steric interactions force the neighboring rings into a nonoptimal geometry.

It remains that there appears to be no distance dependence of H_{ab} in ET through tppz and tpbpz. Table 3.7 shows that k_{en} is the same in Ru•tppz•Os and Ru•tpbpz•Os; if it can be shown that energy transfer takes place via the Dexter exchange mechanism, whose electronic coupling term is the same is that in the Marcus formulation, it provides a third system in which H_{ab} is invariant with distance. First, however, a word must be said about whether or not energy transfer is actually occurring in these compounds. Since the MLCT emission of the energy donor pumps the MLCT absorption of the acceptor, an increase in the intensity of emission due to the acceptor should be seen if energy transfer is taking place. Unfortunately, since no Os-based emission is seen in any compound, this compelling evidence in favor of energy transfer is lacking. However, the near-complete quenching of the Ru-based emission in Ru•tppz•Os and Ru•tpbpz•Os and the lack of quenching in equimolar mixtures of their component monomers strongly suggests that energy transfer is taking place. By making asymmetric Ru dimers, it should be possible to see luminescence sensitization accompanying energy transfer.

The Förster equation gives Equation 6 as formulation for k_{en}:

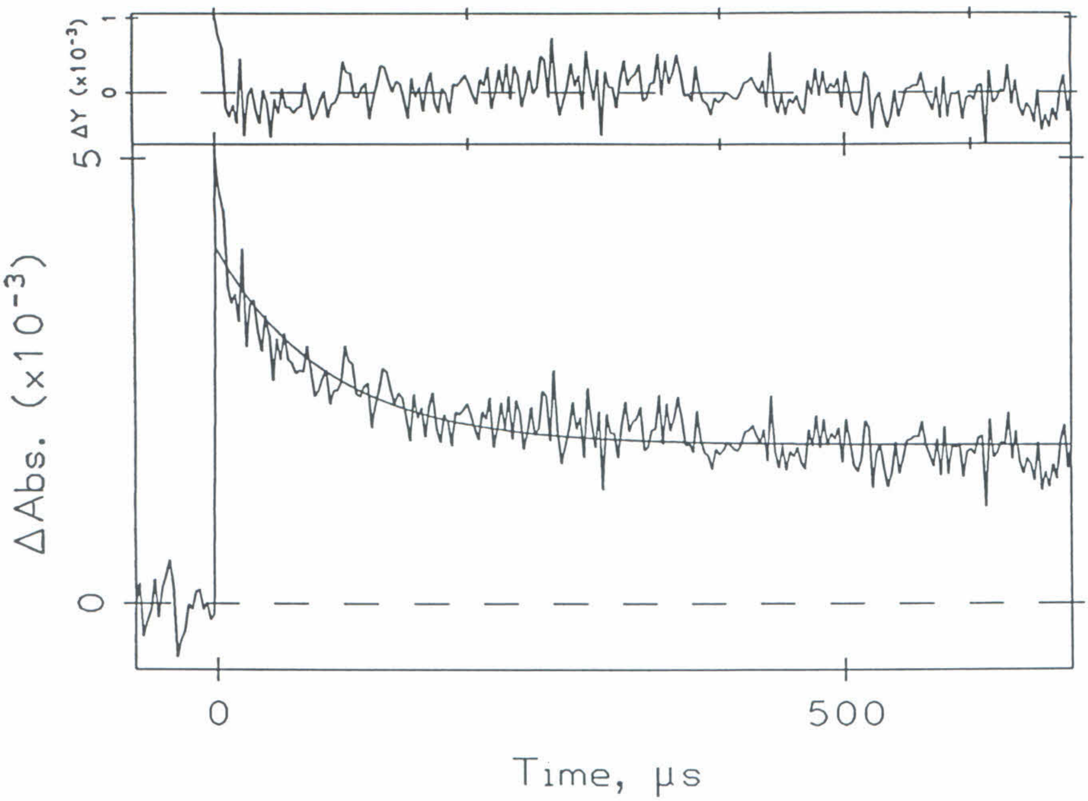
$$k_{en} = 5.87 \times 10^{-25} (\Phi_0/n^4\tau_0 r^6) \text{ (overlap)} \qquad 6.$$

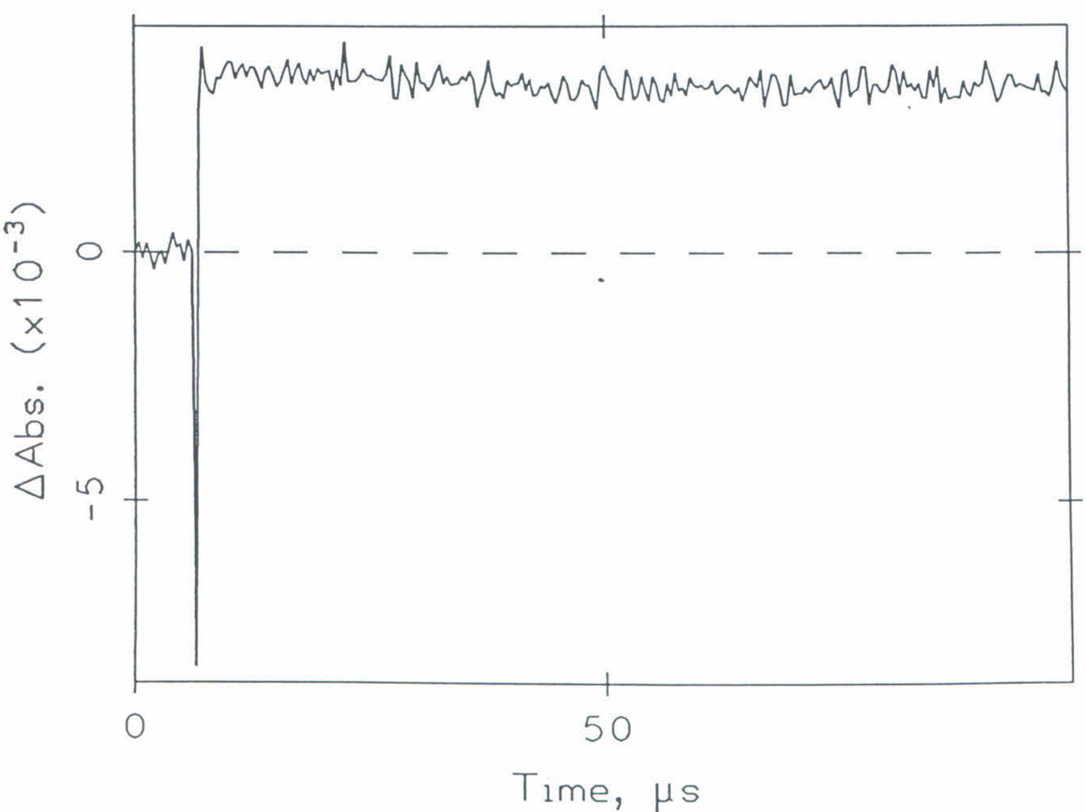
Φ_0 is the emission quantum yield of the model compound, n is the refractive index of the solvent (1.33 for acetonitrile), r is the donor-acceptor separation in cm, (overlap) is the numerical integration of the overlap of the emission band of the energy donor with the absorption band of the acceptor. In a similar Ru-Os system[26b], this integral has a value of 4.3×10^{-14} $\underline{M}$ cm^{-6}. For Ru•tppz•Os, Φ_0=0.06, τ_0=1.2×10^{-6} s, and r = 1.25×10^{-7} cm, yielding k_{en}= 1.0×10^8, in surprisingly good agreement with the experimentally-determined value of 1.2×10^8 s^{-1}. For Ru•tpbpz•Os, Φ_0=0.032, τ_0=5.34×10^{-7} s, and r = 2.0×10^{-7} cm, yielding k_{en}= 7.2×10^6 s^{-1}, at variance by over an order of magnitude from the measured value of k_{en}= 7.6 x 10^7 s^{-1}. Although it cannot be categorically ruled out, it appears that the Förster mechanism is not at work here.

Thus there are three different systems in which H_{ab} seems not to show its expected exponential distance decay. These results, obtained from static emission measurements, need to be independently confirmed by using time-resolved techniques like those employed with Ru•tppz•Cu. Complexes of tatpp need to be examined, as do those of novel related ligands. Perhaps the ultimate test of the lack of distance dependence in ET through tetrapyridophenazines is the synthesis of the hexaazatetrapyridoheptacene. It is accessible via the condensation of phenazinetetramine[34] with phendione. If it is true that H_{ab} in a coplanar π–system is invariant with distance, the same energy- and electron-transfer kinetics should be seen in complexes of this ligands as those that are observed in tppz although the metal-metal separation varies by over 20 Å. Such behavior would be astonishing. The results presented in this chapter would seem to put it in the realm of the possible.

$Ru^{II}Os^{III}$ compounds allow measurement of the rate of thermal charge recombination. Photoinduced ET produces a $Ru^{III}Os^{II}$ compound; the Os^{II}-based MLCT absorbances which disappear when the $Ru^{II}Os^{II}$ is oxidized to the mixed-valence species grow back, giving large transient spectral changes. Transient absorption traces for Ru^{II}•tppz•Os^{III} and Ru^{II}•tpbpz•Os^{III} are presented in Figure 3.38. The observation wavelength is 600 nm, the maximum of the lowest-energy Os^{II}-based MLCT absorption. An optical density increase is seen upon laser excitation, showing that ET from Ru^{II} to Os^{III} takes place. The decays do not return to 0, however, an indication that a net chemical change is taking place. This is surprising; electrochemical measurements show the $Ru^{3+/2+}$ and $Os^{3+/2+}$ couples in these compounds to be completely reversible. Fitting the decay of Ru^{III}•tppz•Os^{II} gives a rate constant of 1.12 x 10^4, reflecting a charge-separated-state lifetime of 89 μs. The back reaction is four orders of magnitude slower than the forward one. As with complexes of bdppz, this slow recombination is a

Figure 3.38. Transient absorption observed at 600 nm after 532 nm laser excitation of Ru^{II}•tppz•Os^{III} (top) and Ru^{II}•tpbpz•Os^{III}.


ΔY (x10⁻³)
1
0
5
0
ΔAbs. (x10⁻³)
0
500
Time, μs


ΔAbs. (x10⁻³)
0
-5
0
50
Time, μs

consequence of the poor ground-state coupling in polypyridophenazines. For comparison, a similar $Ru^{II}Os^{III}$ with a metal-metal separation 5 Å greater than that of Ru^{III}•tppz•Os^{II} has a charge recombination rate of 1 x 10^6, reflecting much better ground-state coupling. The 600 nm transient of Ru^{III}•tpbpz•Os^{II} dips slightly, but is essentially irreversible. If the reaction which competes with charge recombination is the same in both the tppz and tpbpz dimers, it is apparent that the rate of back transfer in Ru^{III}•tppz•Os^{II} is less than 1 x 10^4. It should be possible to develop dimers with reversible ET for measurement of these slow charge recombination rates.

Conclusions

The condensation of phendione with itself or with tetramines allows the synthesis of a series of dinucleating ligands exhibiting varied distance between the two coordination sites. Mononuclear and homo- and heterodinuclear complexes can be made from these ligands. Attaching a $Ru(bpy)_2^{2+}$ moiety gives complexes excited-state energy- and electron-transfer properties. ET can be studied between the Ru chromophore and coordinated Ru^{3+}, Os^{3+}, and Cu^{2+} centers. Preliminary picosecond transient absorption measurements show that ET to Ru^{3+} is very fast. ET to Os^{3+} and Cu^{2+} occurs at the same rate regardless of the metal-metal separation. The rate of energy transfer from Ru to Os^{2+} is also invariant with distance. These results suggest that the usual exponential distance decay of electronic coupling is not operative in these extended planar π-systems. Theory and experiment have previously suggested that such behavior is possible. Additional work should be done to confirm these counterintuitive results. Transient absorption spectroscopy shows that recombination of the thermodynamically-unstable charge-separated states formed by photoinduced ET is slow in bimetallic derivatives of tetrapyridophenazines, in accord with the behavior seen in Chapter 2 for mononuclear dipyridophenazine-based donor-acceptor complexes. In the ground state of these ligands, the bpy portion acts as an insulator, allowing only very poor coupling between donor and acceptor.

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Chapter 4

Toward Multielectron Photochemistry: Complexes of hhtn

Introduction

Most useful chemical transformations do not occur by way of one-electron processes. Respiration, nitrogen fixation, and photosynthesis are biological processes which require multiple electrons. Many industrial processes which convert feedstocks into more useful materials, such as activation of alkenes with transition-metal catalysts, proceed by two-electron changes in the metal oxidation state. A major goal of current work in inorganic photochemistry is the development of systems that will undergo multielectron oxidation-reduction chemistry.[1] Difficulty arises from the fact that, like $Ru(bpy)_3^{2+}$, all inorganic chromophores so far synthesized are capable of only one-electron excited-state processes. Ways must be found around this limitation.

There are two basic approaches that can be taken to overcome the problem. The first of these is to couple photoinduced ET to thermal oxidation or reduction to effect net multielectron chemistry. The reactions of $Rh_2(bridge)_4^{2+}$ (bridge=1,3-diisocyanopropane) in 12 M HCl are shown in equations 1 and 2.[2] Thermal reaction with

$$Rh_2(bridge)_4^{2+} + HCl \xrightarrow{\Delta} Rh_2(bridge)_4Cl^{2+} + 1/2\ H_2 \qquad 1$$

$$Rh_2(bridge)_4Cl^{2+} + HCl \xrightarrow{546\ nm} Rh_2(bridge)_4Cl_2^{2+} + 1/2\ H_2 \qquad 2$$

HCl gives a photoactive intermediate whose excited state reacts with another molecule of HCl, yielding one molecule of H_2 overall. $Rh_2(bridge)_4^{2+}$ acts as a net two-electron reductant, but it does so neither catalytically nor toward a single two-electron oxidant, making it unattractive for practical applications. $Pt_2(pop)_4^{4-}$ (pop=pyrophosphite) suffers from neither of these drawbacks.[3] Its reaction with isopropanol is shown schematically in Figure 4.1. The triplet excited state of $Pt_2(pop)_4^{4-}$ abstracts a hydrogen atom from the alcohol, giving an alcohol radical and an axial monohydride Pt species. The radical then transfers another hydride to $Pt_2(pop)_4H^{4-}$ in a thermal step to give acetone and $Pt_2(pop)_4H_2^{4-}$. Generation of H_2 and regeneration of $Pt_2(pop)_4^{4-}$ occurs upon near-UV irradiation. Net two-electron oxidation of isopropanol is thus achieved photo-catalytically. The general applicability of the reaction scheme is limited by the fact that

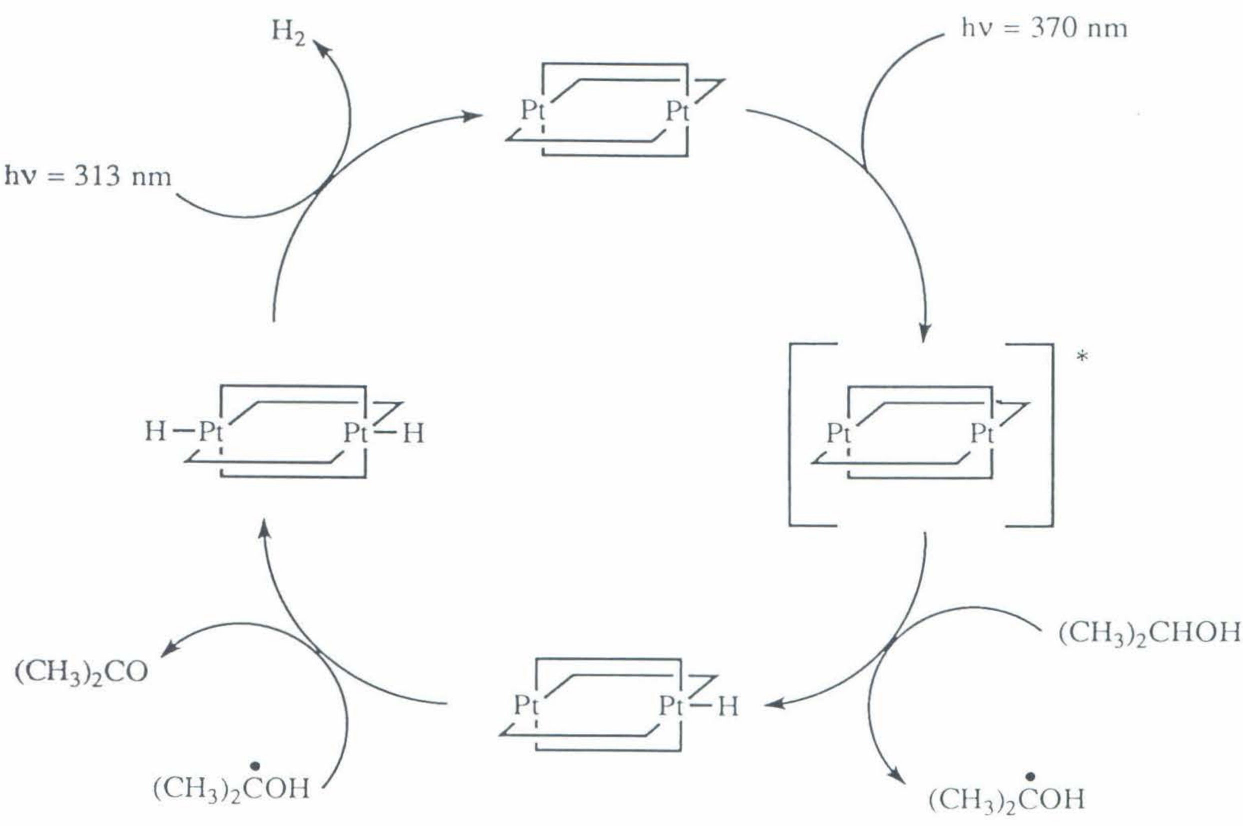


Figure 4.1. Photocatalytic production of H_2 and acetone from isopropanol using $Pt_2(pop)_4^{4-}$.

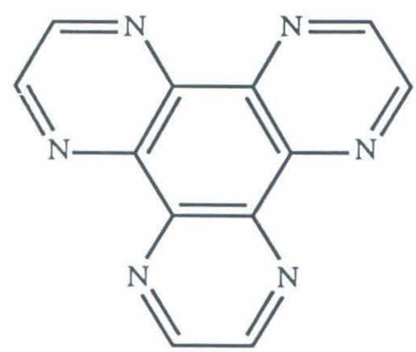
$Pt_2(pop)_4^{4-}$ is only reactive toward relatively weak carbon-hydrogen bonds.

The preceding examples use two metals, one of which undergoes a photon-driven one-electron change accompanied by a thermal one-electron change in the other for a net two-electron process. Both of these processes can take place in a monomeric system if the metal used is unstable to one-electron oxidation or reduction. The one-electron ET quenching of the excited state of a complex of such a metal leaves an unstable oxidation state which may react by further thermal ET to reach a stable configuration. This approach has been employed in studies of luminescent Au(I) complexes.[4] Au(II) is not stable, Au(I) and Au(III) being the metal's stable oxidation states. Oxidative quenching of excited-state $Au(I)_2(dcpe)_3^{2+}$ (dcpe= bis(biscyclohexylphosphino)ethane) gives a transient Au(II) species which can reach a stable state either by disproportionation to Au(I) and Au(III) or, if kinetically competitive with disproportionation, by thermal transfer of another electron to give Au(III) and a doubly-reduced acceptor. While it appears that two-electron reduction is not present in the system, this general approach shows promise.

The other approach to developing multielectron photochemical systems is to couple one-electron photoactive metal centers to a multielectron catalytic site. Nature has chosen to take this route in photosynthesis. The water-oxidizing complex in PS II catalyzes the four-electron oxidation of water to molecular oxyen. O_2 is evolved with every fourth photon absorbed by PS II; the four Mo atoms in the water-oxidizing complex store the four oxidizing equivalents generated by photon absorption.[5] While four-electron systems may be beyond reach, development of two-electron systems may be possible since, as mentioned earlier, monometallic catalysts operate via two-electron processes.

Two one-electron photoactive centers are needed to produce two oxidation or reduction equivalents; thus the system requires a platform capable of coordinating at least three metal atoms. Perhaps the simplest is HAT, shown in figure 4.2 A variety of homo-

Figure 4.2. HAT (1, 4, 5, 8, 9, 12-hexaazatriphenylene).



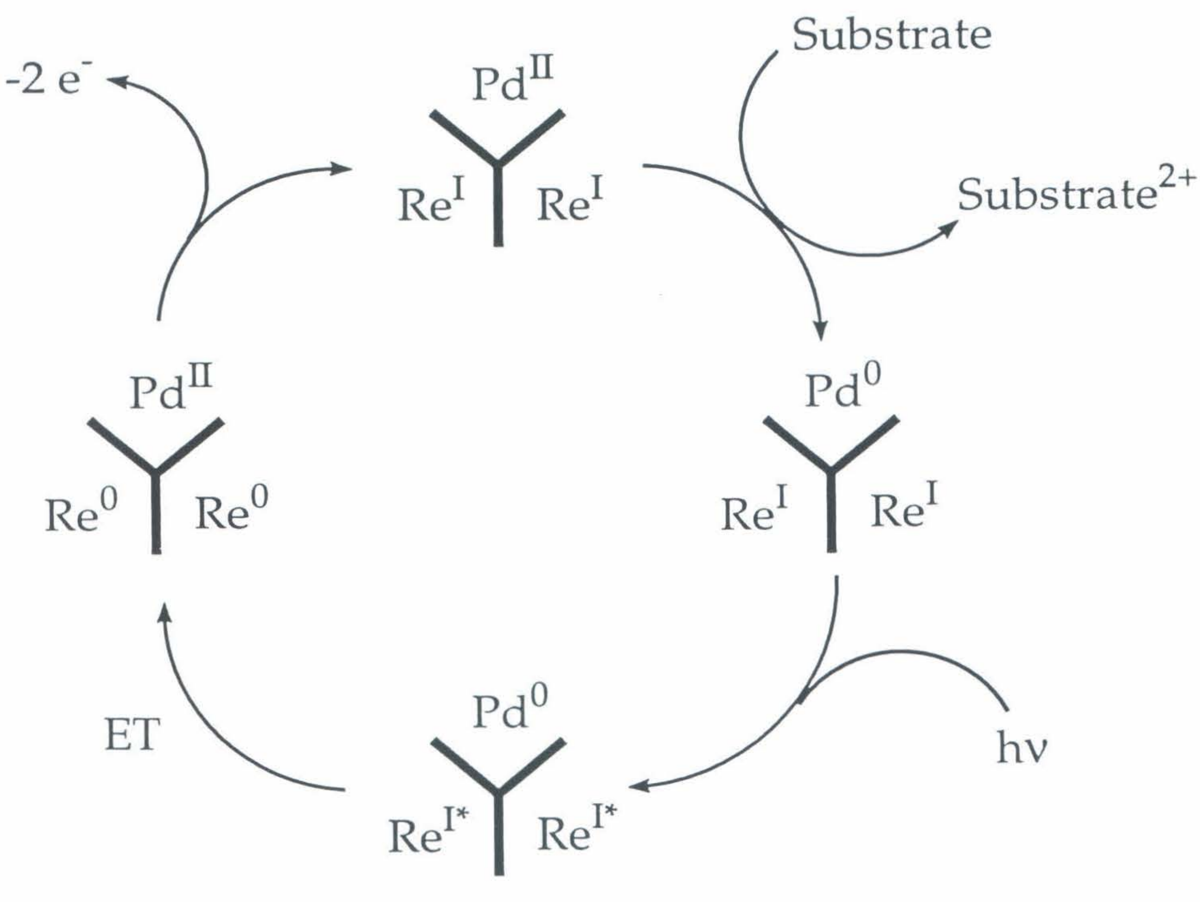
and heteronuclear polymetallic compounds incorporating HAT have been synthesized: $Cr(CO)_4$, $Mo(CO)_4$,[6] $Re(CO)_3Cl$,[7] and $Ru(bpy)_3^{2+}$ [8] fragments have been coordinated.

The ligand has been used as a building block in the construction of sophisticated molecular architectures. Lehn and coworkers have structurally characterized complexes in which six Cu^+ ions serve as a tetrahedral templates to control the assembly of a cylinder with hexaphenyl-HAT ends and quaterpyridine sides.[9] When metal-ligand interactions lead to excited-state properties, this ability to control structure allows the design of supramolecular systems in which light energy can be collected and directed in very specific ways.[10]

Such sophistication may someday lead to systems whose function resembles that of PS II; a more attainable goal is a photochemical system capable of performing two-electron oxidations such as the oxidation of ethylene to acetaldehyde in the presence of Pd, known as the Wacker process.[11] A scheme for the operation of such a system is presented in Figure 4.3. The oxidation of Pd^0 to Pd^{2+} (E^0=0.60 V) is within the excited-state reduction potential of $Ru(bpy)_3^{2+}$ and $Re(CO)_3$phenCl, allowing the system to be turned over by a photooxidant. Two-electron oxidation of the substrate must be rapid relative to the rate of photoinduced reduction of Pd^{2+} to Pd^0, possible since the chromophores are also photoreductants. Means must also be devised to oxidize the photocenters once they have picked up electrons from Pd^0; thermal ET to Pd^{2+} is not a wise choice. It may suffice to operate the system in the presence of oxygen if ET is fast relative to excited-state deactivation of the chromophores by oxygen.

HAT has the three coordination sites required for such a system: one site for the catalytic Pd center, two for the two one-electron photoactive centers responsible for regenerating Pd^{2+} from Pd^0 to turn the system over. Working with HAT has the disadvantage that its synthesis proceeds via substituted trinitrobenzenes which are military explosives.[12] The preceding chapters have shown that condensation of ketones with aromatic amines to give azines is a simple route to new ligands. A natural extension

Figure 4.3. Schematic operation of a two-electron photocatalytic system.

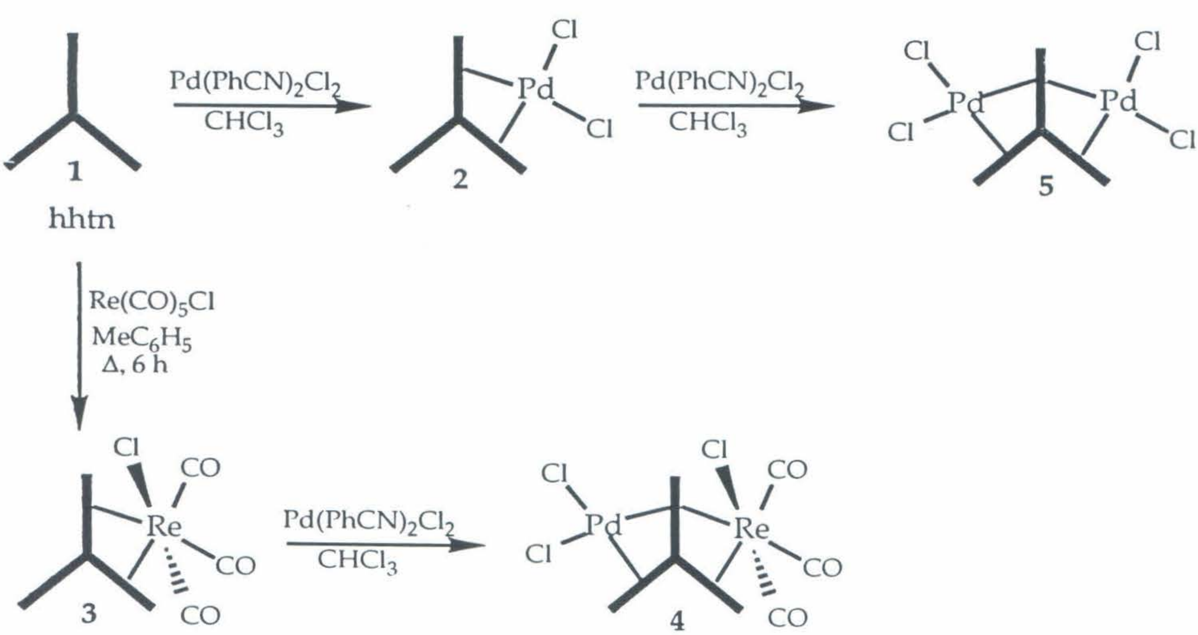

Substrate
-2 e⁻
Pd^II
Re^I Re^I
Substrate^2+
Pd^II
Re^0 Re^0
Pd^0
Re^I Re^I
Pd^0
ET
hν
Re^I* Re^I*

of ligands with one and two coordination sites is the condensation of 4,5-dimethyl-1,2-phenylenediamine with hexaketocyclohexane to give trinucleating hhtn, which was presented in Figure 1.8. The electronic properties of polypyridophenazines which localize electron density on the pz part of the ligand, as demonstrated in Chapter 2, may aid in the development of multielectron systems. In spite of the ease of their synthesis compared to HAT, the coordination properties of hexaazatrinapthalenes like hhtn have never been examined.

Chapter 4 presents the synthesis, structure, and photophysical properties of mono- and dimetallic complexes of hhtn with chromophoric $Re(CO)_3Cl$ and catalytic $PdCl_2$ units. A synthetic scheme for the compounds prepared is shown in Figure 4.4. X-ray crystallographic structure determination shows that these compounds are highly distorted from planarity due to the ligand's congested coordination pocket. Re(I)-containing complexes **3** and **4** do not emit in solution at room temperature as $Re(CO)_3$(phen)Cl does. Re-based emission is observed at 77 K in **3** but not **4**, indicating that Re emission may be quenched by the Pd center in **4**. These results suggest directions that future efforts directed toward multielectron photochemical systems might proceed.

The experimental and results sections in this chapter are adapted excerpts from Catalano, V. J.; Larson, W. E.; Olmstead, M. M.; Gray, H. B. *Inorg. Chem.*, submitted for publication.

Figure 4.4. Synthesis of Re(I) and Pd(II) derivatives of hhtn.


Pd(PhCN)2Cl2
CHCl3
1
hhtn
2
Cl
Pd
5
Re(CO)5Cl
MeC6H5
Δ, 6 h
3
Re
CO
4

Experimental Section

Preparation of Compounds. $(PhCN)_2PdCl_2$ and $Re(CO)_5Cl$ (Strem) and hexaketocyclohexane and 4,5-dimethyl-1,2-phenylenediamine (Aldrich) were used as received. Hhtn was prepared by a modification of a standard procedure.[13] The new compounds reported here are stable to moisture and dioxygen and can be prepared without recourse to inert atmosphere techniques.

5,6,11,12,17,18-hexaza-2,3,8,9,14,15-hexamethyltrinapthalene, (hhtn), 1. To a stirred solution of 200 mL of absolute ethanol were added 1.0 g (3.20 mmol) of hexaketocylohexane octahydrate and 1.44 g (10.5 mmol) of 4,5-dimethyl-1,2-phenylenediamine. The solution was brought to reflux. After a few minutes a greenish-brown color formed. After 12 hours the solution was cooled. A yellow-green precipitate formed and was collected by filtration and dried under vacuum (yield: 85%). ^1H NMR (ppm) (300 MHz $CDCl_3$) δ 2.64 (s, 3H, methyl), δ 8.41(s, 1H, aromatic).

$PdCl_2$(hhtn), 2. An orange solution of 163 mg (0.43 mmol) of $(PhCN)_2PdCl_2$ in 15 mL chloroform was slowly added to a stirred, yellow-green solution of 200 mg (0.43 mmol) of hhtn in 20 mL of chloroform. A deep orange color immediately formed and the solution was stirred for 20 min. The volume was reduced under vacuum to 10 mL. Addition of diethyl ether afforded an orange microcrystalline solid that was collected by filtration, washed with diethyl ether, and dried in air. The compound was recrystallized from dichloromethane and diethyl ether (yield: 94%). ^1H NMR (300 MHz $CDCl_3$) δ 2.67 (s, 3H, methyl), δ 2.69 (s, 3H, methyl), δ 2.70 (s, 3H, methyl), δ 8.42(s, 1H, aromatic), δ 8.45(s, 1H, aromatic), δ 9.28(s, 1H, aromatic).

$Re(CO)_3Cl$(hhtn), 3. To 355 mg (0.76 mmol) of hhtn suspended in 50 mL of toluene were added 273 mg (0.76 mmol) of $Re(CO)_5Cl$. The mixture was brought to reflux. The initial yellow-green color slowly turned deep brown. After 6 hours the solution was cooled, and the toluene was removed under vacuum to yield a brown powder. The powder was dissolved in 30 mL of dichloromethane and filtered through celite. Addition of 20 mL methanol and removal of the dichloromethane under vacuum yielded deep brown-red crystals that were collected by filtration, washed with diethyl ether, and dried in air (yield: 66%). ^{1}H NMR (300 MHz $CDCl_3$) δ 2.61 (s, 3H, methyl), δ 2.71 (s, 3H, methyl), δ 2.77 (s, 3H, methyl), δ 8.44(s, 1H, aromatic), δ 8.55(s, 1H, aromatic), δ 8.84(s, 1H, aromatic).

$(PdCl_2)(Re(CO)_3Cl)$(hhtn), 4. An orange solution of 90 mg (0.23 mmol) of $(PhCN)_2PdCl_2$ in 15 mL dichloromethane was slowly added to a stirred, brown solution of 181 mg (0.23 mmol) of **2** in 20 mL of dichloromethane. The brown solution was stirred for 30 min. An equal volume of methanol was added and the dichloromethane was removed under vacuum to yield a brown microcrystalline solid. The solid was collected by filtration, washed with diethyl ether, and dried in air. The compound was recrystallized from dichloromethane and ether (yield: 83%). ^{1}H NMR (300 MHz $CDCl_3$) δ 2.70 (s, 1H, methyl), δ 2.71 (s, 1H, methyl), δ 2.74 (s, 1H, methyl), δ 2.75 (s, 1H, methyl), δ 2.79 (s, 1H, methyl), δ 2.81 (s, 1H, methyl), δ 8.50(s, 1H, aromatic), δ 8.60(s, 1H, aromatic), δ 8.82(s, 1H, aromatic), δ 8.86(s, 1H, aromatic), δ 9.33(s, 1H, aromatic), δ 9.45(s, 1H, aromatic).

$(PdCl_2)_2$(hhtn), 5. An orange solution of 61 mg (0.16 mmol) of $(PhCN)_2PdCl_2$ in 15 mL chloroform was slowly added to the stirred, orange solution of 100 mg (0.15 mmol) of **2** in 20 mL of chloroform. A deeper orange color appeared, and after 10 min of stirring a deep orange precipitate formed. The precipitate was collected by filtration, washed with diethyl ether, and dried in air (yield: 65%). ^{1}H NMR (300 MHz $CDCl_3$) δ 2.71 (s, 3H, methyl), δ 2.73 (s, 3H, methyl), δ 2.74 (s, 3H, methyl), δ 8.51(s, 1H, aromatic), δ 9.38(s, 1H, aromatic), δ 9.41(s, 1H, aromatic).

Physical Measurements. ^{1}H NMR spectra were recorded on a General Electric QE-300 NMR spectrometer operating at 300 MHz. Infrared measurements were recorded for hydrocarbon mulls on a Beckman IR-4240 spectrometer. Electronic absorption measurements were made with a Hewlett Packard HP-8452A spectrophotometer; emission data were collected on a home-built instrument.[14]

Electrochemical experiments were performed using a Princeton Applied Research (PAR) model 173 potentiostat controlled by a model 175 universal programmer. Cyclic voltammetry was done at ambient temperature with a normal three-electrode configuration consisting of a glassy carbon working electrode, a platinum wire auxiliary electrode, and a AgCl/Ag reference electrode containing 1.0 M KCl. The working compartment of the electrochemical cell was separated from the reference compartment by a modified Luggin capillary. All three compartments contained a 0.1 M solution of supporting electrolyte. Dichloromethane (Burdick and Jackson) was distilled from P_2O_5 prior to use. Tetrabutylammonium hexafluorophosphate ($TBAPF_6$) (Southwestern Analytical) was used as received.

Potentials (vs. aqueous AgCl/Ag) were not corrected for the junction potential. Under conditions identical with those employed here, the ferrocenium/ferrocene couple has an $E^{o\prime}$ of 0.45 V.

X-ray Data Collection

$\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$, 2. Orange needles were obtained by slow diffusion of diethyl ether through a 2 mm layer of methanol into a chlorobenzene solution of the complex. A single crystal was mounted on a glass fiber with silicon grease and placed in the 130 K nitrogen stream of a Siemens R3m/V diffractometer with a modified Enraf-Nonius low-temperature apparatus. Two check reflections showed only random fluctuations (<2%) in intensity throughout the data collection. The data were corrected for Lorentz and polarization effects. Crystal data are given in Table 4.1.

$Re(CO)_3Cl(hhtn) \cdot CH_3OH$, 3. Deep red needles were formed by the slow diffusion of methanol into a tetrahydrofuran solution of the complex. A single crystal was selected and mounted as described above. Two check reflections showed only random fluctuations (<1%) in intensity throughout the data collection. The data were corrected for Lorentz and polarization effects. Crystal data are given in Table 4.1.

$(Re(CO)_3Cl)(PdCl_2)(hhtn) \cdot 2.6\ 1,2\text{-}Cl_2C_6H_4$, 4. Red-brown blocks were formed by the slow diffusion of diethyl ether into 1,2-dichlorobenzene. A single crystal was selected and mounted as described above. There was no decay in the intensities of the two standard check reflections during the course of the data collection. The data were corrected for Lorentz and polarization effects. Crystal data are given in Table 4.1.

Structure Solution and Refinement

$\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$, 2. Calculations were performed using SHELXTL PLUS (PC and VMS versions) software. Scattering factors and corrections for anomalous dispersion were taken from a standard source.[15] An absorption correction was applied.[16] The structure was solved by direct methods. Hydrogen atoms were added geometrically and refined using a riding model with isotropic thermal parameters equal to 0.05Å^2. The Pd and Cl atoms were assigned anisotropic thermal parameters. The largest feature in the final difference map (0.89 e$^-$Å^{-3}) is located 0.97 Å from Pd(2).

$Re(CO)_3Cl(hhtn) \cdot CH_3OH$, 3. The structure was solved in the monoclinic space group $P2_1/n$ using direct methods. Hydrogens were added as described above and refined using isotropic thermal parameters of 0.035Å^2. The hydroxyl hydrogen of the methanol was not located in a Fourier map and was not included in the final model. An absorption correction was applied. All nonhydrogen atoms were refined with anisotropic thermal parameters. The largest peak in the final Fourier difference map corresponded to 3.2 e$^-$Å^{-3} at a distance of 0.9Å from Re. The goodness-of-fit was 1.33.

$(Re(CO)_3Cl)(PdCl_2)(hhtn) \cdot 2.6\ 1,2\text{-}Cl_2C_6H_4$, 4. The structure was solved by a combination of Patterson and difference Fourier methods in the triclinic space group $P\bar{1}$ and refined by full-matrix (based on F^2) least-squares.[17] Hydrogen atoms were added at calculated positions and refined using a riding model with isotropic thermal parameters equal to 1.2 times the equivalent isotropic U of the bonded carbons, except for those of

Table 4.1. Crystal data for complexes **2-4**.

Table 4.1

Crystallographic Data

2, $\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$

$C_{34}H_{30.5}Cl_{2.5}N_6OPd$	FW = 734.1
a = 12.949(3) Å	P$\bar{1}$, triclinic
b = 16.625(4) Å	T = 130K
c = 17.062(4) Å	λ(MoKα) = 0.71073 Å
α = 63.00(2) °	μ(MoKα) = 0.85 mm^{-1}
β = 71.39(2) °	d_{calc} = 1.57 Mg/m^3
γ = 79.78(2) °	transm. factors = 0.86 - 0.90
V = 3099(2) Å^3	
Z = 4	
$R(F_o)$ = 0.059	
$R_w(F_o)$ = 0.060	

3, $Re(CO)_3Cl(hhtn) \cdot CH_3OH$

$C_{34}H_{28}ClN_6O_4Re$	FW = 806.3
a = 10.515(2) Å	$P2_1/n$, monoclinic
b = 27.123(6) Å	T = 130K
c = 11.385(4) Å	λ(MoKα) = 0.71073 Å
β = 110.95(2) °	μ(MoKα) = 4.146 mm^{-1}
V = 3033(2)Å^3	d_{calc} = 1.78 Mg/m^3
Z = 4	transm. factors = 0.47 - 0.75
$R(F_o)$ = 0.052	
$R_w(F_o)$ = 0.052	

4, $(PdCl_2)(Re(CO)_3Cl)(hhtn) \cdot 2.6\ Cl_2C_6H_4$

$C_{48.6}H_{50.4}Cl_{8.2}N_6O_3PdRe$	FW = 1349.84
a = 14.540(4) Å	P$\bar{1}$, triclinic
b = 14.558(3) Å	T = 130K
c = 14.671(4) Å	λ(MoKα) = 0.71073 Å
α = 64.72(2) °	μ(MoKα) = 3.376 mm^{-1}
β = 66.00(2) °	d_{calc} = 1.854 Mg/m^3
γ = 63.30(2) °	transm. factors = 0.66 - 0.89
V = 2418.3 Å^3	
Z = 2	
$R(F^2_o)$ = 0.066	
$wR_2(F^2_o)$ = 0.135	

$R = \Sigma \| F_o | - | F_c \| / \Sigma \|F_o|$; $R_w = \Sigma \| F_o | - | F_c | | w^{1/2} / \Sigma \ | F_o | w^{1/2}$

$wR_2 = [\Sigma[w(F_o^2 - F_c^2)2]/\Sigma[w(F_o^2)^2]]^{1/2}$

the methyl groups, which were assigned multiplicative values of 1.5. Three different sites in the structure with planar electron density were resolved into disordered groupings equivalent to 2.6 molecules of 1,2-dichlorobenzene. An absorption correction was applied.[18] All nonhydrogen atoms of the complex were refined with anisotropic thermal parameters. The largest peak in the final Fourier difference map corresponded to 1.39 e^{-} $Å^{-3}$ in the region of the disordered solvent group.

Results

Synthesis

The green-yellow compound hhtn is synthesized in high yield by the condensation of hexaketocyclohexane with 4,5-dimethyl-1,2-phenylenediamine. When an orange chloroform solution of $Pd(NCPh)_2Cl_2$ is added to the yellow-green chloroform solution of hhtn, a deep orange color appears, and orange microcrystals of $PdCl_2$(hhtn), **2**, can be isolated by addition of diethyl ether. Compound **2** can further react with another equivalent of $Pd(NCPh)_2Cl_2$ to produce the deep orange $(PdCl_2)_2$(hhtn), **5**. Addition of $Re(CO)_5Cl$ to **1** in refluxing toluene affords red-brown crystals of *fac*-$Re(CO)_3Cl$(hhtn), **3**, after 6 hours. The reaction of one equivalent of $Pd(PhCN)_2Cl_2$ with a dichloromethane solution of **3** produces $(Re(CO)_3Cl)(PdCl_2)$(hhtn), **4**, which can be isolated as a brown solid upon addition of diethyl ether.

Hhtn is very soluble in chloroform, moderately soluble in other chlorinated hydrocarbons, slightly soluble in toluene, benzene, and acetone, and insoluble in most alcohols and hydrocarbons. Compounds **2** and **3** are readily soluble in chlorinated hydrocarbons, slightly soluble in acetone, tetrahydrofuran, and acetonitrile, and insoluble in ether, while **4** is considerably less soluble in the aforementioned solvents. $(PdCl_2)_2$(hhtn), **5**, is much less soluble than the previous compounds, but readily dissolves in n-methyl pyrrolidinone. The lack of solubility hindered the isolation and purification of any trinucleated complexes.[19]

Characterization

The ^1H NMR spectrum of each compound displays the appropriate number of signals, all of which are singlets with the proper integration. NMR spectra of **1-5** are shown in Figures 4.5-4.9. Compounds **2, 3,** and **5** show the expected 3 signals for the methyl groups as well as three signals for the aromatic protons in a 3:1 ratio. The

Figure 4.5. 300 MHz ^{1}H NMR spectrum of hhtn, **1**, in CD_3Cl.

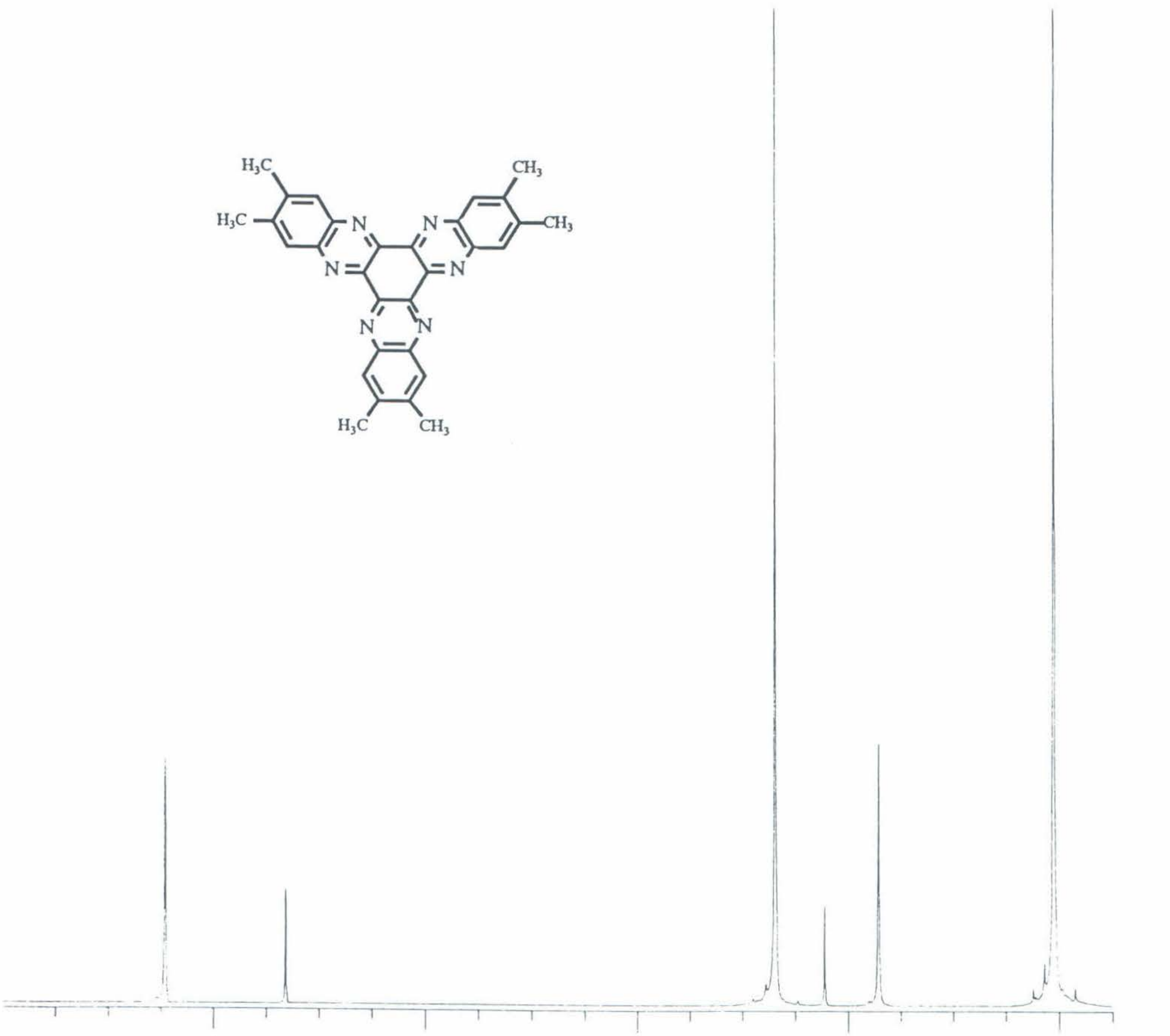
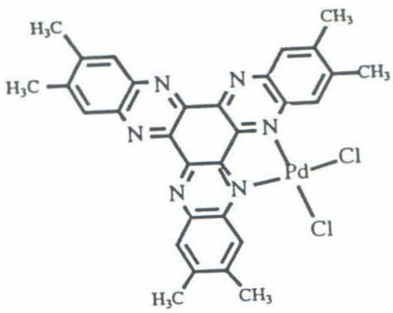

H3C
H3C
CH3
CH3
N
N
N
N
N
N
H3C
CH3
8
6
4
2
0
PPM

Figure 4.6. 300 MHz ^1H NMR spectrum of $(PdCl_2)$hhtn, **2**, in CD_3Cl.


H3C
CH3
H3C
CH3
N
N
N
N
N
N
Pd
Cl
Cl
H3C
CH3

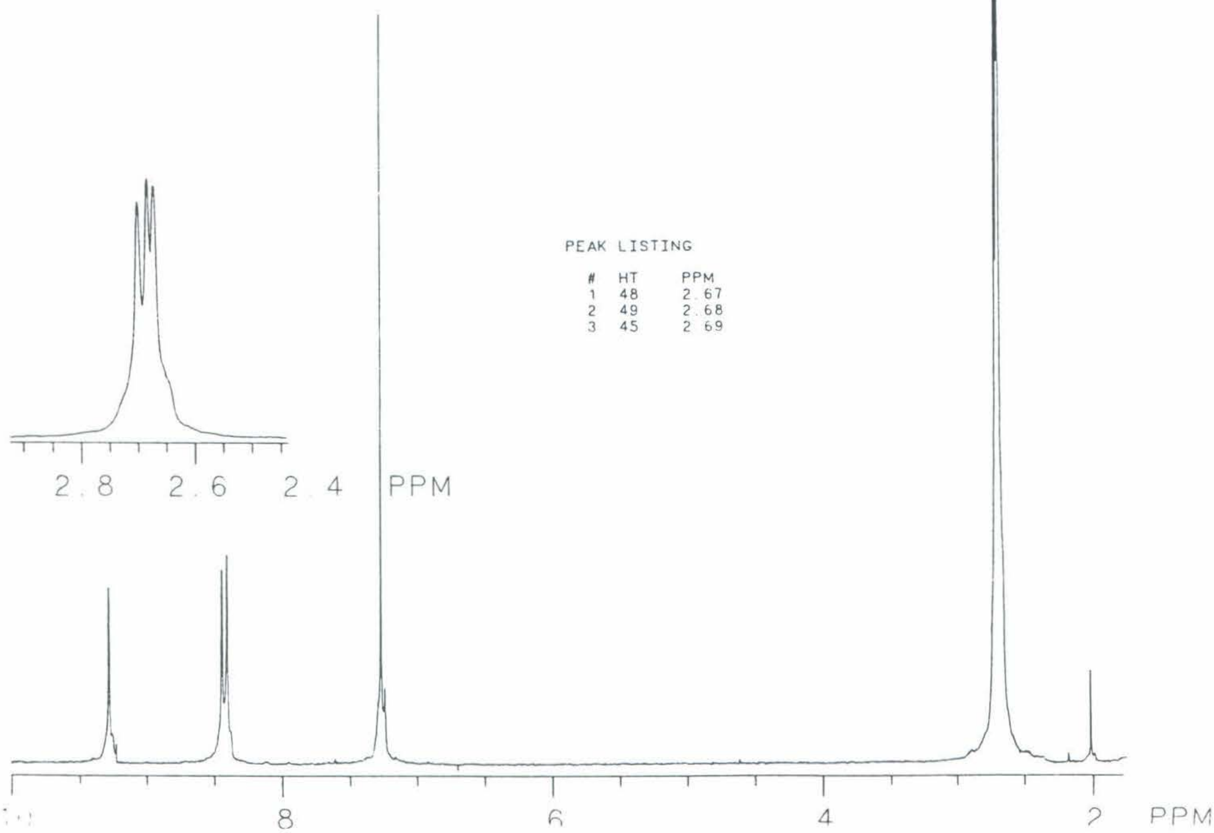

PEAK LISTING
HT PPM
1 48 2.67
2 49 2.68
3 45 2.69
2.8 2.6 2.4 PPM
8
6
4
2 PPM

Figure 4.7. 300 MHz ^{1}H NMR spectrum of $(Re(CO)_3Cl)$hhtn, **3**, in CD_3Cl.

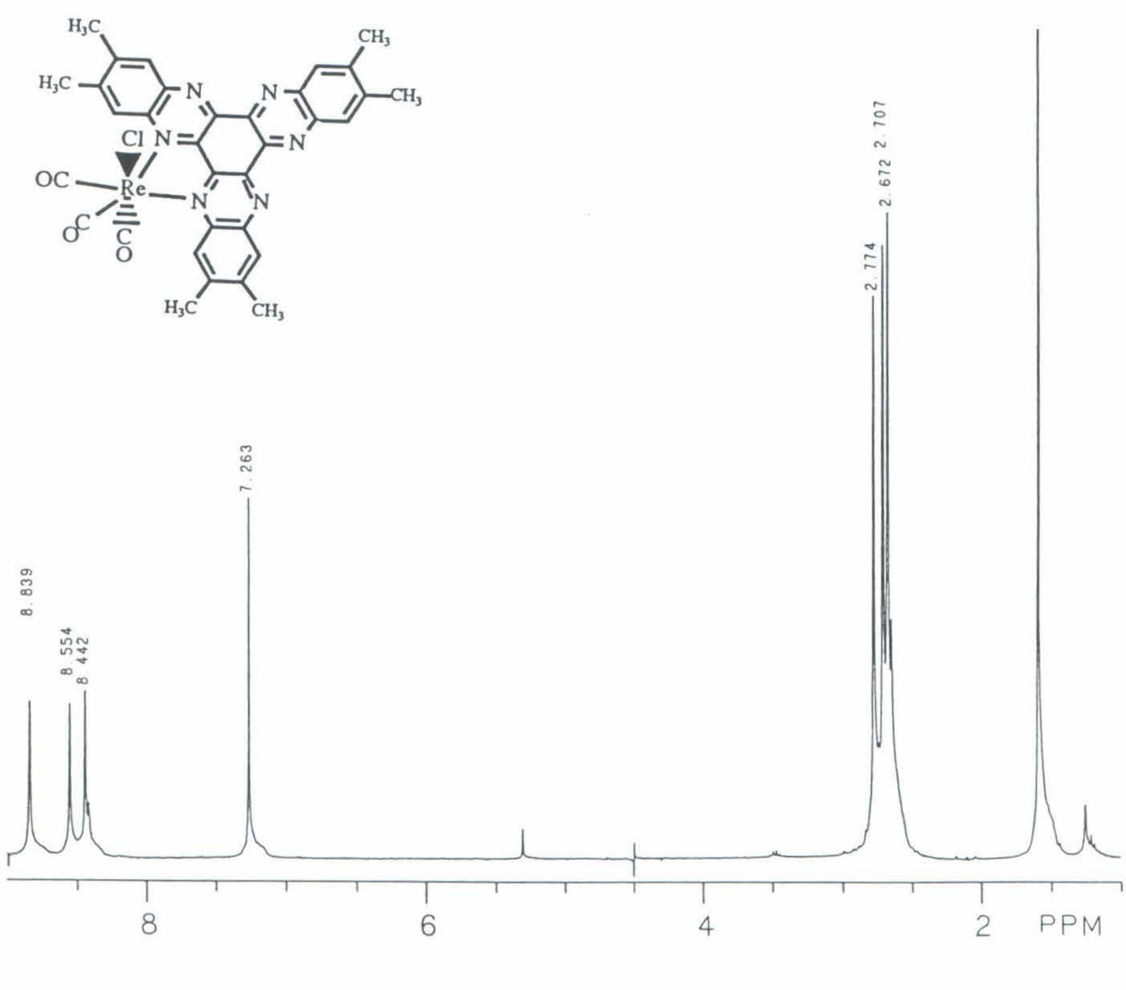
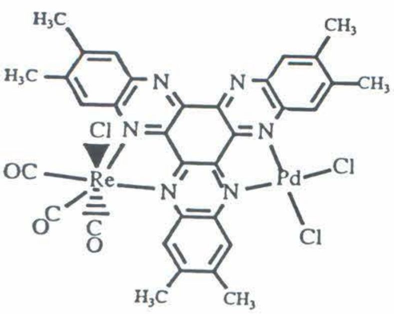
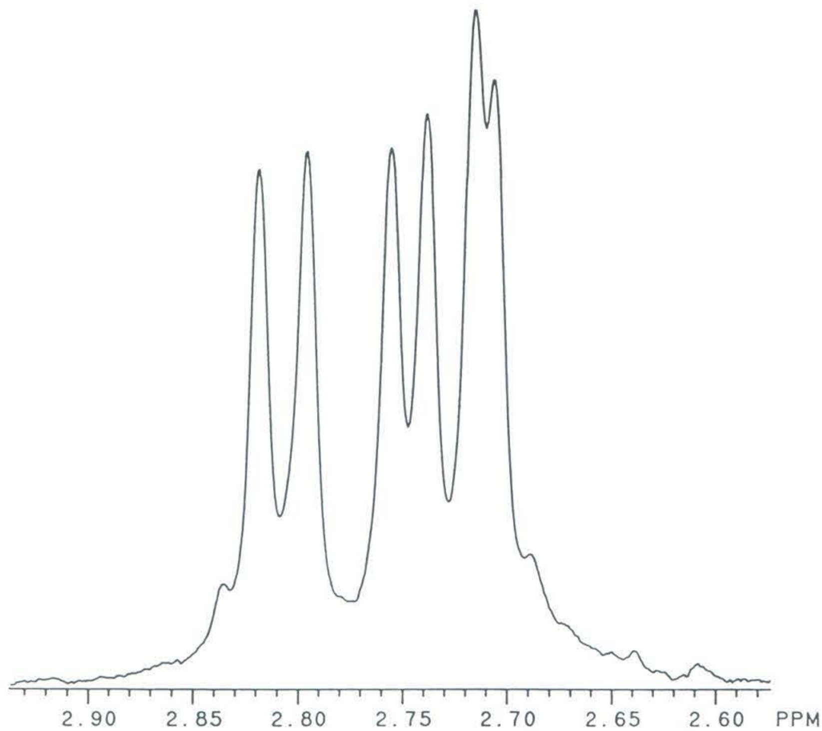

H3C
H3C
CH3
CH3
N
N
N
N
Cl
N
N
OC
Re
OC
CO
H3C
CH3
8.839
8.554
8.442
7.263
2.774
2.672
2.707
8
6
4
2
PPM

Figure 4.8. 300 MHz ^1H NMR spectrum of (Re(CO)$_3$Cl)(PdCl$_2$)hhtn, **4**, in CD$_3$Cl.


H3C
H3C
CH3
CH3
N
N
N
N
N
N
Cl
OC
Re
Pd
Cl
Cl
OC
CO
H3C
CH3


2.90
2.85
2.80
2.75
2.70
2.65
2.60
PPM

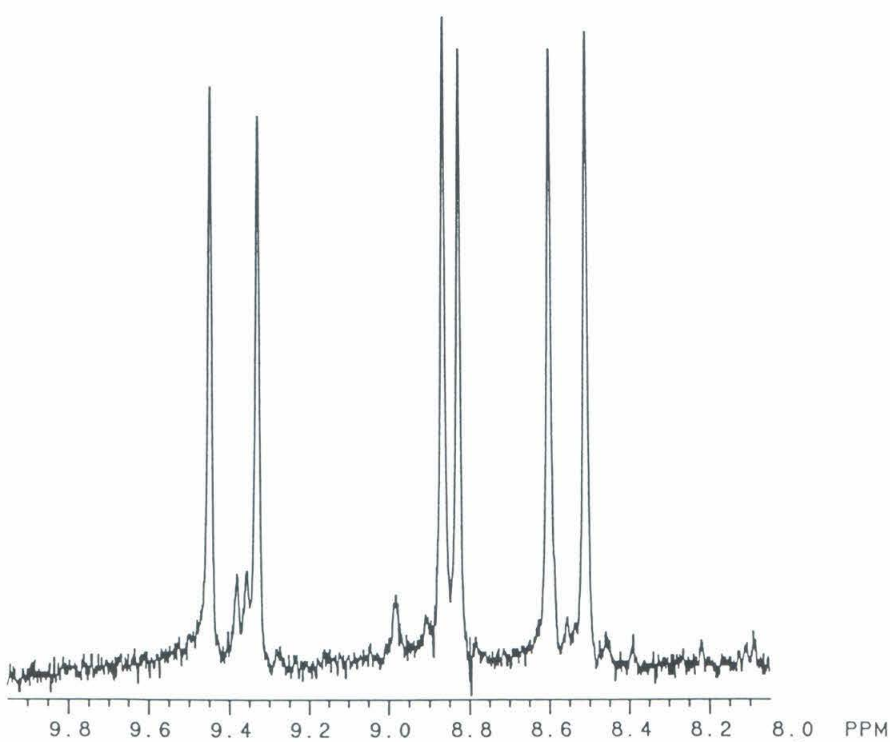
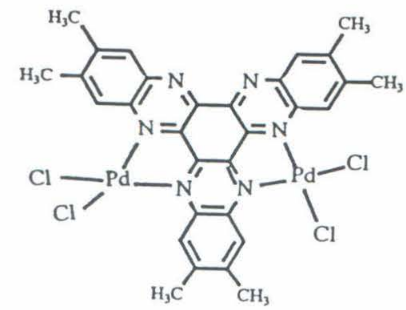
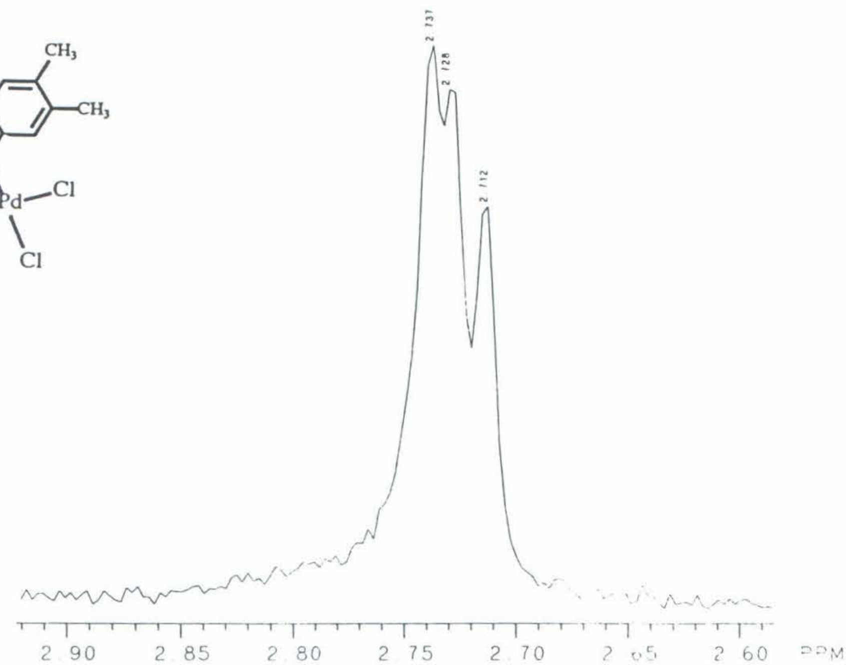
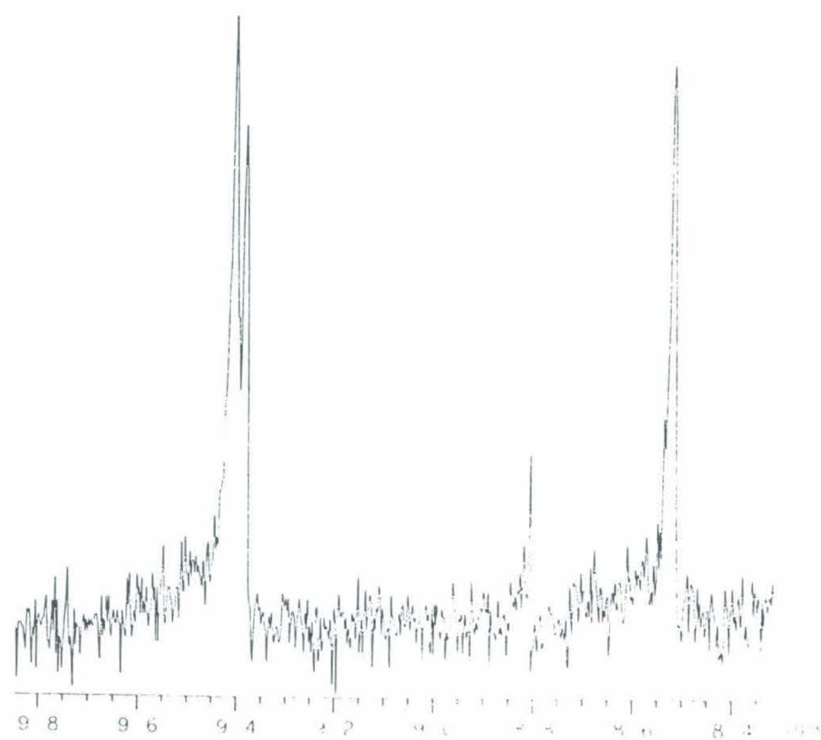

9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
PPM

Figure 4.9. 300 MHz ^{1}H NMR spectrum of $(PdCl_2)_2$hhtn, **5**, in CD_3Cl.


H₃C
CH₃
N
Pd
Cl


2.737
2.728
2.712
2.90
2.85
2.80
2.75
2.70
2.65
2.60
PPM


9.8
9.6
9.4

spectrum of **4** shows six independent signals for the methyl protons along with six signals for the aromatic protons. A downfield shift is seen upon coordination.

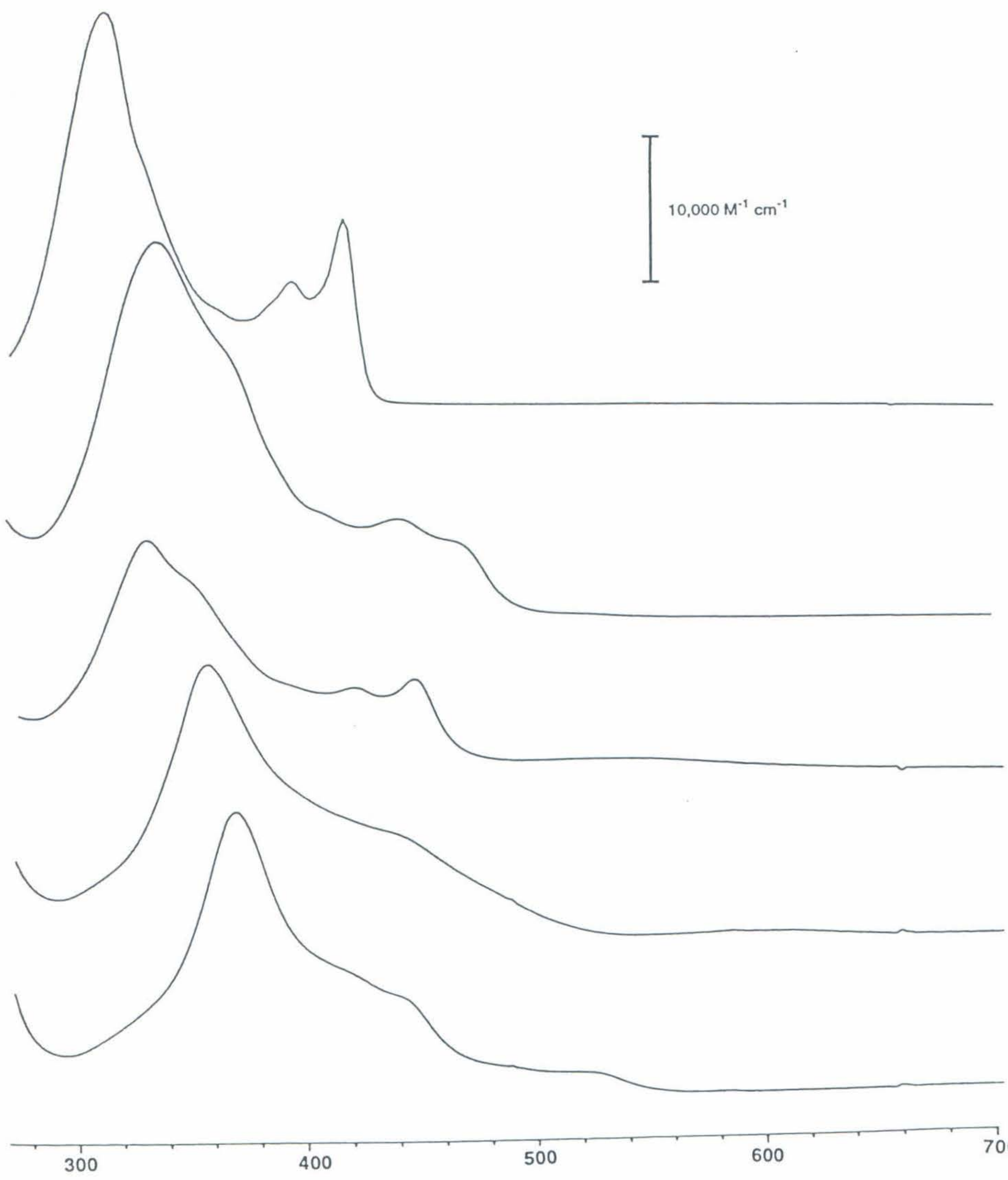
The infrared spectra of compounds **3** and **4** show similar absorptions attributable to CO stretching for the three CO ligands (**3**, 1915, 1977, 2030 cm^{-1}; **4**, 1910, 1980, 2020 cm^{-1}). While these small frequency shifts would seem to indicate that the presence of the $PdCl_2$ unit does not significantly perturb the electronic structure of the Re center, other work has shown that CO stretching is not particularly sensitive of metal-metal coupling in polymetallic systems. This will be addressed in the Discussion Section.

The electronic absorption spectra of chloroform solutions of **1** - **5** are shown in Figure 4.10. The hhtn spectrum is dominated by intense π-π^* absorptions between 300 and 420 nm; these features broaden and red shift in complexes **2** - **5**. In **3** the red shift is not quite as pronounced as in **2**, and the spectrum resembles that of the free ligand more closely. Spectral features become poorly resolved upon coordination of a second metal center.

A chloroform solution of **1** displays a single emission centered at 455 nm (366 nm excitation) at room temperature. The same spectrum is seen for a 77 K frozen solution of **1**. A frozen (77 K) dichloromethane solution of $Re(CO)_3Cl$(hhtn) displays emission at 580 and 710 nm when excited at 436 nm. At 77K, $PdCl_2$(hhtn) shows only one emission band at 620 nm, nearly identical with the 620 nm emission of **5**. At low temperature the heterobinuclear complex, **4**, shows a very broad, asymmetric emission band at 660 nm.

A dichloromethane solution of the hhtn ligand exhibits a reversible reduction at -1.09 V, a quasi-reversible reduction at -1.40 V, and an irreversible oxidation at 1.52 V vs. Ag/AgCl at room temperature. In **3**, the two ligand reductions shift to less negative values, -0.48 and -0.75 V, and 4 new irreversible reduction waves are observed out to the solvent limit. An irreversible oxidation is also observed towards the positive solvent limit. All the palladium-containing compounds (**2**, **4**, **5**) display evidence of decomposition, and reliable cyclic voltammetric data were not obtained.

Figure 4.10. Electronic absorption spectra of **1** (top) - **5** (bottom) in $CHCl_3$ solution: **1,** 312 (91000); 332 (44000); 394 (29000); 416 (51000). **2,** 338 (74000); 336 (54000); 440 (20000); 466 (15000). **3,** 328 (46000); 346 (37000); 416 (17500); 444 (19000). **4,** 358 (59000); 438 (24000); 570 (2800). **5,** 370 (57000); 412 (27500); 440 (21000); 520 nm (5600 M^{-1} cm^{-1}).


10,000 M^{-1} cm^{-1}
300
400
500
600
700
Wavelength (nm)

Structure of $[PdCl_2(hhtn)]_2 \bullet C_6H_5Cl \bullet 2\ CH_3OH$, 2. The asymmetric unit consists of two molecules of the complex, one molecule of chlorobenzene, and two molecules of methanol. A view of the molecule containing Pd(1) is shown in Figure 4.11, while a complete picture of the unit cell is presented in Figure 4.12. Selected atomic coordinates for the Pd(1)-containing species are given in Table 4.2, and selected atomic distances and angles are given in Table 4.3. Atomic coordinates, distances, and angles for the molecule containing Pd(2) are included in Appendix 3.

The complex crystallizes with two crystallographically independent but strongly interacting $PdCl_2$(hhtn) molecules. This intimate association can be seen in Figure 4.13. The coordination environment around the two metal centers is slightly different; the Pd-Cl distances between the two complexes are uniform and within normal ranges while the Pd-N separations are slightly perturbed (Pd(1)-N(1), 2.057(6)Å; Pd(1)-N(6), 2.059(9)Å vs. Pd(2)-N(7), 2.063(7)Å; Pd(2)-N(12), 2.038(8)Å) and there is a slight cant in the coordination plane of Pd(2). The geometry around the Pd center is nearly square planar with the sum of the angles around Pd(1) approaching 359°. There is a contraction of the N(1)-Pd(1)-N(6) angle to 80.7(3)°, owing to the rigid bite of the hhtn ligand. Expansions of the N(1)-Pd(1)-Cl(2) and N(6)-Pd(1)-Cl(1) angles to 95.1(3)° and 95.5(2)° are observed. The deflection of $PdCl_2$ unit from the hhtn ligand plane, measured as the dihedral angle between the normals of the two planes, is 28.1 °. As shown in Figure 4.14, Pd(1) is 1.31Å below the calculated ligand plane. The two Cl atoms are in close contact with the hydrogen atoms on C(2) and C(21) (2.66Å, Cl(1)•••H(2A); and 2.62Å, Cl(2)•••H(21A)).

The 24 aromatic C-C distances from the Pd(1)-containing molecule range from 1.355(15) to 1.474(10)Å (average value of 1.415Å), while the 12 C-N distances are somewhat shorter and more uniform, ranging from 1.319(9) to 1.369(14)Å (average value of 1.344Å). The Pd-Cl distances are within normal ranges .

Figure 4.11. A perspective view of the Pd(1)-containing species of $2PdCl_2(hhtn)$ • C_6H_5Cl • $2CH_3OH$, **2**, with 50% thermal contours.

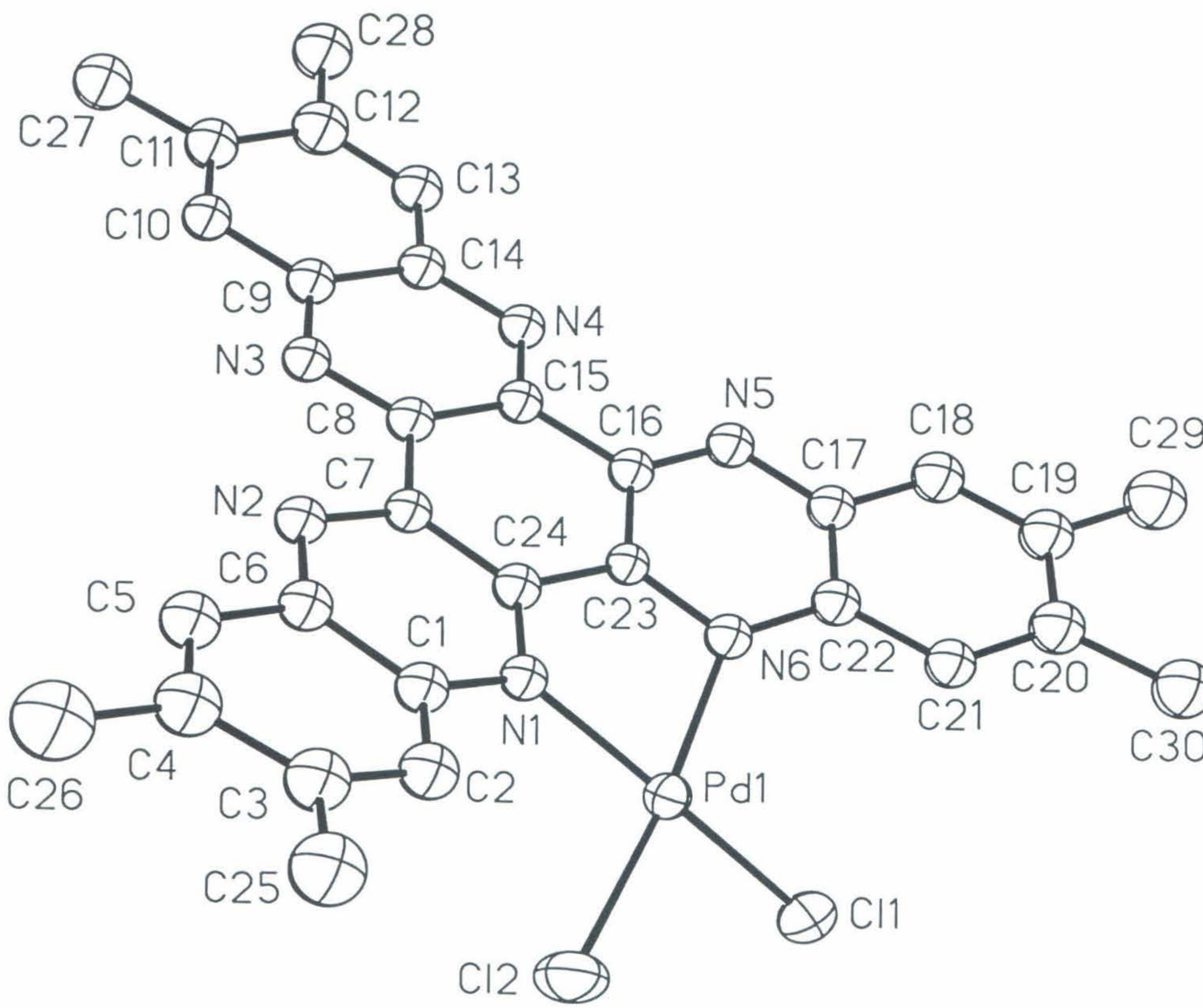

C28
C27
C11
C12
C13
C10
C14
C9
N4
N3
C15
C8
C16
N5
C18
C29
C17
C19
N2
C7
C24
C6
C5
C23
C1
N6
C22
C21
C20
C26
C4
N1
C30
C3
C2
Pd1
C25
Cl1
Cl2

Figure 4.12. Complete asymmetric unit of 2 $PdCl_2$(hhtn) • C_6H_5Cl • 2 CH_3OH, **2**.

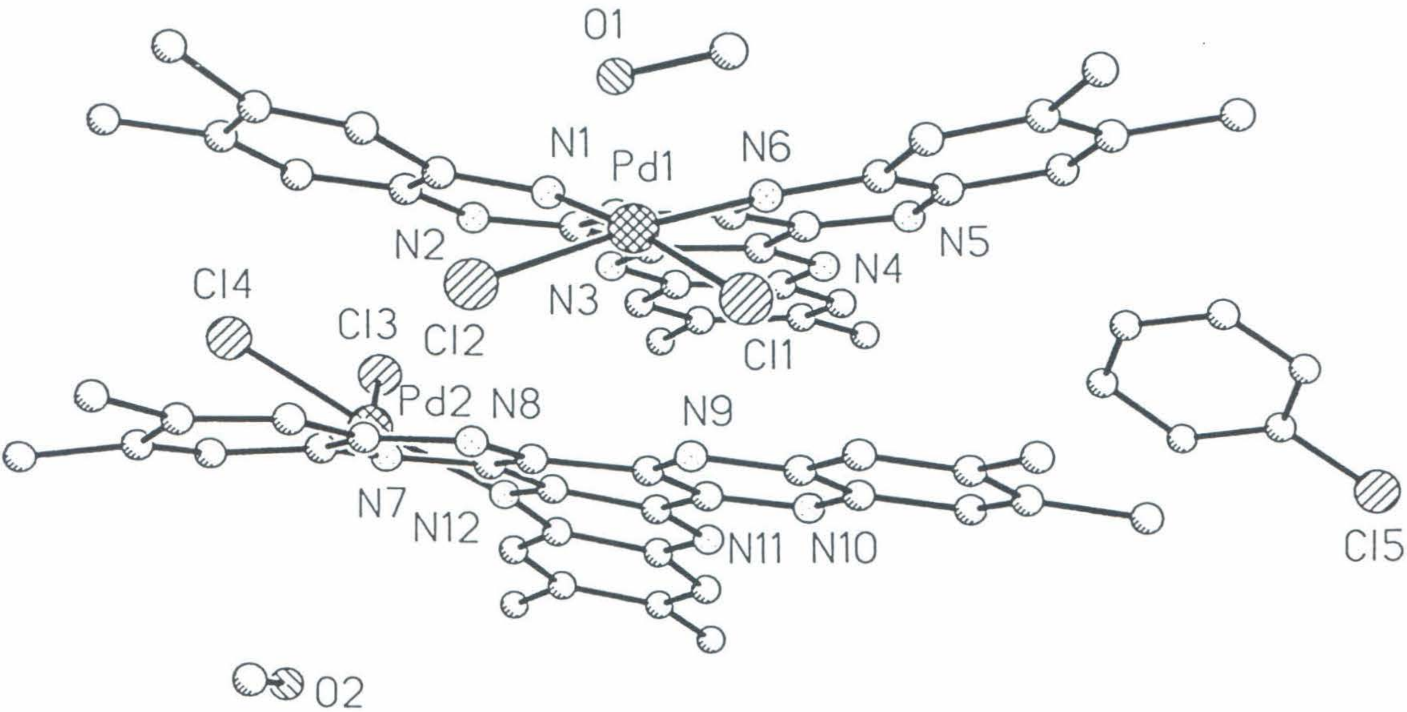

O1
N1
Pd1
N6
N2
N5
N4
Cl4
N3
Cl3
Cl2
Cl1
Pd2
N8
N9
N7
N12
N11
N10
Cl5
O2

Table 4.2. Atomic coordinates and equivalent displacement coefficients for $\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$, **2**.

Table 4.2.

Atomic Coordinates (x 10^4) and Equivalent Displacement Coefficients ($Å^2$ x 10^3) for $\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$, **2**.

	x	y	z	U(eq)
Pd(1)	4529(1)	6907(1)	1847(1)	28(1)*
Cl(1)	3944(2)	8357(2)	1084(2)	43(1)*
Cl(2)	4330(3)	6610(2)	727(2)	51(1)*
N(1)	4788(6)	5577(5)	2694(5)	25(2)
N(2)	4324(6)	3855(5)	4178(5)	29(2)
N(3)	3370(6)	3752(5)	5899(5)	27(2)
N(4)	3130(6)	5309(5)	6225(5)	28(2)
N(5)	3878(6)	6931(5)	4782(5)	28(2)
N(6)	4534(6)	7059(5)	2978(5)	26(2)
C(1)	5087(8)	4813(6)	2551(6)	30(2)
C(2)	5716(8)	4844(7)	1702(6)	35(2)
C(3)	6030(9)	4075(7)	1580(7)	41(2)
C(4)	5658(9)	3210(7)	2317(7)	43(3)
C(5)	5080(8)	3178(7)	3149(7)	37(2)
C(6)	4819(8)	3950(6)	3319(6)	30(2)
C(7)	4127(7)	4614(6)	4299(6)	25(2)
C(8)	3663(7)	4552(6)	5232(6)	27(2)
C(9)	2942(7)	3695(6)	6755(6)	29(2)
C(10)	2608(7)	2857(6)	7491(6)	31(2)
C(11)	2180(8)	2786(7)	8355(7)	38(2)
C(12)	2090(9)	3567(7)	8538(7)	43(3)
C(13)	2372(8)	4384(6)	7832(6)	34(2)
C(14)	2823(7)	4494(6)	6915(6)	28(2)
C(15)	3546(7)	5345(6)	5396(6)	26(2)
C(16)	3888(7)	6223(6)	4623(6)	27(2)
C(17)	4258(7)	7697(6)	4046(6)	28(2)
C(18)	4334(8)	8456(6)	4200(7)	37(2)
C(19)	4750(8)	9249(7)	3476(7)	37(2)
C(20)	5149(8)	9313(7)	2563(7)	38(2)
C(21)	5047(8)	8590(6)	2408(6)	31(2)
C(22)	4602(7)	7778(6)	3141(6)	28(2)

Table 4.2 continued.

C(23)	4246(7)	6269(5)	3722(5)	23(2)
C(24)	4356(7)	5477(6)	3561(6)	28(2)
C(25)	6800(9)	4104(7)	687(7)	51(3)
C(26)	5946(10)	2365(8)	2155(8)	63(3)
C(27)	1794(9)	1893(7)	9126(7)	47(3)
C(28)	1619(9)	3489(7)	9495(7)	50(3)
C(29)	4827(9)	10037(7)	3661(7)	51(3)
C(30)	5653(9)	10172(7)	1793(7)	46(3)

*Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table 4.3. Selected bond lengths and angles for $\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$, **2**.

Table 4.3.

Selected Bond Lengths (Å) and Angles (deg) for $\{PdCl_2(hhtn)\}_2 \cdot C_6H_5Cl \cdot 2CH_3OH$, **2**.

Bond Lengths

Pd(1)-Cl(1)	2.283(2)	Pd(1)-Cl(2)	2.277(4)
Pd(1)-N(1)	2.057(6)	Pd(1)-N(6)	2.059(9)
N(1)-C(1)	1.369(14)	N(1)-C(24)	1.345(12)
N(6)-C(22)	1.367(15)	N(6)-C(23)	1.353(9)

Bond Angles

Cl(1)-Pd(1)-Cl(2)	87.6(1)	Cl(1)-Pd(1)-N(1)	169.9(2)
Cl(2)-Pd(1)-N(1)	95.1(3)	Cl(1)-Pd(1)-N(6)	95.5(2)
Cl(2)-Pd(1)-N(6)	172.1(2)	N(1)-Pd(1)-N(6)	80.7(3)
Pd(1)-N(1)-C(24)	117.8(7)	Pd(1)-N(6)-C(23)	108.1(7)
N(1)-C(24)-C(23)	117.3(7)	N(6)-C(23)-C(24)	116.8(8)

Figure 4.13. A view emphasizing the intermolecular interaction between the $PdCl_2$(hhtn) units of **2.** The solid line represents the distance between the centroids of the hhtn molecule, while the dashed line shows the perpendicular separation between the least squares planes of the hhtn ligands. The Pd(1)' molecule is generated by 1-x, 1-y, 1-z and Pd(2)' is generated by -x, 1-y, 1-z.

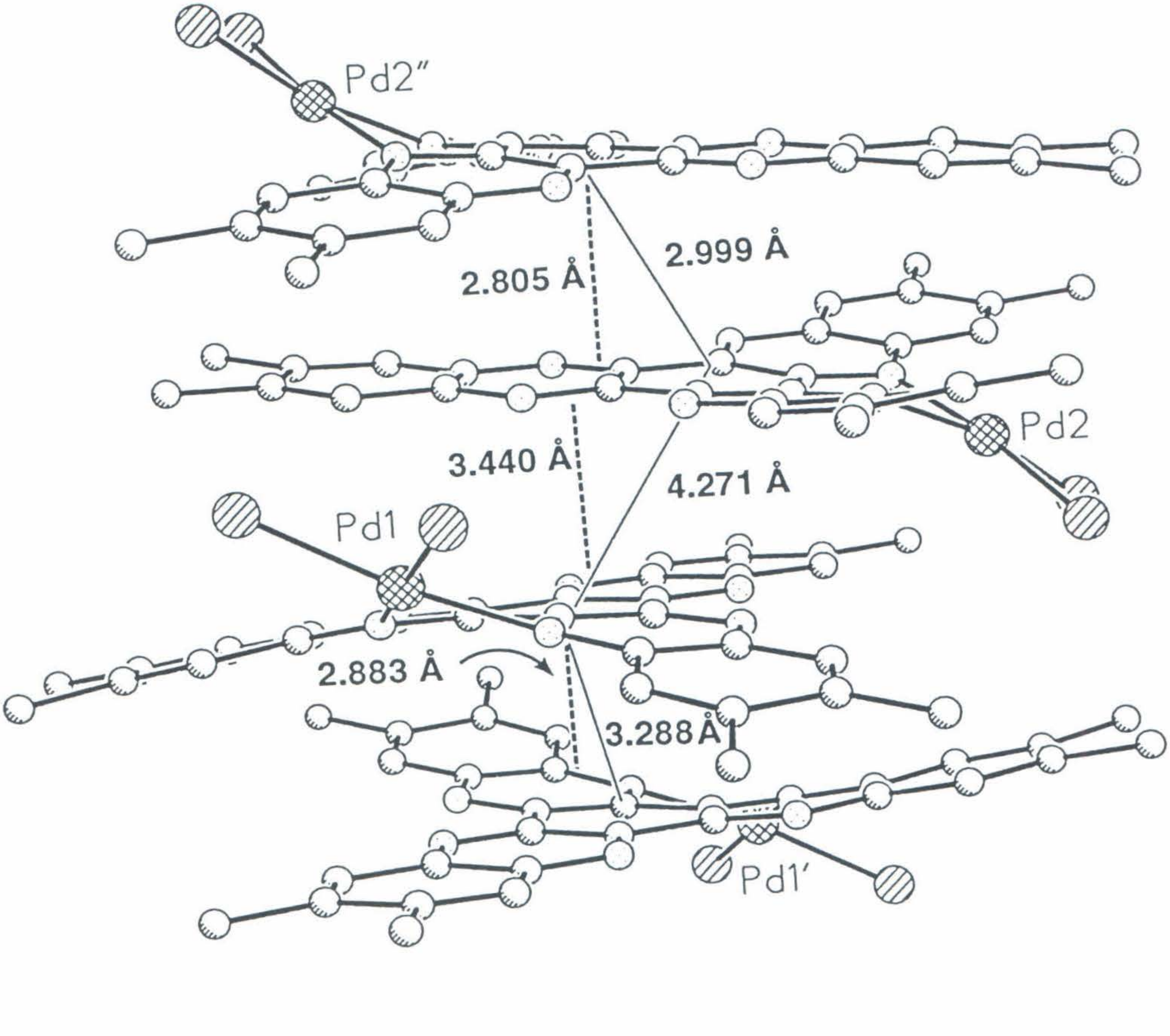
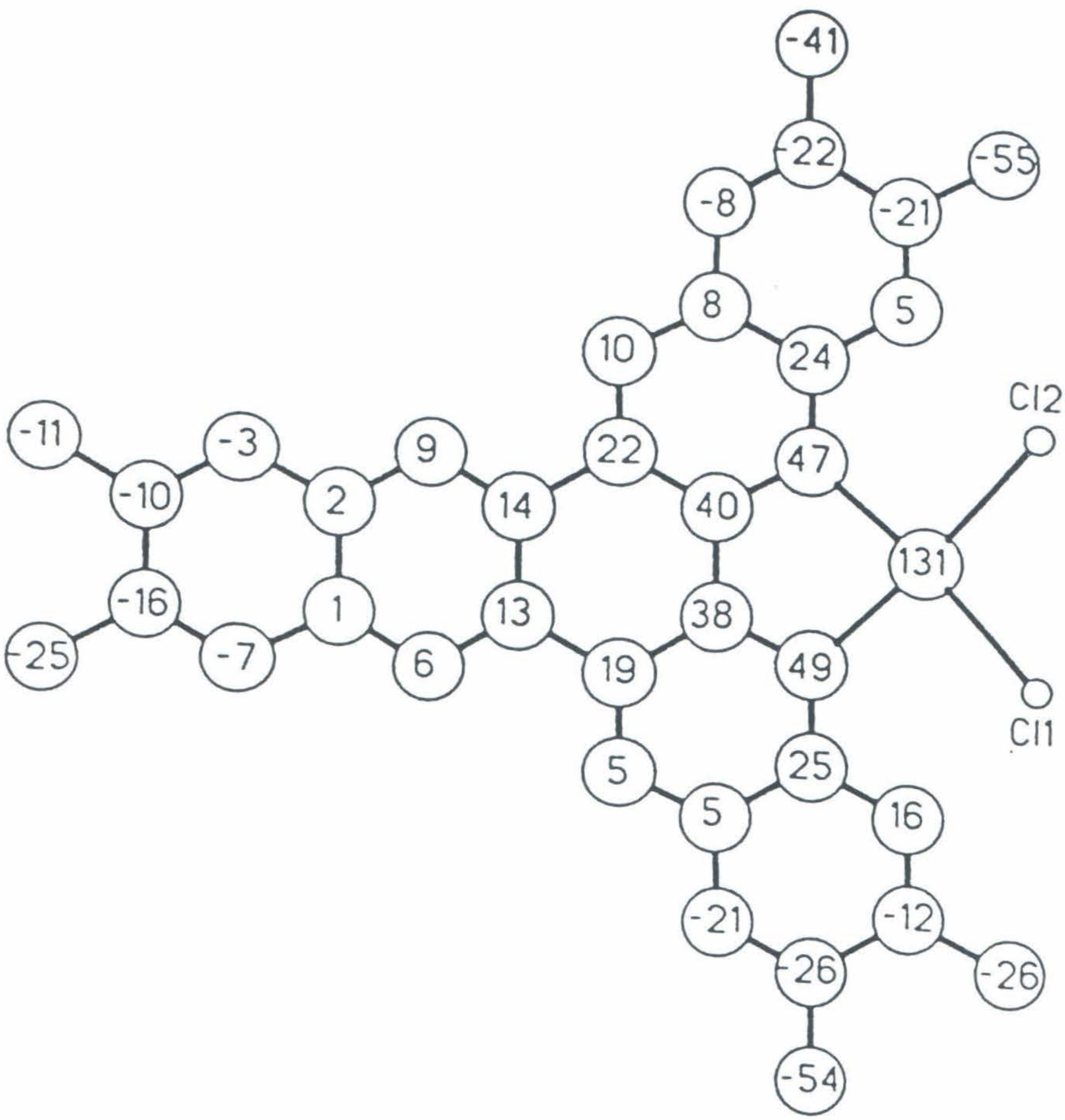

Pd2″
2.805 Å
2.999 Å
Pd2
3.440 Å
4.271 Å
Pd1
2.883 Å
3.288 Å
Pd1′

Figure 4.14. Drawing showing the displacements (0.01Å) from the least-squares plane calculated for the hhtn ligand of **2**.



-41
-22
-55
-8
-21
8
5
10
24
Cl2
-11
-3
9
22
47
-10
2
14
40
131
-16
1
13
38
-25
-7
6
19
49
Cl1
5
25
5
16
-21
-12
-26
-26
-54

The ligands adopt a staggered configuration with respect to hhtn ligands; the $PdCl_2$ portions directed approximately 180°apart from each other. The molecules (Figure 4.13) adopt an alternating convex-concave (CV-CC), concave-convex (CC-CV) relationship. The ligands in the CC-CV relationship are staggered, and in the CV-CC arrangement they are eclipsed and offset from each other. The perpendicular separation between the least-squares-calculated planes is 3.44Å in the CC-CV arrangement; interestingly, this separation is only ca. 2.88Å in the CV-CC geometry. This shorter distance reflects the fact that few atoms actually lie on the least-squares plane. The 3.44Å separation is in the normal range for π-π (ligand-ligand) interactions.[20]

Structure of $Re(CO)_3Cl(hhtn) \cdot CH_3OH$, 3. The asymmetric unit contains one crystallographically independent molecule of this complex and one methanol solvate. A view of the complex is shown in Figure 4.15. Selected atomic coordinates are given in Table 4.4, and selected atomic distances and angles are given in Table 4.5.

The coordination environment around the Re center is roughly octahedral. The Re-C and Re-Cl separations are normal. The Re-N(1) and Re-N(6) distances of 2.222(6) and 2.203(6)Å are within observed ranges. The N(1)-Re-N(6) angle is contracted to 75.5° as a result of the constrained bite of the hhtn ligand. The C-C and C-N separations are very similar to **2** with the 24 aromatic C-C distances ranging from 1.361(11) to 1.478(10)Å (average value of 1.416Å). The 12 C-N separations range from 1.315(10) to 1.379(11)Å (average value of 1.345Å).

The complex crystallizes in an intimate π - π association with a second symmetry-related molecule of the complex. This arrangement is best described as an offset head-to-tail geometry with the mean separation between the planes calculated for the hhtn ligands being 2.94Å. The hhtn ligand in **3** is slightly twisted with an average distortion from planarity of 0.13Å. As shown in Figure 4.16, the Re atom sits 0.61Å beneath the plane as a result of the sterically-hindered coordination pocket. The C(1)•••H(6A) and

Figure 4.15. A perspective view of $Re(CO)_3Cl(hhtn)$, **3**, with 50% thermal contours.

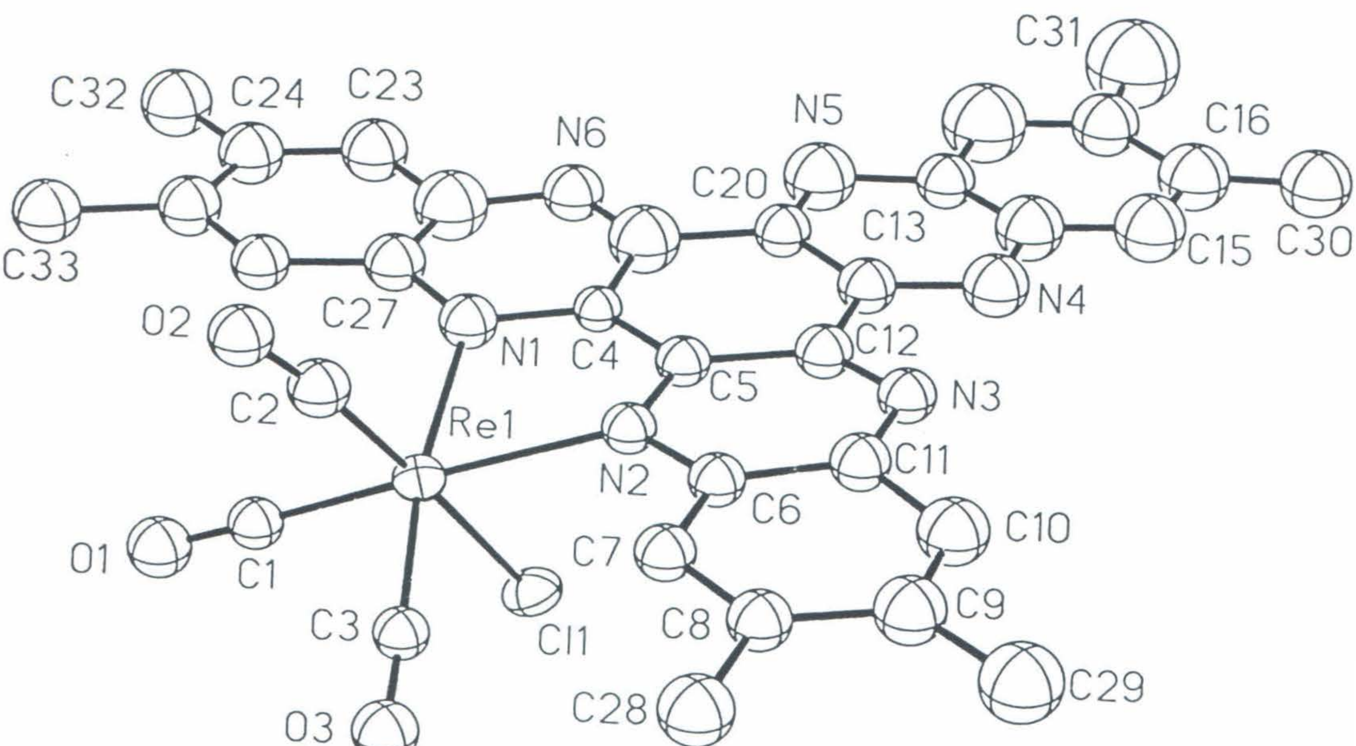

C31
C32
C24
C23
N6
N5
C16
C20
C13
C33
C15
C30
C27
N4
O2
N1
C4
C12
C5
N3
C2
Re1
N2
C11
C6
C10
C7
O1
C1
C9
C3
Cl1
C8
C29
C28
O3

Table 4.4. Atomic coordinates and equivalent displacement coefficients for $Re(CO)_3Cl(hhtn) \bullet CH_3OH$, **3**.

Table 4.4.

Atomic Coordinates (x 10^4) and Equivalent Displacement Coefficients

($Å^2$ x 10^3) for $Re(CO)_3Cl(hhtn) \cdot CH_3OH$, **3**.

	x	y	z	U(eq)*
Re	489(1)	1041(1)	1531(1)	17(1)
Cl	2622(2)	1409(1)	1543(2)	30(1)
O(1)	534(6)	375(2)	-633(5)	29(2)
O(2)	2123(6)	203(2)	3186(5)	32(2)
O(3)	-2020(7)	561(2)	1748(6)	37(3)
N(1)	-393(6)	1716(2)	440(6)	17(2)
N(2)	-772(7)	2675(2)	-606(6)	19(2)
N(3)	-442(6)	3477(2)	908(6)	18(2)
N(4)	723(7)	3356(2)	3571(6)	18(2)
N(5)	1107(7)	2431(2)	4555(6)	20(2)
N(6)	581(6)	1597(2)	2970(6)	19(2)
C(1)	468(8)	624(3)	169(7)	18(2)
C(2)	1502(8)	517(3)	2587(7)	22(3)
C(3)	-1182(9)	756(3)	1649(7)	21(3)
C(4)	-124(8)	2125(3)	1154(7)	18(3)
C(5)	-919(7)	1782(3)	-837(7)	16(2)
C(10)	-1042(8)	2270(3)	-1342(7)	19(3)
C(11)	-332(8)	2600(3)	623(7)	19(3)
C(12)	127(8)	3038(3)	1441(7)	19(3)
C(13)	-174(8)	3867(3)	1693(7)	17(3)
C(18)	441(8)	3815(3)	3015(7)	20(3)
C(19)	418(8)	2975(3)	2772(7)	16(2)
C(21)	1234(8)	1973(3)	5038(7)	18(2)
C(26)	923(8)	1543(3)	4229(7)	18(3)
C(27)	403(7)	2061(6)	2514(7)	15(2)

*Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ij}

Table 4.5. Selected bond lengths and angles for $Re(CO)_3Cl(hhtn) \bullet CH_3OH$, **3**.

Table 4.5.

Selected Bond Lengths (Å) and Angles (deg) for $Re(CO)_3Cl(hhtn) \cdot CH_3OH$, **3**.

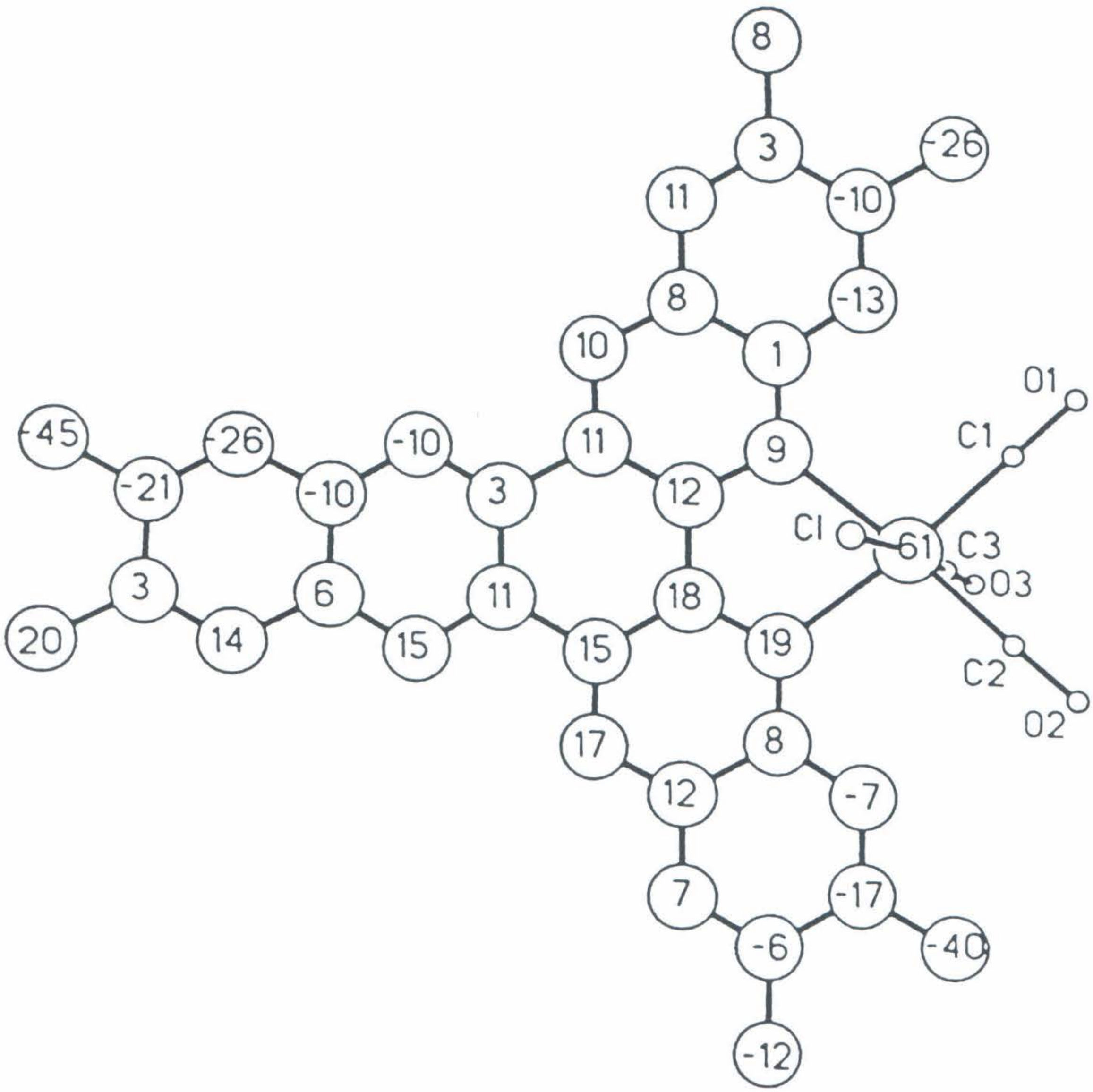
Bond Lengths

Re-Cl	2.241(2)	Re-C(1)	1.913(8)
Re-C(2)	1.918(7)	Re-C(3)	1.967(9)
Re-N(1)	2.222(6)	Re-N(6)	2.203(6)
C(1)-O(1)	1.158(10)	C(2)-O(2)	1.141(9)
C(3)-O(3)	1.069(12)	N(1)-C(4)	1.344(9)
N(1)-C(5)	1.370(9)	N(2)-C(10)	1.3504(9)
N(2)-C(11)	1.323(9)	N(3)-C(12)	1.324(9)
N(3)-C(13)	1.348(9)	N(4)-C(18)	1.379(9)
N(4)-C(19)	1.338(9)	N(5)-C(20)	1.315(10)
N(5)-C(21)	1.347(9)	N(6)-C(26)	1.356(10)
N(6)-C(27)	1.348(9)	C(4)-C(11)	1.406(10)
C(4)-C(27)	1.457(10)	C(5)-C(10)	1.430(10)
C(11)-C(12)	1.477(10)	C(12)-C(19)	1.426(10)
C(13)-C(18)	1.417(11)	C(19)-C(20)	1.478(10)
C(20)-C(27)	1.417(10)	C(21)-C(26)	1.448(10)

Bond Angles

Cl-Re-N(1)	82.2(2)	Cl-Re-N(6)	85.4(2)
Cl-Re-C(1)	89.5(3)	Cl-Re-C(2)	89.8(3)
N(1)-Re-N(6)	75.5(2)	N(1)-Re-C(1)	98.8(3)
N(6)-Re-C(2)	100.0(3)	C(1)-Re-C(2)	85.1(3)
N(1)-C(4)-C(27)	117.5(6)	N(6)-C(27)-C(4)	118.0(6)

Figure 4.16. Drawing showing the displacements (0.01Å) from the least-squares plane calculated for the hhtn ligand of **3**.


O1
C1
Cl
61
C3
O3
C2
O2

C(2)•••H(25A) separations are only 2..38 and 2.43 Å, respectively. It is these proton-carbonyl interactions which probably account for the 19.5° angle between the hhtn ligand and the Re equitorial coordination plane.

Structure of (Re(CO)$_3$Cl)(PdCl$_2$)(hhtn) • 2.6 1,2–Cl$_2$C$_6$H$_4$, 4. The asymmetric unit consists of the heterobinuclear complex and a group equivalent to 2.6 disordered dichlorobenzene molecules. A view of this complex is shown in Figure 4.17, and selected atomic coordinates are given in Table 4.6. Selected atomic distances and angles are set out in Table 4.7. The solvents are π-stacked with the binuclear complex at an average separation of 3.34Å.

The coordination environments around both metals are similar to those of the respective mononuclear complexes. The Pd-N distances are identical at 2.052(10) Å and the Pd-Cl(2) and Pd-Cl(3) distances are nearly equal at 2.277(3) and 2.276(3)Å. The sum of the angles around the Pd metal totals 358.9°. The $PdCl_2$ unit is bent 40.2° out of the hhtn plane and directed to the face opposite Re - Cl. The Re center is more closely coplanar to the hhtn ligand, with the dihedral angle of the normals equaling 10.4°. The Re-N separations (Re-N(1), 2.191(9); Re - N(6), 2.225(10) Å) are nearly identical with those seen in **3**. The Re - Cl and Re - C distances in **3** and **4** are also very similar. The N(1)-Re-N(6) and N(4)-Pd-N(5) angles of 75.6(3) and 79.9(4) °, respectively, are consistent with corresponding values for the mononuclear complexes.

The 24 aromatic C-C bond distances in **4** are similar to those of **2** and **3**. They range from 1.36(2) to 1.45(2)Å (average value of 1.42Å), while the 12 C-N distances range between 1.319(9) and 1.38(2)Å (average value of 1.345Å).

The intermolecular interactions of (Re(CO)$_3$Cl)(PdCl$_2$)(hhtn) including the long-range Pd-Pd' contact of 3.809 Å are shown in Figure 4.18. The hhtn ligand is considerably more distorted in **4** than in either of the mononuclear complexes; the average out-of-plane deviation for the hhtn ligand is 0.38 Å. As shown in Figure 4.19, the Pd atom is a full 1.56 Å above the least-squares plane, while the Re center is

Figure 4.17. A perspective view of $(PdCl_2)(Re(CO)_3Cl)(hhtn)$, **4**, with 50% thermal contours.

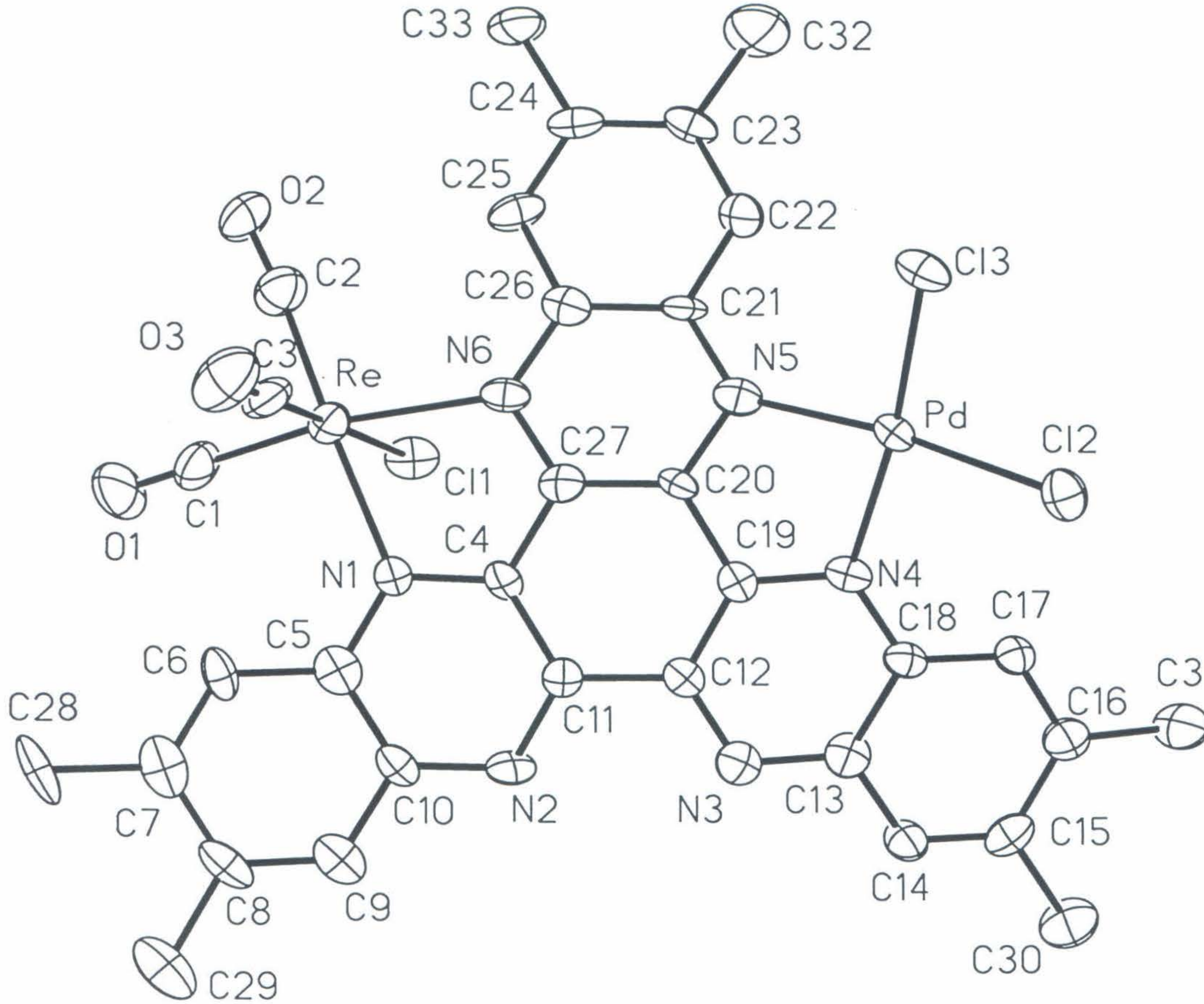

C33
C32
C24
C23
C25
O2
C22
C2
C26
C21
Cl3
O3
C3
Re
N6
N5
Pd
C27
Cl2
Cl1
C20
C1
O1
C4
C19
N1
N4
C5
C18
C17
C6
C12
C31
C28
C11
C16
C10
N2
N3
C13
C15
C7
C14
C8
C9
C30
C29

Table 4.6. Atomic coordinates and equivalent displacement coefficients for $(PdCl_2)(Re(CO)_3Cl)(hhtn) \cdot 2.6Cl_2C_6H_4$, **4**.

Table 4.6.

Atomic Coordinates (x 10^4) and Equivalent Displacement Coefficients ($Å^2$ x 10^3) for $(PdCl_2)(Re(CO)_3Cl)(hhtn) \cdot 2.6Cl_2C_6H_4$, **4.**

	x	y	z	U(eq)*
Re	1540(1)	1955(1)	3316(1)	30(1)
Pd	3695(1)	6108(1)	348(1)	23(1)
Cl(1)	-86(3)	3381(3)	2866(3)	39(1)
Cl(2)	4835(2)	6929(2)	-1000(2)	34(1)
Cl(3)	4494(2)	6016(2)	1449(2)	34(1)
O(1)	494(10)	289(9)	3906(9)	68(4)
O(2)	617(9)	1702(8)	5662(7)	57(3)
O(3)	3641(9)	253(9)	3758(8)	62(3)
N(1)	2164(7)	2155(7)	1634(7)	23(2)
N(2)	2527(7)	2912(8)	-574(7)	25(2)
N(3)	2751(8)	4925(8)	-1644(8)	30(2)
N(4)	3084(7)	5929(7)	-581(7)	22(2)
N(5)	2781(7)	5183(8)	1463(7)	28(2)
N(6)	2093(7)	3365(8)	2655(7)	26(2)
C(1)	899(12)	912(12)	3684(10)	46(4)
C(2)	965(12)	1844(11)	4778(11)	46(4)
C(3)	2889(12)	884(10)	3573(9)	41(3)
C(4)	2352(8)	3079(8)	1065(8)	21(2)
C(5)	2255(8)	1530(9)	1087(10)	28(3)
C(10)	2407(9)	1932(9)	-10(9)	25(2)
C(11)	2549(9)	3449(9)	-52(9)	24(2)
C(12)	2730(9)	4491(9)	-645(9)	24(2)
C(13)	2851(9)	5915(9)	-2116(9)	29(3)
C(18)	3027(9)	6436(9)	-1584(9)	25(2)
C(19)	2884(8)	4986(8)	-101(9)	21(2)
C(21)	2400(9)	4944(9)	2511(8)	25(3)
C(26)	2088(10)	4008(9)	3124(10)	30(3)
C(27)	2376(9)	3683(9)	1609(9)	25(3)

*Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table 4.7. Selected bond lengths and angles for $(PdCl_2)(Re(CO)_3Cl)(hhtn) \cdot 2.6Cl_2C_6H_4$, **4**.

Table 4.7.

Selected Bond Lengths (Å) and Angles (deg) for $(PdCl_2)(Re(CO)_3Cl)(hhtn) \bullet 2.6Cl_2C_6H_4$, **4.**

Bond Lengths

Re-Cl(1)	2.455(3)	Re-N(1)	2.191(9)
Re-N(6)	2.225(10)	Re-C(1)	1.906(14)
Re-C(2)	1.921(14)	Re-C(3)	1.94(2)
Pd-Cl(2)	2.277(3)	Pd-Cl(3)	2.276(3)
Pd-N(4)	2.052(9)	Pd-N(5)	2.052(10)
C(1)-O(1)	1.16(2)	C(2)-O(2)	1.15(2)
C(3)-O(3)	1.11(2)	N(1)-C(4)	1.328(13)
N(1)-C(5)	1.38(2)	N(2)-C(10)	1.360(14)
N(2)-C(11)	1.323(14)	N(3)-C(12)	1.319(14)
N(3)-C(13)	1.353(14)	N(4)-C(18)	1.354(14)
N(4)-C(19)	1.353(13)	N(5)-C(20)	1.326(14)
N(5)-C(21)	1.347(14)	N(6)-C(26)	1.37(2)
N(6)-C(27)	1.338(14)	C(4)-C(11)	1.44(2)
C(4)-C(27)	1.44(2)	C(5)-C(10)	1.42(2)
C(11)-C(12)	1.47(2)	C(12)-C(19)	1.41(2)
C(13)-C(18)	1.45(2)	C(19)-C(20)	1.44(2)
C(20)-C(27)	1.42(2)	C(21)-C(26)	1.43(2)

Bond Angles

Cl(1)-Re-N(1)	84.8(2)	Cl-Re-N(6)	81.1(3)
Cl-Re-C(1)	89.0(5)	Cl-Re-C(2)	93.3(4)
N(1)-Re-N(6)	75.6(3)	N(1)-Re-C(1)	97.7(5)
N(6)-Re-C(2)	102.6(5)	C(1)-Re-C(2)	83.8(6)
N(1)-C(4)-C(27)	117.4(10)	N(6)-C(27)-C(4)	119.1(10)
Cl(3)-Pd-Cl(2)	87.92(12)	N(4)-Pd-Cl(2)	95.4(3)
N(5)-Pd-Cl(3)	95.7(3)	N(5)-Pd-N(4)	79.9(4)
N(5)-Pd-Cl(2)	171.4(3)	N(4)-Pd-Cl(3)	170.9(3)
N(4)-C(19)-C(20)	115.3(10)	N(5)-C(20)-C(19)	117.5(10)
C(11)-N(2)-C(10)	116.5(10)	C(12)-N(3)-C(13)	116.9(10)
C(4)-N(1)-C(5)	116.5(10)	C(11)-N(2)-C(10)	116.5(10)
C(12)-N(3)-C(13)	116.9(10)	C(19)-N(4)-C(18)	117.2(9)
C(20)-N(5)-C(21)	116.5(10)	C(27)-N(6)-C(26)	116.2(10)

Figure 4.18. A view of $(PdCl_2)(Re(CO)_3Cl)$(hhtn) emphasizing the large hhtn distortion and the long-range Pd•••Pd interaction of 3.809 Å.

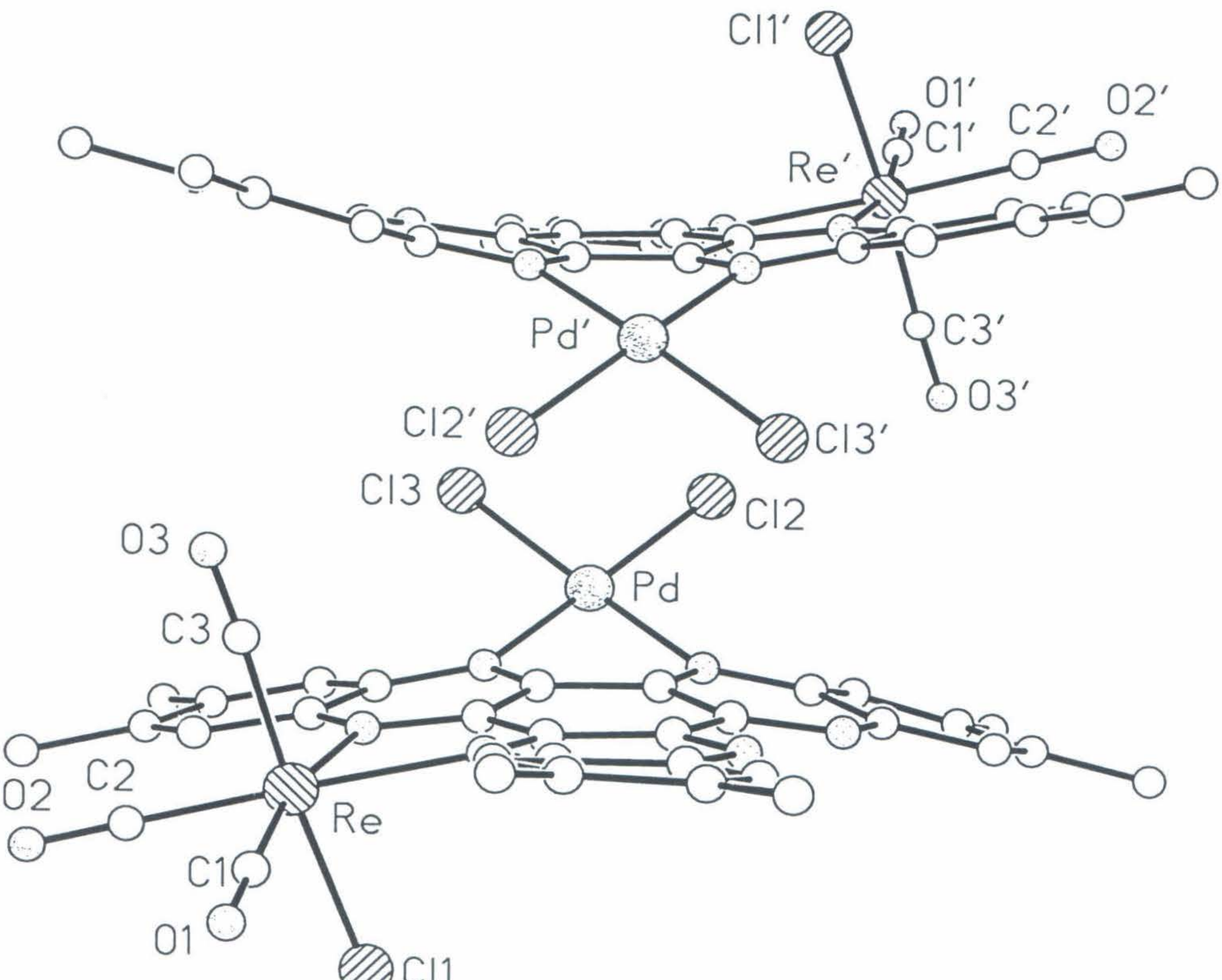
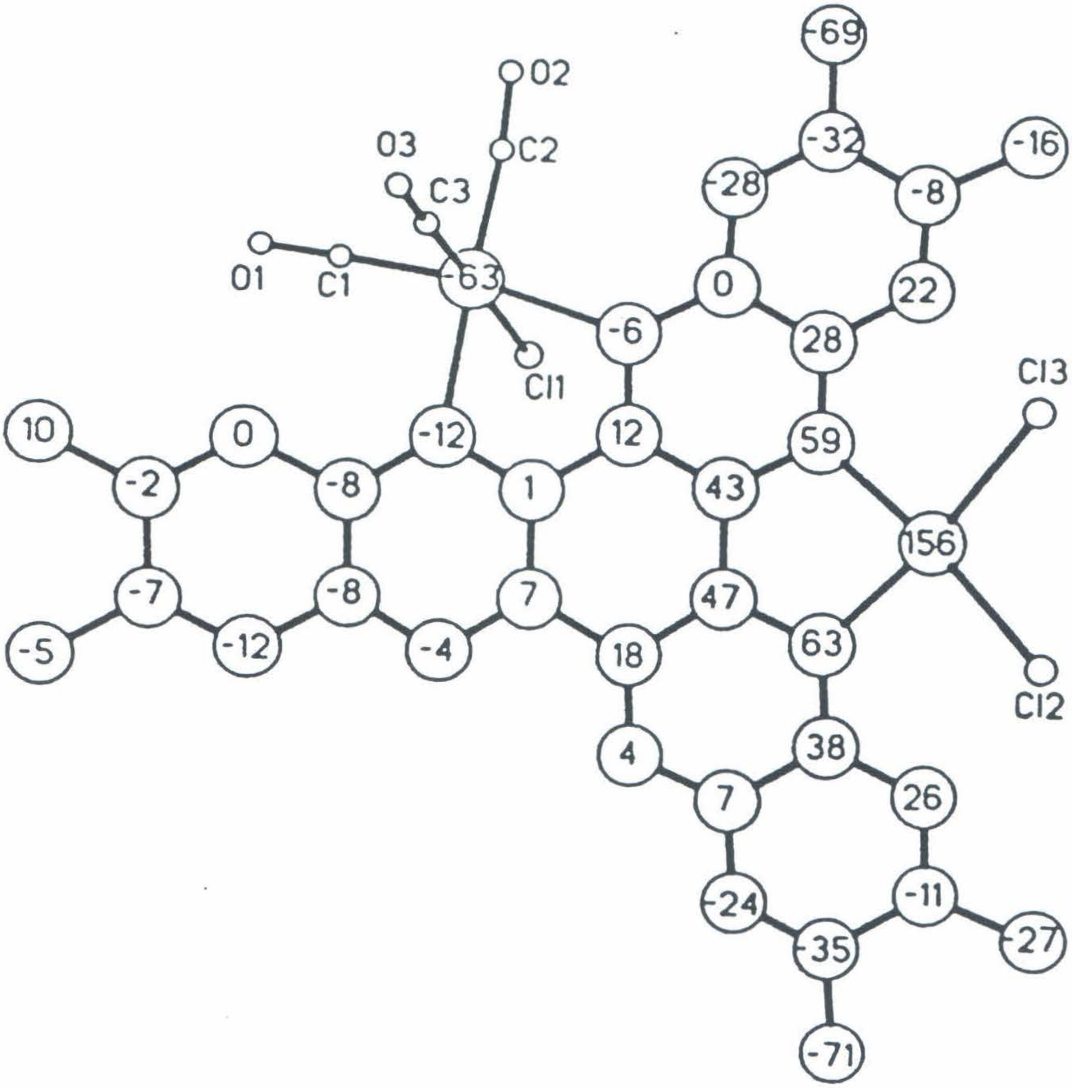

Cl1'
O1'
C1'
C2'
O2'
Re'
Pd'
C3'
O3'
Cl2'
Cl3'
Cl3
Cl2
O3
Pd
C3
C2
O2
Re
C1
O1
Cl1

Figure 4.19. Drawing showing the displacements (0.01Å) from the least-squares plane calculated for the hhtn ligand of **4**.



O2
C2
O3
C3
O1
C1
-63
Cl1
Cl3
Cl2
-69
-32
-16
-28
-8
0
22
-6
28
10
0
-12
12
59
-2
-8
1
43
156
-7
-8
7
47
-5
-12
-4
18
63
4
38
7
26
-24
-11
-35
-27
-71

displaced by 0.63 Å in the opposite direction. The ^{1}H contacts in **4** are similar to those in the mononuclear complexes, with C(1)•••H(5) and C(2)•••H(25) measuring 2.37 and 2.30 Å, while the Cl(2)•••H(17) and Cl(3)•••H(22) separations are 2.69 and 2.68Å, respectively.

Discussion

The straightforward reaction scheme employed to make the hhtn complexes described allows their synthesis in high yield. The high-yield, one-pot synthesis of hhtn is attractive compared to the synthesis of HAT. While the sterically-hindered, dibenzophenanthroline-like coordination does not allow the coordination of the photochemically-active $Ru(bpy)_2^{2+}$ unit, the hhtn ligand is capable of binding transition metals. The trinucleating nature of hhtn allows for the stepwise addition of up to three different metals, making the synthesis of a wide variety of systems possible. While low solubility prohibited isolation of trinuclear compounds in this work, metathesis of the axial Cl^- ion for a neutral ligand such as pyridine allows more soluble ionic species to be made.[21] This should facilitate development of trinuclear compounds.

The structures of **2-4** are very distorted. Owing to severe congestion in the hhtn coordination pocket, the metal center is deflected from the hhtn plane to reduce the unfavorable interaction of ^1H with the equatorial ligands. The large out-of-plane distortions in the structures of **2** (28.1°), **3** (19.5°), and **4** (40.2° for the $PdCl_2$ unit and 10.4° for the $Re(CO)_3Cl$ fragments) are manifestations of these interactions. The displacements in **4** (greater for $PdCl_2$, smaller for $Re(CO)_3Cl$) are due to coupling of the Pd and Re centers. Binding the $Re(CO)_3Cl$ moiety to hhtn induces a significant out-of-plane distortion on N(4) and N(5) (Figure 4.16) that predisposes the incoming $PdCl_2$ center to nitrogen lone pairs that are already greatly displaced out of the hhtn ligand plane; this results in a complex, **4**, where the hhtn ligand is significantly more twisted and cupped compared to **2** and **3**. The twist reduces the steric interaction of the Re equatorial carbonyls, while the cup-like distortion imposes more strain on the Pd center by forcing H(17) and H(22) towards the chlorides. The long-range interatomic Pd•••Pd' contact may also contribute to the large $PdCl_2$ out-of-plane displacement. Structural data on similar highly hindered ligands are lacking; however, in $PdCl_2$(*cis*-2,9-bis[2,2 (methoxycarbonyl) ethyl]-1,10-phenanthroline),[22] the $PdCl_2$ unit is deflected 32.3° out-of-plane. This is presumably due to steric interactions of the methylene protons of the ethyl group with the metal chlorides (H•••Cl separations are 2.66 and 2.58 Å). Using 6,6'-dimethyl-2,2'-bipyridine as the chelating ligand leads to a similar distortion.[23] Likewise, in Pd(η^3-allyl)(8,8'-dimethyl-2,2'-diquinolyl), the Pd atom is deflected 30.5°from a square planar configuration to minimize the allyl-methyl interactions.[24]

The extended π - π interactions in **2**, **3**, and **4** are similar to those of many other π-complexed structures.[6,7,25] The π - π interactions in **2** are the most pronounced because the square planar Pd center allows for close intermolecular packing. The Re axial ligands in **3** and **4** disfavor similar π - π interactions.

The aromatic hhtn ligand is expected to be planar. Crystal structures of phenazine[26] and its Cu(I) and Ag(I)[27] complexes show very little deviation from planarity of the phenazine ligand. Nor does the related complex, $[Cu_3(qpy)_3(Ph_6HAT)]^{3+}$ (qpy is quaterpyridine), show any significant deviation from planarity, with a *maximum* displacement of only 0.19Å for the HAT portion of the ligand including the three Cu atoms.[4] In contrast, the *average* displacements for the hhtn ligand in **2**, **3**, and **4** are 0.32, 0.13, and 0.38 Å, respectively. The deviations in the hhtn complexes are due primarily to the constrained coordination environment.

Coordination of metal centers shifts aromatic ^{1}H NMR resonances downfield relative to free hhtn. The shift in **2**, 0.87 ppm, is likely larger than observed in **3**, 0.43 ppm, due to greater deshielding by Cl relative to CO. The downfield shift is similar to that observed in the related complex *fac*-Re(CO)$_3$Cl[dipyrido(2,3-*a*:2',3'-*h*)phenazine] is 0.83 ppm.[28]

As alluded to earlier, changes in CO IR stretching frequencies are not always a good indicator of perturbation of the electronic structure of Re complexes. Work has shown that the Ru centers in dinuclear $[Ru(bpy)_2]_2(2,2'\text{-bipyrimidine})^{4+}$ are coupled, as evidenced by a NIR IT band in$[Ru(bpy)_2]_2(2,2'\text{-bipyrimidine})^{5+}$.[29] However, only small shifts in IR frequencies are seen in going from Re(CO)$_3$Cl (2,2'-bipryrimidine), whose

CO stretches are at 2033 and 1906 cm^{-1}, to $[Re(CO)_3Cl]_2$ (2,2'-bipryrimidine), in which the frequencies are 2028 and 1908 cm^{-1}.[27] Thus the similar small difference seen upon coordination of $PdCl_2$ to **3** (CO frequencies of 2030 and 1915 cm^{-1}) to give heterobimetallic **4** (CO frequencies of 2020 and 1910 cm^{-1}) may not indicate the degree of coupling between the metal centers.

The spectroscopic features of **2** - **5** are analogous to those observed for Pd(II)[30] and Re(I)[31] complexes containing π-acceptor ligands. The lowest energy band of **3** (514 nm) is assigned as Re(dπ)$\rightarrow$ hhtn(π*) MLCT, while the higher energy bands (300 to 450 nm) are attributed to intraligand transitions. For comparison, the MLCT band of $Re(CO)_3Cl$(phen) is at 409 nm (4000 M^{-1} cm^{-1}).[31] The MLCT bands of **2** and **5** (466 and 520nm, respectively) can be compared to those of $PdCl_2$(phen) [298 (1930) and 357 nm (1280 $M^{-1}cm^{-1}$)].[32] The positions of the MLCT bands in **2**, **3**, and **5** indicate that the π* orbital of hhtn that gives rise to the MLCT lies lower than that of phenanthroline. This finding is supported by CV data: the reduction of **3** occurs at -0.48 and -0.75 V, while $Re(CO)_3Cl$ (phen) is reduced at -1.3 V.[33] The difference between the MLCT energies of **3** (514 nm = 2.41 eV) and $Re(CO)_3Cl$ (phen) (409 nm = 3.03 eV) is 0.62 eV, which is nearly the same as the difference between the second reduction of **3** and the reduction of $Re(CO)_3Cl$ (phen), 0.55 V. This indicates that the MLCT does not involve the LUMO of hhtn. Rather, the excited electron resides in a higher-lying bpy-type orbital, while the reduction at -0.48 V is likely of an orbital possessing pz character. Such behavior is analogous to that seen in complexes of bdppz.

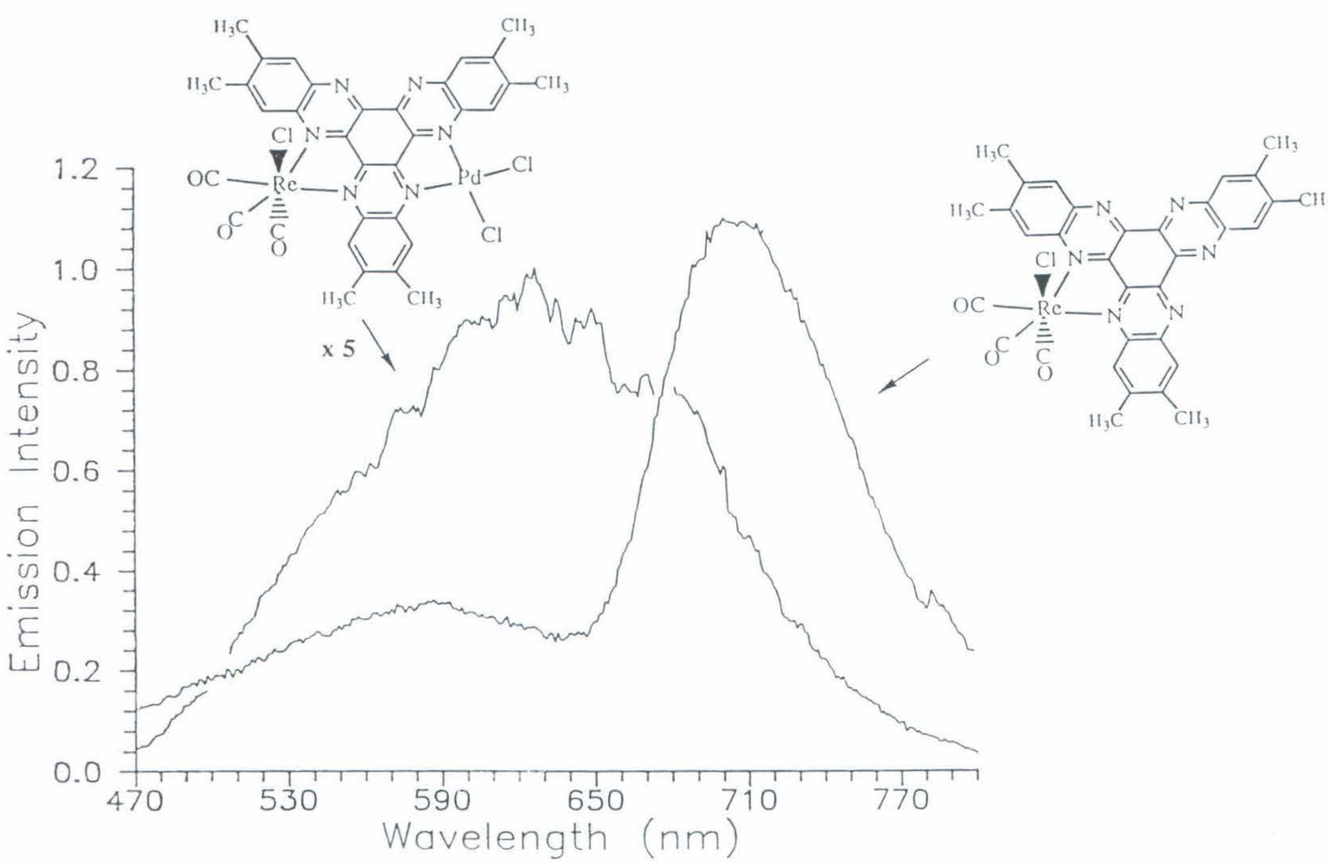
Changes in visible absorption spectra are a better indication of metal-metal interaction than are changes in IR spectra. In Chapter 3 it was demonstrated by the $[Ru(bpy)_2]_n(tppz)^{2n+}$ series that the MLCT energy does not change with n when the metal centers are uncoupled. For the $[Ru(bpy)_2]_n(2,2'\text{-bipyrimidine})^{2n+}$ series the MLCT band shifts from 480 nm for n=1 to 594 nm for n=2. In $[Re(CO)_3Cl]_n$(2,2'-bipryrimidine), the MLCT absorption shifts from 384 to 480 nm when the second metal is coordinated,

indicating that the Re atoms interact much more than one would conclude on the basis of IR data alone. MLCT shifts also show that HAT facilitates electronic communication between coordinated metals; in $[Ru(bpy)_2]_n(HAT)^{2n+}$, the band shifts from 432 nm when n=1 to 580 nm when n=3. The MLCT redshift seen in $(PdCl_2)_2$(hhtn) relative to $PdCl_2$(hhtn) suggests that interaction between the metals is taking place.
The electrochemical behavior of **5** would better indicate the degree of coupling between the $PdCl_2$ moities; the poor CV behavior of Pd complexes in general precludes such a study.

Ground-state interactions between coordinated metals is not desirable in a multielectron photochemical system. Coupling leads to a delocalized electronic structure; while polymetallic, such a complex has a net one-electron excited state, and is not capable of delivering multiple redox equivalents to the catalytic center. Components must retain the properties they exhibited as monomers when brought together in an organized assembly. Thus it appears that hhtn is not an optimal choice as a platform on which to construct such an assembly.

Emission from **3** involving depopulation of the bpy portion of hhtn is shifted to lower energy than that from $Re(CO)_3Cl$ (phen) in a manner consistent with the difference in their MLCT absorbance energies; **3** emits at 710 nm at 77K, whereas emission from $Re(CO)_3Cl$ (phen) is observed at 515 nm at 77K.[10] Lack of emission at room temperature in fluid solution obviously makes homogenous photocatalysis impossible. It is not clear how to remedy the problem, for the luminescence properties of $Re(CO)_3Cl$ (diimine) complexes follow no predictable pattern; some complexes emit while closely-related ones do not. $Re(CO)_3Cl$ (5-Cl-phen) is emissive, $Re(CO)_3Cl$ (5-NO_2phen) is not; $Re(CO)_3Cl$ (bpy) is emissive while $Re(CO)_3Cl$ (2,2'-biquinoline), whose coordination site is like that of hhtn, is not.[33] Weak or nonexistent room-temperature emission also seems to be a general problem in polymetallic systems with metal-metal interactions, particularly those containing Re chromophores.[29]

Figure 4.20. Emission spectra of **3** and **4** in dichloromethane at 77 K upon excitation at 436 nm.


x 5
Emission Intensity
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
470
530
590
650
710
770

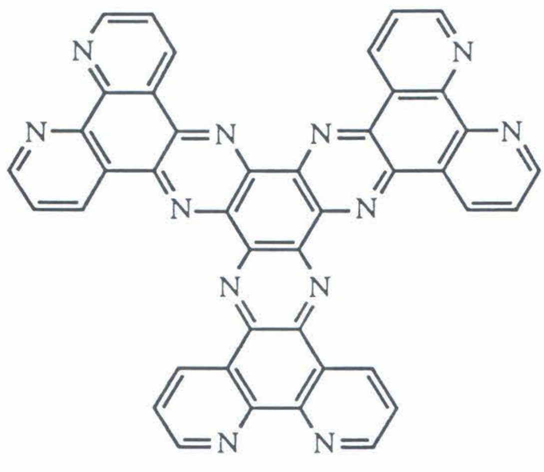
While hhtn is not an ideal ligand on which to base a multielectron photocatalytic system, the emission spectra presented in Figure 4.20 suggest that excited-state interaction between components is present in mixed-metal compound **4**. In the presence of the $PdCl_2$ unit, the emission seen in Re monomer **3** disappears. While it cannot be ruled out on the basis of these data that ground-state Re-Pd coupling destroys the excited-state properties of the Re center, 77 K emission is observed in strongly-interacting $[Re(CO)_3Cl]_2$(2,2'-bipryrimidine). Energy transfer cannot be responsible for the disappearance of Re emission in **4** because no corresponding sensitization of 660 nm Pd-based emission is seen. Therefore it is likely that excited-state ET is taking place, the Re-centered excited-state being oxidatively quenched by the Pd(II) center. Transient absorption spectroscopy may provide insight into the nature of excited-state quenching in **4**.

The luminescence properties of **4** indicate that the polymetallic approach to developing compounds capable of photon-driven multielectron transformations has merit. Two opposing requirements must be met in the design of a platform for such a compound: in a ligand that has at least three coordination sites, metals must be close enough together that excited-state ET is possible yet far enough apart that no deleterious ground-state coupling occurs. HAT and hhtn, with their pyrazine units shared between metals, bring the centers close together, but considerable interaction affects the ability of chromophores to behave as independent one-electron excited-state moities.

The general synthetic approach of condensing polyamines with polyketones, as evidenced by the compounds discussed in this thesis, allows a wide variety of novel ligands to be synthesized. Hexapyridohexaazatrinapthalene, shown in Figure 4.21, should be accessible via the condensation of three equivalents of phendione with one equivalent of hexaketocyclohexane in formamide, in a manner similar to that used for the synthesis of tppz. The compound can also be made from the condensation of phendione

Figure 4.21. Hexapyridohexaazatrinapthalene.

370



with benzenehexamine, which requires the same explosive intermediates used in the synthesis of HAT. While less desirable, this route assures only one product.

Hexapyridohexaazatrinapthalene has three sterically-nonhindered coordination sites in relatively close proximity. The spacer between any two coordination sites is isostructural to tpbpz, whose heterodinuclear Ru compounds were shown in Chapter 3 to have no metal-metal interaction in the ground state yet displayed fast excited-state ET. kinetics. If these properties are retained in trimeric systems of hexapyridohexaaza-trinapthalene, multielectron photochemistry may be possible.

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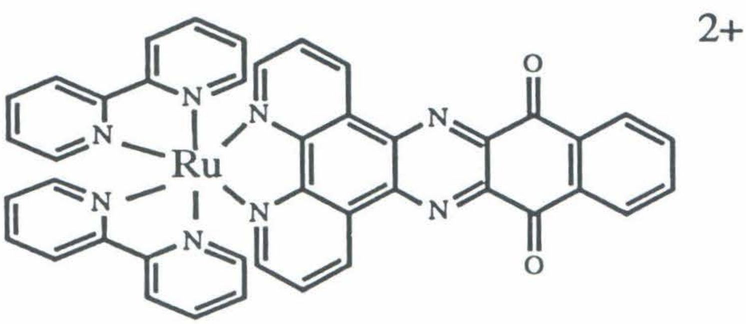
Appendix

Crystal Structure Factor Tables


2+
O
N
Ru
N
O

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
2	0	0	4431	-4157	13
4	0	0	748	812	22
6	0	0	1845	-1825	24
8	0	0	1493	1508	28
10	0	0	579	-553	35
12	0	0	499	571	46
14	0	0	539	-575	47
1	1	0	262	353	-19
2	1	0	384	-198	-22
3	1	0	664	678	20
4	1	0	648	579	23
5	1	0	183	143	-52
6	1	0	145	-113	-67
7	1	0	529	-558	31
8	1	0	667	641	31
9	1	0	129	-19	-129
10	1	0	269	-212	45
11	1	0	185	151	-77
12	1	0	75	75	-75
13	1	0	164	228	-164
14	1	0	189	-139	-79
0	2	0	858	893	16
1	2	0	2848	-2762	15
2	2	0	931	-1057	18
3	2	0	2530	2580	18
4	2	0	348	354	30
5	2	0	848	-857	24
6	2	0	94	175	-94
7	2	0	730	834	29
8	2	0	181	193	-69
9	2	0	1108	-1133	32
10	2	0	123	75	-123
11	2	0	427	480	43
12	2	0	69	-1	-69
13	2	0	633	-635	45
14	2	0	135	-125	-135
1	3	0	534	-531	24
2	3	0	660	659	21
3	3	0	585	-560	23
4	3	0	442	-486	28
5	3	0	144	-156	-87
6	3	0	463	521	31
7	3	0	61	40	-61
8	3	0	340	-292	38
9	3	0	214	-207	47
10	3	0	65	-83	-65
11	3	0	115	-46	-115
12	3	0	211	-110	-71
13	3	0	83	-246	-83
14	3	0	270	-322	62
0	4	0	1380	-1285	21
1	4	0	942	-946	22
2	4	0	1063	1072	22
3	4	0	249	299	37
4	4	0	1299	-1338	24
5	4	0	192	-168	-49

h	k	l	10Fo	10Fc	10s
6	4	0	861	878	28
7	4	0	401	-363	30
8	4	0	774	-765	31
9	4	0	310	300	44
10	4	0	385	402	44
11	4	0	332	-327	52
12	4	0	489	-558	50
13	4	0	184	180	-106
14	4	0	305	385	68
1	5	0	302	305	38
2	5	0	120	-1	-99
3	5	0	399	-408	30
4	5	0	299	-275	37
5	5	0	364	-294	33
6	5	0	220	-213	54
7	5	0	62	57	-62
8	5	0	214	-242	-69
9	5	0	258	-221	49
10	5	0	161	139	-81
11	5	0	207	268	-83
12	5	0	81	-234	-81
13	5	0	81	-114	-81
0	6	0	60	-40	-60
1	6	0	162	-76	-65
2	6	0	507	513	29
3	6	0	1214	-1213	27
4	6	0	1119	-1102	27
5	6	0	1012	1036	29
6	6	0	436	487	37
7	6	0	874	-912	32
8	6	0	230	199	52
9	6	0	780	724	35
10	6	0	260	272	45
11	6	0	648	-646	40
12	6	0	234	-267	-86
13	6	0	526	551	49
1	7	0	855	814	28
2	7	0	213	-203	40
3	7	0	171	125	-51
4	7	0	318	376	38
5	7	0	65	-41	-65
6	7	0	450	-388	34
7	7	0	68	33	-68
8	7	0	221	-258	-70
9	7	0	149	-158	-119
10	7	0	278	255	56
11	7	0	163	-26	-95
12	7	0	363	-325	50
0	8	0	961	929	30
1	8	0	496	439	32
2	8	0	513	-511	33
3	8	0	418	-377	35
4	8	0	591	581	32
5	8	0	375	388	39
6	8	0	868	-917	33
7	8	0	169	157	-83

h	k	l	10Fo	10Fc	10s
8	8	0	115	122	-115
9	8	0	207	243	-58
10	8	0	606	-664	38
11	8	0	129	-239	-129
1	9	0	441	-442	38
2	9	0	68	-37	-68
3	9	0	424	404	38
4	9	0	150	-20	-88
5	9	0	64	-53	-64
6	9	0	59	-17	-59
7	9	0	70	87	-70
8	9	0	182	-196	-60
9	9	0	142	-157	-142
10	9	0	71	-17	-71
11	9	0	79	-143	-79
0	10	0	198	180	-70
1	10	0	847	-908	34
2	10	0	473	-461	38
3	10	0	966	1024	35
4	10	0	68	166	-68
5	10	0	672	-696	36
6	10	0	190	-205	-79
7	10	0	697	684	40
8	10	0	438	468	48
9	10	0	415	-370	43
1	11	0	237	172	54
2	11	0	287	257	44
3	11	0	71	112	-71
4	11	0	70	-190	-70
5	11	0	119	-179	-119
6	11	0	121	97	-121
7	11	0	336	327	53
8	11	0	104	-106	-104
0	12	0	459	-458	39
1	12	0	217	-238	-68
2	12	0	665	675	37
3	12	0	221	431	-63
4	12	0	637	-630	38
5	12	0	524	-523	44
6	12	0	405	375	46
1	13	0	101	-6	-101
-15	0	1	81	-160	-81
-13	0	1	194	-238	-111
-11	0	1	519	-522	43
-9	0	1	1142	1145	31
-7	0	1	1534	-1516	26
-5	0	1	569	532	26
-3	0	1	2164	-2101	16
-1	0	1	2434	2896	10
1	0	1	2052	-2478	11
3	0	1	1516	-1600	18
5	0	1	1215	-1119	23
7	0	1	797	794	28
9	0	1	344	-271	37
11	0	1	956	909	36
13	0	1	663	-648	44

h	k	l	10Fo	10Fc	10s
-15	1	1	85	-124	-85
-14	1	1	84	-39	-84
-12	1	1	185	271	-104
-11	1	1	354	-407	44
-10	1	1	530	-540	37
-9	1	1	432	-431	38
-8	1	1	249	300	40
-7	1	1	62	63	-62
-6	1	1	223	-195	47
-5	1	1	447	-430	29
-4	1	1	1865	1813	20
-3	1	1	1703	-1584	18
-2	1	1	2725	-2834	15
-1	1	1	860	717	13
0	1	1	979	1499	-408
1	1	1	202	43	29
2	1	1	435	527	-21
3	1	1	956	-801	19
4	1	1	320	-271	30
5	1	1	417	-427	29
6	1	1	959	-1010	26
7	1	1	684	670	29
8	1	1	657	695	32
9	1	1	731	-783	33
10	1	1	328	-338	47
11	1	1	542	588	42
12	1	1	405	430	45
13	1	1	352	-437	57
14	1	1	517	-541	45
-14	2	1	348	380	48
-13	2	1	71	10	-71
-12	2	1	371	-334	48
-11	2	1	266	194	47
-10	2	1	307	372	54
-9	2	1	167	199	-81
-8	2	1	964	-919	30
-7	2	1	562	-593	30
-6	2	1	59	66	-59
-5	2	1	166	-187	-62
-4	2	1	1208	-1174	22
-3	2	1	981	-864	21
-2	2	1	1567	1525	17
-1	2	1	667	-729	18
0	2	1	1318	-1299	11
1	2	1	158	-178	-50
2	2	1	85	40	-85
3	2	1	599	-610	23
4	2	1	105	-216	-105
5	2	1	309	-313	34
6	2	1	1161	1117	26
7	2	1	218	-184	47
8	2	1	1173	-1160	29
9	2	1	269	-348	55
10	2	1	737	693	35
11	2	1	310	318	55
12	2	1	488	-433	42

h	k	l	10Fo	10Fc	10s
13	2	1	233	-292	-80
14	2	1	445	373	49
-14	3	1	259	115	54
-13	3	1	211	-214	-97
-12	3	1	256	304	62
-11	3	1	427	-442	44
-10	3	1	378	350	38
-9	3	1	537	622	39
-8	3	1	395	-368	37
-7	3	1	633	-587	31
-6	3	1	695	704	28
-5	3	1	375	364	34
-4	3	1	984	-962	24
-3	3	1	89	-14	-89
-2	3	1	191	169	-49
-1	3	1	994	943	20
0	3	1	1028	1014	18
1	3	1	61	144	-61
2	3	1	1031	1027	20
3	3	1	277	325	33
4	3	1	345	-357	30
5	3	1	825	-814	25
6	3	1	471	504	34
7	3	1	558	623	32
8	3	1	795	-835	32
9	3	1	762	-779	33
10	3	1	712	761	38
11	3	1	763	748	37
12	3	1	82	-212	-82
13	3	1	446	-531	56
14	3	1	91	206	-91
-14	4	1	84	-122	-84
-13	4	1	400	-280	53
-12	4	1	353	449	59
-11	4	1	736	763	39
-10	4	1	73	-166	-73
-9	4	1	468	-519	40
-8	4	1	145	-198	-145
-7	4	1	412	456	41
-6	4	1	66	77	-66
-5	4	1	1021	-980	27
-4	4	1	547	-565	29
-3	4	1	559	570	26
-2	4	1	179	88	-57
-1	4	1	1051	-1036	22
0	4	1	395	379	19
1	4	1	1167	1220	21
2	4	1	142	-88	-65
3	4	1	254	-288	39
4	4	1	170	187	-50
5	4	1	609	608	29
6	4	1	63	101	-63
7	4	1	512	-490	31
8	4	1	271	258	46
9	4	1	464	576	37
10	4	1	870	860	36

Observed and calculated structure factors for $[Ru(bpy)_2(phen\text{-}napthaquinone)](PF_6)_2$

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
11	4	1	73	38	-73	12	6	1	75	210	-75	-5	9	1	339	413	49	-2	12	1	605	605	38	12	1	2	412	-430	50
12	4	1	525	-501	44	13	6	1	205	174	-101	-4	9	1	549	630	38	-1	12	1	457	-428	42	13	1	2	194	-247	-119
13	4	1	225	239	-71	-12	7	1	131	38	-131	-3	9	1	368	-401	40	0	12	1	340	-383	35	14	1	2	256	250	-76
14	4	1	249	144	-72	-11	7	1	147	131	-147	-2	9	1	481	-470	38	1	12	1	65	45	-65	-14	2	2	83	185	-83
-13	5	1	367	-321	52	-10	7	1	404	-336	49	-1	9	1	478	514	35	2	12	1	71	75	-71	-12	2	2	172	49	-91
-12	5	1	207	-255	-83	-9	7	1	506	-509	44	0	9	1	221	-171	37	3	12	1	185	-251	-97	-11	2	2	68	111	-68
-11	5	1	573	664	47	-8	7	1	433	531	50	1	9	1	279	-242	44	4	12	1	72	25	-72	-10	2	2	74	-100	-74
-10	5	1	521	499	44	-7	7	1	774	799	35	2	9	1	68	-136	-68	5	12	1	399	397	49	-9	2	2	271	-277	50
-9	5	1	432	-373	37	-6	7	1	406	-383	38	3	9	1	416	423	41	6	12	1	231	252	-66	-8	2	2	350	340	39
-8	5	1	571	-572	38	-5	7	1	981	-1023	32	4	9	1	659	701	34	-2	13	1	161	122	-112	-7	2	2	904	848	28
-7	5	1	745	710	32	-4	7	1	305	334	44	5	9	1	521	-519	37	-1	13	1	78	-84	-78	-6	2	2	1017	938	27
-6	5	1	1772	1751	29	-3	7	1	321	351	39	6	9	1	453	-545	39	0	13	1	202	-153	-72	-5	2	2	65	-183	-65
-5	5	1	1288	-1322	28	-2	7	1	65	-18	-65	7	9	1	503	499	38	1	13	1	202	150	-64	-4	2	2	372	328	31
-4	5	1	1659	-1590	26	-1	7	1	733	-695	29	8	9	1	64	53	-64	2	13	1	237	218	-62	-3	2	2	259	-218	34
-3	5	1	61	-85	-61	0	7	1	295	-250	31	9	9	1	124	25	-124	3	13	1	230	256	-75	-2	2	2	264	-121	33
-2	5	1	173	266	-55	1	7	1	933	955	28	10	9	1	478	-410	47	-14	0	2	77	-107	-77	-1	2	2	60	-77	-60
-1	5	1	249	-245	35	2	7	1	565	-598	32	-10	10	1	283	402	69	-12	0	2	71	11	-71	0	2	2	214	129	36
0	5	1	922	-915	17	3	7	1	1138	-1159	28	-9	10	1	65	64	-65	-10	0	2	394	427	45	1	2	2	134	106	-64
1	5	1	820	801	24	4	7	1	332	369	37	-8	10	1	215	-185	-75	-8	0	2	463	-423	31	2	2	2	1515	1505	17
2	5	1	1400	1370	24	5	7	1	818	857	31	-7	10	1	139	221	-139	-6	0	2	1298	-1315	24	3	2	2	1153	1206	20
3	5	1	470	-453	28	6	7	1	244	-251	54	-6	10	1	624	673	40	-4	0	2	1628	1572	20	4	2	2	262	-267	38
4	5	1	827	-885	27	7	7	1	908	-972	34	-5	10	1	69	132	-69	-2	0	2	674	462	-16	5	2	2	147	108	-72
5	5	1	1054	1026	28	8	7	1	500	423	39	-4	10	1	704	-731	36	0	0	2	2486	2985	84	6	2	2	198	169	-59
6	5	1	731	724	30	9	7	1	437	403	43	-3	10	1	294	-316	50	2	0	2	1041	-1181	16	7	2	2	404	351	30
7	5	1	455	-437	33	11	7	1	738	-749	42	-2	10	1	900	943	34	4	0	2	760	691	22	8	2	2	554	-570	34
8	5	1	1067	-1121	32	12	7	1	284	318	57	-1	10	1	584	580	36	6	0	2	423	-432	32	9	2	2	729	-763	33
9	5	1	686	693	36	-12	8	1	78	52	-78	0	10	1	584	-595	30	8	0	2	435	423	34	10	2	2	76	-88	-76
10	5	1	1018	973	36	-11	8	1	374	-386	53	1	10	1	452	-495	40	10	0	2	76	-139	-76	11	2	2	149	157	-118
11	5	1	398	-429	50	-10	8	1	75	-16	-75	2	10	1	576	545	38	14	0	2	256	-276	-70	12	2	2	442	427	43
12	5	1	466	-476	48	-9	8	1	170	177	-99	3	10	1	378	437	44	-15	1	2	199	-187	-91	13	2	2	330	-353	52
13	5	1	333	318	53	-8	8	1	71	6	-71	4	10	1	259	-222	52	-14	1	2	189	237	-118	14	2	2	205	-256	-136
-13	6	1	206	-168	-84	-7	8	1	563	-555	39	6	10	1	71	114	-71	-13	1	2	233	357	-89	-14	3	2	377	328	57
-12	6	1	688	654	41	-6	8	1	236	-266	48	7	10	1	541	443	41	-12	1	2	482	-532	46	-13	3	2	545	-575	47
-11	6	1	202	260	-77	-5	8	1	679	692	35	8	10	1	124	-93	-124	-11	1	2	864	-846	37	-12	3	2	201	-7	-85
-10	6	1	216	-245	-75	-4	8	1	74	202	-74	9	10	1	76	-177	-76	-10	1	2	534	572	37	-11	3	2	165	-106	-95
-9	6	1	185	11	-54	-3	8	1	944	-971	31	-8	11	1	180	11	-76	-9	1	2	364	470	46	-10	3	2	670	768	40
-8	6	1	627	604	37	-2	8	1	376	-391	36	-7	11	1	524	-541	42	-8	1	2	510	-534	33	-9	3	2	419	-404	39
-7	6	1	170	221	-100	-1	8	1	1380	1401	30	-6	11	1	71	79	-71	-7	1	2	377	-389	37	-8	3	2	705	-735	33
-6	6	1	473	-426	37	0	8	1	371	338	25	-5	11	1	183	274	-80	-6	1	2	1097	1143	25	-7	3	2	1099	1067	29
-5	6	1	533	-423	34	1	8	1	679	-672	30	-4	11	1	500	-544	41	-5	1	2	951	1004	24	-6	3	2	474	564	31
-4	6	1	725	743	29	2	8	1	514	-546	34	-3	11	1	151	-232	-105	-4	1	2	93	-162	-93	-5	3	2	1440	-1409	25
-3	6	1	66	71	-66	3	8	1	583	598	32	-2	11	1	219	341	-63	-3	1	2	1257	-1166	18	-4	3	2	597	-600	26
-2	6	1	693	-767	28	4	8	1	131	-24	-131	-1	11	1	229	211	-64	-2	1	2	597	672	19	-3	3	2	412	421	28
-1	6	1	294	309	38	5	8	1	707	-709	34	0	11	1	294	-291	34	-1	1	2	375	227	-18	-2	3	2	564	-584	23
0	6	1	537	617	21	6	8	1	297	274	47	1	11	1	148	94	-148	0	1	2	1444	-1459	9	-1	3	2	259	-306	37
1	6	1	206	163	44	7	8	1	320	245	47	2	11	1	401	396	45	1	1	2	138	-3	-50	0	3	2	1254	1201	13
2	6	1	893	-950	27	8	8	1	748	-813	37	3	11	1	445	436	41	2	1	2	944	-1137	17	1	3	2	1246	1228	19
3	6	1	58	1	-58	9	8	1	365	340	47	4	11	1	287	-270	51	3	1	2	125	113	-82	2	3	2	1019	1005	20
4	6	1	656	659	30	10	8	1	215	-194	-72	5	11	1	284	-270	52	4	1	2	1112	-1019	21	3	3	2	515	-611	24
5	6	1	163	-161	-55	11	8	1	106	86	-106	6	11	1	71	114	-71	5	1	2	316	-284	34	4	3	2	770	-769	25
6	6	1	485	-454	35	-11	9	1	315	-288	55	7	11	1	366	372	44	6	1	2	507	558	29	5	3	2	892	872	25
7	6	1	196	267	-58	-10	9	1	267	-243	57	8	11	1	165	-52	-61	7	1	2	191	-93	-51	6	3	2	1200	1221	27
8	6	1	106	-36	-106	-9	9	1	295	424	62	-6	12	1	65	70	-65	8	1	2	251	-270	51	7	3	2	1140	-1121	29
9	6	1	223	179	-58	-8	9	1	196	-309	-112	-5	12	1	287	-283	52	9	1	2	618	-609	34	8	3	2	1049	-996	30
10	6	1	72	-140	-72	-7	9	1	690	-601	38	-4	12	1	469	-505	43	10	1	2	639	666	36	9	3	2	766	739	34
11	6	1	74	-119	-74	-6	9	1	365	-416	45	-3	12	1	414	440	44	11	1	2	583	564	40	10	3	2	906	902	35

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
11	3	2	150	-166	-97
12	3	2	458	-530	46
13	3	2	587	597	43
14	3	2	78	-7	-78
-14	4	2	177	-128	-103
-13	4	2	436	-490	50
-12	4	2	71	76	-71
-11	4	2	383	359	53
-10	4	2	357	-299	41
-9	4	2	186	-317	-89
-8	4	2	270	315	48
-7	4	2	147	224	-84
-6	4	2	719	-637	30
-5	4	2	309	-328	40
-4	4	2	1473	1418	24
-3	4	2	256	-230	39
-2	4	2	663	-703	25
-1	4	2	685	625	24
0	4	2	139	62	-56
1	4	2	246	220	35
2	4	2	444	-412	27
3	4	2	660	-650	25
4	4	2	314	-348	34
5	4	2	61	-40	-61
6	4	2	447	461	30
7	4	2	398	380	35
8	4	2	142	-149	-81
9	4	2	459	-470	41
10	4	2	214	-99	-59
11	4	2	153	-202	-100
12	4	2	259	207	42
13	4	2	150	-76	-150
14	4	2	71	85	-71
-14	5	2	360	-345	59
-13	5	2	481	-495	51
-12	5	2	487	532	43
-11	5	2	907	922	40
-10	5	2	250	-414	-75
-9	5	2	985	-1008	36
-8	5	2	578	612	35
-7	5	2	1017	1026	32
-6	5	2	416	-394	37
-5	5	2	1358	-1320	28
-4	5	2	433	502	35
-3	5	2	229	232	47
-2	5	2	114	-161	-114
-1	5	2	63	-173	-63
0	5	2	632	677	20
1	5	2	613	653	26
2	5	2	817	-843	25
3	5	2	771	-756	26
4	5	2	418	407	33
5	5	2	451	390	30
6	5	2	1138	-1055	29
7	5	2	1167	-1141	30
8	5	2	697	665	34

h	k	l	10Fo	10Fc	10s
9	5	2	1036	1042	35
10	5	2	209	-196	-68
11	5	2	394	-402	51
12	5	2	495	557	45
13	5	2	254	158	-69
-13	6	2	75	-52	-75
-12	6	2	300	249	59
-11	6	2	73	92	-73
-10	6	2	65	60	-65
-8	6	2	167	53	-60
-7	6	2	395	-376	38
-6	6	2	224	-239	50
-5	6	2	965	978	30
-4	6	2	131	116	-131
-3	6	2	914	-922	28
-2	6	2	61	-21	-61
-1	6	2	249	281	41
0	6	2	91	82	-53
1	6	2	1088	1098	26
2	6	2	475	-442	29
3	6	2	392	-395	32
4	6	2	754	-706	29
5	6	2	164	146	-62
6	6	2	188	157	44
7	6	2	365	-313	40
8	6	2	346	-348	41
9	6	2	318	344	53
10	6	2	58	-55	-58
11	6	2	202	77	-54
-12	7	2	495	517	50
-11	7	2	81	-186	-81
-10	7	2	478	-483	44
-9	7	2	378	332	41
-8	7	2	962	933	35
-7	7	2	337	-325	51
-6	7	2	949	-931	34
-5	7	2	689	737	33
-4	7	2	113	156	-113
-3	7	2	822	-888	30
-2	7	2	66	-213	-66
-1	7	2	971	984	28
0	7	2	1060	1054	20
1	7	2	686	-655	28
2	7	2	613	-628	31
3	7	2	692	724	30
4	7	2	716	766	32
5	7	2	459	-496	38
6	7	2	851	-864	32
7	7	2	138	157	-138
8	7	2	490	534	38
9	7	2	116	-34	-116
10	7	2	536	-600	41
11	7	2	206	163	-70
12	7	2	623	606	44
-10	8	2	204	-230	-73
-9	8	2	157	172	-109

h	k	l	10Fo	10Fc	10s
-8	8	2	66	-61	-66
-7	8	2	70	-73	-70
-6	8	2	606	575	37
-5	8	2	352	312	46
-4	8	2	637	-607	34
-3	8	2	241	-249	46
-2	8	2	828	813	31
-1	8	2	72	-92	-72
0	8	2	131	110	-65
1	8	2	178	274	-86
2	8	2	759	-736	31
3	8	2	365	-367	38
4	8	2	666	642	34
5	8	2	159	216	-76
6	8	2	341	-287	43
7	8	2	352	-331	50
8	8	2	177	-197	-72
9	8	2	268	306	61
10	8	2	160	-194	-160
11	8	2	74	79	-74
-11	9	2	576	-519	42
-10	9	2	75	158	-75
-9	9	2	278	323	60
-8	9	2	278	108	49
-7	9	2	73	16	-73
-6	9	2	724	740	36
-5	9	2	887	877	34
-4	9	2	501	-522	39
-3	9	2	631	-563	34
-2	9	2	349	386	42
-1	9	2	680	682	33
0	9	2	678	-652	24
1	9	2	534	-494	37
2	9	2	687	672	34
3	9	2	858	819	33
4	9	2	767	-732	34
5	9	2	475	-456	37
6	9	2	312	290	41
7	9	2	70	242	-70
8	9	2	169	-178	-83
9	9	2	568	-584	39
10	9	2	297	255	54
-10	10	2	75	-105	-75
-9	10	2	74	149	-74
-8	10	2	74	93	-74
-7	10	2	69	-148	-69
-6	10	2	119	47	-119
-5	10	2	73	-119	-73
-4	10	2	415	-411	44
-3	10	2	72	-141	-72
-2	10	2	437	461	46
-1	10	2	65	95	-65
0	10	2	64	-38	-45
1	10	2	73	-104	-73
2	10	2	330	-311	47
3	10	2	286	328	50

h	k	l	10Fo	10Fc	10s
4	10	2	325	377	50
5	10	2	64	86	-64
6	10	2	152	-51	-97
7	10	2	251	208	61
8	10	2	189	-214	-92
9	10	2	72	-180	-72
-8	11	2	633	-612	42
-7	11	2	298	382	56
-6	11	2	368	358	48
-5	11	2	381	-466	46
-4	11	2	854	-925	38
-3	11	2	666	673	37
-2	11	2	149	99	-87
-1	11	2	310	-307	46
0	11	2	178	-108	-57
1	11	2	564	538	38
2	11	2	424	424	42
3	11	2	547	-552	39
4	11	2	698	-697	37
5	11	2	67	25	-67
6	11	2	400	400	47
7	11	2	145	-142	-145
8	11	2	433	-405	47
-5	12	2	65	14	-65
-4	12	2	284	-188	48
-3	12	2	122	189	-122
-1	12	2	74	-111	-74
0	12	2	293	-269	55
1	12	2	154	-141	-126
2	12	2	169	116	-91
3	12	2	121	88	-121
4	12	2	123	-127	-123
5	12	2	269	-190	55
-3	13	2	74	142	-74
-2	13	2	360	-294	47
-1	13	2	238	-233	56
0	13	2	233	281	48
1	13	2	305	287	51
2	13	2	478	-496	43
3	13	2	628	-636	40
-15	0	3	793	-699	48
-13	0	3	410	430	48
-11	0	3	945	-945	36
-9	0	3	780	814	32
-7	0	3	1448	-1398	26
-5	0	3	1267	1219	22
-3	0	3	1797	-1669	17
-1	0	3	847	374	-15
1	0	3	1799	-1361	15
3	0	3	183	130	-51
5	0	3	347	-432	35
7	0	3	1122	1090	28
9	0	3	669	-685	34
11	0	3	679	687	36
13	0	3	422	-427	56
-15	1	3	296	351	67

h	k	l	10Fo	10Fc	10s
-14	1	3	412	409	52
-13	1	3	591	-615	46
-12	1	3	350	-415	44
-11	1	3	438	511	47
-10	1	3	524	449	35
-9	1	3	614	-679	38
-8	1	3	448	-453	35
-7	1	3	919	815	28
-6	1	3	1253	1195	25
-5	1	3	64	74	-64
-4	1	3	565	-551	25
-3	1	3	722	-774	20
-2	1	3	463	-256	-20
-1	1	3	1722	-1830	14
0	1	3	985	-1001	13
1	1	3	894	1042	16
2	1	3	2116	2009	17
3	1	3	140	-70	-65
4	1	3	567	-552	25
5	1	3	60	8	-60
6	1	3	60	-50	-60
7	1	3	232	-207	48
8	1	3	147	-152	-72
9	1	3	68	34	-68
10	1	3	126	67	-126
11	1	3	79	-195	-79
12	1	3	70	32	-70
14	1	3	173	-150	-173
-15	2	3	185	117	-106
-14	2	3	470	440	54
-13	2	3	379	427	53
-12	2	3	559	-541	41
-11	2	3	674	-693	38
-10	2	3	767	744	35
-9	2	3	66	25	-66
-8	2	3	574	-624	34
-7	2	3	417	-395	34
-6	2	3	649	676	27
-5	2	3	65	104	-65
-4	2	3	639	-650	25
-3	2	3	1495	1392	19
-2	2	3	256	-240	35
-1	2	3	631	-568	19
0	2	3	1222	-1278	13
1	2	3	672	700	19
2	2	3	3028	3095	18
3	2	3	600	618	23
4	2	3	1123	-1113	22
5	2	3	170	-221	-65
6	2	3	889	883	27
7	2	3	63	-53	-63
8	2	3	1116	-1135	30
9	2	3	215	-256	-58
10	2	3	608	604	36
12	2	3	76	94	-76
13	2	3	78	-80	-78

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
14	2	3	479	445	49
-14	3	3	237	-180	-66
-13	3	3	588	-621	47
-12	3	3	862	949	41
-11	3	3	225	277	-72
-10	3	3	733	-741	39
-9	3	3	652	-571	33
-8	3	3	651	618	33
-7	3	3	62	38	-62
-6	3	3	605	-632	28
-5	3	3	169	-104	-62
-4	3	3	484	466	30
-3	3	3	395	-344	27
-2	3	3	120	78	-120
-1	3	3	63	42	-63
0	3	3	591	650	15
1	3	3	2027	1955	18
2	3	3	423	-472	27
3	3	3	504	-557	25
4	3	3	138	132	-64
5	3	3	124	69	-124
6	3	3	333	-334	36
7	3	3	445	-478	35
8	3	3	171	166	-76
9	3	3	70	203	-70
10	3	3	170	-27	-109
11	3	3	75	-25	-75
12	3	3	142	50	-142
13	3	3	198	-61	-66
14	3	3	175	-185	-103
-14	4	3	211	141	-82
-13	4	3	81	5	-81
-12	4	3	73	-28	-73
-11	4	3	574	498	41
-10	4	3	458	376	43
-9	4	3	509	-462	38
-8	4	3	312	-259	43
-7	4	3	458	446	33
-6	4	3	252	-184	44
-5	4	3	685	-639	29
-4	4	3	401	379	32
-3	4	3	181	225	-49
-2	4	3	256	-300	42
-1	4	3	1328	-1326	22
0	4	3	113	114	-80
1	4	3	115	-14	-115
2	4	3	1035	-1061	23
3	4	3	541	-594	26
4	4	3	237	201	40
5	4	3	1377	1382	26
6	4	3	234	272	39
7	4	3	630	-562	31
8	4	3	299	-278	43
9	4	3	583	569	37
10	4	3	291	267	49
11	4	3	193	-170	-78

h	k	l	10Fo	10Fc	10s
12	4	3	81	-69	-81
13	4	3	408	355	46
-14	5	3	243	-292	-103
-13	5	3	279	221	62
-12	5	3	472	560	46
-11	5	3	291	-284	64
-10	5	3	569	-610	42
-9	5	3	819	732	35
-8	5	3	638	649	36
-7	5	3	607	-656	35
-6	5	3	184	-112	-60
-5	5	3	182	-106	-61
-4	5	3	65	-95	-65
-3	5	3	107	31	-107
-2	5	3	57	-24	-57
-1	5	3	302	303	34
0	5	3	893	905	17
1	5	3	1055	-1040	24
2	5	3	594	-554	27
3	5	3	599	536	27
4	5	3	532	547	31
5	5	3	590	-646	31
6	5	3	1039	-1111	29
7	5	3	606	682	34
8	5	3	705	776	35
9	5	3	530	-443	39
10	5	3	221	-239	-68
11	5	3	156	-254	-73
12	5	3	193	-166	-86
13	5	3	307	-225	47
-12	6	3	368	314	52
-11	6	3	78	-53	-78
-10	6	3	168	-186	-98
-9	6	3	79	-152	-79
-8	6	3	64	148	-64
-7	6	3	483	-482	37
-6	6	3	231	230	44
-5	6	3	147	250	-147
-4	6	3	288	284	41
-3	6	3	247	-245	43
-2	6	3	1067	-1165	27
-1	6	3	120	-41	-120
0	6	3	1412	1430	18
1	6	3	63	-29	-63
2	6	3	1313	-1276	26
3	6	3	738	637	28
4	6	3	794	840	29
5	6	3	245	313	52
6	6	3	762	-811	32
7	6	3	245	-228	41
8	6	3	420	447	39
9	6	3	72	-168	-72
10	6	3	273	-237	49
11	6	3	336	285	51
12	6	3	681	624	43
-12	7	3	81	-106	-81

h	k	l	10Fo	10Fc	10s
-11	7	3	369	-359	52
-10	7	3	77	116	-77
-9	7	3	397	354	47
-8	7	3	601	-571	38
-7	7	3	530	-547	40
-6	7	3	497	515	36
-5	7	3	414	429	40
-4	7	3	435	-416	39
-3	7	3	307	-389	44
-2	7	3	63	-17	-63
-1	7	3	212	-216	-55
0	7	3	467	-491	28
1	7	3	259	220	37
2	7	3	63	-142	-63
3	7	3	500	542	33
4	7	3	62	-95	-62
5	7	3	908	-921	32
6	7	3	583	558	35
7	7	3	223	-246	53
8	7	3	67	-31	-67
9	7	3	242	-167	50
10	7	3	140	110	-140
11	7	3	336	416	59
12	7	3	229	-172	-69
-12	8	3	82	1	-82
-11	8	3	170	-262	-121
-10	8	3	193	102	-74
-9	8	3	289	280	58
-8	8	3	77	-195	-77
-7	8	3	217	-137	-61
-6	8	3	110	88	-110
-5	8	3	557	598	37
-4	8	3	71	4	-71
-3	8	3	1275	-1260	31
-2	8	3	1077	-1056	31
-1	8	3	1403	1415	30
0	8	3	505	494	24
1	8	3	1136	-1103	29
2	8	3	115	-5	-115
3	8	3	763	752	31
4	8	3	60	-113	-60
5	8	3	443	-449	38
7	8	3	497	489	39
8	8	3	455	-436	39
9	8	3	70	-2	-70
10	8	3	124	-71	-124
11	8	3	510	492	46
-11	9	3	90	217	-90
-10	9	3	236	311	-90
-8	9	3	808	-767	39
-7	9	3	72	91	-72
-6	9	3	690	667	37
-5	9	3	316	-336	42
-4	9	3	534	-556	37
-3	9	3	611	559	34
-2	9	3	273	260	39

h	k	l	10Fo	10Fc	10s
-1	9	3	209	-223	-58
0	9	3	62	-35	-44
1	9	3	329	301	38
2	9	3	326	352	44
3	9	3	294	-334	47
4	9	3	318	-339	44
5	9	3	180	170	-64
6	9	3	321	324	40
8	9	3	456	-450	43
9	9	3	374	304	46
10	9	3	341	333	47
-10	10	3	242	197	59
-9	10	3	258	-359	-70
-8	10	3	240	-317	-63
-7	10	3	62	17	-62
-6	10	3	283	291	53
-5	10	3	117	92	-117
-4	10	3	603	-544	40
-3	10	3	330	-336	50
-2	10	3	782	779	36
-1	10	3	598	575	39
0	10	3	651	-649	26
1	10	3	380	-453	45
2	10	3	822	763	34
3	10	3	460	467	41
4	10	3	293	-298	45
5	10	3	275	-195	49
6	10	3	246	296	53
7	10	3	280	-208	53
8	10	3	529	-514	43
9	10	3	149	-22	-149
-8	11	3	91	193	-91
-7	11	3	371	343	44
-6	11	3	384	-414	54
-5	11	3	640	-628	38
-4	11	3	292	-279	58
-3	11	3	787	768	37
-2	11	3	115	-196	-115
-1	11	3	210	-134	-66
0	11	3	270	303	36
1	11	3	470	540	40
2	11	3	258	-242	52
3	11	3	179	-270	-85
5	11	3	362	439	52
6	11	3	73	54	-73
7	11	3	230	-267	-73
8	11	3	80	93	-80
-6	12	3	295	205	47
-5	12	3	69	-10	-69
-4	12	3	247	-230	49
-2	12	3	197	258	-78
-1	12	3	476	-549	41
0	12	3	505	-459	29
1	12	3	445	434	41
2	12	3	561	596	41
3	12	3	387	-390	46

h	k	l	10Fo	10Fc	10s
4	12	3	74	-120	-74
5	12	3	546	525	42
6	12	3	75	60	-75
-3	13	3	336	-288	48
-2	13	3	69	-70	-69
-1	13	3	229	197	47
0	13	3	190	164	47
1	13	3	217	-132	-62
2	13	3	261	-203	54
-14	0	4	724	806	45
-12	0	4	550	-570	46
-10	0	4	630	666	39
-8	0	4	1225	-1213	29
-6	0	4	1226	1159	25
-4	0	4	2518	-2498	20
-2	0	4	3848	4001	16
0	0	4	3827	-3896	12
2	0	4	1479	1427	18
4	0	4	1281	-1191	22
6	0	4	514	-437	30
8	0	4	839	-845	31
10	0	4	395	422	39
12	0	4	544	-585	45
14	0	4	642	672	45
-15	1	4	165	93	-165
-14	1	4	81	-85	-81
-13	1	4	247	-132	-81
-12	1	4	233	194	-61
-11	1	4	148	-117	-125
-10	1	4	68	46	-68
-9	1	4	242	-258	53
-8	1	4	477	409	34
-7	1	4	65	-112	-65
-6	1	4	1072	1009	25
-5	1	4	211	-252	47
-4	1	4	1647	-1619	21
-3	1	4	1706	1594	18
-2	1	4	1012	1090	18
-1	1	4	248	-157	32
0	1	4	546	450	17
1	1	4	1525	-1460	17
2	1	4	413	-321	25
3	1	4	668	579	22
4	1	4	289	-328	38
5	1	4	228	279	51
6	1	4	503	478	31
7	1	4	320	-270	40
8	1	4	126	-46	-89
9	1	4	280	-266	36
10	1	4	62	68	-62
11	1	4	341	361	48
12	1	4	244	-234	59
13	1	4	305	-392	59
14	1	4	84	134	-84
-15	2	4	642	567	50
-14	2	4	222	296	-74

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

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
-13	2	4	183	-313	-138	14	3	4	223	177	-59	13	5	4	278	282	57	-7	8	4	113	9	-113	6	10	4	322	283	42
-12	2	4	73	18	-73	-14	4	4	462	-544	56	-13	6	4	403	418	60	-6	8	4	1070	1054	34	7	10	4	614	-669	43
-11	2	4	222	195	-71	-13	4	4	441	-407	50	-12	6	4	76	-17	-76	-5	8	4	386	394	44	8	10	4	74	-162	-74
-10	2	4	154	101	-83	-12	4	4	778	707	41	-11	6	4	798	-868	41	-4	8	4	932	-919	33	9	10	4	403	412	47
-9	2	4	505	-538	37	-11	4	4	68	21	-68	-10	6	4	139	56	-139	-3	8	4	235	-255	44	-8	11	4	168	-210	-109
-8	2	4	261	248	44	-10	4	4	920	-973	37	-9	6	4	812	774	36	-2	8	4	1264	1200	31	-7	11	4	70	-62	-70
-7	2	4	638	694	31	-9	4	4	187	-8	-63	-8	6	4	190	-87	-54	-1	8	4	228	261	49	-6	11	4	74	-164	-74
-6	2	4	820	809	28	-8	4	4	703	686	34	-7	6	4	738	-720	36	0	8	4	352	-349	26	-5	11	4	122	-19	-122
-5	2	4	1495	-1402	24	-7	4	4	273	-271	47	-6	6	4	254	-324	55	1	8	4	63	-59	-63	-4	11	4	499	-445	37
-4	2	4	898	-779	24	-6	4	4	622	-659	31	-5	6	4	1083	1091	29	2	8	4	446	491	35	-3	11	4	459	562	43
-3	2	4	1620	1632	20	-5	4	4	500	-475	32	-4	6	4	497	484	33	3	8	4	66	220	-66	-2	11	4	151	147	-115
-2	2	4	1290	1225	19	-4	4	4	2260	2279	24	-3	6	4	812	-854	29	4	8	4	590	-602	34	-1	11	4	64	-83	-64
-1	2	4	4039	-4121	17	-3	4	4	172	263	-61	-2	6	4	450	-498	32	5	8	4	59	-141	-59	0	11	4	151	101	-60
0	2	4	2036	-2088	12	-2	4	4	1465	-1531	23	-1	6	4	897	940	27	6	8	4	316	334	48	1	11	4	75	-21	-75
1	2	4	4037	3939	17	-1	4	4	357	-357	31	0	6	4	424	510	38	7	8	4	173	16	-66	2	11	4	445	-499	44
2	2	4	1415	1360	19	0	4	4	225	312	37	1	6	4	360	-378	34	8	8	4	557	-598	40	3	11	4	320	-287	47
3	2	4	393	-413	29	1	4	4	102	137	-102	2	6	4	883	-840	27	9	8	4	271	-284	54	4	11	4	98	-47	-98
4	2	4	836	-786	24	2	4	4	2119	-2153	22	3	6	4	732	754	29	10	8	4	554	530	45	5	11	4	84	151	-84
5	2	4	1279	1220	24	3	4	4	384	-380	29	4	6	4	471	413	31	11	8	4	347	331	54	7	11	4	273	-330	56
6	2	4	205	238	50	4	4	4	1421	1448	25	5	6	4	1195	-1222	30	-11	9	4	191	200	-67	-6	12	4	332	-296	49
7	2	4	905	-935	29	5	4	4	181	69	-54	7	6	4	903	896	33	-10	9	4	199	-109	-77	-5	12	4	263	-132	46
8	2	4	416	405	38	6	4	4	1045	-1037	28	8	6	4	418	-412	36	-9	9	4	163	121	-132	-4	12	4	374	318	44
9	2	4	514	562	37	7	4	4	97	-95	-97	9	6	4	421	-388	41	-8	9	4	315	287	51	-3	12	4	363	365	41
10	2	4	312	-315	45	8	4	4	701	729	33	10	6	4	283	289	58	-7	9	4	71	153	-71	-2	12	4	639	-595	38
11	2	4	397	-419	41	9	4	4	532	-499	40	11	6	4	598	595	44	-6	9	4	274	-242	53	-1	12	4	384	-376	49
12	2	4	159	240	-159	10	4	4	597	-595	42	12	6	4	81	-220	-81	-5	9	4	654	643	39	0	12	4	652	634	85
13	2	4	379	369	51	11	4	4	155	18	-64	-13	7	4	83	99	-83	-4	9	4	219	-205	-71	1	12	4	280	260	50
14	2	4	77	-70	-77	12	4	4	720	758	41	-11	7	4	76	85	-76	-3	9	4	175	-227	-67	2	12	4	561	-589	41
-14	3	4	80	-137	-80	13	4	4	76	30	-76	-10	7	4	73	-84	-73	-2	9	4	184	-187	-71	3	12	4	76	-210	-76
-13	3	4	200	12	-78	-14	5	4	77	-97	-77	-9	7	4	168	87	-129	-1	9	4	172	171	-68	4	12	4	498	558	43
-12	3	4	86	165	-86	-13	5	4	89	203	-89	-8	7	4	186	142	-74	0	9	4	111	67	-60	5	12	4	206	253	-78
-11	3	4	367	-396	48	-12	5	4	74	1	-74	-7	7	4	178	-166	-56	1	9	4	249	243	56	-3	13	4	69	-105	-69
-10	3	4	77	160	-77	-11	5	4	74	31	-74	-6	7	4	345	-352	44	2	9	4	107	-6	-107	-2	13	4	74	-13	-74
-9	3	4	210	119	-55	-10	5	4	278	232	57	-5	7	4	66	-84	-66	3	9	4	254	-231	53	-1	13	4	178	-156	-88
-8	3	4	191	-154	-51	-9	5	4	158	-196	-91	-4	7	4	1055	1049	30	4	9	4	60	23	-60	0	13	4	170	175	-71
-7	3	4	308	287	42	-8	5	4	137	-186	-137	-3	7	4	65	34	-65	5	9	4	181	114	-65	1	13	4	74	-36	-74
-6	3	4	424	-400	31	-7	5	4	937	827	33	-2	7	4	741	-712	29	6	9	4	71	46	-71	2	13	4	163	-224	-103
-5	3	4	623	-611	27	-6	5	4	176	-211	-74	-1	7	4	151	-10	-63	8	9	4	70	-43	-70	-15	0	5	219	171	-91
-4	3	4	847	-825	24	-5	5	4	779	-755	30	0	7	4	356	393	55	9	9	4	177	-252	-111	-13	0	5	316	-285	54
-3	3	4	371	361	30	-4	5	4	373	425	37	1	7	4	151	-125	-81	10	9	4	72	-2	-72	-11	0	5	71	14	-71
-2	3	4	498	543	25	-3	5	4	436	482	31	2	7	4	259	-253	42	-10	10	4	85	199	-85	-9	0	5	937	-873	32
-1	3	4	435	459	26	-2	5	4	168	-17	-49	3	7	4	60	-73	-60	-9	10	4	309	-352	59	-7	0	5	1414	1423	27
0	3	4	561	634	16	-1	5	4	438	-429	31	4	7	4	430	447	36	-8	10	4	206	-30	-60	-5	0	5	1015	-1106	24
1	3	4	278	-192	34	0	5	4	68	-111	-52	5	7	4	531	539	34	-7	10	4	309	405	49	-3	0	5	4889	4543	18
2	3	4	60	-38	-60	1	5	4	188	-113	-48	6	7	4	134	27	-65	-6	10	4	196	183	-85	-1	0	5	191	229	45
3	3	4	1527	-1472	22	2	5	4	187	116	42	7	7	4	635	-640	34	-5	10	4	1054	-1025	36	1	0	5	443	-456	25
4	3	4	312	-312	34	3	5	4	56	-19	-56	8	7	4	623	597	37	-4	10	4	296	-344	50	3	0	5	408	449	29
5	3	4	506	501	29	4	5	4	207	195	47	9	7	4	180	-146	-79	-3	10	4	889	856	37	5	0	5	512	542	28
6	3	4	154	133	-71	5	5	4	311	295	40	10	7	4	308	-286	52	-2	10	4	500	459	40	7	0	5	60	-134	-60
7	3	4	68	63	-68	6	5	4	62	6	-62	11	7	4	71	104	-71	-1	10	4	812	-823	36	9	0	5	713	682	34
8	3	4	174	95	-59	7	5	4	173	-260	-63	12	7	4	510	465	46	0	10	4	441	-409	28	11	0	5	484	-541	46
9	3	4	492	481	38	8	5	4	193	-107	-71	-12	8	4	426	-484	54	1	10	4	753	797	35	13	0	5	535	457	43
10	3	4	523	545	43	9	5	4	429	422	43	-11	8	4	67	51	-67	2	10	4	203	267	-61	-15	1	5	342	391	69
11	3	4	76	-190	-76	10	5	4	434	-396	46	-10	8	4	622	578	42	3	10	4	490	-458	37	-14	1	5	305	315	61
12	3	4	143	-126	-143	11	5	4	76	83	-76	-9	8	4	283	295	62	4	10	4	280	-268	51	-13	1	5	129	-22	-129
13	3	4	352	341	48	12	5	4	718	690	43	-8	8	4	457	-514	45	5	10	4	465	385	39	-12	1	5	380	-296	49

Observed and calculated structure factors for $[Ru(bpy)_2(phen\text{-}napthaquinone)](PF_6)_2$

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
-11	1	5	231	285	-71	-13	3	5	216	-246	-77	-12	5	5	150	221	-150	-6	7	5	407	399	40	4	9	5	210	-191	52
-10	1	5	417	392	43	-12	3	5	490	508	47	-11	5	5	371	-362	53	-5	7	5	1048	1086	32	6	9	5	655	664	37
-9	1	5	348	-347	44	-11	3	5	228	151	-60	-10	5	5	503	-614	50	-4	7	5	62	1	-62	7	9	5	71	-101	-71
-8	1	5	665	-703	34	-10	3	5	644	-680	39	-9	5	5	439	423	43	-3	7	5	776	-804	31	8	9	5	730	-823	40
-7	1	5	205	142	-58	-9	3	5	648	-589	36	-8	5	5	1134	1062	34	-2	7	5	155	86	-52	9	9	5	127	38	-127
-6	1	5	1621	1607	25	-8	3	5	74	163	-74	-7	5	5	729	-734	34	-1	7	5	734	749	30	10	9	5	599	497	41
-5	1	5	1152	-1230	24	-7	3	5	726	676	30	-6	5	5	1132	-1114	30	0	7	5	257	-259	30	-10	10	5	529	-588	53
-4	1	5	413	-371	30	-6	3	5	1113	-1057	27	-5	5	5	507	567	33	1	7	5	957	-990	29	-9	10	5	393	-385	47
-3	1	5	1276	1264	20	-5	3	5	349	-365	35	-4	5	5	467	485	33	2	7	5	354	353	36	-8	10	5	79	65	-79
-2	1	5	723	630	20	-4	3	5	528	530	29	-3	5	5	705	-637	27	3	7	5	812	746	30	-7	10	5	73	99	-73
-1	1	5	162	39	-56	-3	3	5	836	846	23	-2	5	5	395	-450	32	4	7	5	656	-611	32	-6	10	5	435	-412	42
0	1	5	187	227	37	-2	3	5	685	-653	23	-1	5	5	185	255	-60	5	7	5	1277	-1269	31	-5	10	5	482	-447	42
1	1	5	2286	2176	17	-1	3	5	362	-369	29	0	5	5	1760	1784	17	6	7	5	481	496	36	-4	10	5	752	719	37
2	1	5	230	256	43	0	3	5	235	-197	27	1	5	5	1620	-1612	24	7	7	5	428	394	37	-3	10	5	286	294	61
3	1	5	367	396	29	1	3	5	507	537	24	2	5	5	1231	-1255	25	8	7	5	401	-438	39	-2	10	5	681	-703	39
4	1	5	352	-395	34	2	3	5	1515	-1494	21	3	5	5	1345	1384	26	9	7	5	474	-480	48	-1	10	5	538	-506	37
5	1	5	642	581	27	3	3	5	2249	-2149	22	4	5	5	1176	1138	27	10	7	5	319	347	48	0	10	5	429	432	41
6	1	5	246	270	45	4	3	5	663	666	26	5	5	5	660	-688	30	11	7	5	626	673	44	1	10	5	308	291	46
7	1	5	978	-947	29	5	3	5	808	792	27	6	5	5	973	-997	30	-12	8	5	86	-81	-86	2	10	5	400	-407	42
8	1	5	285	-294	48	6	3	5	694	-692	30	7	5	5	446	473	38	-11	8	5	108	179	-108	3	10	5	207	-210	-68
9	1	5	520	537	37	7	3	5	609	-610	32	8	5	5	1155	1240	34	-10	8	5	76	100	-76	4	10	5	115	40	-115
10	1	5	694	723	36	8	3	5	712	740	33	9	5	5	856	-847	35	-9	8	5	439	-435	44	5	10	5	271	276	51
11	1	5	598	-575	39	9	3	5	1130	1130	33	10	5	5	696	-726	38	-8	8	5	69	-119	-69	6	10	5	169	142	-72
12	1	5	588	-609	41	10	3	5	889	-879	35	12	5	5	234	295	-74	-7	8	5	546	530	37	7	10	5	213	-103	-57
13	1	5	253	279	63	11	3	5	856	-850	38	13	5	5	78	-169	-78	-6	8	5	67	-185	-67	8	10	5	74	84	-74
14	1	5	498	474	53	12	3	5	216	231	-82	-13	6	5	139	165	-139	-5	8	5	494	-504	40	9	10	5	168	-207	-168
-15	2	5	118	49	-118	13	3	5	434	453	50	-12	6	5	682	-603	40	-4	8	5	226	-241	55	-8	11	5	379	377	46
-14	2	5	92	-108	-92	-14	4	5	141	225	-141	-11	6	5	80	64	-80	-3	8	5	549	542	33	-7	11	5	533	537	45
-13	2	5	320	372	66	-13	4	5	660	681	46	-10	6	5	462	551	45	-2	8	5	241	131	47	-6	11	5	362	-244	44
-12	2	5	349	305	47	-12	4	5	126	106	-126	-9	6	5	116	111	-116	-1	8	5	315	-332	40	-5	11	5	414	-431	44
-11	2	5	778	-781	39	-11	4	5	528	-538	47	-8	6	5	68	-13	-68	0	8	5	74	9	-55	-4	11	5	185	175	-115
-10	2	5	201	-129	-63	-10	4	5	76	117	-76	-7	6	5	472	-469	36	1	8	5	191	267	-59	-3	11	5	804	813	39
-9	2	5	472	-477	40	-9	4	5	444	431	40	-6	6	5	406	459	40	2	8	5	533	521	35	-2	11	5	378	-392	50
-8	2	5	291	287	48	-8	4	5	103	146	-103	-5	6	5	477	526	34	3	8	5	753	-795	32	-1	11	5	165	-158	-118
-7	2	5	850	863	30	-7	4	5	412	-537	39	-4	6	5	807	-813	30	4	8	5	148	76	-79	0	11	5	248	308	39
-6	2	5	1408	-1442	26	-6	4	5	444	-417	33	-3	6	5	222	-183	53	5	8	5	139	206	-139	1	11	5	70	89	-70
-5	2	5	1090	-1092	24	-5	4	5	570	590	30	-2	6	5	235	264	40	6	8	5	66	55	-66	2	11	5	71	-105	-71
-4	2	5	2211	2253	22	-4	4	5	1256	1255	25	-1	6	5	166	57	-57	8	8	5	431	-434	46	3	11	5	412	-394	41
-3	2	5	62	45	-62	-3	4	5	1045	-1048	24	0	6	5	817	-830	20	9	8	5	173	177	-79	4	11	5	251	266	61
-2	2	5	1200	-1171	19	-2	4	5	162	-49	-63	1	6	5	506	497	29	10	8	5	374	384	49	5	11	5	447	449	41
-1	2	5	1400	1430	19	-1	4	5	412	381	28	2	6	5	412	437	33	11	8	5	216	-203	-58	6	11	5	204	-301	-81
0	2	5	2831	2856	13	0	4	5	93	-128	-49	3	6	5	245	239	44	-11	9	5	176	222	-114	7	11	5	304	-417	60
1	2	5	163	161	-62	1	4	5	1737	-1693	22	4	6	5	668	-685	31	-10	9	5	131	84	-131	-6	12	5	106	-79	-106
2	2	5	667	596	22	2	4	5	450	-476	30	5	6	5	60	-37	-60	-9	9	5	402	-356	51	-5	12	5	584	538	40
3	2	5	546	505	24	3	4	5	806	846	25	6	6	5	155	-95	-79	-8	9	5	598	-634	38	-4	12	5	72	-17	-72
4	2	5	424	399	29	4	4	5	135	89	-69	7	6	5	183	-272	-81	-7	9	5	169	22	-59	-3	12	5	313	-318	52
5	2	5	207	193	45	5	4	5	432	-453	33	8	6	5	403	408	43	-6	9	5	632	649	39	-2	12	5	292	-222	54
6	2	5	993	-967	27	6	4	5	376	323	34	11	6	5	423	400	43	-5	9	5	386	-386	43	-1	12	5	331	327	49
7	2	5	535	564	33	7	4	5	570	580	33	12	6	5	200	131	-72	-4	9	5	818	-769	34	0	12	5	106	213	-62
8	2	5	533	502	32	8	4	5	147	68	-87	-13	7	5	182	128	-95	-3	9	5	542	557	36	1	12	5	211	-244	-67
9	2	5	172	-255	-78	9	4	5	244	-168	52	-12	7	5	322	-349	62	-2	9	5	376	392	43	2	12	5	223	123	54
10	2	5	476	-437	41	10	4	5	374	-410	48	-11	7	5	367	-422	55	-1	9	5	106	64	-106	3	12	5	258	285	-67
11	2	5	71	-133	-71	11	4	5	184	-58	-56	-10	7	5	204	249	-92	0	9	5	244	-203	33	4	12	5	161	-184	-94
12	2	5	746	755	40	12	4	5	127	284	-127	-9	7	5	789	752	39	1	9	5	381	393	40	5	12	5	75	-126	-75
13	2	5	76	-72	-76	13	4	5	324	-336	61	-8	7	5	332	-393	50	2	9	5	124	123	-124	-2	13	5	244	-289	-67
14	2	5	391	-393	48	-13	5	5	521	561	55	-7	7	5	558	-541	35	3	9	5	73	-204	-73	-1	13	5	429	381	41

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
0	13	5	319	331	46
1	13	5	147	-144	-147
-14	0	6	80	19	-80
-12	0	6	73	75	-73
-10	0	6	64	93	-64
-8	0	6	157	225	-83
-6	0	6	625	625	27
-4	0	6	572	-590	27
-2	0	6	406	162	-28
0	0	6	1945	-1789	13
2	0	6	110	185	-110
4	0	6	770	-721	25
6	0	6	1065	-998	28
8	0	6	246	-196	51
10	0	6	392	446	45
12	0	6	402	-395	45
-15	1	6	375	375	63
-14	1	6	346	-397	68
-13	1	6	384	-354	51
-11	1	6	715	776	38
-10	1	6	625	-607	39
-9	1	6	1124	-1184	33
-8	1	6	584	609	32
-7	1	6	1487	1550	28
-6	1	6	1131	-1099	26
-5	1	6	1111	-1156	24
-4	1	6	1899	1872	22
-3	1	6	412	-346	28
-2	1	6	124	-75	-124
-1	1	6	1096	1018	19
0	1	6	1118	-1048	19
1	1	6	177	-324	-57
2	1	6	397	-426	28
3	1	6	362	-406	32
4	1	6	400	460	31
5	1	6	341	338	33
6	1	6	744	-777	29
7	1	6	299	-309	40
8	1	6	741	707	34
9	1	6	868	844	33
10	1	6	496	-566	43
11	1	6	568	-516	42
12	1	6	318	277	60
-15	2	6	75	11	-75
-14	2	6	78	11	-78
-13	2	6	86	81	-86
-12	2	6	74	136	-74
-11	2	6	778	-815	37
-10	2	6	320	284	54
-9	2	6	122	-87	-122
-8	2	6	439	-408	36
-7	2	6	105	48	-105
-6	2	6	347	-339	34
-5	2	6	400	-381	30
-4	2	6	465	421	29
-3	2	6	61	3	-61

h	k	l	10Fo	10Fc	10s
-2	2	6	169	88	-56
-1	2	6	2610	-2632	19
0	2	6	2679	-2716	15
1	2	6	253	307	37
2	2	6	60	62	-60
3	2	6	798	-824	24
4	2	6	218	207	50
5	2	6	223	185	47
6	2	6	440	-394	34
7	2	6	280	-289	44
8	2	6	62	15	-62
9	2	6	213	196	-60
10	2	6	78	187	-78
11	2	6	497	-441	42
12	2	6	227	-89	-58
13	2	6	150	184	-150
-14	3	6	396	-503	72
-13	3	6	575	538	46
-12	3	6	455	486	46
-11	3	6	670	-716	41
-10	3	6	1111	-1124	36
-9	3	6	470	485	39
-8	3	6	1248	1302	32
-7	3	6	759	-768	30
-6	3	6	1666	-1691	27
-5	3	6	994	990	27
-4	3	6	1043	1043	24
-3	3	6	234	209	40
-2	3	6	904	-879	23
-1	3	6	364	348	28
0	3	6	1461	1453	22
1	3	6	894	-884	22
2	3	6	1914	-1892	22
3	3	6	247	263	43
4	3	6	1410	1392	25
5	3	6	780	-746	27
6	3	6	1107	-1128	28
7	3	6	682	685	33
8	3	6	1105	1189	33
9	3	6	424	-484	43
10	3	6	717	-702	38
11	3	6	276	240	64
12	3	6	229	309	-93
13	3	6	294	-372	67
-14	4	6	86	53	-86
-13	4	6	136	186	-136
-12	4	6	195	151	-77
-11	4	6	68	-2	-68
-10	4	6	371	-351	47
-9	4	6	219	161	-61
-8	4	6	531	-580	38
-7	4	6	595	-556	32
-6	4	6	950	962	29
-5	4	6	345	343	39
-4	4	6	173	-106	-61
-3	4	6	55	-2	-55

h	k	l	10Fo	10Fc	10s
-2	4	6	117	-86	-117
-1	4	6	65	92	-65
0	4	6	555	-542	25
1	4	6	185	-135	-52
2	4	6	62	-176	-62
3	4	6	322	385	35
4	4	6	754	743	27
5	4	6	194	242	-54
6	4	6	431	-458	34
7	4	6	62	-6	-62
8	4	6	338	370	41
9	4	6	74	102	-74
10	4	6	258	-203	57
12	4	6	78	-75	-78
13	4	6	266	230	59
-14	5	6	511	537	52
-13	5	6	412	441	65
-12	5	6	169	-130	-137
-11	5	6	624	-682	44
-10	5	6	387	429	55
-9	5	6	994	1048	36
-8	5	6	506	-514	37
-7	5	6	487	-523	35
-6	5	6	68	16	-68
-5	5	6	58	98	-58
-4	5	6	645	-682	29
-3	5	6	148	-165	-79
-2	5	6	1263	1260	25
-1	5	6	1210	1121	25
0	5	6	58	-68	-41
1	5	6	1588	-1517	25
2	5	6	1114	1166	26
3	5	6	1057	1091	26
4	5	6	137	-94	-73
5	5	6	872	-912	30
6	5	6	465	451	35
7	5	6	1283	1237	31
8	5	6	216	-286	-63
9	5	6	442	-418	42
10	5	6	290	258	55
11	5	6	686	708	39
12	5	6	198	197	-66
-13	6	6	301	228	53
-12	6	6	88	-31	-88
-11	6	6	295	-166	55
-10	6	6	76	46	-76
-9	6	6	213	180	-67
-8	6	6	183	-188	-96
-7	6	6	246	236	51
-6	6	6	265	287	49
-5	6	6	1092	-1076	31
-4	6	6	341	-375	43
-3	6	6	63	150	-63
-2	6	6	61	44	-61
-1	6	6	134	186	-86
0	6	6	143	-107	-39

h	k	l	10Fo	10Fc	10s
1	6	6	134	-109	-104
2	6	6	164	277	-72
3	6	6	206	-129	46
4	6	6	368	-311	36
5	6	6	629	-639	32
6	6	6	324	264	34
7	6	6	359	332	42
8	6	6	274	258	54
9	6	6	68	36	-68
10	6	6	655	659	39
11	6	6	207	-93	-64
12	6	6	202	-120	-67
-13	7	6	201	-259	-86
-12	7	6	439	-421	53
-11	7	6	490	528	46
-10	7	6	561	550	47
-9	7	6	251	-293	-67
-8	7	6	642	-647	39
-7	7	6	357	393	50
-6	7	6	666	636	34
-5	7	6	310	-270	40
-4	7	6	502	-426	33
-3	7	6	445	474	34
-2	7	6	396	385	32
-1	7	6	1080	-1137	30
0	7	6	790	-809	33
1	7	6	675	733	29
2	7	6	304	342	39
3	7	6	727	-768	32
4	7	6	536	-532	35
5	7	6	794	787	34
6	7	6	1002	985	34
7	7	6	658	-686	37
8	7	6	695	-686	38
9	7	6	610	614	39
10	7	6	503	513	42
11	7	6	461	-454	50
-12	8	6	279	-143	58
-11	8	6	79	-57	-79
-10	8	6	166	111	-107
-9	8	6	76	35	-76
-8	8	6	121	98	-121
-7	8	6	149	202	-149
-6	8	6	513	-488	40
-5	8	6	74	-117	-74
-4	8	6	474	473	39
-3	8	6	432	490	41
-2	8	6	177	210	-72
-1	8	6	143	-155	-76
0	8	6	281	-254	29
1	8	6	82	-62	-82
2	8	6	263	320	49
3	8	6	66	104	-66
4	8	6	244	-262	52
5	8	6	702	-701	35
6	8	6	469	486	40

h	k	l	10Fo	10Fc	10s
7	8	6	69	-74	-69
8	8	6	266	-348	49
9	8	6	74	86	-74
-11	9	6	477	467	46
-10	9	6	420	-430	51
-9	9	6	363	-440	52
-8	9	6	258	262	60
-7	9	6	399	451	48
-6	9	6	523	-536	41
-5	9	6	558	-529	37
-4	9	6	454	445	39
-3	9	6	641	605	37
-2	9	6	479	-435	37
-1	9	6	984	-930	33
0	9	6	428	438	27
1	9	6	709	738	35
2	9	6	509	-569	39
3	9	6	417	-423	40
4	9	6	71	-34	-71
5	9	6	285	349	55
7	9	6	644	-740	40
8	9	6	390	356	44
9	9	6	416	469	51
-10	10	6	80	88	-80
-8	10	6	197	229	-102
-7	10	6	260	-144	56
-6	10	6	199	-200	-76
-5	10	6	307	-336	52
-4	10	6	399	513	47
-3	10	6	398	378	45
-2	10	6	314	-340	45
-1	10	6	243	175	53
0	10	6	67	-22	-48
1	10	6	65	178	-65
2	10	6	300	295	44
3	10	6	296	-309	43
4	10	6	292	-319	50
5	10	6	438	483	42
6	10	6	140	156	-140
7	10	6	268	-372	65
8	10	6	266	-250	60
-8	11	6	242	289	-66
-7	11	6	316	-249	60
-6	11	6	292	-319	59
-5	11	6	268	219	52
-4	11	6	345	317	49
-3	11	6	70	-79	-70
-2	11	6	282	-286	51
-1	11	6	305	268	50
0	11	6	278	303	38
1	11	6	167	-279	-138
2	11	6	246	-268	56
3	11	6	170	165	-59
4	11	6	603	595	39
5	11	6	335	-267	49
6	11	6	193	-285	-78

Observed and calculated structure factors for $[Ru(bpy)_2(phen\text{-}napthaquinone)](PF_6)_2$

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
7	11	6	211	240	-84	-15	2	7	84	31	-84	-14	4	7	87	53	-87	-10	6	7	256	276	-65	-3	8	7	1210	1264	33
-6	12	6	151	-32	-151	-14	2	7	352	-327	58	-13	4	7	644	630	50	-9	6	7	135	81	-135	-2	8	7	446	430	37
-5	12	6	104	104	-104	-13	2	7	78	-127	-78	-12	4	7	130	200	-130	-8	6	7	74	150	-74	-1	8	7	1071	-1110	32
-2	12	6	335	-277	51	-12	2	7	552	572	46	-11	4	7	349	-336	50	-7	6	7	176	155	-89	0	8	7	294	-298	32
0	12	6	290	290	50	-11	2	7	275	-135	59	-10	4	7	543	-596	43	-6	6	7	232	-214	55	1	8	7	612	610	34
2	12	6	79	-136	-79	-10	2	7	518	-546	39	-9	4	7	203	196	-69	-5	6	7	172	-175	-93	2	8	7	279	331	44
3	12	6	261	-160	48	-9	2	7	410	-457	40	-8	4	7	355	312	40	-4	6	7	945	-1002	30	3	8	7	445	-450	37
4	12	6	146	273	-146	-8	2	7	1188	1213	31	-7	4	7	669	633	35	-3	6	7	257	254	45	4	8	7	355	-344	42
5	12	6	314	286	57	-7	2	7	142	61	-103	-6	4	7	678	597	32	-2	6	7	1736	1639	28	5	8	7	439	483	37
-2	13	6	235	227	53	-6	2	7	1493	-1485	27	-5	4	7	445	462	31	-1	6	7	59	-9	-59	6	8	7	351	366	45
-1	13	6	392	380	47	-5	2	7	994	993	26	-4	4	7	390	301	31	0	6	7	597	-664	50	7	8	7	578	-615	41
0	13	6	217	-214	33	-4	2	7	985	952	24	-3	4	7	1344	-1444	25	1	6	7	147	165	-68	8	8	7	361	273	46
-15	0	7	404	577	69	-3	2	7	101	81	-101	-2	4	7	144	151	-79	2	6	7	118	102	-118	9	8	7	394	381	46
-13	0	7	273	-250	66	-2	2	7	531	-550	26	-1	4	7	378	442	30	3	6	7	858	-868	29	10	8	7	72	-23	-72
-11	0	7	428	422	41	-1	2	7	1644	1579	20	0	4	7	726	711	18	4	6	7	1344	-1261	29	-11	9	7	331	-224	51
-9	0	7	994	-995	33	0	2	7	2796	2833	22	1	4	7	1245	-1169	24	5	6	7	57	-40	-57	-10	9	7	661	-669	46
-7	0	7	1015	1056	29	1	2	7	513	-491	24	2	4	7	693	668	28	6	6	7	457	408	37	-9	9	7	318	383	66
-5	0	7	690	-693	27	2	2	7	1424	-1421	22	3	4	7	2145	2100	25	7	6	7	467	-441	37	-8	9	7	532	554	45
-3	0	7	192	286	-56	3	2	7	373	399	31	4	4	7	374	357	31	8	6	7	572	599	41	-7	9	7	336	-303	48
-1	0	7	923	726	21	4	2	7	1469	1572	25	5	4	7	345	-457	36	9	6	7	224	-144	53	-6	9	7	313	-326	60
1	0	7	1680	1648	21	5	2	7	462	-461	31	6	4	7	414	-413	36	10	6	7	187	-119	-77	-5	9	7	200	229	-53
3	0	7	1026	-1012	24	6	2	7	895	-939	29	7	4	7	475	411	34	11	6	7	73	11	-73	-4	9	7	709	717	38
5	0	7	1393	1368	27	7	2	7	137	-46	-89	8	4	7	320	293	51	12	6	7	326	-283	60	-3	9	7	418	-381	39
7	0	7	1093	-1051	30	8	2	7	481	484	36	9	4	7	574	-543	40	-12	7	7	382	329	58	-1	9	7	525	506	36
9	0	7	1046	1067	35	9	2	7	434	483	38	10	4	7	66	117	-66	-11	7	7	216	385	-105	0	9	7	391	349	27
11	0	7	810	-758	39	10	2	7	823	-839	37	12	4	7	74	33	-74	-10	7	7	387	-360	47	1	9	7	358	-355	44
13	0	7	352	348	45	11	2	7	207	28	-58	13	4	7	445	-359	52	-9	7	7	433	-448	50	2	9	7	167	-221	-91
-15	1	7	208	-269	-95	12	2	7	701	706	42	-14	5	7	205	310	-144	-8	7	7	506	492	39	4	9	7	56	91	-56
-14	1	7	468	-465	63	13	2	7	84	93	-84	-13	5	7	85	64	-85	-7	7	7	78	197	-78	5	9	7	66	11	-66
-13	1	7	655	735	47	-14	3	7	356	345	59	-12	5	7	533	-534	47	-6	7	7	622	-571	36	6	9	7	333	-247	46
-12	1	7	81	99	-81	-13	3	7	364	359	55	-11	5	7	263	224	59	-5	7	7	105	217	-105	7	9	7	252	154	49
-11	1	7	445	-409	48	-12	3	7	321	-355	52	-10	5	7	324	383	56	-4	7	7	431	425	36	8	9	7	329	321	56
-10	1	7	400	-377	47	-11	3	7	320	-314	59	-9	5	7	567	-580	40	-3	7	7	63	59	-63	9	9	7	211	-219	-66
-9	1	7	289	323	56	-10	3	7	485	480	46	-8	5	7	377	-355	40	-2	7	7	187	-76	-50	-10	10	7	457	-522	53
-8	1	7	70	200	-70	-9	3	7	441	457	41	-7	5	7	198	237	-75	-1	7	7	214	-158	-55	-8	10	7	130	208	-130
-7	1	7	149	-133	-71	-8	3	7	504	-504	36	-6	5	7	592	-669	33	0	7	7	259	307	42	-7	10	7	252	233	-66
-6	1	7	940	-924	27	-7	3	7	200	-118	-69	-5	5	7	62	-174	-62	1	7	7	110	-86	-110	-6	10	7	275	-250	55
-5	1	7	485	473	30	-6	3	7	182	156	-68	-4	5	7	65	133	-65	2	7	7	195	-128	47	-5	10	7	399	-362	39
-4	1	7	708	622	25	-5	3	7	381	362	35	-3	5	7	326	309	34	3	7	7	425	-410	35	-4	10	7	670	737	41
-3	1	7	1414	-1340	21	-4	3	7	441	436	30	-2	5	7	59	-48	-59	4	7	7	61	-54	-61	-3	10	7	945	876	36
-2	1	7	374	416	30	-3	3	7	186	150	-49	-1	5	7	883	-845	26	5	7	7	290	278	43	-2	10	7	983	-970	36
-1	1	7	1061	975	20	-2	3	7	465	439	28	0	5	7	368	-417	40	6	7	7	68	-4	-68	-1	10	7	622	-684	38
0	1	7	188	253	39	-1	3	7	601	593	25	1	5	7	306	328	39	7	7	7	849	-835	34	0	10	7	530	635	36
1	1	7	437	-372	25	0	3	7	911	-988	27	2	5	7	385	411	32	8	7	7	261	244	45	1	10	7	404	423	39
2	1	7	1661	-1670	21	1	3	7	980	-985	23	3	5	7	217	179	45	9	7	7	489	445	43	2	10	7	162	-240	-99
3	1	7	771	793	25	2	3	7	298	304	34	4	5	7	598	-528	29	10	7	7	251	-174	58	3	10	7	275	-281	53
4	1	7	1041	1084	25	3	3	7	200	189	48	5	5	7	157	-172	-62	11	7	7	75	-3	-75	4	10	7	413	372	42
5	1	7	58	36	-58	4	3	7	200	-235	-55	6	5	7	473	374	33	-12	8	7	80	113	-80	5	10	7	71	-28	-71
6	1	7	682	-691	30	5	3	7	677	-703	29	7	5	7	74	-185	-74	-11	8	7	87	238	-87	6	10	7	728	-661	38
7	1	7	63	74	-63	6	3	7	589	570	30	8	5	7	64	-57	-64	-10	8	7	77	-42	-77	7	10	7	126	-80	-126
8	1	7	67	191	-67	7	3	7	242	185	35	9	5	7	161	131	-114	-9	8	7	229	-214	-69	8	10	7	494	567	44
9	1	7	74	0	-74	8	3	7	226	-165	-59	10	5	7	207	-219	-69	-8	8	7	72	-22	-72	-8	11	7	371	378	56
10	1	7	73	-16	-73	9	3	7	253	162	51	12	5	7	79	16	-79	-7	8	7	214	229	-61	-7	11	7	250	-263	-71
11	1	7	76	193	-76	10	3	7	70	78	-70	-13	6	7	142	-275	-142	-6	8	7	78	145	-78	-5	11	7	382	316	47
12	1	7	143	-157	-143	11	3	7	479	-429	44	-12	6	7	460	-381	47	-5	8	7	612	-661	37	-4	11	7	266	-251	54
13	1	7	301	-245	50	13	3	7	78	13	-78	-11	6	7	91	-298	-91	-4	8	7	483	-450	37	-3	11	7	71	-103	-71

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

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	11	7	277	264	52	11	1	8	509	-531	43	10	3	8	719	-688	38	-13	6	8	184	-204	-184	-5	8	8	477	-479	39
-1	11	7	457	455	44	12	1	8	324	369	56	11	3	8	458	433	41	-12	6	8	136	-188	-136	-4	8	8	1041	1089	34
0	11	7	184	-92	-48	13	1	8	74	28	-74	12	3	8	70	47	-70	-11	6	8	617	604	48	-3	8	8	383	365	41
1	11	7	138	-124	-138	-15	2	8	439	-584	75	-14	4	8	729	737	49	-10	6	8	78	26	-78	-2	8	8	1041	-1048	32
2	11	7	137	130	-137	-14	2	8	258	-207	-74	-13	4	8	226	255	-76	-9	6	8	646	-602	38	-1	8	8	280	-344	49
4	11	7	71	-59	-71	-13	2	8	459	540	51	-12	4	8	421	-436	52	-8	6	8	71	162	-71	0	8	8	419	403	42
5	11	7	80	85	-80	-12	2	8	79	-30	-79	-11	4	8	75	-3	-75	-7	6	8	794	796	35	1	8	8	189	142	-57
-6	12	7	73	-111	-73	-11	2	8	670	-710	42	-10	4	8	583	642	42	-6	6	8	72	6	-72	2	8	8	67	-26	-67
-5	12	7	199	228	-82	-10	2	8	76	-79	-76	-9	4	8	275	-367	59	-5	6	8	1571	-1611	31	3	8	8	185	163	-64
-4	12	7	222	-25	55	-9	2	8	547	584	37	-8	4	8	791	-749	34	-4	6	8	318	-345	43	4	8	8	703	743	35
-3	12	7	617	-719	45	-8	2	8	64	-10	-64	-7	4	8	101	81	-101	-3	6	8	1625	1604	29	6	8	8	747	-740	35
-1	12	7	420	426	47	-7	2	8	1522	-1487	29	-6	4	8	110	109	-110	-2	6	8	194	350	-62	7	8	8	327	-304	46
0	12	7	444	428	57	-6	2	8	618	648	30	-5	4	8	61	-11	-61	-1	6	8	973	-990	28	8	8	8	609	675	41
1	12	7	493	-492	41	-5	2	8	1561	1500	25	-4	4	8	1679	-1648	26	0	6	8	74	-144	-53	9	8	8	192	178	-89
2	12	7	260	-312	-66	-4	2	8	494	-504	27	-3	4	8	348	-311	32	1	6	8	340	415	37	10	8	8	406	-511	51
3	12	7	629	651	41	-3	2	8	749	-774	24	-2	4	8	1395	1463	25	2	6	8	122	79	-85	-11	9	8	163	-105	-163
-14	0	8	625	-642	50	-2	2	8	775	-714	23	-1	4	8	404	390	32	3	6	8	1172	-1126	29	-10	9	8	76	91	-76
-12	0	8	125	123	-125	-1	2	8	142	-91	-88	0	4	8	1349	-1498	19	4	6	8	480	-509	36	-9	9	8	214	-86	-59
-10	0	8	145	-188	-145	0	2	8	1156	-1153	16	1	4	8	779	-845	26	5	6	8	601	606	34	-8	9	8	86	-116	-86
-8	0	8	279	336	47	1	2	8	1513	-1612	22	2	4	8	2162	2135	25	6	6	8	60	53	-60	-7	9	8	213	115	-78
-6	0	8	895	-931	28	2	2	8	132	-203	-79	3	4	8	131	-60	-84	7	6	8	747	-664	34	-6	9	8	155	68	-124
-4	0	8	779	832	26	3	2	8	1445	1466	25	4	4	8	596	-588	29	8	6	8	791	884	37	-5	9	8	575	-581	41
-2	0	8	1435	-1271	22	4	2	8	59	67	-59	5	4	8	381	-365	35	9	6	8	537	551	42	-4	9	8	416	395	43
0	0	8	2191	1988	17	5	2	8	386	-389	33	6	4	8	391	334	38	10	6	8	343	318	55	-3	9	8	214	195	45
2	0	8	1449	-1461	23	6	2	8	134	164	-134	7	4	8	215	-267	-64	11	6	8	650	-591	44	-2	9	8	68	-122	-68
4	0	8	467	441	33	7	2	8	98	-112	-98	8	4	8	153	-88	-101	-12	7	8	79	-59	-79	-1	9	8	245	-249	48
6	0	8	744	-713	31	8	2	8	452	-452	43	9	4	8	687	713	36	-11	7	8	85	-90	-85	0	9	8	263	-169	53
8	0	8	659	653	33	9	2	8	462	-448	39	10	4	8	443	439	41	-10	7	8	149	83	-149	1	9	8	509	-481	38
10	0	8	751	-730	38	10	2	8	489	455	38	11	4	8	190	-166	-93	-9	7	8	77	94	-77	2	9	8	67	-74	-67
12	0	8	144	58	-144	11	2	8	655	641	39	12	4	8	554	-453	44	-8	7	8	433	-438	44	3	9	8	60	-58	-60
-15	1	8	93	-196	-93	12	2	8	146	-102	-146	-14	5	8	147	217	-147	-7	7	8	70	64	-70	4	9	8	115	4	-115
-14	1	8	85	24	-85	13	2	8	477	-519	59	-13	5	8	162	4	-104	-6	7	8	975	930	34	5	9	8	242	274	47
-13	1	8	448	406	58	-14	3	8	247	-158	-87	-12	5	8	219	275	-92	-5	7	8	71	-169	-71	6	9	8	120	-46	-120
-12	1	8	554	-581	47	-13	3	8	192	149	-90	-10	5	8	171	-134	-99	-4	7	8	632	-660	33	7	9	8	299	-253	50
-11	1	8	350	268	48	-12	3	8	149	137	-149	-9	5	8	189	267	-98	-3	7	8	266	280	48	8	9	8	178	260	-103
-10	1	8	68	-51	-68	-11	3	8	80	41	-80	-8	5	8	432	-411	41	-2	7	8	198	278	-68	9	9	8	130	166	-130
-9	1	8	252	-199	40	-10	3	8	562	-539	40	-7	5	8	736	-734	35	-1	7	8	169	-315	-73	-9	10	8	281	355	68
-8	1	8	565	546	34	-9	3	8	252	234	58	-6	5	8	830	806	32	0	7	8	245	-207	38	-8	10	8	321	345	49
-7	1	8	435	-411	34	-8	3	8	486	548	38	-5	5	8	632	598	32	1	7	8	67	44	-67	-7	10	8	813	-732	42
-6	1	8	195	-141	-51	-7	3	8	639	-637	31	-4	5	8	63	-205	-63	2	7	8	236	231	47	-6	10	8	203	-94	-73
-5	1	8	851	861	26	-6	3	8	1383	-1293	28	-3	5	8	565	-513	30	3	7	8	101	37	-101	-5	10	8	677	678	41
-4	1	8	194	-213	-54	-5	3	8	1292	1349	27	-2	5	8	188	-109	46	4	7	8	239	267	50	-4	10	8	383	458	51
-3	1	8	453	410	28	-4	3	8	617	574	28	-1	5	8	398	408	29	5	7	8	325	399	47	-3	10	8	622	-641	41
-2	1	8	332	-306	34	-3	3	8	60	-32	-60	0	5	8	73	64	-51	6	7	8	156	138	-126	-2	10	8	465	-514	44
-1	1	8	506	-461	25	-2	3	8	933	-886	24	1	5	8	901	-961	27	7	7	8	73	-144	-73	-1	10	8	769	762	36
0	1	8	106	48	-53	-1	3	8	361	-341	31	2	5	8	371	353	31	8	7	8	335	-362	50	0	10	8	201	147	47
1	1	8	587	-517	25	0	3	8	2200	2141	25	3	5	8	794	805	28	9	7	8	79	102	-79	1	10	8	248	-263	55
2	1	8	189	198	-53	1	3	8	107	95	-107	4	5	8	297	-303	40	10	7	8	458	438	43	2	10	8	78	91	-78
3	1	8	312	-351	34	2	3	8	999	-947	24	5	5	8	713	-719	31	11	7	8	445	-456	51	3	10	8	262	212	41
4	1	8	63	-97	-63	3	3	8	585	565	28	6	5	8	186	-200	-72	-12	8	8	649	620	45	4	10	8	274	-268	48
5	1	8	552	568	31	4	3	8	374	421	33	7	5	8	720	718	35	-11	8	8	113	-161	-113	5	10	8	426	-456	48
6	1	8	61	33	-61	5	3	8	242	202	49	8	5	8	308	-235	49	-10	8	8	780	-781	43	7	10	8	491	540	46
7	1	8	66	-114	-66	6	3	8	384	-359	37	9	5	8	535	-559	42	-9	8	8	70	76	-70	8	10	8	73	204	-73
8	1	8	420	396	37	7	3	8	154	87	-69	10	5	8	503	493	42	-8	8	8	529	537	42	-8	11	8	174	-261	-113
9	1	8	463	485	37	8	3	8	705	708	36	11	5	8	318	433	64	-7	8	8	193	147	-80	-7	11	8	285	-355	67
10	1	8	280	-282	51	9	3	8	506	-471	38	12	5	8	186	-217	-78	-6	8	8	863	-814	36	-6	11	8	77	-13	-77

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
-5	11	8	73	-171	-73
-4	11	8	74	121	-74
-3	11	8	175	91	-73
-2	11	8	69	95	-69
-1	11	8	71	80	-71
0	11	8	71	55	-50
1	11	8	79	-177	-79
2	11	8	210	277	-83
3	11	8	159	109	-113
4	11	8	65	27	-65
5	11	8	193	-318	-74
6	11	8	247	-183	58
-5	12	8	186	207	-79
-4	12	8	674	-684	44
-3	12	8	166	-106	-115
-2	12	8	711	660	40
-1	12	8	291	271	55
0	12	8	363	-412	37
1	12	8	325	-283	51
2	12	8	635	713	41
3	12	8	245	190	-71
4	12	8	588	-630	41
-15	0	9	149	-198	-149
-13	0	9	81	-84	-81
-11	0	9	169	185	-169
-9	0	9	926	892	35
-7	0	9	923	-903	30
-5	0	9	1156	1127	26
-3	0	9	363	-360	30
-1	0	9	254	248	41
1	0	9	494	459	29
3	0	9	1224	-1137	26
5	0	9	700	664	29
7	0	9	67	-102	-67
9	0	9	326	-333	55
11	0	9	593	632	42
13	0	9	74	75	-74
-15	1	9	88	-111	-88
-14	1	9	402	-450	68
-13	1	9	461	389	54
-12	1	9	92	-252	-92
-11	1	9	579	-595	45
-10	1	9	294	-316	67
-9	1	9	735	746	36
-8	1	9	426	503	43
-7	1	9	1097	-1122	30
-6	1	9	745	-618	29
-5	1	9	809	769	28
-4	1	9	432	505	31
-3	1	9	388	-425	31
-2	1	9	691	-719	25
-1	1	9	581	556	26
0	1	9	125	43	-60
1	1	9	139	23	-80
2	1	9	529	-499	29
3	1	9	339	418	35

h	k	l	10Fo	10Fc	10s
4	1	9	835	848	28
5	1	9	566	-527	30
6	1	9	810	-816	31
7	1	9	486	521	37
8	1	9	536	454	37
9	1	9	695	-735	39
10	1	9	867	-889	37
11	1	9	591	651	41
12	1	9	507	585	44
13	1	9	286	-412	-87
-15	2	9	81	89	-81
-14	2	9	298	332	67
-13	2	9	235	-292	-71
-12	2	9	148	218	-148
-11	2	9	142	83	-101
-10	2	9	164	100	-107
-9	2	9	700	615	36
-8	2	9	934	-921	32
-7	2	9	710	-722	32
-6	2	9	1109	1179	29
-5	2	9	979	935	27
-4	2	9	895	-906	26
-3	2	9	191	61	47
-2	2	9	977	994	24
-1	2	9	62	149	-62
0	2	9	194	235	44
1	2	9	161	-4	-65
2	2	9	736	700	26
3	2	9	610	-639	27
4	2	9	626	641	29
5	2	9	435	467	34
6	2	9	296	-339	42
7	2	9	219	-332	-55
8	2	9	468	-429	34
9	2	9	193	237	-89
10	2	9	294	253	54
11	2	9	173	-189	-121
12	2	9	376	-360	49
13	2	9	255	-201	-67
-14	3	9	264	349	-87
-13	3	9	347	366	63
-12	3	9	337	-376	58
-11	3	9	549	-556	46
-10	3	9	528	536	43
-9	3	9	625	697	40
-8	3	9	925	-951	33
-7	3	9	466	-388	36
-6	3	9	317	374	41
-5	3	9	559	552	32
-4	3	9	287	259	40
-3	3	9	290	-298	36
-2	3	9	1229	1213	25
-1	3	9	1035	1061	24
0	3	9	2325	-2259	20
1	3	9	1596	-1667	24
2	3	9	989	886	26

h	k	l	10Fo	10Fc	10s
3	3	9	851	814	27
4	3	9	58	-80	-58
5	3	9	217	-183	51
6	3	9	955	910	31
7	3	9	576	595	37
8	3	9	765	-726	34
9	3	9	876	-813	36
10	3	9	537	517	42
11	3	9	520	560	48
12	3	9	149	-87	-149
-14	4	9	94	-156	-94
-13	4	9	242	-164	-73
-12	4	9	88	-57	-88
-11	4	9	450	519	52
-10	4	9	120	-88	-120
-9	4	9	246	-151	50
-8	4	9	538	-504	36
-7	4	9	738	686	34
-6	4	9	753	768	31
-5	4	9	1282	-1325	29
-4	4	9	730	-758	29
-3	4	9	653	677	28
-2	4	9	63	232	-63
-1	4	9	505	-514	30
0	4	9	143	137	-64
1	4	9	514	491	30
2	4	9	432	373	32
3	4	9	476	-445	32
4	4	9	58	-20	-58
5	4	9	193	211	-67
6	4	9	66	-130	-66
7	4	9	65	181	-65
8	4	9	285	256	50
9	4	9	77	135	-77
10	4	9	78	153	-78
11	4	9	205	-247	-64
12	4	9	354	-322	51
-14	5	9	91	250	-91
-13	5	9	272	-342	-74
-12	5	9	383	-394	55
-11	5	9	235	191	-76
-10	5	9	558	527	41
-9	5	9	642	-588	40
-8	5	9	647	-612	38
-7	5	9	593	544	35
-6	5	9	263	319	51
-5	5	9	639	-653	33
-4	5	9	864	-905	30
-3	5	9	698	684	31
-2	5	9	588	645	29
-1	5	9	634	-759	29
0	5	9	1098	-1198	28
1	5	9	446	386	31
2	5	9	704	790	30
3	5	9	608	-652	32
4	5	9	889	-896	31

h	k	l	10Fo	10Fc	10s
5	5	9	289	318	40
6	5	9	669	614	33
7	5	9	395	-429	39
8	5	9	767	-735	37
9	5	9	494	521	39
10	5	9	648	612	41
11	5	9	76	35	-76
12	5	9	421	-443	53
-13	6	9	442	-440	53
-12	6	9	523	518	51
-11	6	9	81	89	-81
-10	6	9	357	-329	47
-9	6	9	79	-128	-79
-8	6	9	478	466	43
-7	6	9	271	243	48
-6	6	9	394	-374	39
-5	6	9	530	-612	37
-4	6	9	1034	1052	31
-3	6	9	658	656	32
-2	6	9	246	-240	44
-1	6	9	62	-63	-62
0	6	9	354	332	31
1	6	9	60	34	-60
2	6	9	948	-997	29
3	6	9	434	-399	34
4	6	9	344	367	39
5	6	9	65	-69	-65
6	6	9	72	88	-72
7	6	9	72	-131	-72
8	6	9	601	577	40
9	6	9	209	-329	-66
10	6	9	270	-237	57
11	6	9	238	-251	-90
-12	7	9	141	327	-141
-11	7	9	501	491	51
-9	7	9	867	-859	40
-8	7	9	317	338	55
-7	7	9	987	979	36
-6	7	9	295	-246	52
-5	7	9	556	-568	35
-4	7	9	723	685	33
-3	7	9	117	220	-117
-2	7	9	373	-339	38
-1	7	9	784	-897	31
0	7	9	321	358	32
1	7	9	873	835	31
2	7	9	379	-360	35
3	7	9	721	-727	34
4	7	9	617	614	33
5	7	9	1038	1122	34
6	7	9	365	-339	45
7	7	9	1026	-986	36
8	7	9	259	330	63
9	7	9	774	833	39
-11	8	9	454	-537	61
-10	8	9	70	-56	-70

h	k	l	10Fo	10Fc	10s
-9	8	9	541	515	46
-8	8	9	160	-102	-93
-7	8	9	154	-188	-74
-6	8	9	73	-74	-73
-5	8	9	412	342	39
-4	8	9	142	189	-93
-3	8	9	242	-231	44
-2	8	9	138	-162	-138
-1	8	9	570	525	35
0	8	9	255	196	-93
1	8	9	479	-489	37
2	8	9	62	26	-62
3	8	9	176	165	-71
4	8	9	75	83	-75
5	8	9	307	-410	60
6	8	9	277	-181	48
7	8	9	73	106	-73
8	8	9	189	98	-68
9	8	9	105	-30	-105
10	8	9	133	-37	-133
-11	9	9	184	-182	-184
-10	9	9	489	-464	52
-9	9	9	399	339	45
-8	9	9	862	852	43
-7	9	9	305	-329	49
-6	9	9	564	-618	40
-5	9	9	71	72	-71
-4	9	9	1210	1229	35
-3	9	9	435	-440	43
-2	9	9	183	-204	-92
-1	9	9	256	366	63
0	9	9	132	-24	-55
1	9	9	71	-150	-71
3	9	9	237	199	51
4	9	9	864	844	37
5	9	9	431	-438	42
6	9	9	1120	-1092	37
7	9	9	568	273	41
8	9	9	766	757	41
9	9	9	304	-325	58
-9	10	9	158	198	-158
-8	10	9	287	-234	53
-7	10	9	182	153	-84
-6	10	9	242	253	57
-5	10	9	142	-199	-142
-4	10	9	76	-71	-76
-3	10	9	350	369	52
-2	10	9	360	350	43
-1	10	9	76	-108	-76
0	10	9	285	-235	47
1	10	9	252	245	49
2	10	9	153	-242	-86
3	10	9	227	-195	-65
5	10	9	212	191	-68
6	10	9	76	6	-76
7	10	9	104	58	-104

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
-8	11	9	159	-58	-101
-7	11	9	506	-428	53
-6	11	9	329	342	46
-5	11	9	331	307	54
-4	11	9	253	-241	56
-3	11	9	367	-475	57
-2	11	9	325	343	54
-1	11	9	255	238	53
0	11	9	288	-255	49
1	11	9	331	-315	44
2	11	9	487	445	42
3	11	9	204	257	-81
4	11	9	229	-278	-75
5	11	9	490	-517	45
6	11	9	73	58	-73
-5	12	9	510	-557	44
-4	12	9	215	107	-81
-3	12	9	237	203	-71
-2	12	9	165	171	-96
-1	12	9	74	-193	-74
0	12	9	217	-175	-64
1	12	9	128	95	-128
2	12	9	77	-24	-77
3	12	9	280	-288	64
-14	0	10	81	-53	-81
-12	0	10	643	-690	44
-10	0	10	163	299	-163
-8	0	10	119	153	-119
-6	0	10	573	-615	31
-4	0	10	1028	1032	26
-2	0	10	165	-132	-67
0	0	10	980	1011	18
2	0	10	1505	-1507	25
4	0	10	719	680	29
6	0	10	235	256	49
8	0	10	278	231	49
10	0	10	262	-306	62
12	0	10	368	380	51
-15	1	10	402	-457	69
-14	1	10	322	348	76
-13	1	10	675	706	49
-12	1	10	1145	-1191	41
-11	1	10	561	-570	45
-10	1	10	1071	1066	37
-9	1	10	1516	1474	33
-8	1	10	1002	-1068	34
-7	1	10	823	-795	31
-6	1	10	1805	1807	28
-5	1	10	883	934	28
-4	1	10	1025	-984	26
-3	1	10	997	-904	25
-2	1	10	1115	1149	25
-1	1	10	394	375	32
0	1	10	156	-114	-51
1	1	10	392	-352	32
2	1	10	660	588	27

h	k	l	10Fo	10Fc	10s
3	1	10	846	873	27
4	1	10	1629	-1559	27
5	1	10	1071	-1056	29
6	1	10	978	994	31
7	1	10	1195	1157	31
8	1	10	816	-806	35
9	1	10	634	-658	38
10	1	10	748	740	37
11	1	10	301	326	55
12	1	10	245	-23	51
-14	2	10	346	-295	55
-13	2	10	308	267	64
-12	2	10	199	-198	-88
-11	2	10	319	-371	53
-10	2	10	382	501	47
-9	2	10	230	-256	-72
-8	2	10	347	-303	46
-7	2	10	489	575	38
-6	2	10	584	-617	33
-5	2	10	1029	994	28
-4	2	10	578	-488	29
-3	2	10	95	-213	-95
-2	2	10	159	-202	-67
-1	2	10	948	925	26
0	2	10	651	665	19
1	2	10	59	34	-59
2	2	10	61	-39	-61
3	2	10	589	637	31
4	2	10	147	-178	-82
5	2	10	310	-273	36
6	2	10	567	580	33
7	2	10	72	107	-72
8	2	10	226	-103	51
9	2	10	420	-403	40
10	2	10	374	-308	51
11	2	10	611	590	41
12	2	10	223	-224	-67
-14	3	10	480	370	52
-13	3	10	360	-371	60
-12	3	10	432	-441	45
-11	3	10	76	1	-76
-10	3	10	1192	1239	37
-9	3	10	633	-561	38
-8	3	10	1203	-1233	34
-7	3	10	650	685	35
-6	3	10	483	537	35
-5	3	10	582	-612	31
-4	3	10	502	-496	31
-3	3	10	392	436	30
-2	3	10	550	587	29
-1	3	10	993	-959	26
0	3	10	895	-847	19
1	3	10	1897	1912	25
2	3	10	1523	1421	25
3	3	10	858	-869	28
4	3	10	502	-561	33

h	k	l	10Fo	10Fc	10s
5	3	10	519	519	31
6	3	10	866	906	32
7	3	10	421	-461	40
8	3	10	810	-789	35
9	3	10	72	124	-72
10	3	10	309	386	52
11	3	10	76	-60	-76
12	3	10	458	-465	45
-14	4	10	86	218	-86
-13	4	10	231	-169	-78
-12	4	10	134	-177	-134
-11	4	10	148	193	-148
-10	4	10	73	-53	-73
-9	4	10	428	-410	45
-8	4	10	247	-278	51
-7	4	10	65	15	-65
-6	4	10	465	-421	37
-5	4	10	66	19	-66
-4	4	10	168	194	-66
-3	4	10	223	-240	49
-2	4	10	591	635	30
-1	4	10	377	391	35
0	4	10	68	-156	-50
1	4	10	1060	-1035	27
2	4	10	455	405	31
3	4	10	471	-469	32
4	4	10	509	-449	32
5	4	10	396	451	37
6	4	10	684	697	35
7	4	10	175	-162	-69
8	4	10	159	-126	-112
9	4	10	71	-3	-71
10	4	10	70	-75	-70
11	4	10	73	-103	-73
12	4	10	108	-146	-108
-13	5	10	478	-391	49
-12	5	10	286	248	70
-11	5	10	501	541	52
-10	5	10	313	-390	52
-9	5	10	669	-694	39
-8	5	10	92	97	-92
-7	5	10	477	491	40
-6	5	10	70	53	-70
-5	5	10	265	-320	47
-4	5	10	319	371	38
-3	5	10	718	676	30
-2	5	10	650	-597	29
-1	5	10	982	-973	28
0	5	10	280	216	37
1	5	10	876	818	29
2	5	10	370	-350	33
3	5	10	521	-487	32
4	5	10	58	10	-58
5	5	10	687	703	33
6	5	10	792	-761	33
7	5	10	291	-261	46

h	k	l	10Fo	10Fc	10s
8	5	10	297	246	47
9	5	10	76	227	-76
10	5	10	189	-162	-79
11	5	10	402	-478	47
-13	6	10	75	-17	-75
-12	6	10	83	64	-83
-11	6	10	299	349	66
-10	6	10	377	276	48
-9	6	10	187	-80	-72
-8	6	10	272	192	53
-7	6	10	145	-200	-145
-6	6	10	396	-419	39
-5	6	10	105	137	-105
-4	6	10	304	264	41
-3	6	10	255	246	46
-2	6	10	97	14	-97
-1	6	10	432	-459	37
0	6	10	62	87	-44
1	6	10	261	-242	42
2	6	10	204	-163	-57
3	6	10	337	-377	42
4	6	10	259	274	46
5	6	10	1025	1020	33
6	6	10	142	189	-100
7	6	10	359	-347	42
8	6	10	472	477	42
9	6	10	186	143	-56
10	6	10	68	-23	-68
11	6	10	252	-277	60
-12	7	10	537	567	51
-11	7	10	442	-446	53
-10	7	10	395	-430	52
-9	7	10	242	320	-77
-8	7	10	598	584	42
-7	7	10	135	-95	-135
-6	7	10	340	-401	44
-5	7	10	156	233	-89
-4	7	10	581	592	36
-3	7	10	891	-883	33
-2	7	10	933	-899	32
-1	7	10	598	566	32
0	7	10	840	818	32
1	7	10	600	-625	32
2	7	10	576	-563	35
3	7	10	575	652	36
4	7	10	969	938	33
5	7	10	343	-397	50
6	7	10	836	-827	36
7	7	10	371	312	40
8	7	10	530	572	43
9	7	10	230	-137	-75
10	7	10	368	-444	53
-11	8	10	163	-52	-123
-10	8	10	110	-103	-110
-9	8	10	79	-136	-79
-8	8	10	71	120	-71

h	k	l	10Fo	10Fc	10s
-7	8	10	198	-59	-58
-5	8	10	265	234	57
-4	8	10	224	-149	54
-3	8	10	68	-208	-68
-2	8	10	72	-110	-72
-1	8	10	205	181	-56
0	8	10	210	159	41
1	8	10	152	-174	-92
2	8	10	579	-591	36
3	8	10	110	-52	-110
4	8	10	707	621	36
5	8	10	230	-146	56
6	8	10	661	-726	41
7	8	10	71	89	-71
8	8	10	83	240	-83
9	8	10	63	-22	-63
-10	9	10	255	227	-65
-9	9	10	389	420	58
-8	9	10	90	-186	-90
-7	9	10	531	-536	45
-6	9	10	333	316	49
-5	9	10	310	262	45
-4	9	10	567	545	40
-3	9	10	984	-1038	37
-2	9	10	263	333	59
-1	9	10	369	333	46
0	9	10	82	-120	-61
1	9	10	185	-250	-77
2	9	10	187	16	-62
3	9	10	427	469	43
4	9	10	571	-565	39
5	9	10	1096	-1130	37
6	9	10	300	319	58
7	9	10	669	646	41
8	9	10	167	-204	-116
-9	10	10	84	-90	-84
-8	10	10	74	-166	-74
-7	10	10	321	-355	62
-6	10	10	76	5	-76
-4	10	10	265	-195	58
-3	10	10	184	-127	-72
-2	10	10	70	61	-70
-1	10	10	136	204	-136
0	10	10	218	182	-95
1	10	10	507	-421	38
2	10	10	309	-295	46
3	10	10	583	533	41
4	10	10	510	527	44
5	10	10	250	-260	55
6	10	10	221	-191	-66
7	10	10	212	176	-58
-7	11	10	84	84	-84
-6	11	10	230	281	-76
-5	11	10	238	-268	-78
-4	11	10	490	-500	47
-3	11	10	532	465	42

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

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	11	10	296	383	49	-13	2	11	115	22	-115	-11	4	11	376	340	52	-4	6	11	1267	1293	32	7	8	11	214	267	-95
-1	11	10	102	-117	-102	-12	2	11	563	-627	46	-10	4	11	237	223	-78	-3	6	11	67	-17	-67	8	8	11	76	-43	-76
0	11	10	416	-387	41	-11	2	11	192	133	-79	-9	4	11	192	-146	-80	-2	6	11	1219	-1180	31	9	8	11	169	-202	-88
2	11	10	590	592	42	-10	2	11	607	635	42	-8	4	11	349	-342	47	-1	6	11	179	-168	-62	-10	9	11	356	333	57
3	11	10	301	-293	56	-9	2	11	77	-1	-77	-7	4	11	608	605	35	0	6	11	699	732	33	-9	9	11	194	-69	-88
4	11	10	465	-492	49	-8	2	11	898	-943	35	-6	4	11	251	240	52	1	6	11	563	560	33	-8	9	11	79	-175	-79
5	11	10	73	132	-73	-7	2	11	249	207	44	-5	4	11	1190	-1178	30	2	6	11	974	-979	31	-6	9	11	289	285	48
-5	12	10	76	-21	-76	-6	2	11	783	866	31	-4	4	11	450	-424	33	3	6	11	133	43	-133	-5	9	11	244	-278	-74
-4	12	10	70	-22	-70	-5	2	11	213	176	-54	-3	4	11	1429	1455	28	4	6	11	776	813	34	-4	9	11	71	196	-71
-3	12	10	132	-98	-132	-4	2	11	1140	-1134	27	-2	4	11	505	460	30	5	6	11	354	409	45	-3	9	11	203	149	-71
-2	12	10	417	351	47	-3	2	11	58	1	-58	-1	4	11	2030	-2147	27	6	6	11	194	-88	-58	-2	9	11	342	303	45
-1	12	10	167	83	-107	-2	2	11	740	792	28	0	4	11	290	-284	27	7	6	11	78	-184	-78	-1	9	11	163	27	-69
0	12	10	313	-280	51	-1	2	11	371	-364	34	1	4	11	741	793	29	8	6	11	277	258	51	0	9	11	106	62	-56
1	12	10	198	-309	-91	0	2	11	1761	-1842	20	2	4	11	184	-182	-58	9	6	11	80	112	-80	1	9	11	370	-376	46
2	12	10	334	326	56	1	2	11	61	-90	-61	3	4	11	895	-949	30	10	6	11	386	-390	51	2	9	11	300	-267	46
-15	0	11	103	-327	-103	2	2	11	1575	1556	27	4	4	11	61	58	-61	-12	7	11	223	-57	-85	3	9	11	74	-45	-74
-13	0	11	239	206	-79	3	2	11	537	-539	32	5	4	11	505	506	34	-11	7	11	412	-418	55	4	9	11	377	-378	45
-11	0	11	589	571	41	4	2	11	1217	-1214	28	6	4	11	202	217	-58	-10	7	11	623	608	47	5	9	11	365	395	53
-9	0	11	1036	979	35	5	2	11	178	-97	-64	7	4	11	66	67	-66	-9	7	11	278	228	52	6	9	11	305	341	54
-7	0	11	1389	-1490	31	6	2	11	419	396	35	8	4	11	256	-241	44	-8	7	11	365	-414	48	7	9	11	83	254	-83
-5	0	11	1514	1446	27	7	2	11	212	170	-53	9	4	11	70	100	-70	-7	7	11	73	2	-73	8	9	11	185	-19	-72
-3	0	11	465	-439	30	8	2	11	763	-795	35	10	4	11	70	20	-70	-6	7	11	346	291	46	-8	10	11	536	-492	45
-1	0	11	328	325	34	9	2	11	221	-296	-68	11	4	11	608	-550	41	-5	7	11	112	-22	-112	-7	10	11	75	51	-75
1	0	11	864	-752	27	10	2	11	609	678	43	-13	5	11	85	19	-85	-4	7	11	457	-398	37	-6	10	11	525	562	46
3	0	11	977	990	29	11	2	11	76	-3	-76	-12	5	11	267	259	-72	-3	7	11	557	-593	39	-5	10	11	78	112	-78
5	0	11	1458	-1428	29	12	2	11	398	-432	49	-11	5	11	335	-276	60	-2	7	11	65	63	-65	-4	10	11	125	-37	-125
7	0	11	1055	975	32	-14	3	11	285	-271	-78	-10	5	11	180	31	-110	-1	7	11	63	4	-63	-3	10	11	68	-17	-68
9	0	11	893	-899	36	-13	3	11	491	-412	56	-9	5	11	197	169	-91	0	7	11	139	173	-63	-2	10	11	539	562	43
11	0	11	1032	1117	39	-12	3	11	279	-374	-75	-8	5	11	306	338	55	1	7	11	330	-405	42	-1	10	11	74	63	-74
-14	1	11	239	269	-89	-11	3	11	639	651	43	-7	5	11	545	-530	39	2	7	11	137	230	-89	0	10	11	522	-549	33
-13	1	11	424	-517	58	-10	3	11	402	-324	46	-6	5	11	122	61	-122	3	7	11	392	379	40	1	10	11	381	-360	40
-12	1	11	625	-598	50	-9	3	11	274	-262	58	-5	5	11	244	324	-63	4	7	11	154	172	-94	2	10	11	654	568	39
-11	1	11	160	94	-160	-8	3	11	562	556	40	-4	5	11	171	-151	-64	5	7	11	205	-130	-68	3	10	11	245	239	-67
-10	1	11	705	688	42	-7	3	11	323	-287	40	-3	5	11	64	217	-64	6	7	11	65	-57	-65	4	10	11	508	-436	40
-9	1	11	365	-298	48	-6	3	11	69	-128	-69	-2	5	11	305	-312	44	7	7	11	182	56	-50	5	10	11	242	-151	50
-8	1	11	68	10	-68	-5	3	11	279	-319	49	-1	5	11	259	398	45	8	7	11	75	-25	-75	6	10	11	447	525	47
-7	1	11	174	130	-66	-4	3	11	189	149	-60	0	5	11	643	647	23	9	7	11	67	155	-67	-6	11	11	220	52	-59
-6	1	11	173	-88	-73	-3	3	11	718	719	29	1	5	11	66	-5	-66	10	7	11	253	221	56	-5	11	11	332	-437	68
-5	1	11	434	-425	34	-2	3	11	496	-497	31	2	5	11	125	41	-125	-11	8	11	460	-469	56	-4	11	11	198	241	-92
-4	1	11	780	-746	29	-1	3	11	215	-243	48	3	5	11	62	-56	-62	-10	8	11	92	-144	-92	-3	11	11	288	356	55
-3	1	11	200	-164	-52	0	3	11	623	-621	20	4	5	11	374	423	38	-9	8	11	440	405	51	-2	11	11	231	-293	-69
-2	1	11	373	356	36	1	3	11	664	641	29	5	5	11	326	311	40	-8	8	11	181	183	-112	-1	11	11	71	-56	-71
-1	1	11	546	-557	30	2	3	11	236	-211	43	6	5	11	764	-732	35	-7	8	11	505	-526	42	0	11	11	75	41	-53
0	1	11	354	-344	33	3	3	11	945	-973	29	7	5	11	458	509	42	-6	8	11	249	-242	-67	1	11	11	262	242	59
1	1	11	429	521	34	4	3	11	301	-217	41	8	5	11	261	263	64	-5	8	11	1096	1090	37	2	11	11	164	108	-117
2	1	11	1347	1398	27	5	3	11	537	582	33	9	5	11	343	-384	55	-4	8	11	302	258	46	3	11	11	444	-470	49
3	1	11	976	-1032	28	6	3	11	68	149	-68	10	5	11	333	273	49	-3	8	11	976	-1031	36	5	11	11	152	157	-116
4	1	11	1306	-1281	29	7	3	11	68	32	-68	11	5	11	226	180	56	-2	8	11	338	-390	47	-4	12	11	156	-150	-156
5	1	11	371	365	36	8	3	11	172	-119	-57	-12	6	11	385	407	57	-1	8	11	876	900	35	-3	12	11	593	498	42
6	1	11	498	511	37	9	3	11	134	-49	-134	-11	6	11	305	307	60	0	8	11	80	158	-58	-2	12	11	481	427	45
7	1	11	291	-262	43	10	3	11	172	11	-66	-10	6	11	376	-310	50	1	8	11	863	-959	34	-1	12	11	284	-391	-72
8	1	11	167	55	-96	11	3	11	127	44	-127	-9	6	11	145	-198	-145	2	8	11	420	-416	38	0	12	11	376	-395	49
9	1	11	219	109	-63	12	3	11	202	-92	-66	-8	6	11	208	226	-89	3	8	11	612	632	36	1	12	11	422	478	50
10	1	11	73	-97	-73	-14	4	11	196	83	-123	-7	6	11	163	-177	-91	4	8	11	174	19	-47	2	12	11	294	335	58
12	1	11	212	-130	-61	-13	4	11	484	-532	51	-6	6	11	300	-301	49	5	8	11	630	-627	38	-14	0	12	532	616	54
-14	2	11	504	559	58	-12	4	11	194	-197	-101	-5	6	11	69	-108	-69	6	8	11	71	-15	-71	-12	0	12	1382	-1384	41

Observed and calculated structure factors for $[Ru(bpy)_2(phen\text{-}napthaquinone)](PF_6)_2$

h	k	l	10Fo	10Fc	10s
-10	0	12	391	-349	46
-8	0	12	352	-345	42
-6	0	12	799	779	32
-4	0	12	61	-149	-61
-2	0	12	207	-93	50
0	0	12	1147	-1258	19
2	0	12	1595	1630	28
4	0	12	971	-900	31
6	0	12	68	85	-68
8	0	12	766	-690	35
10	0	12	616	520	40
12	0	12	344	-308	52
-14	1	12	86	-98	-86
-13	1	12	282	-266	-83
-12	1	12	607	-538	48
-11	1	12	79	-119	-79
-10	1	12	865	862	40
-9	1	12	488	557	44
-8	1	12	375	-366	42
-7	1	12	246	-220	51
-6	1	12	669	604	32
-5	1	12	69	-121	-69
-4	1	12	562	-530	31
-3	1	12	333	-376	38
-2	1	12	67	2	-67
-1	1	12	710	719	28
0	1	12	217	-201	35
1	1	12	112	-148	-112
2	1	12	65	-18	-65
3	1	12	333	381	43
4	1	12	698	-663	31
5	1	12	1003	-924	31
6	1	12	735	805	34
7	1	12	779	732	36
8	1	12	366	-290	44
9	1	12	499	-535	42
10	1	12	140	-1	-140
11	1	12	272	219	55
12	1	12	428	-475	53
-14	2	12	85	17	-85
-13	2	12	479	-467	47
-12	2	12	85	-13	-85
-11	2	12	182	188	-89
-10	2	12	77	-29	-77
-9	2	12	853	-859	36
-8	2	12	719	713	35
-7	2	12	528	461	35
-6	2	12	485	-456	37
-5	2	12	265	156	44
-4	2	12	67	3	-67
-3	2	12	980	1032	28
-2	2	12	248	-268	46
-1	2	12	697	-671	28
0	2	12	180	213	-49
1	2	12	1448	1453	27
2	2	12	272	322	41

h	k	l	10Fo	10Fc	10s
3	2	12	341	-386	36
4	2	12	316	312	37
5	2	12	434	432	35
6	2	12	443	460	37
7	2	12	376	-394	43
8	2	12	113	177	-113
9	2	12	470	437	44
10	2	12	234	-179	49
11	2	12	254	-339	62
12	2	12	79	-150	-79
-14	3	12	195	236	-195
-13	3	12	300	-301	-84
-12	3	12	158	-35	-158
-11	3	12	390	434	52
-10	3	12	73	-7	-73
-9	3	12	166	-239	-125
-8	3	12	429	-383	44
-7	3	12	253	307	-64
-6	3	12	796	781	32
-5	3	12	427	-391	34
-4	3	12	255	-250	43
-3	3	12	175	-128	-65
-2	3	12	742	828	29
-1	3	12	64	-46	-64
0	3	12	416	-395	30
1	3	12	534	609	32
2	3	12	185	191	-52
3	3	12	239	140	42
4	3	12	494	-514	35
5	3	12	65	73	-65
6	3	12	485	566	37
7	3	12	142	-165	-142
8	3	12	611	-536	36
9	3	12	314	300	52
10	3	12	276	244	55
11	3	12	210	-282	-83
-14	4	12	281	-338	-88
-13	4	12	293	-336	-82
-12	4	12	138	171	-138
-11	4	12	202	194	-78
-10	4	12	424	-422	51
-9	4	12	367	334	51
-8	4	12	785	833	38
-7	4	12	71	-184	-71
-6	4	12	1164	-1177	32
-5	4	12	176	266	-74
-4	4	12	1170	1161	30
-3	4	12	351	396	38
-2	4	12	985	-893	29
-1	4	12	749	848	30
0	4	12	1858	1901	20
1	4	12	617	-536	31
2	4	12	431	-425	34
3	4	12	138	7	-73
4	4	12	260	250	45
5	4	12	105	33	-105

h	k	l	10Fo	10Fc	10s
6	4	12	74	-150	-74
7	4	12	646	675	37
8	4	12	65	8	-65
9	4	12	288	-326	55
10	4	12	531	-570	43
11	4	12	169	117	-96
-13	5	12	150	-10	-150
-11	5	12	248	126	-63
-10	5	12	211	265	-75
-9	5	12	421	-475	48
-8	5	12	75	152	-75
-7	5	12	806	808	35
-6	5	12	69	-81	-69
-5	5	12	552	-614	38
-4	5	12	185	191	-58
-3	5	12	229	259	47
-2	5	12	112	-30	-112
-1	5	12	485	-504	33
0	5	12	486	-441	33
1	5	12	742	762	31
2	5	12	140	-40	-102
3	5	12	325	-350	40
4	5	12	105	-82	-105
5	5	12	544	562	36
6	5	12	362	-237	42
7	5	12	413	-444	42
8	5	12	357	409	51
9	5	12	421	410	50
10	5	12	448	-424	45
11	5	12	478	-541	49
-13	6	12	391	358	66
-12	6	12	79	47	-79
-11	6	12	588	-498	50
-9	6	12	776	705	43
-8	6	12	71	20	-71
-7	6	12	807	-815	39
-6	6	12	173	-78	-79
-5	6	12	1148	1133	34
-4	6	12	253	363	63
-3	6	12	1557	-1501	31
-2	6	12	458	-463	35
-1	6	12	809	872	32
0	6	12	338	326	41
1	6	12	587	-560	33
2	6	12	239	-242	49
3	6	12	592	566	35
4	6	12	140	42	-110
5	6	12	213	-164	-58
6	6	12	114	-85	-114
7	6	12	513	519	41
8	6	12	140	-85	-77
9	6	12	455	-422	45
-12	7	12	85	34	-85
-11	7	12	201	-104	-100
-10	7	12	208	-141	-109
-9	7	12	151	-65	-118

h	k	l	10Fo	10Fc	10s
-8	7	12	309	297	59
-7	7	12	377	-356	47
-6	7	12	580	-596	39
-5	7	12	280	201	53
-4	7	12	395	382	40
-3	7	12	563	-523	37
-2	7	12	417	-391	41
-1	7	12	260	286	42
0	7	12	155	214	-67
1	7	12	124	-133	-124
2	7	12	166	-178	-95
3	7	12	109	-152	-109
4	7	12	65	-97	-65
5	7	12	248	-213	55
6	7	12	505	-551	43
7	7	12	140	135	-140
8	7	12	464	485	49
9	7	12	317	-347	58
-11	8	12	86	-113	-86
-10	8	12	485	507	53
-9	8	12	83	218	-83
-8	8	12	830	-742	43
-7	8	12	80	-192	-80
-6	8	12	898	956	39
-5	8	12	486	525	42
-4	8	12	654	-604	38
-3	8	12	897	-913	37
-2	8	12	858	841	35
-1	8	12	113	163	-113
0	8	12	379	-401	44
1	8	12	129	66	-129
2	8	12	340	381	50
3	8	12	69	-85	-69
4	8	12	451	-419	41
5	8	12	74	-103	-74
6	8	12	67	47	-67
7	8	12	178	148	-81
8	8	12	408	-352	45
-10	9	12	144	-3	-144
-9	9	12	455	509	60
-8	9	12	190	28	-81
-7	9	12	238	-339	-65
-6	9	12	82	63	-82
-5	9	12	80	178	-80
-4	9	12	76	239	-76
-3	9	12	98	-225	-98
-2	9	12	76	245	-76
-1	9	12	287	285	46
0	9	12	317	-347	51
1	9	12	203	-216	-78
2	9	12	313	261	48
3	9	12	68	-2	-68
4	9	12	210	-363	-77
5	9	12	175	-118	-68
6	9	12	506	497	48
7	9	12	485	494	48

h	k	l	10Fo	10Fc	10s
-9	10	12	562	-606	49
-8	10	12	179	-104	-104
-7	10	12	524	545	50
-6	10	12	186	232	-109
-5	10	12	522	-464	46
-4	10	12	242	-189	57
-3	10	12	568	631	40
-2	10	12	303	-313	52
-1	10	12	265	-350	-79
0	10	12	236	-176	47
1	10	12	430	407	47
2	10	12	142	-6	-142
3	10	12	742	-711	42
4	10	12	318	350	56
5	10	12	765	791	42
6	10	12	84	122	-84
-7	11	12	81	108	-81
-6	11	12	138	121	-138
-5	11	12	219	121	-64
-4	11	12	74	-46	-74
-3	11	12	70	5	-70
-2	11	12	498	542	44
-1	11	12	77	-10	-77
0	11	12	206	-163	-56
1	11	12	74	119	-74
2	11	12	166	-116	-96
3	11	12	168	-172	-109
4	11	12	151	-186	-151
-3	12	12	82	109	-82
-2	12	12	536	-458	43
-1	12	12	362	-384	47
0	12	12	610	633	31
-13	0	13	90	-49	-90
-11	0	13	210	287	-83
-9	0	13	501	-457	41
-7	0	13	781	828	35
-5	0	13	186	-137	-63
-3	0	13	168	-169	-87
-1	0	13	431	-412	36
1	0	13	635	-666	31
3	0	13	1244	1276	30
5	0	13	1466	-1426	32
7	0	13	155	-46	-84
9	0	13	70	71	-70
11	0	13	452	412	46
-14	1	13	409	302	59
-13	1	13	530	-461	50
-12	1	13	176	-174	-176
-11	1	13	447	479	54
-10	1	13	638	633	42
-9	1	13	344	-348	46
-8	1	13	357	-339	49
-7	1	13	305	301	41
-6	1	13	1008	1034	32
-5	1	13	720	-715	33
-4	1	13	1418	-1421	29

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
-3	1	13	254	178	39
-2	1	13	927	940	28
-1	1	13	285	-317	45
0	1	13	513	-495	37
1	1	13	726	684	30
2	1	13	797	815	30
3	1	13	604	-583	32
4	1	13	1044	-1070	32
5	1	13	1098	1069	32
6	1	13	823	783	32
7	1	13	582	-606	39
8	1	13	766	-717	37
9	1	13	247	253	60
10	1	13	725	594	40
11	1	13	369	-268	54
-14	2	13	197	-246	-127
-13	2	13	93	-152	-93
-12	2	13	177	-163	-128
-11	2	13	226	300	-90
-10	2	13	424	-468	48
-9	2	13	64	109	-64
-8	2	13	778	734	37
-7	2	13	277	265	51
-6	2	13	308	-350	58
-5	2	13	64	13	-64
-4	2	13	123	72	-123
-3	2	13	233	-191	50
-2	2	13	709	-731	30
-1	2	13	216	-265	54
0	2	13	66	-103	-47
1	2	13	282	218	42
2	2	13	733	698	32
3	2	13	453	433	35
4	2	13	935	-987	32
5	2	13	418	-400	41
7	2	13	169	186	-80
8	2	13	67	40	-67
9	2	13	68	-30	-68
10	2	13	267	-204	45
11	2	13	211	-244	-74
-14	3	13	356	-250	67
-13	3	13	487	-565	59
-12	3	13	502	466	50
-10	3	13	839	-902	40
-9	3	13	476	-467	43
-8	3	13	761	761	37
-7	3	13	459	483	39
-6	3	13	290	-293	43
-5	3	13	484	-441	36
-4	3	13	480	435	35
-3	3	13	964	918	29
-2	3	13	872	-909	31
-1	3	13	553	-611	32
0	3	13	177	-146	-45
1	3	13	242	372	50
2	3	13	529	460	33
3	3	13	757	-775	31
4	3	13	274	227	41
5	3	13	680	676	35
6	3	13	415	-389	39
7	3	13	405	-381	42
8	3	13	213	233	-67
9	3	13	447	459	42
10	3	13	340	-324	48
11	3	13	481	-486	45
-13	4	13	149	162	-149
-12	4	13	142	95	-142
-11	4	13	292	-368	-85
-10	4	13	268	294	52
-9	4	13	309	322	56
-8	4	13	80	-137	-80
-7	4	13	760	-773	35
-6	4	13	323	-358	51
-5	4	13	635	584	34
-4	4	13	682	680	34
-3	4	13	780	-841	32
-2	4	13	1058	-1043	30
-1	4	13	481	-473	32
0	4	13	556	-552	23
1	4	13	148	181	-72
2	4	13	291	288	45
3	4	13	117	88	-117
4	4	13	247	-249	55
5	4	13	247	185	48
6	4	13	69	23	-69
7	4	13	295	309	51
8	4	13	400	-388	43
9	4	13	142	-247	-142
10	4	13	80	-163	-80
11	4	13	132	84	-132
-13	5	13	487	424	57
-12	5	13	250	340	-87
-11	5	13	328	-343	57
-10	5	13	436	-441	54
-9	5	13	534	496	43
-8	5	13	650	639	41
-7	5	13	693	-695	36
-6	5	13	758	-677	36
-5	5	13	224	244	-73
-4	5	13	565	566	37
-3	5	13	712	-700	33
-2	5	13	621	-589	33
-1	5	13	978	979	31
0	5	13	967	998	24
1	5	13	384	-436	39
2	5	13	575	-648	35
3	5	13	618	638	35
4	5	13	721	747	36
5	5	13	512	-472	37
6	5	13	817	-817	36
7	5	13	778	819	38
8	5	13	745	791	40
9	5	13	469	-500	45
10	5	13	603	-584	45
-12	6	13	458	-428	52
-11	6	13	89	148	-89
-10	6	13	492	498	47
-9	6	13	77	-16	-77
-8	6	13	466	-454	45
-7	6	13	497	-419	43
-6	6	13	241	338	-61
-5	6	13	342	374	49
-4	6	13	498	-542	41
-3	6	13	456	-465	37
-2	6	13	265	256	46
-1	6	13	225	-269	53
0	6	13	580	-568	25
1	6	13	367	280	39
2	6	13	261	133	46
3	6	13	225	-173	-59
4	6	13	278	-272	46
5	6	13	75	159	-75
6	6	13	74	-2	-74
7	6	13	240	-81	53
8	6	13	73	40	-73
9	6	13	267	216	52
10	6	13	84	160	-84
-12	7	13	230	-185	-83
-11	7	13	704	-716	53
-10	7	13	453	519	57
-9	7	13	693	719	47
-8	7	13	433	-511	49
-7	7	13	458	-476	44
-6	7	13	600	549	41
-5	7	13	610	611	39
-4	7	13	640	-678	38
-3	7	13	204	-129	-58
-2	7	13	355	440	41
-1	7	13	418	414	41
0	7	13	308	-288	31
1	7	13	455	-396	37
2	7	13	320	267	44
3	7	13	511	465	38
4	7	13	374	-357	43
5	7	13	862	-824	37
6	7	13	278	299	53
7	7	13	826	859	38
8	7	13	410	-409	49
9	7	13	303	-318	57
-11	8	13	171	101	-171
-10	8	13	75	122	-75
-9	8	13	318	-270	63
-8	8	13	108	-51	-108
-7	8	13	246	245	-73
-6	8	13	82	-13	-82
-5	8	13	321	293	55
-4	8	13	206	-248	-86
-3	8	13	375	-313	46
-2	8	13	371	360	44
-1	8	13	72	30	-72
0	8	13	112	100	-62
1	8	13	199	148	-73
2	8	13	70	-110	-70
3	8	13	262	-222	50
6	8	13	78	12	-78
7	8	13	72	39	-72
8	8	13	132	56	-132
-10	9	13	605	657	55
-9	9	13	164	-192	-164
-8	9	13	662	-686	46
-7	9	13	399	394	52
-6	9	13	326	406	59
-5	9	13	231	-378	-75
-4	9	13	71	135	-71
-3	9	13	315	178	45
-2	9	13	140	-13	-140
-1	9	13	708	-707	38
0	9	13	299	-311	46
1	9	13	508	561	44
2	9	13	355	374	48
3	9	13	315	-203	50
4	9	13	520	-495	41
5	9	13	555	651	45
6	9	13	864	874	40
7	9	13	215	-176	-72
-8	10	13	79	53	-79
-7	10	13	138	28	-138
-6	10	13	190	33	-80
-4	10	13	247	377	-62
-3	10	13	389	-416	50
-2	10	13	379	-300	44
-1	10	13	191	147	-99
0	10	13	148	-141	-69
1	10	13	75	88	-75
3	10	13	164	-31	-69
4	10	13	106	271	-106
5	10	13	293	-204	53
-6	11	13	214	-282	-94
-5	11	13	193	-259	-119
-3	11	13	435	471	50
-2	11	13	169	-372	-169
-1	11	13	446	-401	47
0	11	13	78	144	-55
1	11	13	412	369	48
2	11	13	251	-255	-66
3	11	13	557	-606	45
-14	0	14	197	141	-127
-12	0	14	772	-829	48
-10	0	14	83	13	-83
-8	0	14	71	52	-71
-6	0	14	1376	1289	33
-4	0	14	992	-857	31
-2	0	14	156	-101	-75
0	0	14	1387	-1352	28
2	0	14	1236	1292	30
4	0	14	1276	-1273	32
6	0	14	314	272	40
8	0	14	95	-21	-95
10	0	14	508	504	45
-14	1	14	555	-607	59
-13	1	14	1038	-983	47
-12	1	14	409	407	52
-11	1	14	838	890	44
-10	1	14	144	34	-144
-9	1	14	834	-788	39
-8	1	14	784	784	36
-7	1	14	413	495	43
-6	1	14	415	-453	42
-5	1	14	865	-894	33
-4	1	14	762	733	32
-3	1	14	700	691	31
-2	1	14	460	-504	35
-1	1	14	431	-458	36
0	1	14	400	389	26
1	1	14	474	454	33
2	1	14	818	-847	31
3	1	14	842	-819	32
4	1	14	1178	1180	32
5	1	14	964	967	33
6	1	14	815	-796	35
7	1	14	732	-766	37
8	1	14	78	188	-78
9	1	14	467	489	42
10	1	14	68	-23	-68
11	1	14	149	-281	-149
-14	2	14	128	-109	-128
-13	2	14	92	-209	-92
-12	2	14	637	654	48
-11	2	14	256	-233	63
-10	2	14	394	-398	51
-9	2	14	288	201	50
-8	2	14	188	41	-74
-7	2	14	365	316	42
-6	2	14	260	257	49
-5	2	14	277	-329	52
-4	2	14	172	-147	-62
-3	2	14	534	483	34
-2	2	14	656	634	32
-1	2	14	355	-316	36
0	2	14	446	-456	32
1	2	14	1521	1584	29
2	2	14	60	-4	-60
3	2	14	678	-654	33
4	2	14	658	680	35
5	2	14	294	301	53
6	2	14	141	-234	-141
7	2	14	278	-248	49
8	2	14	303	-272	43
9	2	14	233	230	-61
10	2	14	162	-80	-162

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$ Page 15

h	k	l	10Fo	10Fc	10s
11	2	14	213	-242	-72
-14	3	14	622	-646	60
-13	3	14	334	382	80
-12	3	14	328	351	62
-11	3	14	524	-626	49
-10	3	14	608	-622	47
-9	3	14	425	473	50
-8	3	14	806	823	39
-7	3	14	384	-312	45
-6	3	14	929	-941	35
-5	3	14	542	590	36
-4	3	14	834	906	32
-3	3	14	697	-776	34
-2	3	14	621	-578	33
-1	3	14	710	720	32
0	3	14	334	385	28
1	3	14	225	-274	47
2	3	14	281	-349	49
3	3	14	652	637	34
4	3	14	769	713	34
5	3	14	553	-529	36
6	3	14	942	-978	35
7	3	14	175	12	-77
8	3	14	256	371	-65
9	3	14	213	-244	53
10	3	14	337	-344	46
11	3	14	264	295	64
-13	4	14	278	214	-94
-12	4	14	264	256	-83
-11	4	14	309	-247	67
-10	4	14	79	-91	-79
-9	4	14	177	245	-177
-8	4	14	120	58	-120
-7	4	14	148	76	-125
-6	4	14	256	-209	61
-5	4	14	73	144	-73
-4	4	14	522	444	34
-3	4	14	65	83	-65
-2	4	14	201	-129	-50
-1	4	14	616	659	35
0	4	14	611	654	25
1	4	14	116	151	-116
2	4	14	349	-355	45
3	4	14	269	264	45
4	4	14	663	657	35
5	4	14	291	-357	46
6	4	14	453	-447	38
7	4	14	769	748	37
8	4	14	198	-110	-78
10	4	14	478	-479	43
-13	5	14	282	323	-85
-12	5	14	120	-177	-120
-11	5	14	467	-436	52
-10	5	14	205	244	-90
-9	5	14	481	495	52
-8	5	14	311	-358	58

h	k	l	10Fo	10Fc	10s
-7	5	14	483	-538	45
-6	5	14	391	404	49
-5	5	14	452	383	39
-4	5	14	452	-496	40
-3	5	14	515	-511	35
-2	5	14	674	635	35
-1	5	14	346	393	39
0	5	14	1286	-1188	26
1	5	14	368	-434	43
2	5	14	430	479	42
3	5	14	615	563	36
4	5	14	502	-479	36
5	5	14	363	-328	42
6	5	14	328	259	48
7	5	14	365	301	46
8	5	14	73	2	-73
9	5	14	329	-409	52
10	5	14	75	70	-75
-12	6	14	94	-78	-94
-11	6	14	249	-240	-87
-10	6	14	85	-30	-85
-9	6	14	253	228	-76
-8	6	14	86	274	-86
-7	6	14	173	25	-79
-6	6	14	216	-53	-62
-5	6	14	163	68	-123
-4	6	14	71	-1	-71
-3	6	14	502	-533	38
-2	6	14	365	-308	43
-1	6	14	339	332	40
0	6	14	555	570	25
1	6	14	335	-298	47
2	6	14	155	-136	-77
3	6	14	536	519	37
4	6	14	114	-115	-114
5	6	14	299	-226	49
6	6	14	182	-138	-69
7	6	14	591	588	41
8	6	14	147	-218	-147
9	6	14	405	-360	46
-11	7	14	318	275	56
-10	7	14	578	539	48
-9	7	14	294	-247	66
-8	7	14	509	-563	55
-7	7	14	81	174	-81
-6	7	14	436	438	47
-5	7	14	77	143	-77
-4	7	14	605	-622	41
-3	7	14	219	144	-58
-2	7	14	269	257	52
-1	7	14	371	-458	47
0	7	14	699	-705	30
1	7	14	304	322	54
2	7	14	672	678	39
3	7	14	436	-445	40
4	7	14	454	-431	42

h	k	l	10Fo	10Fc	10s
5	7	14	80	177	-80
6	7	14	284	334	58
7	7	14	125	-166	-125
8	7	14	300	-271	61
-10	8	14	251	336	-83
-9	8	14	181	251	-181
-8	8	14	247	-195	-71
-7	8	14	214	154	-72
-6	8	14	265	214	58
-4	8	14	157	250	-157
-3	8	14	69	-44	-69
-2	8	14	403	409	47
-1	8	14	166	96	-63
0	8	14	567	-590	35
1	8	14	74	-122	-74
2	8	14	348	233	44
3	8	14	219	236	-78
4	8	14	253	-262	55
5	8	14	161	-228	-113
6	8	14	571	573	43
7	8	14	71	134	-71
-9	9	14	382	-452	55
-8	9	14	198	152	-111
-7	9	14	260	361	-83
-6	9	14	73	-128	-73
-5	9	14	76	-98	-76
-3	9	14	571	542	40
-2	9	14	294	-293	65
-1	9	14	499	-443	44
0	9	14	188	97	-61
1	9	14	785	808	41
2	9	14	444	-488	44
3	9	14	854	-892	41
4	9	14	162	229	-120
5	9	14	792	749	41
6	9	14	200	-120	-73
-8	10	14	205	82	-87
-7	10	14	243	234	-64
-6	10	14	251	-94	52
-4	10	14	170	-82	-170
-3	10	14	237	197	49
-2	10	14	166	183	-96
-1	10	14	477	-561	47
0	10	14	91	-110	-65
1	10	14	721	761	41
2	10	14	246	195	-73
3	10	14	660	-642	42
4	10	14	262	-254	48
5	10	14	448	368	47
-5	11	14	300	311	71
-4	11	14	426	429	45
-3	11	14	135	-138	-135
-2	11	14	78	-127	-78
-1	11	14	79	105	-79
0	11	14	423	461	33
1	11	14	132	92	-132

h	k	l	10Fo	10Fc	10s
2	11	14	494	-558	47
-13	0	15	283	-302	-74
-11	0	15	589	550	46
-9	0	15	298	-372	62
-7	0	15	1378	1423	34
-5	0	15	1595	-1493	32
-3	0	15	172	-183	-91
-1	0	15	1074	-1070	31
1	0	15	1320	1313	31
3	0	15	663	-716	35
5	0	15	1128	1038	33
7	0	15	638	-617	39
9	0	15	399	444	48
11	0	15	488	-532	44
-14	1	15	98	-188	-98
-13	1	15	430	395	69
-12	1	15	762	694	47
-11	1	15	92	63	-92
-10	1	15	78	-148	-78
-9	1	15	173	287	-114
-8	1	15	71	-40	-71
-7	1	15	144	-245	-144
-6	1	15	336	338	50
-5	1	15	756	689	34
-4	1	15	205	-190	-65
-3	1	15	264	-337	46
-2	1	15	126	-164	-126
-1	1	15	622	573	32
0	1	15	758	745	24
1	1	15	388	-396	42
2	1	15	1262	-1300	31
3	1	15	649	647	34
4	1	15	908	878	34
5	1	15	273	-234	52
6	1	15	78	-165	-78
7	1	15	297	266	53
8	1	15	70	13	-70
9	1	15	158	263	-158
11	1	15	321	-206	49
-14	2	15	419	-390	73
-13	2	15	82	92	-82
-12	2	15	164	252	-164
-11	2	15	394	-313	52
-10	2	15	389	-328	55
-9	2	15	594	-554	43
-8	2	15	776	826	39
-7	2	15	160	141	-98
-6	2	15	1085	-1080	34
-5	2	15	194	-170	-87
-4	2	15	1275	1287	32
-3	2	15	543	523	36
-2	2	15	729	-850	33
-1	2	15	66	11	-66
0	2	15	779	852	22
1	2	15	216	93	-56
2	2	15	1311	-1318	31

h	k	l	10Fo	10Fc	10s
3	2	15	215	188	-69
4	2	15	692	698	35
5	2	15	155	51	-71
6	2	15	598	-632	38
7	2	15	428	-415	40
8	2	15	366	413	48
9	2	15	65	55	-65
10	2	15	537	-503	42
-13	3	15	543	541	63
-12	3	15	187	-59	-79
-11	3	15	319	-373	74
-10	3	15	263	161	64
-9	3	15	82	90	-82
-8	3	15	418	-413	46
-7	3	15	312	253	46
-6	3	15	578	633	37
-5	3	15	71	47	-71
-4	3	15	60	-45	-60
-3	3	15	464	-491	41
-2	3	15	68	88	-68
-1	3	15	347	372	40
0	3	15	67	-147	-47
1	3	15	433	-505	39
2	3	15	286	277	49
3	3	15	605	561	33
4	3	15	310	-299	44
5	3	15	332	-401	55
6	3	15	271	268	46
7	3	15	151	5	-87
8	3	15	82	-160	-82
9	3	15	192	155	-53
10	3	15	83	44	-83
-13	4	15	530	552	59
-12	4	15	98	-227	-98
-11	4	15	460	-463	55
-10	4	15	84	-138	-84
-9	4	15	676	699	43
-8	4	15	246	275	-80
-7	4	15	925	-966	39
-6	4	15	342	-387	54
-5	4	15	1090	1132	35
-4	4	15	71	113	-71
-3	4	15	1512	-1589	32
-2	4	15	428	-443	38
-1	4	15	1055	1108	32
0	4	15	77	-69	-58
1	4	15	729	-727	36
2	4	15	122	-29	-122
3	4	15	827	852	35
4	4	15	68	30	-68
5	4	15	456	-471	42
6	4	15	348	-343	43
7	4	15	930	900	38
8	4	15	75	-238	-75
9	4	15	685	-644	41
10	4	15	82	-40	-82

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
-13	5	15	86	-55	-86
-12	5	15	246	-234	-97
-11	5	15	87	202	-87
-9	5	15	240	-342	-92
-8	5	15	79	-91	-79
-7	5	15	156	169	-132
-6	5	15	75	-64	-75
-5	5	15	71	-9	-71
-4	5	15	181	-200	-74
-3	5	15	72	-34	-72
-2	5	15	206	129	-60
-1	5	15	194	65	-61
0	5	15	333	313	38
1	5	15	70	134	-70
2	5	15	198	212	-54
3	5	15	317	202	44
5	5	15	134	-200	-134
6	5	15	119	13	-119
7	5	15	157	84	-83
8	5	15	77	56	-77
9	5	15	71	-90	-71
-12	6	15	501	-575	65
-10	6	15	459	592	62
-9	6	15	77	-71	-77
-8	6	15	573	-590	45
-7	6	15	289	-337	69
-6	6	15	638	653	40
-5	6	15	226	322	-69
-4	6	15	1251	-1307	35
-3	6	15	291	-235	51
-2	6	15	1212	1209	35
-1	6	15	509	586	40
0	6	15	1421	-1500	49
1	6	15	231	-206	-64
2	6	15	835	838	36
3	6	15	132	-85	-70
4	6	15	560	-531	37
5	6	15	69	-89	-69
6	6	15	359	260	45
7	6	15	239	235	46
8	6	15	401	-410	47
9	6	15	153	-69	-153
-11	7	15	88	90	-88
-9	7	15	85	-132	-85
-8	7	15	155	185	-155
-7	7	15	472	447	50
-6	7	15	229	-189	-72
-5	7	15	435	362	49
-4	7	15	668	-681	38
-3	7	15	253	209	49
-2	7	15	70	160	-70
-1	7	15	75	-218	-75
0	7	15	75	116	-75
1	7	15	326	315	44
2	7	15	62	63	-62
3	7	15	71	144	-71
4	7	15	155	-159	-112
5	7	15	74	151	-74
6	7	15	250	283	-63
7	7	15	77	149	-77
8	7	15	132	-181	-132
-10	8	15	209	254	-113
-9	8	15	396	-423	58
-8	8	15	240	-44	-80
-7	8	15	573	498	48
-6	8	15	83	-48	-83
-5	8	15	146	-301	-146
-4	8	15	71	40	-71
-3	8	15	123	171	-123
-2	8	15	122	144	-122
-1	8	15	1344	-1393	37
0	8	15	304	-303	51
1	8	15	716	687	40
2	8	15	414	471	45
3	8	15	78	-164	-78
5	8	15	283	396	-71
7	8	15	411	-370	50
-9	9	15	209	102	-95
-8	9	15	142	76	-142
-7	9	15	265	206	55
-6	9	15	366	-288	47
-5	9	15	83	-59	-83
-4	9	15	211	190	-71
-3	9	15	128	-66	-128
-2	9	15	145	-175	-145
-1	9	15	239	-209	-71
0	9	15	80	67	-80
1	9	15	78	57	-78
2	9	15	535	-587	43
3	9	15	232	195	-59
4	9	15	223	210	-66
5	9	15	75	57	-75
6	9	15	76	26	-76
-7	10	15	77	-18	-77
-6	10	15	379	-354	52
-5	10	15	79	-23	-79
-4	10	15	291	244	53
-3	10	15	547	476	48
-2	10	15	891	-892	41
-1	10	15	361	-374	54
0	10	15	809	802	46
1	10	15	397	450	52
2	10	15	551	-597	41
3	10	15	241	-280	-66
4	10	15	354	400	60
-4	11	15	162	-247	-103
-3	11	15	159	-46	-121
-2	11	15	81	-40	-81
-1	11	15	75	186	-75
0	11	15	95	124	-69
1	11	15	234	-234	-79
-14	0	16	354	-395	68
-12	0	16	470	467	56
-10	0	16	199	125	-83
-8	0	16	553	556	41
-6	0	16	386	347	42
-4	0	16	161	313	-161
-2	0	16	512	-530	36
0	0	16	1118	1140	28
2	0	16	629	-747	37
4	0	16	482	440	38
6	0	16	546	-574	40
8	0	16	287	324	52
10	0	16	104	70	-104
-14	1	16	346	-310	73
-13	1	16	317	-372	-80
-12	1	16	222	165	-119
-11	1	16	751	748	48
-10	1	16	228	-198	-71
-9	1	16	688	-643	40
-8	1	16	405	440	48
-7	1	16	313	266	49
-6	1	16	144	-166	-144
-5	1	16	613	-612	39
-4	1	16	137	-46	-137
-3	1	16	409	390	38
-2	1	16	229	-295	51
-1	1	16	68	106	-68
0	1	16	494	452	26
1	1	16	214	313	-70
2	1	16	276	-292	57
3	1	16	794	-756	35
4	1	16	583	515	38
5	1	16	891	903	35
6	1	16	330	-343	45
7	1	16	508	-527	46
8	1	16	68	-5	-68
10	1	16	258	-246	-65
-13	2	16	462	541	60
-12	2	16	327	350	67
-11	2	16	332	-321	64
-10	2	16	307	-247	64
-9	2	16	422	372	46
-8	2	16	289	-213	64
-7	2	16	674	-645	40
-6	2	16	298	341	51
-5	2	16	543	569	37
-4	2	16	174	35	-84
-3	2	16	610	-643	34
-2	2	16	512	-500	34
-1	2	16	724	708	33
0	2	16	140	-42	-61
1	2	16	292	-286	51
2	2	16	402	-391	41
3	2	16	380	392	45
4	2	16	190	98	-60
5	2	16	388	-333	42
6	2	16	393	-379	45
7	2	16	65	-73	-65
8	2	16	70	-22	-70
9	2	16	77	-179	-77
10	2	16	238	147	57
-13	3	16	202	277	-202
-12	3	16	172	-99	-93
-11	3	16	283	-306	-77
-10	3	16	454	-533	59
-9	3	16	80	46	-80
-8	3	16	540	498	42
-7	3	16	168	-267	-110
-6	3	16	574	-542	36
-5	3	16	380	439	46
-4	3	16	369	370	38
-3	3	16	281	-299	51
-2	3	16	201	-368	-70
-1	3	16	180	-135	-69
0	3	16	63	-41	-44
1	3	16	392	-430	39
2	3	16	261	-277	50
3	3	16	286	194	44
4	3	16	574	617	39
5	3	16	410	-515	42
6	3	16	441	-410	48
7	3	16	324	218	50
8	3	16	124	198	-124
9	3	16	195	-241	-85
10	3	16	394	-373	50
-13	4	16	88	66	-88
-12	4	16	359	-323	59
-11	4	16	221	189	-78
-10	4	16	635	600	45
-9	4	16	80	44	-80
-8	4	16	756	-773	43
-7	4	16	221	44	-60
-6	4	16	987	948	37
-5	4	16	237	222	-66
-4	4	16	1356	-1365	34
-3	4	16	125	213	-125
-2	4	16	1062	1053	33
-1	4	16	70	65	-70
0	4	16	529	-564	26
1	4	16	66	-72	-66
2	4	16	166	221	-108
3	4	16	211	142	-53
4	4	16	244	-383	-66
5	4	16	116	-174	-116
6	4	16	314	313	52
7	4	16	434	482	48
8	4	16	634	-682	42
9	4	16	197	63	-76
-12	5	16	96	-197	-96
-11	5	16	94	-21	-94
-10	5	16	199	-48	-84
-9	5	16	221	143	-77
-8	5	16	74	-85	-74
-7	5	16	610	-614	41
-6	5	16	457	561	48
-5	5	16	558	536	41
-4	5	16	593	-626	38
-3	5	16	289	216	46
-2	5	16	640	587	36
-1	5	16	77	-58	-77
0	5	16	708	-752	37
1	5	16	318	-375	43
3	5	16	292	291	51
4	5	16	69	-14	-69
5	5	16	298	-274	55
6	5	16	186	281	-66
7	5	16	387	441	46
8	5	16	439	-385	46
9	5	16	425	-387	51
-11	6	16	398	467	65
-10	6	16	82	57	-82
-9	6	16	663	-608	47
-8	6	16	76	23	-76
-7	6	16	1104	1147	40
-6	6	16	76	94	-76
-5	6	16	1250	-1208	37
-4	6	16	75	-255	-75
-3	6	16	910	894	37
-2	6	16	517	483	39
-1	6	16	998	-1064	35
0	6	16	84	158	-62
1	6	16	599	628	40
2	6	16	188	231	-83
3	6	16	71	-33	-71
4	6	16	283	-266	55
5	6	16	243	236	58
6	6	16	125	84	-125
7	6	16	447	-434	48
-11	7	16	235	215	-83
-10	7	16	341	284	52
-9	7	16	284	116	55
-8	7	16	250	-256	-68
-7	7	16	82	85	-82
-6	7	16	167	-128	-167
-5	7	16	76	-160	-76
-4	7	16	820	-808	39
-3	7	16	713	635	38
-2	7	16	79	158	-79
-1	7	16	205	133	-64
0	7	16	213	-193	45
1	7	16	236	171	51
2	7	16	68	45	-68
3	7	16	121	-142	-121
4	7	16	159	-12	-110
5	7	16	82	265	-82
6	7	16	577	556	42
7	7	16	283	-297	68
-10	8	16	503	-545	58
-9	8	16	83	-165	-83

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

h	k	l	10Fo	10Fc	10s
-8	8	16	510	518	54
-7	8	16	224	193	-83
-6	8	16	172	-280	-172
-5	8	16	336	-193	51
-4	8	16	459	481	48
-3	8	16	71	-56	-71
-2	8	16	964	-966	41
-1	8	16	142	66	-142
0	8	16	549	587	30
1	8	16	73	40	-73
2	8	16	286	-263	48
3	8	16	229	191	-61
4	8	16	146	190	-146
5	8	16	64	28	-64
6	8	16	314	-423	64
-7	9	16	295	327	69
-6	9	16	287	-295	59
-5	9	16	81	-178	-81
-4	9	16	82	146	-82
-3	9	16	310	346	69
-2	9	16	388	-390	52
-1	9	16	506	-576	48
0	9	16	240	171	51
1	9	16	148	106	-148
2	9	16	128	-213	-128
3	9	16	225	-153	-79
4	9	16	331	333	63
5	9	16	415	414	47
-7	10	16	560	-491	50
-5	10	16	589	603	49
-4	10	16	225	214	-75
-3	10	16	407	-344	50
-2	10	16	301	-274	69
-1	10	16	639	644	46
0	10	16	199	137	-64
1	10	16	508	-467	46
2	10	16	73	-42	-73
3	10	16	157	188	-157
-3	11	16	182	14	-67
-2	11	16	254	-298	61
-1	11	16	239	306	-80
-13	0	17	127	-16	-127
-11	0	17	268	150	67
-9	0	17	287	397	64
-7	0	17	582	-563	40
-5	0	17	266	-273	53
-3	0	17	495	-457	36
-1	0	17	413	382	39
1	0	17	784	762	37
3	0	17	931	-944	36
5	0	17	78	-164	-78
7	0	17	207	117	-54
9	0	17	450	387	44
-13	1	17	412	455	67
-12	1	17	824	774	48
-11	1	17	710	-683	49

h	k	l	10Fo	10Fc	10s
-10	1	17	412	-496	57
-9	1	17	224	248	-77
-8	1	17	364	288	51
-7	1	17	731	-722	41
-6	1	17	960	-946	36
-5	1	17	746	739	37
-4	1	17	950	1048	36
-3	1	17	415	-389	37
-2	1	17	682	-683	34
-1	1	17	447	475	39
0	1	17	1043	1029	23
1	1	17	510	-573	41
2	1	17	1451	-1423	33
3	1	17	811	812	34
4	1	17	934	961	36
5	1	17	568	-561	40
6	1	17	630	-620	39
7	1	17	68	-73	-68
8	1	17	201	285	-85
9	1	17	344	-335	52
10	1	17	227	-215	-90
-13	2	17	96	-65	-96
-12	2	17	547	-439	53
-11	2	17	91	-196	-91
-10	2	17	76	-23	-76
-9	2	17	354	-383	59
-8	2	17	204	-267	-93
-7	2	17	76	151	-76
-6	2	17	558	576	39
-5	2	17	113	-169	-113
-4	2	17	389	-338	42
-3	2	17	341	-322	43
-2	2	17	314	299	46
-1	2	17	319	320	40
0	2	17	135	44	-63
1	2	17	303	309	51
2	2	17	601	-610	37
3	2	17	254	-189	50
4	2	17	304	319	51
5	2	17	220	202	-58
6	2	17	297	-248	50
7	2	17	231	-207	55
8	2	17	102	-1	-102
-13	3	17	402	223	61
-12	3	17	392	-397	73
-11	3	17	187	-193	-152
-10	3	17	239	236	-84
-9	3	17	849	840	42
-8	3	17	353	-327	59
-7	3	17	212	-179	-80
-6	3	17	542	467	39
-5	3	17	650	674	40
-4	3	17	78	-92	-78
-3	3	17	601	-570	36
-2	3	17	235	245	56
-1	3	17	304	281	50

h	k	l	10Fo	10Fc	10s
0	3	17	122	-85	-56
1	3	17	534	-541	39
2	3	17	561	537	39
3	3	17	538	582	38
4	3	17	301	-354	54
5	3	17	710	-731	37
6	3	17	1011	954	37
7	3	17	459	462	42
8	3	17	694	-683	40
9	3	17	260	-236	60
-11	4	17	240	288	-86
-10	4	17	82	-29	-82
-9	4	17	191	-243	-191
-8	4	17	86	44	-86
-7	4	17	338	231	48
-6	4	17	70	44	-70
-5	4	17	325	-337	51
-4	4	17	219	-371	-90
-3	4	17	160	250	-160
-2	4	17	74	141	-74
-1	4	17	767	805	35
0	4	17	405	404	41
1	4	17	111	-139	-111
2	4	17	243	-199	53
3	4	17	322	260	47
4	4	17	341	369	47
5	4	17	73	63	-73
6	4	17	233	83	-66
7	4	17	176	128	-88
8	4	17	72	-53	-72
-12	5	17	314	-416	-80
-11	5	17	722	719	51
-10	5	17	235	282	-114
-9	5	17	592	-660	50
-8	5	17	696	-673	42
-7	5	17	644	673	44
-6	5	17	668	679	41
-5	5	17	628	-592	40
-4	5	17	522	-447	43
-3	5	17	275	336	58
-2	5	17	132	-34	-132
-1	5	17	285	260	55
0	5	17	73	-30	-51
1	5	17	388	490	44
2	5	17	339	377	47
3	5	17	232	-300	-66
4	5	17	548	-504	39
5	5	17	384	403	47
6	5	17	560	478	40
7	5	17	446	-484	45
8	5	17	717	-598	42
-10	6	17	255	-158	58
-9	6	17	85	-144	-85
-8	6	17	387	221	50
-7	6	17	357	316	49
-6	6	17	127	-58	-127

h	k	l	10Fo	10Fc	10s
-5	6	17	401	-336	48
-4	6	17	69	-235	-69
-3	6	17	430	465	48
-2	6	17	273	134	52
-1	6	17	70	274	-70
0	6	17	286	-289	56
1	6	17	449	-426	44
2	6	17	137	122	-137
3	6	17	277	190	50
4	6	17	73	38	-73
5	6	17	177	-174	-73
6	6	17	220	188	-62
8	6	17	78	-74	-78
-11	7	17	445	453	68
-9	7	17	403	-476	60
-8	7	17	314	163	47
-7	7	17	392	478	63
-6	7	17	403	-401	56
-5	7	17	278	307	65
-4	7	17	178	-69	-127
-3	7	17	74	-76	-74
-1	7	17	525	-590	45
0	7	17	161	190	-63
1	7	17	384	389	53
2	7	17	245	-296	-72
3	7	17	378	-363	50
4	7	17	193	286	-84
5	7	17	674	567	42
6	7	17	518	-458	45
7	7	17	659	-615	44
-9	8	17	287	276	-76
-8	8	17	187	199	-187
-6	8	17	417	-437	51
-5	8	17	189	-102	-73
-4	8	17	185	33	-64
-3	8	17	315	-312	61
-2	8	17	194	278	-91
-1	8	17	192	209	-81
0	8	17	207	-210	43
1	8	17	205	-153	-70
2	8	17	79	71	-79
3	8	17	67	83	-67
4	8	17	198	-201	-92
5	8	17	85	-189	-85
6	8	17	73	99	-73
-8	9	17	355	359	64
-7	9	17	313	-247	76
-6	9	17	476	-410	52
-5	9	17	479	420	52
-4	9	17	358	327	58
-3	9	17	393	-444	48
-2	9	17	382	-422	49
-1	9	17	513	581	48
0	9	17	234	198	42
1	9	17	238	-129	-64
2	9	17	516	-596	47

h	k	l	10Fo	10Fc	10s
3	9	17	360	315	51
4	9	17	554	599	48
-5	10	17	86	-171	-86
-4	10	17	89	-95	-89
-3	10	17	77	114	-77
-2	10	17	77	78	-77
-1	10	17	81	-12	-81
0	10	17	93	-13	-68
-12	0	18	347	338	66
-10	0	18	82	13	-82
-8	0	18	78	130	-78
-6	0	18	168	-30	-88
-4	0	18	737	705	38
-2	0	18	759	-694	36
0	0	18	1636	1579	24
2	0	18	1436	-1444	35
4	0	18	78	164	-78
6	0	18	68	5	-68
8	0	18	338	365	49
-13	1	18	617	634	59
-12	1	18	361	-464	74
-10	1	18	565	425	46
-9	1	18	325	278	54
-8	1	18	588	-624	46
-7	1	18	448	-473	47
-6	1	18	587	610	43
-5	1	18	642	665	38
-4	1	18	715	-704	38
-3	1	18	483	-460	38
-2	1	18	330	398	53
-1	1	18	75	95	-75
0	1	18	189	-198	-52
1	1	18	615	-605	38
2	1	18	463	460	43
3	1	18	722	673	36
4	1	18	748	-725	37
5	1	18	528	-543	44
6	1	18	71	212	-71
7	1	18	187	110	-87
8	1	18	162	-65	-132
9	1	18	211	-47	-67
-13	2	18	185	313	-185
-12	2	18	560	516	58
-10	2	18	79	-103	-79
-9	2	18	79	-18	-79
-8	2	18	181	206	-112
-7	2	18	189	-114	-83
-6	2	18	333	-413	55
-5	2	18	724	712	40
-4	2	18	209	208	-76
-3	2	18	683	-620	38
-2	2	18	181	-140	-83
-1	2	18	826	879	37
0	2	18	80	30	-60
1	2	18	764	-829	37
2	2	18	172	-187	-97

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$ Page 18

h	k	l	10Fo	10Fc	10s
3	2	18	285	325	59
4	2	18	70	-198	-70
5	2	18	554	-560	40
6	2	18	261	194	59
7	2	18	143	212	-143
8	2	18	71	-29	-71
9	2	18	292	-316	56
-13	3	18	267	-360	-106
-12	3	18	458	-459	58
-11	3	18	95	106	-95
-10	3	18	357	512	81
-9	3	18	135	-239	-135
-8	3	18	312	-354	64
-7	3	18	498	476	45
-6	3	18	559	463	39
-5	3	18	205	-243	-75
-4	3	18	448	-543	44
-3	3	18	161	207	-84
-2	3	18	68	81	-68
-1	3	18	472	-465	42
0	3	18	81	-212	-60
1	3	18	791	801	36
2	3	18	359	438	47
3	3	18	474	-457	41
4	3	18	179	-279	-79
5	3	18	75	17	-75
6	3	18	631	544	41
7	3	18	81	-208	-81
8	3	18	514	-520	43
9	3	18	374	301	53
-12	4	18	289	-145	-91
-11	4	18	214	209	-115
-10	4	18	373	409	62
-9	4	18	86	-66	-86
-8	4	18	529	-572	47
-7	4	18	82	-96	-82
-6	4	18	191	191	-93
-5	4	18	140	14	-140
-4	4	18	621	-603	39
-3	4	18	212	-143	-77
-2	4	18	1007	937	36
-1	4	18	301	183	49
0	4	18	698	-694	26
1	4	18	447	-438	43
2	4	18	555	642	41
3	4	18	79	-205	-79
4	4	18	652	-687	41
5	4	18	68	52	-68
6	4	18	329	337	49
8	4	18	478	-432	48
-12	5	18	294	284	66
-11	5	18	367	405	69
-10	5	18	466	-528	55
-9	5	18	737	-673	47
-8	5	18	158	123	-158
-7	5	18	584	582	44

h	k	l	10Fo	10Fc	10s
-6	5	18	484	-499	48
-5	5	18	227	-338	-62
-4	5	18	121	244	-121
-3	5	18	120	126	-120
-2	5	18	152	-131	-91
-1	5	18	552	-557	42
0	5	18	277	220	48
1	5	18	458	494	43
2	5	18	342	-303	43
3	5	18	249	-277	58
4	5	18	199	137	-66
5	5	18	144	245	-144
6	5	18	127	-19	-127
7	5	18	585	-580	46
-11	6	18	341	442	-89
-10	6	18	83	84	-83
-9	6	18	278	-290	66
-7	6	18	428	379	50
-6	6	18	72	-58	-72
-5	6	18	568	-634	41
-4	6	18	445	-502	53
-3	6	18	545	523	41
-2	6	18	141	5	-141
-1	6	18	671	-776	42
0	6	18	364	-358	34
1	6	18	710	718	39
2	6	18	78	60	-78
3	6	18	267	-300	61
4	6	18	204	-83	-60
5	6	18	442	445	51
6	6	18	75	117	-75
7	6	18	520	-609	49
-10	7	18	253	-345	-95
-8	7	18	492	430	56
-7	7	18	228	-279	-90
-6	7	18	407	-312	54
-5	7	18	358	387	52
-4	7	18	83	-224	-83
-3	7	18	79	-141	-79
-2	7	18	535	-535	44
-1	7	18	668	726	42
0	7	18	649	624	30
1	7	18	456	-498	49
2	7	18	370	-323	45
3	7	18	232	328	-87
4	7	18	349	400	53
5	7	18	200	-217	-65
6	7	18	204	-203	-73
-9	8	18	198	-9	-83
-8	8	18	210	171	-96
-7	8	18	89	-115	-89
-6	8	18	75	-30	-75
-5	8	18	83	89	-83
-4	8	18	245	161	-73
-3	8	18	83	133	-83
-2	8	18	292	-298	64

h	k	l	10Fo	10Fc	10s
-1	8	18	423	-434	48
0	8	18	405	427	38
1	8	18	258	224	-70
2	8	18	606	-502	43
3	8	18	185	-56	-93
4	8	18	326	324	60
-7	9	18	122	-122	-122
-6	9	18	301	290	59
-5	9	18	383	289	51
-4	9	18	227	-280	-95
-3	9	18	325	-329	56
-2	9	18	332	301	55
-1	9	18	410	431	55
0	9	18	124	-87	-89
1	9	18	609	-618	49
2	9	18	88	179	-88
3	9	18	665	645	48
-5	10	18	293	335	71
-4	10	18	80	-3	-80
-3	10	18	328	-246	62
-2	10	18	77	-8	-77
-1	10	18	569	509	47
0	10	18	179	-12	-96
1	10	18	453	-453	51
-13	0	19	247	343	-96
-11	0	19	282	-411	-90
-9	0	19	584	555	48
-7	0	19	1392	-1325	38
-5	0	19	604	587	42
-3	0	19	767	-876	38
-1	0	19	876	879	37
1	0	19	1394	-1397	35
3	0	19	732	770	38
5	0	19	195	-222	-71
7	0	19	190	196	-80
9	0	19	427	-408	45
-13	1	19	111	-251	-111
-12	1	19	98	-91	-98
-11	1	19	88	-151	-88
-10	1	19	165	-178	-165
-7	1	19	263	210	61
-6	1	19	361	-414	52
-5	1	19	71	81	-71
-4	1	19	152	79	-152
-3	1	19	317	-269	54
-2	1	19	66	47	-66
-1	1	19	438	-459	42
0	1	19	73	-145	-51
1	1	19	449	425	43
2	1	19	324	428	50
3	1	19	231	-269	-78
4	1	19	392	-309	48
5	1	19	74	70	-74
6	1	19	67	-114	-67
7	1	19	192	23	-64
8	1	19	331	297	54

h	k	l	10Fo	10Fc	10s
9	1	19	71	-109	-71
-13	2	19	101	-65	-101
-12	2	19	753	-743	55
-11	2	19	96	-128	-96
-10	2	19	555	495	53
-9	2	19	86	246	-86
-8	2	19	507	-529	49
-7	2	19	129	-137	-129
-6	2	19	1056	1113	39
-5	2	19	312	220	47
-4	2	19	1000	-995	38
-3	2	19	74	0	-74
-2	2	19	939	1021	37
-1	2	19	174	-117	-91
0	2	19	948	-946	25
1	2	19	132	98	-132
2	2	19	749	708	37
3	2	19	277	-250	60
4	2	19	521	-510	43
5	2	19	70	32	-70
6	2	19	807	775	41
7	2	19	146	-257	-146
8	2	19	461	-440	47
-12	3	19	96	152	-96
-11	3	19	384	403	61
-10	3	19	168	-111	-106
-9	3	19	162	295	-162
-8	3	19	156	244	-156
-7	3	19	76	-66	-76
-6	3	19	125	-153	-125
-5	3	19	324	314	60
-4	3	19	259	209	58
-3	3	19	191	-81	-61
-2	3	19	77	-15	-77
-1	3	19	134	-199	-134
0	3	19	89	132	-67
1	3	19	487	424	40
2	3	19	118	85	-118
3	3	19	76	-96	-76
4	3	19	98	45	-98
5	3	19	265	-273	60
6	3	19	161	133	-87
7	3	19	128	162	-128
-11	4	19	559	562	57
-10	4	19	243	-50	60
-9	4	19	698	-652	46
-8	4	19	364	-386	59
-7	4	19	518	475	47
-6	4	19	74	141	-74
-5	4	19	979	-1018	41
-4	4	19	80	-148	-80
-3	4	19	1492	1525	37
-2	4	19	343	403	52
-1	4	19	271	-360	62
0	4	19	84	5	-61
1	4	19	593	643	41

h	k	l	10Fo	10Fc	10s
2	4	19	195	-63	-78
3	4	19	677	-588	38
4	4	19	78	63	-78
5	4	19	766	750	40
6	4	19	303	359	60
7	4	19	720	-734	42
8	4	19	288	-167	58
-11	5	19	342	244	66
-10	5	19	262	-256	-88
-9	5	19	238	-256	-104
-8	5	19	215	205	-94
-7	5	19	235	-121	-79
-6	5	19	72	108	-72
-5	5	19	79	-37	-79
-4	5	19	161	-86	-95
-3	5	19	224	286	-79
-2	5	19	122	-91	-122
-1	5	19	77	143	-77
0	5	19	289	354	-73
1	5	19	78	-57	-78
2	5	19	200	-109	-63
3	5	19	72	-180	-72
4	5	19	77	-14	-77
5	5	19	71	10	-71
6	5	19	300	-298	61
7	5	19	75	-73	-75
-11	6	19	81	138	-81
-10	6	19	456	-521	64
-9	6	19	193	-179	-123
-8	6	19	661	681	50
-7	6	19	140	94	-140
-6	6	19	340	-470	64
-5	6	19	295	-241	57
-4	6	19	332	383	62
-3	6	19	859	909	41
-2	6	19	703	-628	41
-1	6	19	176	-111	-80
0	6	19	896	982	42
1	6	19	176	-81	-73
2	6	19	161	-207	-130
4	6	19	450	517	47
5	6	19	184	98	-100
6	6	19	585	-559	47
-10	7	19	205	-67	-134
-9	7	19	265	294	-101
-8	7	19	91	69	-91
-7	7	19	143	-89	-143
-6	7	19	198	-174	-90
-5	7	19	78	-93	-78
-4	7	19	203	-241	-79
-3	7	19	362	-336	50
-2	7	19	224	164	-59
-1	7	19	197	167	-95
0	7	19	89	-130	-65
1	7	19	77	77	-77
3	7	19	69	-201	-69

Observed and calculated structure factors for $[Ru(bpy)_2(phen\text{-}napthaquinone)](PF_6)_2$

h	k	l	10Fo	10Fc	10s
4	7	19	201	182	-88
-8	8	19	196	74	-127
-7	8	19	417	-283	49
-6	8	19	89	-109	-89
-5	8	19	752	710	45
-4	8	19	84	122	-84
-3	8	19	878	-930	43
-2	8	19	490	-480	51
-1	8	19	927	976	41
0	8	19	500	521	72
1	8	19	780	-817	44
2	8	19	299	-353	64
3	8	19	640	745	48
4	8	19	82	81	-82
-6	9	19	309	234	69
-5	9	19	251	-114	52
-3	9	19	181	-3	-105
-2	9	19	161	47	-161
-1	9	19	194	-119	-81
0	9	19	238	-182	59
1	9	19	82	54	-82
2	9	19	72	24	-72
-12	0	20	447	-384	63
-10	0	20	494	431	52
-8	0	20	867	-817	44
-6	0	20	508	561	48
-4	0	20	665	-653	38
-2	0	20	694	734	41
0	0	20	587	-578	29
2	0	20	765	785	39
4	0	20	270	-304	54
8	0	20	77	102	-77
-11	1	20	363	-395	71
-10	1	20	546	493	52
-9	1	20	610	645	49
-8	1	20	78	-16	-78
-7	1	20	75	-189	-75
-6	1	20	326	337	52
-5	1	20	175	-23	-60
-4	1	20	500	-509	45
-3	1	20	66	-156	-66
-2	1	20	72	197	-72
-1	1	20	73	145	-73
0	1	20	415	-445	38
1	1	20	178	-181	-80
2	1	20	254	294	57
3	1	20	154	254	-154
4	1	20	288	-263	50
5	1	20	444	-453	50
6	1	20	452	446	47
7	1	20	295	253	61
8	1	20	362	-348	51
-12	2	20	161	201	-161
-11	2	20	678	595	52
-10	2	20	148	-58	-148
-9	2	20	337	-382	65

h	k	l	10Fo	10Fc	10s
-8	2	20	208	191	-91
-7	2	20	697	684	44
-6	2	20	87	-111	-87
-5	2	20	687	-701	41
-4	2	20	245	139	-67
-3	2	20	497	551	43
-2	2	20	81	189	-81
-1	2	20	391	-375	49
0	2	20	175	-208	-73
1	2	20	347	387	54
2	2	20	65	36	-65
3	2	20	170	-240	-121
4	2	20	74	3	-74
6	2	20	461	368	48
7	2	20	582	-618	43
-12	3	20	354	-342	55
-11	3	20	202	-182	-157
-10	3	20	299	395	72
-9	3	20	219	-37	-84
-8	3	20	526	-478	45
-7	3	20	267	264	58
-6	3	20	444	398	43
-5	3	20	426	-522	48
-4	3	20	236	-336	-75
-3	3	20	657	639	39
-2	3	20	78	-60	-78
-1	3	20	322	-434	57
0	3	20	372	317	31
1	3	20	229	209	-63
2	3	20	583	551	39
3	3	20	344	-356	47
4	3	20	701	-664	41
5	3	20	205	208	-78
6	3	20	437	477	47
7	3	20	73	-128	-73
-11	4	20	206	213	-96
-10	4	20	615	-581	53
-9	4	20	147	-36	-147
-8	4	20	337	258	54
-7	4	20	315	-227	62
-6	4	20	809	-796	44
-5	4	20	78	-7	-78
-4	4	20	863	780	40
-3	4	20	79	60	-79
-2	4	20	425	-415	43
-1	4	20	408	-476	50
0	4	20	425	408	33
1	4	20	70	-65	-70
2	4	20	449	-443	45
3	4	20	226	-272	-74
4	4	20	370	358	45
5	4	20	80	-21	-80
6	4	20	199	-240	-83
7	4	20	335	-307	51
-11	5	20	248	253	-90
-10	5	20	492	-424	54

h	k	l	10Fo	10Fc	10s
-9	5	20	245	-314	-91
-8	5	20	409	307	52
-7	5	20	377	431	61
-6	5	20	247	-232	59
-5	5	20	471	-414	46
-4	5	20	567	449	46
-3	5	20	146	49	-146
-2	5	20	252	-272	-66
-1	5	20	79	68	-79
0	5	20	75	54	-53
1	5	20	268	334	46
2	5	20	492	-488	42
3	5	20	432	-421	47
4	5	20	149	184	-149
5	5	20	426	422	44
6	5	20	171	-25	-123
-10	6	20	183	-289	-183
-9	6	20	375	330	65
-8	6	20	191	202	-125
-7	6	20	666	-684	48
-6	6	20	197	127	-106
-5	6	20	752	740	45
-4	6	20	84	-107	-84
-3	6	20	538	-626	48
-2	6	20	533	-606	46
-1	6	20	244	242	-61
0	6	20	88	-81	-65
2	6	20	82	34	-82
3	6	20	290	293	60
4	6	20	274	122	50
5	6	20	409	-508	49
6	6	20	236	-215	-70
-9	7	20	352	227	59
-8	7	20	248	128	61
-7	7	20	618	-614	51
-6	7	20	635	-546	46
-5	7	20	370	336	53
-4	7	20	335	413	61
-3	7	20	440	-400	53
-1	7	20	703	626	43
0	7	20	612	712	49
1	7	20	493	-561	51
2	7	20	153	-147	-153
3	7	20	327	366	56
4	7	20	398	302	47
5	7	20	317	-342	59
-8	8	20	650	-639	52
-6	8	20	632	632	47
-5	8	20	82	67	-82
-4	8	20	894	-847	45
-3	8	20	161	-180	-161
-2	8	20	712	725	47
-1	8	20	177	-78	-91
0	8	20	416	-444	36
-5	9	20	171	183	-130
-4	9	20	422	-327	53

h	k	l	10Fo	10Fc	10s
-3	9	20	276	-287	-97
-1	9	20	270	342	64
0	9	20	83	-60	-83
1	9	20	414	-380	54
-11	0	21	97	17	-97
-9	0	21	90	-320	-90
-7	0	21	487	525	47
-5	0	21	310	-203	59
-3	0	21	78	150	-78
-1	0	21	230	-259	-60
1	0	21	454	-528	46
3	0	21	253	122	49
5	0	21	440	-384	42
7	0	21	343	363	53
-12	1	21	377	-457	88
-11	1	21	518	558	55
-10	1	21	624	573	53
-9	1	21	299	-322	-75
-8	1	21	588	-526	44
-7	1	21	329	270	46
-6	1	21	345	330	62
-5	1	21	361	-398	56
-4	1	21	609	-594	45
-3	1	21	538	528	42
-2	1	21	1044	1043	38
-1	1	21	723	-740	41
0	1	21	688	-689	28
1	1	21	1006	1027	40
2	1	21	390	412	49
3	1	21	622	-645	41
4	1	21	238	-318	-74
5	1	21	356	378	45
6	1	21	209	298	-78
7	1	21	588	-528	46
-10	2	21	123	-12	-123
-9	2	21	87	123	-87
-8	2	21	139	136	-139
-7	2	21	192	153	-109
-6	2	21	169	-56	-169
-5	2	21	246	-137	-64
-4	2	21	73	91	-73
-3	2	21	467	385	49
-2	2	21	212	284	-95
-1	2	21	322	-456	59
0	2	21	157	-78	-61
2	2	21	264	279	56
3	2	21	79	22	-79
4	2	21	489	-479	44
5	2	21	74	-40	-74
6	2	21	308	421	61
7	2	21	294	-349	61
-11	3	21	565	513	60
-10	3	21	417	-456	61
-9	3	21	452	-384	53
-8	3	21	378	380	67
-7	3	21	251	205	56

h	k	l	10Fo	10Fc	10s
-6	3	21	753	-676	46
-5	3	21	500	-549	52
-4	3	21	321	388	57
-3	3	21	369	397	56
-2	3	21	386	-408	50
-1	3	21	224	-214	-80
0	3	21	151	205	-73
1	3	21	532	602	44
2	3	21	399	-455	50
3	3	21	586	-593	45
4	3	21	413	400	46
5	3	21	279	320	65
6	3	21	330	-431	56
7	3	21	370	-438	51
-11	4	21	251	-123	-117
-10	4	21	96	-112	-96
-8	4	21	79	0	-79
-7	4	21	472	-391	51
-6	4	21	157	28	-157
-5	4	21	80	138	-80
-4	4	21	352	377	58
-3	4	21	322	360	58
-2	4	21	351	-335	51
-1	4	21	204	-332	-93
0	4	21	144	-56	-70
1	4	21	126	80	-126
2	4	21	219	170	-83
3	4	21	75	-86	-75
4	4	21	79	116	-79
5	4	21	75	-42	-75
6	4	21	75	32	-75
-10	5	21	185	-373	-185
-9	5	21	294	314	-81
-8	5	21	608	627	54
-7	5	21	332	-383	75
-6	5	21	115	-133	-115
-5	5	21	193	-163	-110
-4	5	21	421	389	52
-3	5	21	82	201	-82
-2	5	21	73	-51	-73
-1	5	21	209	-124	-67
0	5	21	477	454	33
1	5	21	377	-550	60
2	5	21	388	-380	51
3	5	21	462	416	45
4	5	21	348	417	55
5	5	21	328	-448	62
6	5	21	538	-545	48
-9	6	21	407	417	61
-8	6	21	91	56	-91
-7	6	21	147	65	-147
-6	6	21	309	123	58
-5	6	21	84	58	-84
-4	6	21	344	-362	59
-3	6	21	268	380	-76
-2	6	21	82	-19	-82

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$

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	6	21	81	71	-81	6	1	22	311	-365	62	-7	5	22	76	-138	-76	-8	1	23	92	-191	-92	0	4	23	301	282	40
0	6	21	341	343	52	7	1	22	77	-201	-77	-6	5	22	462	426	59	-7	1	23	88	272	-88	1	4	23	684	-672	43
1	6	21	186	195	-105	-10	2	22	85	-95	-85	-5	5	22	243	-258	-73	-6	1	23	289	216	56	2	4	23	77	-7	-77
2	6	21	75	10	-75	-9	2	22	229	-244	-75	-4	5	22	274	349	-71	-5	1	23	221	-169	-92	3	4	23	478	425	45
4	6	21	71	-22	-71	-8	2	22	88	-27	-88	-3	5	22	86	-110	-86	-4	1	23	217	-187	-87	5	4	23	594	-559	48
5	6	21	75	79	-75	-7	2	22	81	117	-81	-2	5	22	154	160	-121	-3	1	23	226	230	-83	-9	5	23	84	-98	-84
-8	7	21	423	-448	60	-6	2	22	86	-218	-86	-1	5	22	545	520	45	-2	1	23	210	23	53	-8	5	23	128	19	-128
-7	7	21	720	-652	51	-5	2	22	698	-700	45	0	5	22	359	-336	55	-1	1	23	346	-304	54	-7	5	23	87	13	-87
-6	7	21	318	396	65	-4	2	22	168	122	-120	1	5	22	215	-233	-77	0	1	23	141	121	-73	-6	5	23	122	59	-122
-5	7	21	321	279	69	-3	2	22	968	971	41	2	5	22	360	528	65	1	1	23	276	222	67	-5	5	23	529	-482	50
-3	7	21	240	-137	-80	-2	2	22	69	5	-69	3	5	22	109	177	-109	2	1	23	195	71	-77	-4	5	23	305	183	60
-2	7	21	274	236	60	-1	2	22	847	-913	41	4	5	22	206	-228	-85	3	1	23	74	-19	-74	-3	5	23	290	345	-73
-1	7	21	80	47	-80	0	2	22	119	210	-67	5	5	22	80	-146	-80	4	1	23	446	-345	48	-2	5	23	82	62	-82
0	7	21	338	-391	50	1	2	22	228	296	-76	-9	6	22	350	464	83	5	1	23	388	430	51	-1	5	23	78	-75	-78
1	7	21	449	-481	48	2	2	22	399	284	48	-8	6	22	97	92	-97	6	1	23	85	83	-85	0	5	23	79	-79	-56
2	7	21	351	317	54	3	2	22	690	-668	42	-7	6	22	471	-501	58	-11	2	23	136	-98	-136	1	5	23	78	-145	-78
3	7	21	554	544	46	4	2	22	166	84	-117	-6	6	22	518	-378	48	-10	2	23	403	-376	69	2	5	23	82	-74	-82
4	7	21	348	-387	59	5	2	22	405	357	50	-5	6	22	220	143	-85	-9	2	23	90	-84	-90	4	5	23	113	6	-113
-7	8	21	90	161	-90	6	2	22	216	142	-62	-4	6	22	140	29	-140	-8	2	23	493	577	58	-8	6	23	536	-550	60
-5	8	21	84	-55	-84	-11	3	22	745	-682	56	-3	6	22	559	-575	47	-7	2	23	263	178	-72	-7	6	23	371	-326	64
-4	8	21	187	162	-78	-10	3	22	316	-268	70	-2	6	22	263	-331	-82	-6	2	23	622	-617	47	-6	6	23	340	366	57
-3	8	21	298	-190	64	-9	3	22	176	208	-176	-1	6	22	664	680	46	-5	2	23	81	-53	-81	-5	6	23	172	215	-172
-2	8	21	183	-132	-96	-8	3	22	79	180	-79	0	6	22	443	454	56	-4	2	23	1058	1085	43	-4	6	23	739	-761	48
-1	8	21	269	166	-70	-7	3	22	201	-138	-84	1	6	22	455	-442	50	-3	2	23	240	19	-61	-3	6	23	86	-59	-86
0	8	21	466	492	44	-6	3	22	89	-264	-89	3	6	22	536	547	49	-2	2	23	811	-806	42	-2	6	23	707	731	49
1	8	21	268	-173	-72	-5	3	22	246	319	-77	4	6	22	178	55	-74	-1	2	23	166	52	-96	-1	6	23	181	34	-93
-3	9	21	256	268	-82	-4	3	22	82	311	-82	-7	7	22	270	97	-81	0	2	23	450	455	33	0	6	23	635	-710	48
-2	9	21	327	274	70	-3	3	22	197	-142	-72	-6	7	22	90	172	-90	2	2	23	713	-758	43	1	6	23	79	23	-79
-1	9	21	236	-251	-74	-2	3	22	196	-225	-91	-5	7	22	410	-354	67	4	2	23	520	566	45	2	6	23	713	781	48
-12	0	22	235	-409	-144	-1	3	22	85	258	-85	-4	7	22	144	-191	-144	5	2	23	108	-7	-108	-5	7	23	92	-11	-92
-10	0	22	96	178	-96	0	3	22	407	374	34	-3	7	22	90	59	-90	6	2	23	292	-341	-85	-4	7	23	173	246	-173
-8	0	22	80	48	-80	1	3	22	543	-582	45	-2	7	22	424	391	54	-10	3	23	103	-36	-103	-2	7	23	78	1	-78
-6	0	22	327	366	65	2	3	22	338	-344	56	-1	7	22	139	-3	-139	-9	3	23	222	-94	-118	-1	7	23	82	-175	-82
-4	0	22	1010	-1035	42	3	3	22	245	276	-76	0	7	22	83	-36	-83	-8	3	23	214	196	-115	0	7	23	82	-158	-58
-2	0	22	854	807	40	4	3	22	225	200	-64	1	7	22	160	3	-100	-7	3	23	208	160	-136	1	7	23	84	-223	-84
0	0	22	488	-500	33	5	3	22	79	-203	-79	2	7	22	404	389	53	-6	3	23	86	-2	-86	-10	0	24	525	-533	50
2	0	22	176	176	-92	6	3	22	299	-261	55	3	7	22	87	-188	-87	-5	3	23	321	-345	63	-8	0	24	546	509	55
4	0	22	180	-187	-101	-10	4	22	492	-477	59	-5	8	22	233	199	-109	-4	3	23	304	307	56	-6	0	24	469	-502	54
6	0	22	374	351	39	-9	4	22	92	6	-92	-4	8	22	323	-320	68	-3	3	23	82	-156	-82	-4	0	24	437	484	58
-11	1	22	382	394	63	-8	4	22	406	335	54	-3	8	22	148	-265	-148	-2	3	23	216	-110	-69	-2	0	24	365	-404	59
-10	1	22	217	-307	-117	-7	4	22	90	87	-90	-2	8	22	412	410	60	-1	3	23	78	14	-78	0	0	24	185	264	-79
-9	1	22	241	-255	-87	-6	4	22	406	-378	49	-1	8	22	145	243	-145	0	3	23	168	-185	-75	2	0	24	107	-85	-107
-8	1	22	444	558	59	-5	4	22	158	-235	-158	0	8	22	826	-804	51	1	3	23	151	-59	-95	4	0	24	153	96	-153
-7	1	22	309	332	68	-4	4	22	970	969	43	1	8	22	262	-310	-70	2	3	23	70	3	-70	-10	1	24	248	-214	-97
-6	1	22	73	-112	-73	-3	4	22	285	265	65	-11	0	23	556	588	60	3	3	23	71	-155	-71	-9	1	24	478	-487	62
-5	1	22	568	-582	46	-2	4	22	465	-506	47	-9	0	23	514	-437	56	4	3	23	77	153	-77	-8	1	24	461	460	59
-4	1	22	235	207	-64	-1	4	22	258	-191	-68	-7	0	23	839	849	44	5	3	23	81	128	-81	-7	1	24	121	58	-121
-3	1	22	515	520	43	0	4	22	436	389	51	-5	0	23	994	-1014	43	-10	4	23	103	-194	-103	-6	1	24	494	-460	53
-2	1	22	451	-407	46	1	4	22	407	318	53	-3	0	23	920	952	42	-9	4	23	452	550	71	-5	1	24	197	-211	-113
-1	1	22	336	-316	63	2	4	22	586	-670	48	-1	0	23	902	-949	43	-7	4	23	285	-425	-85	-4	1	24	396	373	57
0	1	22	319	299	43	3	4	22	79	-112	-79	1	0	23	79	-124	-79	-6	4	23	264	-232	-87	-3	1	24	84	117	-84
1	1	22	143	100	-143	4	4	22	404	474	47	3	0	23	180	-95	-104	-5	4	23	880	883	45	-2	1	24	614	-574	46
2	1	22	544	-495	42	6	4	22	386	-378	50	5	0	23	293	275	65	-4	4	23	524	482	53	-1	1	24	228	170	-86
3	1	22	177	-89	-94	-10	5	22	285	144	70	-11	1	23	301	-107	72	-3	4	23	850	-868	44	0	1	24	474	498	35
4	1	22	73	113	-73	-9	5	22	429	358	61	-10	1	23	86	25	-86	-2	4	23	311	-247	59	1	1	24	186	-33	-66
5	1	22	166	195	-166	-8	5	22	152	-116	-152	-9	1	23	89	-34	-89	-1	4	23	435	455	55	3	1	24	475	-520	49

Observed and calculated structure factors for [Ru(bpy)$_2$(phen-napthaquinone)](PF$_6$)$_2$ Page 21

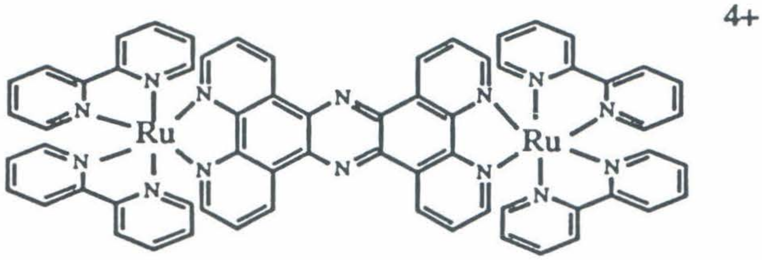
h	k	l	10Fo	10Fc	10s
4	1	24	309	264	61
5	1	24	647	711	45
-10	2	24	98	-66	-98
-9	2	24	366	366	70
-8	2	24	250	-2	-105
-7	2	24	392	-549	71
-6	2	24	87	-224	-87
-5	2	24	316	354	68
-4	2	24	310	215	60
-3	2	24	436	-538	51
-2	2	24	290	-222	53
-1	2	24	153	246	-153
0	2	24	75	32	-57
1	2	24	375	-354	53
2	2	24	133	59	-133
3	2	24	79	235	-79
5	2	24	137	-221	-137
-10	3	24	273	-383	-98
-9	3	24	466	506	57
-8	3	24	220	305	-135
-7	3	24	261	-317	65
-6	3	24	170	-189	-170
-5	3	24	614	582	53
-4	3	24	362	309	59
-3	3	24	470	-440	48
-1	3	24	81	186	-81
0	3	24	243	224	-65
1	3	24	347	-338	60
2	3	24	675	-627	45
3	3	24	494	479	47
4	3	24	479	446	54
-9	4	24	93	156	-93
-8	4	24	243	-237	-157
-7	4	24	85	-25	-85
-6	4	24	635	637	51
-5	4	24	83	-151	-83
-4	4	24	78	-149	-78
-2	4	24	161	205	-161
-1	4	24	81	112	-81
0	4	24	229	-243	-59
2	4	24	489	473	52
3	4	24	77	14	-77
4	4	24	240	-203	-76
-8	5	24	187	-86	-142
-7	5	24	444	-410	63
-6	5	24	306	381	67
-5	5	24	91	-22	-91
-4	5	24	169	-119	-127

h	k	l	10Fo	10Fc	10s
-3	5	24	89	79	-89
-2	5	24	385	530	60
0	5	24	374	-379	49
1	5	24	410	-384	52
2	5	24	324	302	52
3	5	24	256	313	-66
-7	6	24	245	321	-101
-6	6	24	92	-102	-92
-5	6	24	661	-543	51
-4	6	24	80	0	-80
-3	6	24	398	449	58
-1	6	24	117	10	-117
0	6	24	75	8	-75
1	6	24	94	277	-94
2	6	24	80	93	-80
-4	7	24	250	-169	-74
-3	7	24	360	319	60
-2	7	24	414	438	68
-1	7	24	319	-171	64
-9	0	25	97	235	-97
-7	0	25	89	-23	-89
-5	0	25	79	104	-79
-3	0	25	137	-13	-137
-1	0	25	204	-205	-73
1	0	25	188	192	-101
3	0	25	77	-122	-77
-9	1	25	308	362	-95
-8	1	25	156	249	-156
-7	1	25	96	-215	-96
-6	1	25	240	-204	-75
-5	1	25	165	293	-165
-4	1	25	461	535	55
-3	1	25	730	-729	46
-2	1	25	439	-507	50
-1	1	25	367	464	57
0	1	25	215	159	-85
1	1	25	190	85	-88
2	1	25	365	-383	48
3	1	25	447	442	48
4	1	25	395	389	52
-9	2	25	98	82	-98
-8	2	25	157	4	-157
-7	2	25	176	-81	-176
-6	2	25	97	203	-97
-5	2	25	357	321	57
-4	2	25	218	234	-96
-3	2	25	369	-451	58
-2	2	25	76	-50	-76

h	k	l	10Fo	10Fc	10s
0	2	25	80	32	-57
1	2	25	158	198	-158
2	2	25	386	-339	45
3	2	25	223	-176	-66
4	2	25	264	275	58
-9	3	25	419	499	76
-8	3	25	263	-236	-88
-7	3	25	284	-220	68
-6	3	25	445	368	53
-5	3	25	296	298	-84
-4	3	25	288	-215	60
-3	3	25	418	-525	62
-2	3	25	292	274	57
-1	3	25	487	532	51
0	3	25	326	-320	65
1	3	25	752	-758	47
2	3	25	480	453	52
3	3	25	393	350	49
-8	4	25	88	-94	-88
-7	4	25	92	96	-92
-6	4	25	81	-136	-81
-5	4	25	213	-78	-113
-4	4	25	208	244	-120
-3	4	25	264	-263	-83
-2	4	25	84	35	-84
-1	4	25	336	338	69
0	4	25	73	59	-73
1	4	25	243	-71	-68
2	4	25	244	-256	-73
3	4	25	116	142	-116
-7	5	25	99	137	-99
-6	5	25	455	383	57
-5	5	25	435	-471	53
-4	5	25	313	-236	71
-3	5	25	435	384	56
-2	5	25	293	200	71
-1	5	25	513	-457	50
0	5	25	520	-551	36
1	5	25	460	483	56
-5	6	25	87	-20	-87
-4	6	25	81	-111	-81
-3	6	25	152	-140	-152
-2	6	25	312	258	67
0	6	25	311	-296	41
-8	0	26	482	351	56
-6	0	26	431	-393	56
-4	0	26	550	482	54
-2	0	26	590	-593	49

h	k	l	10Fo	10Fc	10s
0	0	26	375	357	46
2	0	26	306	-298	59
-9	1	26	166	135	-166
-8	1	26	90	-17	-90
-7	1	26	200	-258	-116
-6	1	26	81	-10	-81
-5	1	26	362	376	58
-4	1	26	265	-349	-87
-3	1	26	348	-354	66
-2	1	26	389	345	57
0	1	26	75	-31	-75
2	1	26	240	138	58
3	1	26	138	218	-138
-7	2	26	489	-473	53
-6	2	26	87	-36	-87
-5	2	26	759	821	51
-4	2	26	98	-15	-98
-3	2	26	544	-662	58
-2	2	26	83	-118	-83
-1	2	26	345	377	59
0	2	26	78	45	-78
1	2	26	456	-537	53
2	2	26	228	-298	-77
3	2	26	352	472	62
-8	3	26	271	-260	-109
-7	3	26	132	-30	-132
-6	3	26	337	368	77
-5	3	26	92	215	-92
-4	3	26	309	-230	61
-3	3	26	145	105	-145
-2	3	26	251	195	-66
-1	3	26	233	-379	-98
0	3	26	233	-177	-60
1	3	26	259	280	-70
2	3	26	201	148	-93
-7	4	26	90	73	-90
-6	4	26	400	402	70
-5	4	26	201	-190	-157
-4	4	26	350	-290	63
-3	4	26	99	-214	-99
-2	4	26	681	704	51
-1	4	26	188	151	-121
0	4	26	518	-508	48
1	4	26	83	-167	-83
-5	5	26	275	27	-72
-3	5	26	316	287	58
-2	5	26	174	-211	-132
-1	5	26	353	-372	79

h	k	l	10Fo	10Fc	10s
0	5	26	81	114	-81
-7	0	27	705	-724	54
-5	0	27	416	491	56
-3	0	27	493	-533	51
-1	0	27	383	386	57
-7	1	27	244	-262	-106
-6	1	27	238	-76	-84
-5	1	27	87	49	-87
-4	1	27	82	98	-82
-3	1	27	223	-280	-121
-2	1	27	344	-377	66
0	1	27	401	434	39
1	1	27	78	104	-78
-7	2	27	230	-158	-106
-6	2	27	723	743	51
-5	2	27	252	177	-67
-4	2	27	752	-877	54
-3	2	27	88	-5	-88
-2	2	27	447	433	64
-1	2	27	313	246	72
0	2	27	360	-310	42
1	2	27	166	-179	-166
-6	3	27	88	55	-88
-5	3	27	222	213	-110
-3	3	27	174	-277	-174
-2	3	27	171	-154	-130
-1	3	27	86	174	-86
0	3	27	185	-288	-85
-5	4	27	633	-630	55
-4	4	27	285	283	-86
-3	4	27	468	486	51
-2	4	27	97	96	-97
-1	4	27	579	-606	54
-6	0	28	76	132	-76
-4	0	28	262	-336	-117
-2	0	28	189	71	-90
0	0	28	212	-325	-69
-6	1	28	206	204	-149
-5	1	28	93	171	-93
-4	1	28	307	-294	71
-3	1	28	193	-308	-193
-2	1	28	148	224	-148
-1	1	28	424	400	58
-5	2	28	204	-194	-204
-4	2	28	220	187	-101
-3	2	28	152	171	-152
-2	2	28	229	-152	-76
-1	2	28	88	-171	-88


4+
Ru
Ru
N

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
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6	0	0	76	66	-76
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10	0	0	201	-92	-88
12	0	0	1837	-1859	20
14	0	0	2210	2098	21
16	0	0	390	190	51
18	0	0	3597	-3292	23
20	0	0	1986	-1756	26
22	0	0	779	820	36
24	0	0	492	524	47
26	0	0	846	-745	34
28	0	0	532	-537	41
30	0	0	3290	3103	30
32	0	0	166	-280	-166
34	0	0	2012	-1890	32
36	0	0	460	446	51
38	0	0	666	-633	39
40	0	0	1256	-1329	33
42	0	0	491	-428	40
1	1	0	2653	2825	9
3	1	0	1656	1798	11
5	1	0	1556	-1224	14
7	1	0	285	284	44
9	1	0	2479	-2197	17
11	1	0	1519	-1474	20
13	1	0	1406	1562	21
15	1	0	1802	1761	22
17	1	0	1594	-1483	24
19	1	0	1150	-1070	26
21	1	0	1190	-1165	27
23	1	0	312	-273	48
25	1	0	168	-20	-97
27	1	0	353	-300	45
29	1	0	742	719	36
31	1	0	360	331	51
33	1	0	388	382	57
35	1	0	772	-793	36
37	1	0	307	-341	56
39	1	0	215	-126	-60
41	1	0	987	-955	32
2	2	0	915	-944	15
4	2	0	4125	4083	13
6	2	0	329	-442	37
8	2	0	2752	-2637	16
10	2	0	4028	3897	18
12	2	0	999	1066	23
14	2	0	1277	-1320	22
16	2	0	3241	-3163	22
18	2	0	1926	1899	24
20	2	0	1490	1460	26
22	2	0	1694	-1638	27
24	2	0	158	-22	-127
26	2	0	1154	1069	30
28	2	0	509	-501	38
30	2	0	1501	-1469	32

h	k	l	10Fo	10Fc	10s
32	2	0	205	269	-92
34	2	0	1586	1527	33
36	2	0	158	22	-158
38	2	0	828	-831	35
40	2	0	569	637	37
42	2	0	334	314	46
3	3	0	431	-252	30
5	3	0	4835	4775	16
7	3	0	410	387	32
9	3	0	894	829	23
11	3	0	320	-272	44
13	3	0	522	-539	32
15	3	0	1687	-1734	24
17	3	0	998	931	28
19	3	0	2433	2440	26
21	3	0	894	891	31
23	3	0	891	-883	31
25	3	0	214	239	-81
27	3	0	1226	1234	32
29	3	0	1442	-1374	32
31	3	0	1087	-1142	35
33	3	0	954	923	36
35	3	0	336	343	56
37	3	0	133	138	-133
39	3	0	80	162	-80
41	3	0	1227	1204	30
0	4	0	6228	-5887	18
2	4	0	2957	-3007	18
4	4	0	3772	-3788	18
6	4	0	167	133	-105
8	4	0	1158	1212	22
10	4	0	437	-408	37
12	4	0	1143	-1145	25
14	4	0	1146	1244	27
16	4	0	1292	1250	26
18	4	0	582	-624	33
20	4	0	1900	1787	28
22	4	0	1532	1550	30
24	4	0	169	87	-142
26	4	0	1264	-1321	33
28	4	0	525	498	42
30	4	0	84	66	-84
32	4	0	505	-557	44
34	4	0	85	-182	-85
36	4	0	394	-383	50
38	4	0	1563	1533	32
40	4	0	365	330	40
1	5	0	1748	1932	22
3	5	0	4593	-4799	21
5	5	0	1252	-1203	25
7	5	0	1924	2031	23
9	5	0	2074	2007	24
11	5	0	3016	-3067	24
13	5	0	143	146	-143
15	5	0	2166	2170	26
17	5	0	750	729	32

h	k	l	10Fo	10Fc	10s
19	5	0	969	-1010	31
21	5	0	168	-19	-141
23	5	0	1880	1925	31
25	5	0	935	-951	37
27	5	0	1077	-1079	35
29	5	0	1193	1232	35
31	5	0	809	773	37
33	5	0	1361	-1279	35
35	5	0	80	11	-80
37	5	0	837	842	35
39	5	0	112	270	-112
0	6	0	281	-344	63
2	6	0	365	240	45
4	6	0	850	-835	28
6	6	0	1463	-1444	27
8	6	0	1539	1518	27
10	6	0	188	66	-91
12	6	0	82	-7	-82
14	6	0	1606	1536	29
16	6	0	670	689	35
18	6	0	645	-606	41
20	6	0	655	-678	40
22	6	0	1077	-1143	36
24	6	0	489	559	54
26	6	0	229	-224	-100
28	6	0	518	531	45
30	6	0	280	-209	-74
32	6	0	87	-7	-87
34	6	0	393	347	47
36	6	0	75	-84	-75
38	6	0	403	352	41
1	7	0	577	-603	40
3	7	0	2899	2989	28
5	7	0	1356	1384	31
7	7	0	2375	-2465	29
9	7	0	2006	-2023	30
11	7	0	2378	2299	31
13	7	0	346	287	56
15	7	0	1382	-1508	35
17	7	0	266	-198	-83
19	7	0	802	806	40
21	7	0	1252	-1348	38
23	7	0	1051	-1046	38
25	7	0	922	940	41
27	7	0	1034	1106	38
29	7	0	620	-688	47
31	7	0	778	-834	41
33	7	0	948	1082	39
35	7	0	264	216	61
0	8	0	1826	1679	33
2	8	0	1587	1616	34
4	8	0	2803	2672	33
6	8	0	94	229	-94
8	8	0	1691	-1593	34
10	8	0	1048	1046	39
12	8	0	498	-409	48

h	k	l	10Fo	10Fc	10s
14	8	0	1144	-1136	38
16	8	0	1387	-1329	38
18	8	0	258	-122	-90
20	8	0	294	366	-91
22	8	0	555	-555	48
24	8	0	248	-382	-118
26	8	0	892	865	43
28	8	0	528	547	52
30	8	0	807	-800	41
32	8	0	271	-242	-71
34	8	0	279	250	62
1	9	0	163	177	-163
3	9	0	395	350	63
5	9	0	682	-623	49
7	9	0	2305	2299	39
9	9	0	668	596	52
11	9	0	1624	-1616	41
13	9	0	199	-168	-199
15	9	0	100	-37	-100
17	9	0	405	-370	66
19	9	0	1063	-1053	41
21	9	0	691	660	50
23	9	0	1198	1204	43
25	9	0	1066	-1109	41
27	9	0	817	-886	45
29	9	0	897	945	43
31	9	0	82	16	-82
0	10	0	1893	1712	43
2	10	0	1205	-1161	46
4	10	0	908	-899	52
6	10	0	919	937	51
8	10	0	1492	1352	45
10	10	0	230	77	-166
12	10	0	1773	-1663	45
14	10	0	286	291	-118
16	10	0	479	520	68
18	10	0	590	-568	52
20	10	0	100	68	-100
22	10	0	671	596	53
24	10	0	263	258	-101
26	10	0	932	-911	47
28	10	0	711	-704	42
1	11	0	378	-362	88
3	11	0	247	-318	-184
5	11	0	111	100	-111
7	11	0	489	-484	83
9	11	0	116	-204	-116
11	11	0	117	83	-117
13	11	0	113	186	-113
15	11	0	120	319	-120
17	11	0	600	659	61
19	11	0	293	306	-103
21	11	0	359	-338	89
23	11	0	267	-103	-88
0	12	0	866	-802	64
2	12	0	119	-151	-119

h	k	l	10Fo	10Fc	10s
4	12	0	125	194	-125
6	12	0	1572	-1352	55
8	12	0	1924	-1683	54
10	12	0	694	663	75
12	12	0	1372	1276	58
14	12	0	127	-182	-127
16	12	0	298	-48	-100
18	12	0	1098	1039	55
1	13	0	384	-410	-111
3	13	0	130	279	-130
5	13	0	129	-288	-129
7	13	0	1037	-1004	71
9	13	0	301	-123	-136
11	13	0	506	511	90
-41	1	1	308	-324	48
-39	1	1	1736	1639	32
-37	1	1	292	-242	62
-35	1	1	301	-263	61
-33	1	1	472	-426	44
-31	1	1	638	580	39
-29	1	1	1441	-1400	32
-27	1	1	1778	-1698	30
-25	1	1	1361	1373	30
-23	1	1	1028	1046	29
-21	1	1	2441	-2234	26
-19	1	1	2391	-2171	25
-17	1	1	3777	3626	23
-15	1	1	455	322	37
-13	1	1	4141	-3893	20
-11	1	1	1115	1054	22
-7	1	1	2966	-2858	15
-5	1	1	1931	-1630	14
-3	1	1	685	649	15
-1	1	1	2686	2971	9
1	1	1	2244	-2162	9
3	1	1	3197	-3017	10
7	1	1	1686	1692	15
9	1	1	1380	-1403	17
11	1	1	995	-1074	21
13	1	1	274	192	49
15	1	1	540	510	32
17	1	1	2668	-2601	22
19	1	1	715	-655	29
21	1	1	2747	2800	25
23	1	1	180	-265	-114
25	1	1	1255	-1300	29
27	1	1	613	580	34
29	1	1	544	-512	38
31	1	1	791	-753	35
33	1	1	203	-176	-95
35	1	1	1421	1394	32
37	1	1	902	906	35
39	1	1	1661	-1606	31
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-42	2	1	479	-516	35
-40	2	1	78	35	-78

Observed and calculated structure factors for {[Ru(bipy)$_2$]$_2$L}(PF$_6$)$_4$

h	k	l	10Fo	10Fc	10s
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-34	2	1	473	-529	48
-32	2	1	785	686	36
-30	2	1	1126	-1113	34
-28	2	1	637	-608	37
-26	2	1	581	557	40
-24	2	1	857	895	31
-22	2	1	1182	-1143	29
-20	2	1	2304	-2046	26
-18	2	1	1093	-1054	28
-16	2	1	2679	2567	24
-14	2	1	2285	2100	22
-12	2	1	1461	-1367	22
-10	2	1	771	704	25
-6	2	1	978	1005	20
-4	2	1	2621	-2688	14
-2	2	1	2962	2891	13
0	2	1	577	-670	20
2	2	1	831	-645	16
4	2	1	853	690	17
6	2	1	880	-769	19
8	2	1	2615	2514	16
10	2	1	1170	-1034	20
12	2	1	202	10	-70
14	2	1	637	617	27
16	2	1	292	-366	53
18	2	1	1572	-1479	24
20	2	1	1058	1141	27
22	2	1	400	367	43
24	2	1	708	-715	32
26	2	1	1489	-1549	30
28	2	1	125	174	-125
30	2	1	356	-369	48
32	2	1	1507	-1493	32
34	2	1	1072	1014	33
36	2	1	651	582	37
38	2	1	200	88	-72
40	2	1	921	-899	32
42	2	1	165	-217	-111
-41	3	1	133	103	-133
-39	3	1	599	-585	39
-37	3	1	872	-847	35
-35	3	1	599	570	41
-33	3	1	604	-554	41
-31	3	1	895	-893	36
-29	3	1	952	951	35
-27	3	1	1271	1250	33
-25	3	1	1617	-1583	31
-23	3	1	1371	-1269	30
-21	3	1	957	916	30
-19	3	1	699	704	34
-17	3	1	1918	-1910	26
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-11	3	1	1158	1108	24
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-3	3	1	776	724	22
-1	3	1	1221	-1190	17
1	3	1	4921	4899	15
3	3	1	983	-921	19
5	3	1	369	-290	33
7	3	1	1679	-1741	18
9	3	1	519	564	28
11	3	1	914	-912	24
13	3	1	864	-836	24
15	3	1	78	-145	-78
17	3	1	2269	2405	24
19	3	1	997	1039	28
21	3	1	2134	-2228	27
23	3	1	189	274	-93
25	3	1	978	1101	32
27	3	1	602	-630	38
29	3	1	1453	-1422	32
31	3	1	1237	1274	33
33	3	1	704	-747	38
35	3	1	553	-499	40
37	3	1	81	40	-81
39	3	1	638	644	35
41	3	1	746	765	33
-40	4	1	798	-771	33
-38	4	1	356	-365	48
-36	4	1	333	241	53
-34	4	1	397	298	45
-32	4	1	543	-582	46
-30	4	1	139	-220	-139
-28	4	1	1624	1617	33
-26	4	1	207	39	-93
-24	4	1	2206	-2124	31
-22	4	1	481	-507	42
-20	4	1	2002	1930	29
-18	4	1	87	1	-87
-16	4	1	1884	-1758	27
-14	4	1	1641	1641	26
-12	4	1	2701	2610	24
-10	4	1	2238	-2212	23
-8	4	1	1830	-1710	22
-6	4	1	2085	2061	20
-4	4	1	1899	1875	20
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2	4	1	1794	1692	19
4	4	1	918	884	22
6	4	1	1600	-1712	20
8	4	1	1271	-1214	22
10	4	1	2761	2668	21
12	4	1	1282	-1225	24
14	4	1	1678	-1711	24
16	4	1	1843	1888	25
18	4	1	1197	1130	27
20	4	1	1112	-1106	28
22	4	1	1668	-1688	28
24	4	1	818	850	32
26	4	1	732	720	35
28	4	1	1011	-925	34
30	4	1	341	297	56
32	4	1	998	962	34
34	4	1	560	-599	42
36	4	1	970	-919	34
38	4	1	256	294	62
40	4	1	1006	989	31
-39	5	1	373	352	43
-37	5	1	82	123	-82
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-31	5	1	605	600	44
-29	5	1	276	229	66
-27	5	1	593	-613	44
-25	5	1	195	-63	-102
-23	5	1	374	350	61
-21	5	1	174	175	-174
-19	5	1	754	672	34
-17	5	1	1008	1066	32
-15	5	1	82	96	-82
-13	5	1	706	-754	33
-11	5	1	1157	-1063	28
-9	5	1	395	383	45
-7	5	1	1167	1126	25
-5	5	1	372	-402	42
-3	5	1	3224	-3220	22
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5	5	1	2940	2989	22
7	5	1	174	183	-82
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11	5	1	238	235	-69
13	5	1	566	585	33
15	5	1	287	-265	53
17	5	1	83	124	-83
19	5	1	748	-750	32
21	5	1	222	215	-77
23	5	1	222	-146	-82
25	5	1	89	-192	-89
27	5	1	389	351	50
29	5	1	910	945	36
31	5	1	80	61	-80
33	5	1	358	-451	58
35	5	1	209	201	-105
37	5	1	226	285	-71
39	5	1	71	-6	-71
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-36	6	1	787	-795	39
-34	6	1	590	-552	41
-32	6	1	906	926	39
-30	6	1	207	214	-108
-28	6	1	1270	-1258	37
-26	6	1	838	823	42
-24	6	1	1918	1922	36
-22	6	1	140	8	-140
-20	6	1	1379	-1357	33
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-16	6	1	874	853	36
-14	6	1	1525	-1478	31
-12	6	1	2797	-2711	29
-10	6	1	1517	1548	29
-8	6	1	988	898	30
-6	6	1	3039	-2971	26
-4	6	1	1334	-1259	27
-2	6	1	1301	1253	27
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4	6	1	431	400	41
6	6	1	3012	2993	25
8	6	1	1157	-1128	28
10	6	1	1605	-1619	28
12	6	1	615	-560	35
14	6	1	2121	2124	28
16	6	1	1042	-1041	30
18	6	1	1105	-1121	33
20	6	1	1780	1770	32
22	6	1	981	997	34
24	6	1	739	-755	38
26	6	1	154	-21	-154
28	6	1	766	751	40
30	6	1	654	626	42
32	6	1	791	-784	38
34	6	1	204	227	-107
36	6	1	1091	1138	35
38	6	1	485	-407	36
-35	7	1	731	-682	38
-33	7	1	653	618	41
-31	7	1	295	273	60
-29	7	1	1047	-959	37
-27	7	1	656	680	45
-25	7	1	1056	1075	39
-23	7	1	633	594	45
-21	7	1	228	145	-104
-19	7	1	717	-732	43
-17	7	1	95	139	-95
-15	7	1	394	-342	54
-13	7	1	1074	-1049	35
-11	7	1	91	-8	-91
-9	7	1	90	263	-90
-7	7	1	582	587	40
-5	7	1	2137	-2167	30
-3	7	1	88	-207	-88
-1	7	1	1644	1672	30
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5	7	1	1550	-1527	30
7	7	1	314	-306	57
9	7	1	512	470	43
11	7	1	797	-823	36
13	7	1	446	333	46
15	7	1	465	453	46
17	7	1	609	-611	43
19	7	1	560	542	44
21	7	1	91	172	-91
23	7	1	650	678	44
25	7	1	333	-365	64
27	7	1	440	-513	54
29	7	1	1224	1197	37
31	7	1	1391	-1384	36
33	7	1	152	148	-152
35	7	1	777	873	37
-34	8	1	658	822	42
-32	8	1	1159	-1142	38
-30	8	1	164	-80	-164
-28	8	1	527	503	47
-26	8	1	96	-177	-96
-24	8	1	273	-216	-92
-22	8	1	94	96	-94
-20	8	1	1683	1739	39
-18	8	1	1500	-1537	39
-16	8	1	1930	-1882	37
-14	8	1	1499	1493	38
-12	8	1	968	809	39
-10	8	1	732	-681	44
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-6	8	1	539	515	48
-4	8	1	2285	2229	34
-2	8	1	1661	-1718	35
0	8	1	1989	1965	23
2	8	1	1611	1504	34
4	8	1	1665	-1624	34
6	8	1	1006	-1064	37
8	8	1	794	718	39
10	8	1	2712	2717	34
12	8	1	685	-628	43
14	8	1	2310	-2307	35
16	8	1	1072	1082	39
18	8	1	392	344	63
20	8	1	588	-618	51
22	8	1	280	225	-84
24	8	1	675	712	44
26	8	1	91	89	-91
28	8	1	931	-890	41
30	8	1	93	90	-93
32	8	1	1007	982	36
34	8	1	359	-354	52
-31	9	1	493	-504	49
-29	9	1	304	265	67
-27	9	1	101	196	-101
-25	9	1	1262	-1335	44
-23	9	1	624	-673	51
-21	9	1	164	142	-164
-19	9	1	897	974	48

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
-17	9	1	644	-633	51
-15	9	1	379	-370	75
-13	9	1	1276	1305	43
-11	9	1	717	642	49
-9	9	1	2148	-2089	40
-7	9	1	645	562	48
-5	9	1	1230	1283	42
-3	9	1	698	658	43
-1	9	1	956	-964	43
1	9	1	539	599	58
3	9	1	875	881	44
5	9	1	1225	-1322	41
7	9	1	1081	-1068	42
9	9	1	1351	1335	41
11	9	1	1243	1243	41
13	9	1	797	-829	45
15	9	1	212	-63	-171
17	9	1	247	94	-89
19	9	1	175	-199	-175
21	9	1	1249	-1341	43
23	9	1	97	234	-97
25	9	1	1075	1090	41
27	9	1	194	-213	-138
29	9	1	792	-831	43
31	9	1	495	590	50
-28	10	1	469	-515	54
-26	10	1	727	-712	50
-24	10	1	313	219	72
-22	10	1	680	-669	57
-20	10	1	951	-881	47
-18	10	1	963	1017	51
-16	10	1	793	771	53
-14	10	1	104	-81	-104
-12	10	1	369	-342	-96
-10	10	1	108	140	-108
-8	10	1	105	43	-105
-6	10	1	109	-105	-109
-4	10	1	1113	1111	51
-2	10	1	1014	1024	49
0	10	1	416	386	53
2	10	1	110	-45	-110
4	10	1	722	-696	54
6	10	1	168	187	-168
8	10	1	541	-516	60
10	10	1	866	-795	52
12	10	1	1456	1406	47
14	10	1	889	803	48
16	10	1	637	-669	55
18	10	1	861	-809	49
20	10	1	103	199	-103
22	10	1	104	-156	-104
24	10	1	489	-554	58
26	10	1	312	-261	74
28	10	1	579	546	47
-23	11	1	257	187	-92
-21	11	1	937	-992	53

h	k	l	10Fo	10Fc	10s
-19	11	1	396	-301	79
-17	11	1	846	893	56
-15	11	1	599	573	69
-13	11	1	1274	-1278	53
-11	11	1	292	-287	-158
-9	11	1	1905	1857	51
-7	11	1	602	-620	66
-5	11	1	121	-10	-121
-3	11	1	899	850	59
-1	11	1	889	798	59
1	11	1	218	120	-218
3	11	1	830	-699	56
5	11	1	369	256	-96
7	11	1	802	899	62
9	11	1	1241	-1288	53
11	11	1	886	-957	58
13	11	1	1322	1296	51
15	11	1	893	917	55
17	11	1	897	-946	56
19	11	1	431	-457	75
21	11	1	1210	1241	49
23	11	1	536	-611	61
-18	12	1	278	183	-105
-16	12	1	109	-10	-109
-14	12	1	282	-352	-133
-12	12	1	262	418	-262
-10	12	1	736	775	71
-8	12	1	426	472	106
-6	12	1	124	13	-124
-4	12	1	704	-687	74
-2	12	1	641	-626	70
0	12	1	578	-553	57
2	12	1	251	39	-147
4	12	1	308	-135	-147
6	12	1	440	339	92
8	12	1	278	245	-169
10	12	1	276	-47	-130
12	12	1	907	-903	60
14	12	1	107	40	-107
16	12	1	365	251	84
18	12	1	177	21	-177
-11	13	1	122	397	-122
-9	13	1	385	-475	-115
-7	13	1	377	-41	-98
-5	13	1	648	422	79
-3	13	1	1183	-1110	63
-1	13	1	1627	-1521	63
1	13	1	308	301	-180
3	13	1	750	719	80
5	13	1	125	78	-125
7	13	1	130	76	-130
9	13	1	1047	1069	63
11	13	1	250	-57	-219
-42	0	2	327	331	47
-40	0	2	884	-813	34
-38	0	2	940	917	35

h	k	l	10Fo	10Fc	10s
-36	0	2	1275	1242	34
-34	0	2	2938	-2914	32
-32	0	2	355	-274	51
-30	0	2	588	521	39
-28	0	2	929	951	32
-26	0	2	1031	-961	31
-24	0	2	620	-573	34
-22	0	2	1844	1851	27
-20	0	2	1112	999	27
-18	0	2	2143	-1979	24
-16	0	2	1630	1583	23
-14	0	2	1302	1284	22
-12	0	2	115	91	-115
-10	0	2	2211	2332	18
-8	0	2	2308	2391	15
-6	0	2	1610	1477	14
2	0	2	149	54	-44
4	0	2	242	126	30
6	0	2	406	354	24
8	0	2	357	-243	31
10	0	2	102	-114	-102
12	0	2	4144	-4153	18
14	0	2	1482	1450	20
16	0	2	568	526	28
18	0	2	771	-786	28
20	0	2	470	-491	35
22	0	2	1161	1076	27
24	0	2	841	840	29
26	0	2	2269	-2235	28
28	0	2	1470	-1518	30
30	0	2	1631	1612	31
32	0	2	82	16	-82
34	0	2	358	411	55
36	0	2	74	-33	-74
38	0	2	760	714	34
40	0	2	509	-435	36
42	0	2	1280	-1256	29
-41	1	2	74	-132	-74
-39	1	2	458	445	46
-37	1	2	350	-257	47
-35	1	2	219	-292	-87
-33	1	2	721	-723	39
-31	1	2	674	-618	39
-29	1	2	1498	1434	32
-27	1	2	89	-185	-89
-25	1	2	154	93	-154
-23	1	2	215	177	-78
-21	1	2	272	120	60
-19	1	2	294	-315	52
-17	1	2	579	-492	33
-15	1	2	1633	1611	23
-13	1	2	1731	1654	21
-11	1	2	3444	-3429	19
-9	1	2	1324	-1361	19
-7	1	2	147	-203	-136
-5	1	2	1004	1059	16

h	k	l	10Fo	10Fc	10s
-3	1	2	1838	-1895	12
-1	1	2	3180	-3343	10
1	1	2	3753	3667	10
3	1	2	364	354	22
5	1	2	991	1054	15
7	1	2	3534	3641	14
9	1	2	2682	-2697	16
11	1	2	626	-594	25
13	1	2	228	30	53
15	1	2	1163	1160	22
17	1	2	926	980	25
19	1	2	587	-613	31
21	1	2	846	890	27
23	1	2	426	-339	38
25	1	2	966	-994	30
27	1	2	320	-329	53
29	1	2	334	-364	51
31	1	2	1018	1007	32
33	1	2	84	-45	-84
35	1	2	484	-460	39
37	1	2	947	918	33
39	1	2	125	139	-125
41	1	2	150	-122	-75
-42	2	2	538	519	37
-40	2	2	468	452	44
-38	2	2	1221	-1198	34
-36	2	2	622	-591	37
-34	2	2	808	794	38
-32	2	2	1475	1454	34
-30	2	2	469	-409	46
-28	2	2	1158	-1106	33
-26	2	2	1884	1835	30
-24	2	2	231	-283	-75
-22	2	2	2875	-2798	27
-20	2	2	691	654	34
-18	2	2	2052	2000	26
-16	2	2	1795	-1794	24
-14	2	2	1064	-1096	25
-12	2	2	2722	2535	21
-10	2	2	1553	1558	20
-8	2	2	2888	-2897	17
-6	2	2	545	363	25
-4	2	2	835	822	18
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6	2	2	1461	-1313	16
8	2	2	1453	-1454	17
10	2	2	72	-9	-72
12	2	2	2837	2692	19
14	2	2	807	810	24
16	2	2	247	-132	51
18	2	2	310	396	50
20	2	2	944	845	28
22	2	2	2762	-2720	25

h	k	l	10Fo	10Fc	10s
24	2	2	373	-413	45
26	2	2	1621	1630	29
28	2	2	911	882	33
30	2	2	1697	-1667	31
32	2	2	87	-271	-87
34	2	2	719	785	37
36	2	2	84	65	-84
38	2	2	461	-445	39
40	2	2	172	-21	-88
42	2	2	1038	956	29
-41	3	2	627	607	35
-39	3	2	520	-469	40
-37	3	2	413	-358	47
-35	3	2	426	318	48
-33	3	2	1389	1396	34
-31	3	2	359	318	59
-29	3	2	1981	-1948	33
-27	3	2	827	854	36
-25	3	2	493	396	42
-23	3	2	806	-755	34
-21	3	2	2720	-2611	28
-19	3	2	1694	1600	27
-17	3	2	2867	2816	25
-15	3	2	1901	-1804	24
-13	3	2	1916	-1760	23
-11	3	2	1586	1557	23
-9	3	2	466	-345	32
-7	3	2	332	-190	40
-5	3	2	1473	1653	19
-3	3	2	3072	2997	16
-1	3	2	112	198	-112
1	3	2	1819	-1844	16
3	3	2	1350	-1361	17
5	3	2	335	186	33
7	3	2	926	-965	20
9	3	2	752	-791	23
11	3	2	632	597	26
13	3	2	1321	1387	22
15	3	2	2401	-2487	22
17	3	2	196	-165	-80
19	3	2	986	1022	27
21	3	2	849	-813	30
23	3	2	1078	-1046	30
25	3	2	772	681	33
27	3	2	1989	2069	30
29	3	2	81	-127	-81
31	3	2	1471	-1467	32
33	3	2	387	325	49
35	3	2	363	360	47
37	3	2	1026	-991	33
39	3	2	463	-508	43
41	3	2	859	798	31
-40	4	2	369	-403	46
-38	4	2	737	798	36
-36	4	2	83	195	-83
-34	4	2	462	429	47

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
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-24	4	2	807	-711	36
-22	4	2	2888	2846	30
-20	4	2	710	661	36
-18	4	2	2149	-2165	28
-16	4	2	353	316	48
-14	4	2	624	-651	33
-12	4	2	976	-1012	28
-10	4	2	2220	-2328	23
-8	4	2	1394	1266	23
-6	4	2	389	227	36
-4	4	2	650	-619	24
-2	4	2	74	-187	-74
0	4	2	1315	1283	27
2	4	2	1560	1610	19
4	4	2	556	-511	26
6	4	2	74	131	-74
8	4	2	3060	3019	20
10	4	2	389	-260	35
12	4	2	1662	-1592	23
14	4	2	567	556	31
16	4	2	589	-514	32
18	4	2	1172	-1182	27
20	4	2	86	-168	-86
22	4	2	1607	1655	29
24	4	2	826	816	35
26	4	2	269	-250	-79
28	4	2	336	329	59
30	4	2	246	339	-83
32	4	2	85	91	-85
34	4	2	656	-653	38
36	4	2	397	-459	48
38	4	2	398	385	39
40	4	2	70	2	-70
-39	5	2	79	-153	-79
-37	5	2	1668	1670	32
-35	5	2	278	-282	68
-33	5	2	1016	-951	36
-31	5	2	213	-96	-98
-29	5	2	887	882	38
-27	5	2	458	398	49
-25	5	2	1272	-1292	35
-23	5	2	741	654	38
-21	5	2	1288	1319	33
-19	5	2	1614	-1595	31
-17	5	2	1768	-1771	30
-15	5	2	1287	1278	30
-13	5	2	1492	1581	28
-11	5	2	2677	-2491	26
-9	5	2	1636	1650	26
-7	5	2	3784	3956	23
-5	5	2	719	-680	28
-3	5	2	2107	-2202	22

h	k	l	10Fo	10Fc	10s
-1	5	2	762	786	26
1	5	2	1104	1086	23
3	5	2	955	-970	24
5	5	2	2059	-2032	23
7	5	2	451	348	34
9	5	2	1881	1836	24
11	5	2	1209	-1301	26
13	5	2	1310	-1404	27
15	5	2	1236	1240	28
17	5	2	290	-269	53
19	5	2	1132	-1199	30
21	5	2	663	675	34
23	5	2	2132	2214	31
25	5	2	600	-685	39
27	5	2	1897	-1934	32
29	5	2	732	727	38
31	5	2	1304	1253	35
33	5	2	88	-216	-88
35	5	2	824	-826	34
37	5	2	78	-79	-78
39	5	2	566	584	35
-38	6	2	83	-177	-83
-36	6	2	419	-497	48
-34	6	2	379	355	53
-32	6	2	183	-157	-160
-30	6	2	88	-148	-88
-28	6	2	86	17	-86
-26	6	2	377	406	58
-24	6	2	996	957	38
-22	6	2	367	323	56
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8	6	2	280	-242	53
10	6	2	495	460	36
12	6	2	871	-862	31
14	6	2	81	37	-81
16	6	2	197	-77	-100
18	6	2	981	986	33
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22	6	2	616	651	41
24	6	2	960	-924	35
26	6	2	216	-168	-93
28	6	2	258	149	-68
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h	k	l	10Fo	10Fc	10s
32	6	2	214	-239	-87
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36	6	2	627	662	39
38	6	2	218	220	-79
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7	7	2	761	-806	35
9	7	2	85	-8	-85
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13	7	2	498	469	41
15	7	2	968	-979	35
17	7	2	891	-807	36
19	7	2	1220	1319	36
21	7	2	522	570	48
23	7	2	1124	-1162	37
25	7	2	93	179	-93
27	7	2	311	243	66
29	7	2	84	-2	-84
31	7	2	915	-968	38
33	7	2	658	698	41
35	7	2	926	923	34
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-26	8	2	646	578	45
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-20	8	2	242	172	-91
-18	8	2	1755	1789	40
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-10	8	2	1089	1050	39
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-6	8	2	152	-195	-152
-4	8	2	150	107	-150

h	k	l	10Fo	10Fc	10s
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6	8	2	289	322	-74
8	8	2	649	-652	42
10	8	2	375	321	59
12	8	2	905	807	41
14	8	2	271	-361	-82
16	8	2	1539	-1578	37
18	8	2	900	911	39
20	8	2	176	-99	-176
22	8	2	1212	-1198	38
24	8	2	658	719	48
26	8	2	525	503	49
28	8	2	470	460	51
30	8	2	714	-831	42
32	8	2	502	-467	45
34	8	2	631	663	40
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-29	9	2	1019	1087	42
-27	9	2	925	-948	44
-25	9	2	546	-523	51
-23	9	2	434	320	60
-21	9	2	296	133	-77
-19	9	2	101	71	-101
-17	9	2	107	-169	-107
-15	9	2	1421	1428	43
-13	9	2	299	-207	-91
-11	9	2	2583	-2503	40
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-7	9	2	556	459	52
-5	9	2	447	-310	61
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3	9	2	1075	-1101	42
5	9	2	1031	-1119	43
7	9	2	758	773	44
9	9	2	461	422	54
11	9	2	260	194	-86
13	9	2	287	193	-89
15	9	2	558	542	57
17	9	2	95	87	-95
19	9	2	1534	-1602	40
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23	9	2	615	564	49
25	9	2	277	-417	-101
27	9	2	89	-86	-89
29	9	2	146	-232	-146
31	9	2	780	794	38
-28	10	2	690	731	50
-26	10	2	974	-1116	46
-24	10	2	591	-708	58
-22	10	2	586	552	59
-20	10	2	203	-46	-203

h	k	l	10Fo	10Fc	10s
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-16	10	2	647	605	58
-14	10	2	861	882	52
-12	10	2	106	-162	-106
-10	10	2	961	-961	53
-8	10	2	812	758	49
-6	10	2	1411	1418	48
-4	10	2	968	-1009	51
-2	10	2	353	-382	83
0	10	2	1158	1214	48
2	10	2	183	101	-183
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6	10	2	821	-778	50
8	10	2	1114	974	46
10	10	2	349	320	86
12	10	2	1669	-1653	45
14	10	2	1387	1469	46
16	10	2	1637	1646	45
18	10	2	1021	-1050	45
20	10	2	612	-622	56
22	10	2	98	32	-98
24	10	2	870	855	47
26	10	2	968	-955	42
28	10	2	368	-495	65
-23	11	2	99	-22	-99
-21	11	2	474	-639	75
-19	11	2	111	-91	-111
-17	11	2	421	-361	76
-15	11	2	107	79	-107
-13	11	2	398	407	80
-11	11	2	110	156	-110
-9	11	2	510	475	73
-7	11	2	651	-670	68
-5	11	2	588	542	67
-3	11	2	116	285	-116
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1	11	2	296	294	-127
3	11	2	409	549	93
5	11	2	773	900	62
7	11	2	447	-349	78
9	11	2	776	-716	57
11	11	2	114	-4	-114
13	11	2	690	-713	57
15	11	2	442	-289	70
17	11	2	605	556	54
19	11	2	554	495	55
21	11	2	209	2	-149
23	11	2	105	-305	-105
-18	12	2	625	587	67
-16	12	2	688	-616	64
-14	12	2	931	-820	60
-12	12	2	126	245	-126
-10	12	2	1567	1584	58
-8	12	2	730	-583	67
-6	12	2	953	-883	63
-4	12	2	378	236	-108

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$ Page 5

h	k	l	10Fo	10Fc	10s
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6	12	2	945	822	56
8	12	2	1448	-1370	55
10	12	2	394	-421	-103
12	12	2	610	749	83
14	12	2	738	-752	61
16	12	2	494	-503	79
18	12	2	696	623	55
-9	13	2	337	228	-118
-7	13	2	118	-64	-118
-5	13	2	128	32	-128
-3	13	2	118	156	-118
-1	13	2	119	-15	-119
1	13	2	125	-290	-125
3	13	2	328	105	-116
5	13	2	470	356	74
7	13	2	123	-353	-123
9	13	2	498	-478	86
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-37	1	3	818	803	38
-35	1	3	640	-603	39
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-31	1	3	1656	1598	33
-29	1	3	939	-864	34
-27	1	3	1628	-1570	32
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-23	1	3	829	835	32
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-17	1	3	3131	3102	24
-15	1	3	871	889	26
-13	1	3	973	-976	23
-11	1	3	1573	1674	20
-9	1	3	1817	1872	18
-7	1	3	806	853	19
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-3	1	3	925	-983	15
-1	1	3	3478	3203	12
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5	1	3	2554	2557	13
7	1	3	1327	1189	16
9	1	3	465	480	25
11	1	3	232	-189	47
13	1	3	1821	1931	19
15	1	3	1488	1588	21
17	1	3	2489	-2586	22
19	1	3	983	-1023	25
21	1	3	1996	2041	25
23	1	3	70	75	-70
25	1	3	377	-278	46
27	1	3	353	-288	45
29	1	3	1093	1151	32

h	k	l	10Fo	10Fc	10s
31	1	3	421	-363	45
33	1	3	1413	-1354	31
35	1	3	530	560	39
37	1	3	1263	1208	31
39	1	3	608	-562	32
41	1	3	533	-556	32
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-34	2	3	650	621	42
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-30	2	3	406	-379	53
-28	2	3	1217	-1248	33
-26	2	3	652	-671	37
-24	2	3	2947	2816	29
-22	2	3	86	-34	-86
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-18	2	3	229	-104	-66
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-14	2	3	503	-472	34
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-10	2	3	158	-94	-105
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-6	2	3	381	-287	31
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-2	2	3	2242	2315	14
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2	2	3	1415	-1193	15
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10	2	3	2389	-2335	18
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16	2	3	2231	-2307	22
18	2	3	601	-589	31
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24	2	3	812	-808	30
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38	2	3	492	509	41
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h	k	l	10Fo	10Fc	10s
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9	3	3	1121	1096	21
11	3	3	601	660	26
13	3	3	2656	-2723	21
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19	3	3	1632	1758	25
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27	3	3	923	-887	32
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33	3	3	754	761	35
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37	3	3	470	-489	38
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-26	4	3	1616	1568	33
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h	k	l	10Fo	10Fc	10s
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26	4	3	516	495	37
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15	5	3	512	467	35
17	5	3	749	710	31
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25	5	3	530	-530	39
27	5	3	81	6	-81
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31	5	3	303	217	54
33	5	3	378	-410	47
35	5	3	218	319	-80
37	5	3	433	394	38

h	k	l	10Fo	10Fc	10s
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24	6	3	408	-387	52
26	6	3	1021	-976	36
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-31	7	3	87	-101	-87
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-5	7	3	1180	-1266	33
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Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$ Page 6

h	k	l	10Fo	10Fc	10s
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11	7	3	602	-560	39
13	7	3	888	881	34
15	7	3	851	-919	37
17	7	3	226	-174	-82
19	7	3	538	-534	42
21	7	3	250	218	-77
23	7	3	527	526	46
25	7	3	231	-331	-108
27	7	3	601	637	42
29	7	3	167	58	-167
31	7	3	672	-699	41
33	7	3	293	-361	62
35	7	3	180	150	-94
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-26	8	3	173	34	-173
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-22	8	3	188	-194	-188
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-18	8	3	97	19	-97
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-14	8	3	316	-383	-83
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12	8	3	190	9	-129
14	8	3	966	-964	38
16	8	3	282	-283	-85
18	8	3	146	205	-146
20	8	3	93	168	-93
22	8	3	1023	-983	40
24	8	3	763	656	42
26	8	3	546	539	45
28	8	3	778	-868	41
30	8	3	90	190	-90
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-27	9	3	1081	1089	40
-25	9	3	1014	-944	42
-23	9	3	1147	-1050	42
-21	9	3	347	242	73

h	k	l	10Fo	10Fc	10s
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-15	9	3	872	-896	46
-13	9	3	1481	1445	42
-11	9	3	562	566	59
-9	9	3	1018	-1043	45
-7	9	3	328	-264	82
-5	9	3	1182	1228	45
-3	9	3	496	532	61
-1	9	3	1785	-1918	40
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3	9	3	1049	1008	43
5	9	3	1265	-1246	41
7	9	3	503	-529	57
9	9	3	668	632	47
11	9	3	480	434	59
13	9	3	739	-641	43
15	9	3	304	239	-89
17	9	3	1427	1525	40
19	9	3	99	-189	-99
21	9	3	1548	-1650	39
23	9	3	390	593	70
25	9	3	304	193	74
27	9	3	336	360	64
29	9	3	899	-898	39
-26	10	3	275	-23	-91
-24	10	3	732	708	50
-22	10	3	465	-488	69
-20	10	3	599	-563	64
-18	10	3	206	-55	-206
-16	10	3	508	458	60
-14	10	3	111	248	-111
-12	10	3	108	-177	-108
-10	10	3	368	356	88
-8	10	3	849	823	55
-6	10	3	1161	-1057	47
-4	10	3	396	-269	66
-2	10	3	725	657	51
0	10	3	339	-433	74
2	10	3	511	536	62
4	10	3	184	68	-184
6	10	3	350	-310	74
8	10	3	237	-115	-128
10	10	3	1496	-1402	45
12	10	3	377	-209	86
14	10	3	167	192	-167
16	10	3	476	425	66
18	10	3	337	-216	64
20	10	3	298	-221	-98
22	10	3	804	739	45
24	10	3	678	-652	48
26	10	3	333	-336	64
-23	11	3	894	941	48
-21	11	3	545	-595	68
-19	11	3	1166	-1181	50
-17	11	3	929	943	54

h	k	l	10Fo	10Fc	10s
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-13	11	3	805	-751	57
-11	11	3	117	-32	-117
-9	11	3	1511	1402	50
-7	11	3	371	370	-95
-5	11	3	844	-904	62
-3	11	3	201	96	-201
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1	11	3	200	64	-200
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5	11	3	721	686	61
7	11	3	787	766	59
9	11	3	1361	-1301	49
11	11	3	1725	-1743	48
13	11	3	1210	1200	49
15	11	3	557	549	60
17	11	3	868	-882	50
19	11	3	103	121	-103
21	11	3	1070	1105	46
23	11	3	94	-35	-94
-18	12	3	335	217	-94
-16	12	3	317	-173	-96
-14	12	3	419	-321	80
-12	12	3	116	-2	-116
-10	12	3	290	176	-118
-8	12	3	277	298	-161
-6	12	3	214	-149	-214
-4	12	3	317	-168	-107
-2	12	3	114	-116	-114
0	12	3	344	210	-87
2	12	3	194	214	-194
4	12	3	636	-565	64
6	12	3	115	-122	-115
8	12	3	269	325	-148
10	12	3	168	112	-168
12	12	3	185	51	-185
14	12	3	265	62	-119
16	12	3	112	12	-112
-7	13	3	345	-312	-95
-5	13	3	1381	1470	63
-3	13	3	130	145	-130
-1	13	3	1310	-1224	62
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3	13	3	968	943	68
5	13	3	961	-872	63
7	13	3	705	-675	74
-40	0	4	1495	-1497	32
-38	0	4	1155	1073	33
-36	0	4	1476	1477	34
-34	0	4	173	-168	-129
-32	0	4	1148	-1073	34
-30	0	4	835	765	36
-28	0	4	1707	1595	31
-26	0	4	2014	-1986	30
-24	0	4	693	-656	34
-22	0	4	1600	1530	28

h	k	l	10Fo	10Fc	10s
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-18	0	4	723	-721	29
-16	0	4	725	-702	28
-14	0	4	3302	3260	21
-12	0	4	529	564	28
-10	0	4	4026	-4234	18
-8	0	4	1699	1740	17
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2	0	4	4388	4258	13
6	0	4	2138	2226	15
8	0	4	2591	2688	16
10	0	4	1100	-1087	18
12	0	4	1616	-1568	19
14	0	4	609	639	26
16	0	4	217	93	-56
18	0	4	1027	1058	25
20	0	4	2904	-2862	24
22	0	4	1623	1560	26
24	0	4	3319	3321	26
26	0	4	1911	-1904	28
28	0	4	1462	-1491	30
30	0	4	335	244	51
32	0	4	714	721	35
34	0	4	893	-911	32
36	0	4	77	-138	-77
38	0	4	1247	1209	31
40	0	4	332	328	43
-41	1	4	173	-19	-98
-39	1	4	82	-152	-82
-37	1	4	582	539	41
-35	1	4	419	382	42
-33	1	4	719	-677	39
-31	1	4	285	283	65
-29	1	4	788	749	36
-27	1	4	758	-741	33
-25	1	4	83	117	-83
-23	1	4	81	82	-81
-21	1	4	1053	-1021	29
-19	1	4	576	-526	31
-17	1	4	1864	-1878	24
-15	1	4	844	947	26
-13	1	4	1019	1061	23
-11	1	4	571	-554	26
-9	1	4	810	930	21
-7	1	4	350	-309	29
-5	1	4	2792	2912	15
-3	1	4	927	-898	16
-1	1	4	1736	-1718	14
1	1	4	3191	3350	13
3	1	4	3671	-3703	14
5	1	4	732	819	18
7	1	4	492	425	22
9	1	4	564	587	22

h	k	l	10Fo	10Fc	10s
11	1	4	443	495	27
13	1	4	2237	-2405	19
15	1	4	1329	1396	22
17	1	4	263	-316	50
19	1	4	172	-230	-78
21	1	4	2261	2271	25
23	1	4	966	-987	28
25	1	4	155	131	-108
27	1	4	680	-613	32
29	1	4	416	-462	45
31	1	4	920	921	32
33	1	4	254	-257	-65
35	1	4	226	-221	-75
37	1	4	372	388	43
39	1	4	422	410	40
41	1	4	69	-66	-69
-40	2	4	816	831	34
-38	2	4	584	-620	40
-36	2	4	1360	-1347	34
-34	2	4	660	607	39
-32	2	4	1132	1083	35
-30	2	4	883	-894	38
-28	2	4	865	-828	37
-26	2	4	1842	1759	31
-24	2	4	678	732	37
-22	2	4	800	-783	33
-20	2	4	858	-797	31
-18	2	4	922	907	29
-16	2	4	640	-574	31
-14	2	4	2796	-2868	23
-12	2	4	2159	2231	22
-10	2	4	1689	1718	20
-8	2	4	882	-959	21
-6	2	4	2456	-2444	17
-4	2	4	1739	1752	16
-2	2	4	1395	1305	16
0	2	4	237	195	27
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4	2	4	1756	1637	16
6	2	4	842	839	19
8	2	4	1960	-1969	17
10	2	4	1446	-1447	19
12	2	4	180	-45	-67
14	2	4	826	779	23
16	2	4	889	-863	24
18	2	4	634	636	30
20	2	4	2875	2859	25
22	2	4	1067	-1061	27
24	2	4	2060	-1983	27
26	2	4	492	499	38
28	2	4	1137	1096	29
30	2	4	1268	-1194	31
32	2	4	728	-756	35
34	2	4	1310	1240	32
36	2	4	126	121	-126
38	2	4	938	-929	31

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
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-39	3	4	206	281	-84
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-35	3	4	427	-393	47
-33	3	4	1110	1065	35
-31	3	4	348	-334	61
-29	3	4	1392	-1330	34
-27	3	4	1244	1289	34
-25	3	4	1563	1620	32
-23	3	4	1155	-1181	32
-21	3	4	1924	-1914	29
-19	3	4	2183	2122	28
-17	3	4	1212	1245	27
-15	3	4	511	-565	34
-13	3	4	567	574	33
-11	3	4	292	-245	48
-9	3	4	1291	1266	22
-7	3	4	2579	-2776	19
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-3	3	4	1360	1356	18
-1	3	4	1111	1122	18
1	3	4	732	-663	21
3	3	4	524	483	23
5	3	4	770	776	21
7	3	4	897	-903	21
9	3	4	1415	-1447	20
11	3	4	1636	1562	21
13	3	4	931	937	24
15	3	4	1214	-1198	24
17	3	4	73	-69	-73
19	3	4	1735	1758	25
21	3	4	493	-472	33
23	3	4	1732	-1777	28
25	3	4	584	-627	35
27	3	4	1570	1598	31
29	3	4	676	708	38
31	3	4	1126	-1117	32
33	3	4	191	334	-105
35	3	4	813	737	34
37	3	4	1102	-1174	31
39	3	4	526	-552	35
-38	4	4	79	161	-79
-36	4	4	122	214	-122
-34	4	4	771	-826	39
-32	4	4	261	107	61
-30	4	4	305	208	67
-28	4	4	91	99	-91
-26	4	4	1115	-1095	35
-24	4	4	968	-901	36
-22	4	4	796	745	35
-20	4	4	461	499	48
-18	4	4	574	-603	40
-16	4	4	1079	1064	30
-14	4	4	1535	1486	27
-12	4	4	702	-635	31
-10	4	4	1264	-1228	25

h	k	l	10Fo	10Fc	10s
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-6	4	4	334	412	40
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-2	4	4	849	-874	23
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8	4	4	592	596	26
10	4	4	724	695	26
12	4	4	151	-200	-151
14	4	4	1046	1097	25
16	4	4	695	701	29
18	4	4	1607	-1634	27
20	4	4	1803	-1849	28
22	4	4	827	-810	32
24	4	4	1154	1176	30
26	4	4	311	375	60
28	4	4	208	-220	-91
30	4	4	1112	1174	32
32	4	4	336	302	51
34	4	4	454	-433	42
36	4	4	499	-510	38
38	4	4	346	356	43
-37	5	4	1714	1772	33
-35	5	4	82	-76	-82
-33	5	4	1162	-1156	36
-31	5	4	1051	-1032	37
-29	5	4	1349	1421	37
-27	5	4	85	64	-85
-25	5	4	1923	-1942	35
-23	5	4	1461	1509	34
-21	5	4	2119	2140	32
-19	5	4	216	-117	-89
-17	5	4	185	-225	-147
-15	5	4	330	322	58
-13	5	4	555	560	35
-11	5	4	3041	-3007	26
-9	5	4	1268	-1288	27
-7	5	4	2969	3169	24
-5	5	4	230	-94	55
-3	5	4	2100	-2224	23
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3	5	4	652	-665	27
5	5	4	1776	-1782	23
7	5	4	1296	1304	24
9	5	4	1781	1743	24
11	5	4	946	-929	27
13	5	4	1175	-1249	27
15	5	4	1568	1586	27
17	5	4	362	-295	46
19	5	4	2345	-2400	28
21	5	4	538	-647	42
23	5	4	2728	2833	30
25	5	4	309	328	63

h	k	l	10Fo	10Fc	10s
27	5	4	1875	-1965	32
29	5	4	347	335	50
31	5	4	782	794	36
33	5	4	281	-299	62
35	5	4	852	-912	35
37	5	4	356	358	39
-36	6	4	353	291	52
-34	6	4	226	137	-74
-32	6	4	296	272	72
-30	6	4	362	-378	60
-28	6	4	87	-187	-87
-26	6	4	497	-442	50
-24	6	4	254	109	-78
-22	6	4	1256	1281	36
-20	6	4	979	1006	39
-18	6	4	86	-91	-86
-16	6	4	1944	-1946	32
-14	6	4	338	-350	59
-12	6	4	1021	-972	32
-10	6	4	435	491	47
-8	6	4	749	732	32
-6	6	4	1990	1995	27
-4	6	4	401	-371	40
-2	6	4	246	-328	-67
0	6	4	505	-434	25
2	6	4	970	-967	28
4	6	4	397	417	41
6	6	4	369	-312	38
8	6	4	509	504	35
10	6	4	957	915	29
12	6	4	848	-806	31
14	6	4	546	-474	36
16	6	4	732	681	34
18	6	4	917	-889	33
20	6	4	694	702	36
22	6	4	616	602	39
24	6	4	171	-135	-171
26	6	4	490	562	48
28	6	4	122	-45	-122
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32	6	4	610	-608	38
34	6	4	83	247	-83
36	6	4	559	578	35
-35	7	4	317	-279	55
-33	7	4	1447	1517	35
-31	7	4	208	-35	-106
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-25	7	4	412	418	62
-23	7	4	193	-209	-193
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-19	7	4	633	663	43
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-13	7	4	1227	-1258	36
-11	7	4	1324	1307	34

h	k	l	10Fo	10Fc	10s
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7	7	4	723	-700	35
9	7	4	1283	-1256	32
11	7	4	1370	1306	31
13	7	4	1319	1278	32
15	7	4	1537	-1546	32
17	7	4	1664	-1721	33
19	7	4	1437	1513	34
21	7	4	782	744	38
23	7	4	1152	-1166	35
25	7	4	253	112	-64
27	7	4	554	601	44
29	7	4	83	113	-83
31	7	4	1034	-1081	35
33	7	4	313	369	56
-32	8	4	940	996	39
-30	8	4	240	-111	-88
-28	8	4	92	-168	-92
-26	8	4	693	606	46
-24	8	4	201	-252	-201
-22	8	4	1247	-1186	41
-20	8	4	586	-618	53
-18	8	4	1294	1226	40
-16	8	4	607	530	50
-14	8	4	287	-276	-92
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-8	8	4	328	-218	67
-6	8	4	1436	-1406	37
-4	8	4	224	-172	-84
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6	8	4	517	-591	49
8	8	4	869	-847	39
10	8	4	699	-668	42
12	8	4	1350	1310	36
14	8	4	98	163	-98
16	8	4	429	-261	48
18	8	4	614	607	44
20	8	4	293	-257	62
22	8	4	861	-877	40
24	8	4	88	-164	-88
26	8	4	268	260	-72
28	8	4	878	848	40
30	8	4	502	-430	44
32	8	4	697	-711	38
-29	9	4	770	811	42

h	k	l	10Fo	10Fc	10s
-27	9	4	230	138	-109
-25	9	4	321	-339	-83
-23	9	4	263	-404	-117
-21	9	4	103	-129	-103
-19	9	4	946	-964	44
-17	9	4	973	-888	44
-15	9	4	1698	1657	42
-13	9	4	473	404	55
-11	9	4	399	-459	73
-9	9	4	110	50	-110
-7	9	4	272	157	-93
-5	9	4	949	953	46
-3	9	4	1359	-1406	40
-1	9	4	503	475	55
1	9	4	2001	1961	39
3	9	4	436	-410	60
5	9	4	879	-833	42
7	9	4	779	-797	47
9	9	4	433	364	57
11	9	4	437	303	59
13	9	4	1175	-1116	41
15	9	4	1221	1202	41
17	9	4	608	709	51
19	9	4	229	-351	-134
21	9	4	94	-120	-94
23	9	4	151	17	-151
25	9	4	248	307	-82
27	9	4	797	-835	40
29	9	4	83	-117	-83
-26	10	4	771	-908	49
-24	10	4	442	-305	65
-22	10	4	1080	1023	47
-20	10	4	228	5	-128
-18	10	4	1095	-1070	47
-16	10	4	234	-428	-207
-14	10	4	680	740	64
-12	10	4	717	709	56
-10	10	4	2038	-1887	46
-8	10	4	997	949	48
-6	10	4	1136	1195	50
-4	10	4	929	-857	49
-2	10	4	271	-282	-106
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2	10	4	863	754	49
4	10	4	1071	-908	46
6	10	4	439	233	60
8	10	4	614	483	54
10	10	4	555	-497	54
12	10	4	1778	-1662	43
14	10	4	555	641	59
16	10	4	1157	1227	45
18	10	4	204	204	-199
20	10	4	1207	-1212	42
22	10	4	475	447	55
24	10	4	855	905	46
26	10	4	990	-1033	41

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
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-19	11	4	106	148	-106
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-15	11	4	110	20	-110
-13	11	4	258	273	-132
-11	11	4	110	-1	-110
-9	11	4	814	725	56
-7	11	4	587	-474	65
-5	11	4	121	201	-121
-3	11	4	199	168	-199
-1	11	4	269	-133	-98
1	11	4	107	35	-107
3	11	4	610	-659	63
5	11	4	101	-96	-101
7	11	4	521	629	70
9	11	4	327	286	-88
11	11	4	371	336	85
13	11	4	113	-346	-113
15	11	4	575	-552	58
17	11	4	101	22	-101
19	11	4	323	255	79
21	11	4	813	802	47
-16	12	4	197	335	-197
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-12	12	4	414	192	82
-10	12	4	1419	1278	56
-8	12	4	486	-494	88
-6	12	4	1265	-1282	58
-4	12	4	1294	1303	57
-2	12	4	452	468	96
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h	k	l	10Fo	10Fc	10s
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Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$ Page 9

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Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
-11	3	6	340	410	40
-9	3	6	1124	1255	24
-7	3	6	1886	-1945	22
-5	3	6	1030	-1035	23
-3	3	6	272	151	35
-1	3	6	401	369	29
1	3	6	2128	-2135	20
3	3	6	123	-71	-123
5	3	6	1479	1449	20
7	3	6	814	-812	22
9	3	6	2062	-2001	21
11	3	6	1064	-1033	24
13	3	6	727	714	25
15	3	6	880	-925	27
17	3	6	303	-251	43
19	3	6	1367	1324	27
21	3	6	1601	1604	27
23	3	6	1521	-1514	28
25	3	6	1440	-1517	30
27	3	6	1097	1094	31
29	3	6	1581	1592	30
31	3	6	437	-388	40
33	3	6	74	-11	-74
35	3	6	995	1011	31
37	3	6	413	-388	38
-38	4	6	88	85	-88
-36	4	6	625	635	41
-34	4	6	288	-289	-78
-32	4	6	84	181	-84
-30	4	6	579	570	44
-28	4	6	952	948	36
-26	4	6	1294	1272	36
-24	4	6	1297	-1256	34
-22	4	6	798	871	37
-20	4	6	198	182	-102
-18	4	6	1223	-1252	32
-16	4	6	1088	1073	31
-14	4	6	734	688	32
-12	4	6	695	704	30
-10	4	6	1663	-1673	25
-8	4	6	824	-780	27
-6	4	6	1339	1345	24
-4	4	6	218	167	-57
-2	4	6	1836	-1836	22
0	4	6	1810	-1690	19
2	4	6	1589	1647	22
4	4	6	752	-784	24
6	4	6	507	-434	28
8	4	6	172	124	-73
10	4	6	231	-158	52
12	4	6	3125	-3041	24
14	4	6	946	951	26
16	4	6	1928	1914	26
18	4	6	468	476	37
20	4	6	166	-131	-109
22	4	6	755	-791	33

h	k	l	10Fo	10Fc	10s
24	4	6	1087	1091	30
26	4	6	359	-360	48
28	4	6	497	482	40
30	4	6	1195	1211	32
32	4	6	934	962	33
34	4	6	350	-287	43
36	4	6	445	-420	38
-35	5	6	1125	1129	35
-33	5	6	86	42	-86
-31	5	6	504	-541	53
-29	5	6	1137	1052	37
-27	5	6	935	927	38
-25	5	6	1059	-1112	36
-23	5	6	407	-343	50
-21	5	6	625	656	44
-19	5	6	532	547	42
-17	5	6	1512	-1609	33
-15	5	6	676	725	36
-13	5	6	1682	1845	30
-11	5	6	2362	-2343	28
-9	5	6	2439	-2524	27
-7	5	6	1439	1442	27
-5	5	6	731	767	29
-3	5	6	522	-592	34
-1	5	6	163	60	-94
1	5	6	432	238	35
3	5	6	732	-772	26
5	5	6	2913	-2836	24
7	5	6	1018	-1047	26
9	5	6	1853	1861	26
11	5	6	170	-163	-80
13	5	6	1623	-1633	27
15	5	6	603	586	34
17	5	6	2185	2237	29
19	5	6	2037	-2095	29
21	5	6	1416	-1496	30
23	5	6	1230	1313	32
25	5	6	1109	1092	32
27	5	6	261	-147	61
29	5	6	116	-123	-116
31	5	6	1181	1215	32
33	5	6	272	272	61
35	5	6	918	-880	30
-34	6	6	451	412	47
-32	6	6	569	585	46
-30	6	6	785	-842	43
-28	6	6	83	-108	-83
-26	6	6	176	-138	-176
-24	6	6	920	-849	38
-22	6	6	741	750	43
-20	6	6	533	566	47
-18	6	6	654	616	41
-16	6	6	1205	1220	35
-14	6	6	989	-1048	35
-12	6	6	401	-366	50
-10	6	6	1724	-1786	30

h	k	l	10Fo	10Fc	10s
-8	6	6	172	43	-119
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-4	6	6	424	-415	41
-2	6	6	1551	1555	28
0	6	6	680	678	40
2	6	6	166	-51	-97
4	6	6	1580	-1458	28
6	6	6	1429	-1315	28
8	6	6	333	360	50
10	6	6	1193	1157	29
12	6	6	217	133	-76
14	6	6	396	411	40
16	6	6	460	-481	44
18	6	6	465	-439	43
20	6	6	83	-49	-83
22	6	6	604	-604	38
24	6	6	1105	1092	34
26	6	6	572	616	42
28	6	6	74	8	-74
30	6	6	507	-475	41
32	6	6	476	-485	41
34	6	6	326	-244	43
-33	7	6	451	392	48
-31	7	6	246	312	-99
-29	7	6	1488	-1545	38
-27	7	6	1018	-1018	40
-25	7	6	1048	977	40
-23	7	6	204	-92	-115
-21	7	6	428	-465	60
-19	7	6	250	210	-96
-17	7	6	1165	1187	40
-15	7	6	867	-934	43
-13	7	6	730	-731	40
-11	7	6	1317	1296	36
-9	7	6	1413	1423	35
-7	7	6	1092	-1146	36
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-3	7	6	1511	1541	32
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1	7	6	1024	-1014	33
3	7	6	1799	-1745	30
5	7	6	2081	2044	30
7	7	6	310	275	62
9	7	6	1102	-1037	32
11	7	6	1637	1729	33
13	7	6	1514	1525	33
15	7	6	566	-567	41
17	7	6	2019	-2009	33
19	7	6	583	561	40
21	7	6	1122	1187	36
23	7	6	423	-463	52
25	7	6	871	-941	38
27	7	6	525	562	45
29	7	6	155	-129	-155
31	7	6	1156	-1146	33
-30	8	6	555	-612	55

h	k	l	10Fo	10Fc	10s
-28	8	6	924	-927	41
-26	8	6	314	-180	73
-24	8	6	677	697	52
-22	8	6	922	-860	45
-20	8	6	530	-510	55
-18	8	6	94	-22	-94
-16	8	6	100	84	-100
-14	8	6	464	-388	62
-12	8	6	255	-39	-97
-10	8	6	1521	1564	39
-8	8	6	1221	1226	39
-6	8	6	865	-877	40
-4	8	6	517	494	49
-2	8	6	89	112	-89
0	8	6	1645	-1631	27
2	8	6	665	-583	39
4	8	6	1649	1592	35
6	8	6	1897	1825	34
8	8	6	177	-172	-177
10	8	6	811	-765	41
12	8	6	1155	1083	37
14	8	6	156	118	-156
16	8	6	692	-702	42
18	8	6	193	205	-119
20	8	6	475	453	44
22	8	6	89	-84	-89
24	8	6	1267	-1237	36
26	8	6	504	-502	42
28	8	6	187	-282	-111
30	8	6	196	-161	-80
-27	9	6	487	386	47
-25	9	6	871	-839	44
-23	9	6	97	73	-97
-21	9	6	883	843	45
-19	9	6	596	-734	52
-17	9	6	635	-600	55
-15	9	6	538	574	56
-13	9	6	752	850	49
-11	9	6	252	112	-113
-9	9	6	762	-778	49
-7	9	6	1037	1109	45
-5	9	6	667	670	49
-3	9	6	1281	-1372	42
-1	9	6	392	-390	64
1	9	6	1139	1101	40
3	9	6	920	841	43
5	9	6	97	186	-97
7	9	6	91	-31	-91
9	9	6	1437	1464	39
11	9	6	299	-296	-88
13	9	6	1794	-1732	38
15	9	6	816	774	44
17	9	6	632	643	46
19	9	6	370	381	64
21	9	6	657	-569	44
23	9	6	181	153	-129

h	k	l	10Fo	10Fc	10s
25	9	6	152	205	-152
27	9	6	1506	-1518	34
-24	10	6	895	-971	44
-22	10	6	391	455	70
-20	10	6	274	241	-96
-18	10	6	416	-346	63
-16	10	6	813	-793	52
-14	10	6	1349	1426	47
-12	10	6	106	-139	-106
-10	10	6	1476	-1469	47
-8	10	6	104	-39	-104
-6	10	6	1047	1062	49
-4	10	6	310	232	-90
-2	10	6	854	-956	54
0	10	6	278	199	-109
2	10	6	1625	1569	43
4	10	6	428	-450	65
6	10	6	291	-92	68
8	10	6	364	259	76
10	10	6	398	-471	71
12	10	6	989	-928	44
14	10	6	582	-623	56
16	10	6	1778	1788	41
18	10	6	205	18	-119
20	10	6	1275	-1324	39
22	10	6	302	299	61
-17	11	6	292	279	-97
-15	11	6	100	-47	-100
-13	11	6	595	-603	65
-11	11	6	106	73	-106
-9	11	6	450	396	69
-7	11	6	690	-729	60
-5	11	6	984	-999	52
-3	11	6	333	246	-88
-1	11	6	619	728	62
1	11	6	452	534	71
3	11	6	336	-361	-95
5	11	6	599	-628	61
7	11	6	583	-504	57
9	11	6	302	-237	-92
11	11	6	423	340	69
13	11	6	101	193	-101
15	11	6	432	-452	63
17	11	6	249	-227	-90
-10	12	6	432	479	87
-8	12	6	107	109	-107
-6	12	6	1128	-1234	58
-4	12	6	292	137	-112
-2	12	6	765	682	58
0	12	6	400	-347	63
2	12	6	914	-867	58
4	12	6	237	321	-237
6	12	6	453	354	66
8	12	6	1000	-1011	53
10	12	6	777	-759	54
-37	1	7	353	383	61

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
-35	1	7	700	-653	37
-33	1	7	1336	-1334	34
-31	1	7	246	-20	-69
-29	1	7	136	214	-136
-27	1	7	499	-479	48
-25	1	7	226	-236	-90
-23	1	7	2151	2276	30
-21	1	7	495	-479	38
-19	1	7	1251	-1310	28
-17	1	7	663	-684	31
-15	1	7	1560	1644	25
-13	1	7	801	737	26
-11	1	7	1786	-1867	23
-9	1	7	2649	2493	21
-7	1	7	1492	1514	21
-5	1	7	2121	-2060	20
-3	1	7	1313	-1290	20
-1	1	7	2361	2318	19
1	1	7	2099	2128	19
3	1	7	3373	-3339	19
5	1	7	1653	-1673	19
7	1	7	3957	4006	19
9	1	7	332	-373	33
11	1	7	1557	-1551	21
13	1	7	312	371	35
15	1	7	757	785	26
17	1	7	736	706	27
19	1	7	1417	-1356	26
21	1	7	179	119	-74
23	1	7	1802	1797	27
25	1	7	2323	-2304	28
27	1	7	947	-1029	32
29	1	7	551	525	37
31	1	7	320	208	43
33	1	7	942	-1000	31
35	1	7	490	414	34
37	1	7	1010	995	29
-38	2	7	624	592	37
-36	2	7	165	-12	-165
-34	2	7	1293	-1254	35
-32	2	7	871	-950	38
-30	2	7	970	-971	37
-28	2	7	755	-770	39
-26	2	7	88	-144	-88
-24	2	7	698	689	37
-22	2	7	669	623	36
-20	2	7	202	-39	-86
-18	2	7	1922	-1899	28
-16	2	7	1942	1928	26
-14	2	7	832	808	27
-12	2	7	506	457	33
-10	2	7	1423	1308	23
-8	2	7	610	602	26
-6	2	7	440	-417	30
-4	2	7	1448	-1361	21
-2	2	7	64	-67	-64

h	k	l	10Fo	10Fc	10s
0	2	7	339	327	57
2	2	7	516	-477	25
4	2	7	355	-363	31
6	2	7	1197	1117	21
8	2	7	2004	2000	21
10	2	7	458	341	28
12	2	7	1513	-1502	23
14	2	7	561	536	28
16	2	7	1535	1516	25
18	2	7	1090	-1066	26
20	2	7	1299	1235	27
22	2	7	218	224	-58
24	2	7	686	-638	33
26	2	7	842	-834	32
28	2	7	921	-929	31
30	2	7	175	222	-101
32	2	7	71	-73	-71
34	2	7	634	-549	33
36	2	7	198	248	-57
-37	3	7	265	-202	-74
-35	3	7	500	438	45
-33	3	7	162	-182	-162
-31	3	7	1099	-1157	36
-29	3	7	1090	-1078	36
-27	3	7	571	513	39
-25	3	7	490	434	45
-23	3	7	318	-278	61
-21	3	7	1062	-1033	32
-19	3	7	1320	1424	31
-17	3	7	1048	1078	31
-15	3	7	1877	-1938	27
-13	3	7	1604	1735	26
-11	3	7	1110	1120	26
-9	3	7	245	-240	49
-7	3	7	72	-120	-72
-5	3	7	1519	1556	22
-3	3	7	695	-662	25
-1	3	7	2501	-2448	21
1	3	7	1712	-1708	21
3	3	7	2262	2226	21
5	3	7	1354	1344	22
7	3	7	1000	-968	23
9	3	7	651	615	26
11	3	7	1236	1236	24
13	3	7	849	869	27
15	3	7	2280	-2294	25
17	3	7	751	813	30
19	3	7	151	-1	-113
21	3	7	1122	-1174	29
23	3	7	831	-770	32
25	3	7	245	280	-66
27	3	7	482	470	41
29	3	7	1133	-1183	31
31	3	7	253	-330	59
33	3	7	1031	1078	31
35	3	7	65	-38	-65

h	k	l	10Fo	10Fc	10s
-36	4	7	84	-35	-84
-34	4	7	591	653	46
-32	4	7	297	316	68
-30	4	7	662	-600	42
-28	4	7	433	-533	56
-26	4	7	1277	1187	35
-24	4	7	1395	-1384	34
-22	4	7	948	-912	36
-20	4	7	1768	1881	32
-18	4	7	1371	1403	32
-16	4	7	466	-468	41
-14	4	7	788	-790	32
-12	4	7	411	-392	42
-10	4	7	409	410	37
-8	4	7	2108	-2085	25
-6	4	7	1250	1199	25
-4	4	7	3030	3100	23
-2	4	7	138	96	-118
0	4	7	2881	-2850	18
2	4	7	470	-445	31
4	4	7	1493	1396	23
6	4	7	465	-473	31
8	4	7	698	-634	28
10	4	7	874	894	27
12	4	7	1202	1205	26
14	4	7	865	-860	27
16	4	7	1181	-1174	29
18	4	7	1011	991	29
20	4	7	206	209	-73
22	4	7	1348	-1350	30
24	4	7	185	159	-96
26	4	7	1816	1736	30
28	4	7	195	135	-81
30	4	7	991	-993	32
32	4	7	190	221	-66
34	4	7	204	57	-54
-35	5	7	209	-165	-107
-33	5	7	425	419	48
-31	5	7	1402	1371	35
-29	5	7	758	788	43
-27	5	7	665	-716	45
-25	5	7	346	-360	60
-23	5	7	290	-427	-84
-21	5	7	456	497	48
-19	5	7	160	222	-160
-17	5	7	243	57	-68
-15	5	7	241	133	-80
-13	5	7	1445	-1470	31
-11	5	7	1456	-1437	30
-9	5	7	1126	-1092	29
-7	5	7	805	873	30
-5	5	7	1862	1864	27
-3	5	7	144	63	-108
-1	5	7	670	660	29
1	5	7	134	115	-134
3	5	7	1520	-1608	25

h	k	l	10Fo	10Fc	10s
5	5	7	610	-638	33
7	5	7	252	-270	60
9	5	7	584	-570	32
11	5	7	239	128	54
13	5	7	663	713	32
15	5	7	76	-87	-76
17	5	7	325	-327	45
19	5	7	472	-463	39
21	5	7	343	400	49
23	5	7	361	370	50
25	5	7	300	392	58
27	5	7	326	399	58
29	5	7	676	710	35
31	5	7	111	-63	-111
33	5	7	739	-776	33
-32	6	7	819	915	40
-30	6	7	1799	1793	36
-28	6	7	225	348	-126
-26	6	7	873	-872	41
-24	6	7	540	598	51
-22	6	7	608	531	45
-20	6	7	1156	-1162	37
-18	6	7	637	-630	41
-16	6	7	396	326	53
-14	6	7	180	233	-139
-12	6	7	1114	-1077	35
-10	6	7	1336	-1370	33
-8	6	7	1222	1219	32
-6	6	7	255	327	-71
-4	6	7	1868	-1942	29
-2	6	7	481	489	42
0	6	7	2310	2302	66
2	6	7	453	-448	35
4	6	7	2224	-2165	28
6	6	7	414	481	43
8	6	7	1474	1407	29
10	6	7	2012	-1928	29
12	6	7	1391	-1449	31
14	6	7	905	917	33
16	6	7	570	546	38
18	6	7	661	-600	35
20	6	7	1036	-1045	34
22	6	7	1240	1245	33
24	6	7	360	297	48
26	6	7	915	-953	35
28	6	7	861	880	34
30	6	7	1342	1347	31
32	6	7	194	-225	-85
-31	7	7	413	415	57
-29	7	7	95	193	-95
-27	7	7	89	-25	-89
-25	7	7	708	745	44
-23	7	7	97	-30	-97
-21	7	7	278	-435	-100
-19	7	7	794	-798	41
-17	7	7	482	-540	59

h	k	l	10Fo	10Fc	10s
-15	7	7	729	732	42
-13	7	7	560	-603	47
-11	7	7	1001	1040	39
-9	7	7	555	546	43
-7	7	7	680	-708	41
-5	7	7	1473	-1546	34
-3	7	7	1136	-1240	35
-1	7	7	1195	1229	32
1	7	7	788	733	36
3	7	7	86	132	-86
5	7	7	722	749	36
7	7	7	447	-388	45
9	7	7	219	-219	-71
11	7	7	532	-529	43
13	7	7	1299	-1304	34
15	7	7	1447	1464	34
17	7	7	82	-59	-82
19	7	7	90	165	-90
21	7	7	390	451	55
23	7	7	243	250	-68
25	7	7	216	186	-73
27	7	7	473	-467	42
29	7	7	126	131	-126
-28	8	7	390	330	58
-26	8	7	1086	1110	39
-24	8	7	181	160	-181
-22	8	7	727	-713	46
-20	8	7	209	-260	-175
-18	8	7	171	247	-171
-16	8	7	1095	-1122	41
-14	8	7	574	-538	48
-12	8	7	1785	1764	39
-10	8	7	279	194	-87
-8	8	7	859	-778	42
-6	8	7	678	-728	43
-4	8	7	706	650	41
-2	8	7	317	-322	74
0	8	7	1418	-1388	47
2	8	7	1526	1444	35
4	8	7	2112	1996	34
6	8	7	1374	-1339	36
8	8	7	1373	-1325	35
10	8	7	332	399	69
12	8	7	1309	1284	37
14	8	7	1263	-1221	36
16	8	7	574	-595	44
18	8	7	1540	1616	36
20	8	7	154	-129	-154
22	8	7	590	-510	38
24	8	7	161	104	-121
26	8	7	80	165	-80
28	8	7	499	-552	41
-25	9	7	401	446	73
-23	9	7	776	-797	45
-21	9	7	568	651	49
-19	9	7	752	719	51

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
-17	9	7	515	-496	57
-15	9	7	512	-490	60
-13	9	7	314	242	-82
-11	9	7	1394	1449	43
-9	9	7	319	-387	-81
-7	9	7	1314	-1344	41
-5	9	7	727	782	48
-3	9	7	880	929	45
-1	9	7	592	-618	49
1	9	7	99	-84	-99
3	9	7	877	840	41
5	9	7	235	-205	-112
7	9	7	883	-886	44
9	9	7	650	648	45
11	9	7	789	771	43
13	9	7	276	-118	67
15	9	7	592	-586	47
17	9	7	92	17	-92
19	9	7	748	850	42
21	9	7	245	-207	-63
23	9	7	383	-428	54
25	9	7	86	141	-86
-20	10	7	90	-155	-90
-18	10	7	100	19	-100
-16	10	7	945	945	47
-14	10	7	247	-78	-116
-12	10	7	103	21	-103
-10	10	7	107	52	-107
-8	10	7	431	416	65
-6	10	7	621	505	52
-4	10	7	839	-830	50
-2	10	7	451	408	64
0	10	7	133	134	-86
2	10	7	451	-389	62
4	10	7	98	-95	-98
6	10	7	143	2	-143
8	10	7	883	936	48
10	10	7	98	207	-98
12	10	7	298	-202	-80
14	10	7	1136	1121	41
16	10	7	233	-196	-84
18	10	7	712	-686	43
20	10	7	88	-5	-88
-15	11	7	914	1035	53
-13	11	7	226	-122	-135
-11	11	7	995	-945	51
-9	11	7	487	278	59
-7	11	7	1131	1101	48
-5	11	7	690	-747	58
-3	11	7	295	-224	-98
-1	11	7	339	161	79
1	11	7	101	61	-101
3	11	7	549	-436	61
5	11	7	475	-424	62
7	11	7	1308	1253	46
9	11	7	454	409	61

h	k	l	10Fo	10Fc	10s
11	11	7	834	-733	47
13	11	7	155	65	-155
15	11	7	690	620	45
-2	12	7	107	-13	-107
0	12	7	105	39	-74
2	12	7	151	53	-151
-36	0	8	757	712	35
-34	0	8	87	167	-87
-32	0	8	1057	-997	35
-30	0	8	86	88	-86
-28	0	8	1160	1176	34
-26	0	8	507	-508	42
-24	0	8	1192	-1144	33
-22	0	8	401	-422	45
-20	0	8	1391	1446	30
-18	0	8	1606	-1597	28
-16	0	8	1310	-1220	27
-14	0	8	4228	4123	25
-12	0	8	813	816	26
-10	0	8	2471	-2358	23
-8	0	8	730	-777	26
-6	0	8	2851	2624	21
-4	0	8	376	396	30
-2	0	8	2494	-2517	20
0	0	8	1309	-1361	21
2	0	8	2476	2495	20
4	0	8	1484	-1612	21
6	0	8	1674	-1713	21
8	0	8	1480	1510	22
10	0	8	1063	1090	23
12	0	8	1135	-1162	24
14	0	8	1540	-1553	24
16	0	8	3480	3468	24
18	0	8	137	41	-137
20	0	8	768	-710	30
22	0	8	401	-458	40
24	0	8	307	282	47
26	0	8	78	95	-78
28	0	8	1257	-1175	30
30	0	8	1074	1028	31
32	0	8	966	952	31
34	0	8	933	-954	30
36	0	8	67	5	-67
-37	1	8	79	98	-79
-35	1	8	193	265	-106
-33	1	8	349	-391	59
-31	1	8	83	-23	-83
-29	1	8	502	467	47
-27	1	8	383	417	54
-25	1	8	712	-735	39
-23	1	8	223	32	-75
-21	1	8	81	126	-81
-19	1	8	428	-469	43
-17	1	8	883	878	30
-15	1	8	1563	-1590	27
-13	1	8	1438	1436	26

h	k	l	10Fo	10Fc	10s
-11	1	8	825	782	26
-9	1	8	794	-765	26
-7	1	8	1043	960	23
-5	1	8	64	1	-64
-3	1	8	506	-487	26
-1	1	8	1909	-1904	20
1	1	8	1065	997	22
3	1	8	220	277	46
5	1	8	709	-694	23
7	1	8	755	830	24
9	1	8	200	-72	43
11	1	8	507	-524	29
13	1	8	240	189	44
15	1	8	70	107	-70
17	1	8	543	554	33
19	1	8	69	-24	-69
21	1	8	1348	-1295	28
23	1	8	77	177	-77
25	1	8	69	-125	-69
27	1	8	383	-354	43
29	1	8	68	-88	-68
31	1	8	68	-49	-68
33	1	8	496	476	35
35	1	8	174	-80	-66
-36	2	8	626	-595	38
-34	2	8	288	-250	63
-32	2	8	432	376	46
-30	2	8	435	-481	48
-28	2	8	987	-1010	36
-26	2	8	89	53	-89
-24	2	8	1828	1757	32
-22	2	8	872	-801	34
-20	2	8	958	-975	32
-18	2	8	1433	1433	30
-16	2	8	1059	1051	29
-14	2	8	1537	-1537	27
-12	2	8	1353	-1279	26
-10	2	8	1751	1671	24
-8	2	8	1000	1056	25
-6	2	8	2447	-2423	22
-4	2	8	487	419	28
-2	2	8	707	742	25
0	2	8	1338	-1341	15
2	2	8	197	84	-53
4	2	8	64	-100	-64
6	2	8	3005	3046	22
8	2	8	809	-874	24
10	2	8	1360	-1387	24
12	2	8	776	798	27
14	2	8	254	258	49
16	2	8	1238	-1222	26
18	2	8	1166	-1165	28
20	2	8	1574	1597	28
22	2	8	918	1023	31
24	2	8	1537	-1490	29
26	2	8	327	305	46

h	k	l	10Fo	10Fc	10s
28	2	8	943	964	31
30	2	8	506	-571	36
32	2	8	683	-674	32
34	2	8	480	487	35
-35	3	8	536	-533	41
-33	3	8	514	537	45
-31	3	8	388	263	51
-29	3	8	1035	-927	37
-27	3	8	753	-683	37
-25	3	8	983	987	37
-23	3	8	448	486	51
-21	3	8	559	-602	43
-19	3	8	334	264	50
-17	3	8	854	801	33
-15	3	8	85	-192	-85
-13	3	8	2323	-2451	27
-11	3	8	260	273	53
-9	3	8	1575	1492	26
-7	3	8	193	59	-67
-5	3	8	969	-945	25
-3	3	8	728	688	25
-1	3	8	1420	1444	23
1	3	8	1140	-1135	23
3	3	8	803	-785	25
5	3	8	827	899	25
7	3	8	564	570	27
9	3	8	169	-153	-73
11	3	8	140	36	-95
13	3	8	510	491	33
15	3	8	176	85	-80
17	3	8	1661	-1677	27
19	3	8	76	74	-76
21	3	8	1861	1834	28
23	3	8	475	-389	34
25	3	8	74	-68	-74
27	3	8	754	761	33
29	3	8	144	237	-144
31	3	8	950	-990	31
33	3	8	844	-804	31
35	3	8	1204	1152	27
-34	4	8	201	93	-113
-32	4	8	226	111	-90
-30	4	8	305	134	56
-28	4	8	754	637	39
-26	4	8	782	738	38
-24	4	8	1213	-1205	35
-22	4	8	711	696	38
-20	4	8	214	26	-89
-18	4	8	272	-170	59
-16	4	8	1005	-1017	34
-14	4	8	292	-251	62
-12	4	8	901	918	31
-10	4	8	2185	-2091	27
-8	4	8	321	299	49
-6	4	8	1042	1027	27
-4	4	8	1508	1507	25

h	k	l	10Fo	10Fc	10s
-2	4	8	185	-177	-64
0	4	8	188	272	-47
2	4	8	497	499	31
4	4	8	1205	-1135	25
6	4	8	1040	-1027	26
8	4	8	908	841	27
10	4	8	743	757	29
12	4	8	421	-392	38
14	4	8	248	-285	54
16	4	8	486	452	35
18	4	8	82	133	-82
20	4	8	685	-709	33
22	4	8	386	-345	40
24	4	8	952	991	33
26	4	8	78	-143	-78
28	4	8	763	-766	34
30	4	8	72	26	-72
32	4	8	197	204	-77
34	4	8	194	-128	-64
-33	5	8	658	-536	37
-31	5	8	90	-31	-90
-29	5	8	343	389	64
-27	5	8	639	723	41
-25	5	8	904	-871	39
-23	5	8	759	-738	41
-21	5	8	1441	1512	35
-19	5	8	313	363	64
-17	5	8	2599	-2644	32
-15	5	8	898	930	34
-13	5	8	2093	2214	31
-11	5	8	273	-237	64
-9	5	8	2516	-2642	29
-7	5	8	189	-279	-117
-5	5	8	1394	1344	28
-3	5	8	998	-1009	29
-1	5	8	338	185	39
1	5	8	1705	1646	27
3	5	8	1345	1331	27
5	5	8	1957	-1944	27
7	5	8	1266	-1245	28
9	5	8	1024	1047	29
11	5	8	398	407	43
13	5	8	1993	-2003	28
15	5	8	667	722	33
17	5	8	1836	1907	30
19	5	8	839	-789	32
21	5	8	712	-687	34
23	5	8	342	410	51
25	5	8	1003	975	32
27	5	8	609	-522	35
29	5	8	233	-220	-65
31	5	8	1043	1042	30
-32	6	8	94	252	-94
-30	6	8	138	38	-138
-28	6	8	453	531	54
-26	6	8	195	116	-173

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
-24	6	8	489	-515	51
-22	6	8	525	563	49
-20	6	8	919	-976	39
-18	6	8	580	610	47
-16	6	8	280	307	65
-14	6	8	212	111	-103
-12	6	8	596	510	41
-10	6	8	859	-781	36
-8	6	8	321	287	53
-6	6	8	487	-406	43
-4	6	8	1219	-1291	32
-2	6	8	196	195	-80
0	6	8	1068	1098	51
2	6	8	912	967	33
4	6	8	570	537	36
6	6	8	709	-645	33
8	6	8	810	-842	33
10	6	8	705	-674	35
12	6	8	716	651	36
14	6	8	80	-64	-80
16	6	8	129	99	-129
18	6	8	468	484	44
20	6	8	583	-538	36
22	6	8	79	34	-79
24	6	8	193	-235	-102
26	6	8	480	-422	38
28	6	8	305	251	54
30	6	8	899	833	30
-29	7	8	915	-962	41
-27	7	8	531	-595	54
-25	7	8	778	825	45
-23	7	8	90	-89	-90
-21	7	8	97	-55	-97
-19	7	8	537	-580	52
-17	7	8	1047	1050	39
-15	7	8	131	92	-131
-13	7	8	1317	-1340	37
-11	7	8	681	663	46
-9	7	8	1365	1536	37
-7	7	8	1215	-1234	36
-5	7	8	1635	-1695	35
-3	7	8	1290	1253	34
-1	7	8	1276	1356	33
1	7	8	1231	-1185	34
3	7	8	1235	-1168	33
5	7	8	1375	1365	34
7	7	8	359	-345	53
9	7	8	1675	-1629	33
11	7	8	276	332	-69
13	7	8	1278	1304	34
15	7	8	170	130	-170
17	7	8	1434	-1410	34
19	7	8	289	305	60
21	7	8	1062	1081	34
23	7	8	862	-879	34
25	7	8	622	-594	38

h	k	l	10Fo	10Fc	10s
27	7	8	519	487	38
-26	8	8	214	-150	-105
-24	8	8	510	469	53
-22	8	8	817	-765	45
-20	8	8	193	67	-193
-18	8	8	753	815	44
-16	8	8	95	101	-95
-14	8	8	290	-332	-84
-12	8	8	831	-784	45
-10	8	8	704	812	49
-8	8	8	333	441	73
-6	8	8	146	33	-146
-4	8	8	284	219	-76
-2	8	8	272	156	-72
0	8	8	486	-587	36
2	8	8	1274	-1330	36
4	8	8	492	-516	47
6	8	8	748	693	41
8	8	8	156	-152	-156
10	8	8	271	119	-69
12	8	8	409	433	54
14	8	8	389	432	48
16	8	8	321	-378	61
18	8	8	656	-663	41
20	8	8	682	615	39
22	8	8	345	401	51
24	8	8	662	-740	39
26	8	8	464	453	40
-23	9	8	337	247	73
-21	9	8	694	592	50
-19	9	8	98	-59	-98
-17	9	8	379	-365	73
-15	9	8	531	-561	54
-13	9	8	973	984	44
-11	9	8	105	-17	-105
-9	9	8	693	-690	45
-7	9	8	740	784	46
-5	9	8	497	587	63
-3	9	8	465	-453	54
-1	9	8	746	-766	47
1	9	8	488	423	48
3	9	8	151	-92	-151
5	9	8	1189	-1122	40
7	9	8	941	879	40
9	9	8	1430	1454	38
11	9	8	90	-104	-90
13	9	8	779	-734	44
15	9	8	367	-359	60
17	9	8	383	435	63
19	9	8	233	-125	-82
21	9	8	819	-830	38
-18	10	8	715	-754	53
-16	10	8	310	-398	-104
-14	10	8	956	991	47
-12	10	8	344	366	-90
-10	10	8	775	-799	53

h	k	l	10Fo	10Fc	10s
-8	10	8	542	-532	60
-6	10	8	834	908	50
-4	10	8	487	439	64
-2	10	8	1541	-1603	44
0	10	8	325	-210	52
2	10	8	758	767	52
4	10	8	283	244	-90
6	10	8	197	276	-197
8	10	8	91	8	-91
10	10	8	624	477	45
12	10	8	346	-253	67
14	10	8	1462	-1385	39
16	10	8	1081	1092	39
-11	11	8	285	188	-116
-9	11	8	112	43	-112
-7	11	8	345	318	85
-5	11	8	687	-717	57
-3	11	8	105	-32	-105
-1	11	8	554	462	53
1	11	8	93	-21	-93
3	11	8	531	518	57
5	11	8	98	110	-98
7	11	8	313	-205	72
9	11	8	94	-46	-94
-35	1	9	454	-407	39
-33	1	9	1169	-1264	35
-31	1	9	180	105	-111
-29	1	9	604	599	39
-27	1	9	905	-928	35
-25	1	9	86	-99	-86
-23	1	9	1924	2019	32
-21	1	9	871	886	34
-19	1	9	1275	-1236	31
-17	1	9	1367	-1410	29
-15	1	9	1356	1341	29
-13	1	9	536	-573	33
-11	1	9	2125	-2057	26
-9	1	9	1960	1851	25
-7	1	9	871	840	26
-5	1	9	917	-873	24
-3	1	9	1495	-1533	23
-1	1	9	1410	1409	23
1	1	9	1837	1850	22
3	1	9	877	-845	24
5	1	9	2283	-2336	23
7	1	9	2377	2413	23
9	1	9	245	-218	43
11	1	9	2084	-2130	24
13	1	9	1270	-1270	26
15	1	9	421	457	34
17	1	9	345	-362	43
19	1	9	1102	-1059	28
21	1	9	1504	1432	28
23	1	9	1222	1239	29
25	1	9	648	-529	32
27	1	9	527	-552	35

h	k	l	10Fo	10Fc	10s
29	1	9	347	358	42
31	1	9	708	690	31
33	1	9	367	-372	41
-34	2	9	695	-673	36
-32	2	9	204	-169	-83
-30	2	9	227	215	-80
-28	2	9	182	210	-116
-26	2	9	546	-517	40
-24	2	9	159	146	-159
-22	2	9	2417	2344	31
-20	2	9	624	-534	38
-18	2	9	1568	-1517	31
-16	2	9	541	516	37
-14	2	9	371	-345	40
-12	2	9	369	402	46
-10	2	9	648	-652	31
-8	2	9	1209	1246	26
-6	2	9	1291	1254	25
-4	2	9	421	-412	34
-2	2	9	480	527	31
0	2	9	435	429	23
2	2	9	663	690	27
4	2	9	1985	-1987	23
6	2	9	244	300	51
8	2	9	1478	1467	24
10	2	9	69	81	-69
12	2	9	1597	-1582	26
14	2	9	594	590	31
16	2	9	515	-536	34
18	2	9	1009	-1036	29
20	2	9	138	44	-138
22	2	9	1302	1237	29
24	2	9	270	240	55
26	2	9	1138	-1117	30
28	2	9	66	43	-66
30	2	9	857	861	30
32	2	9	363	399	43
-33	3	9	1078	1149	34
-31	3	9	645	-624	38
-29	3	9	728	-676	37
-27	3	9	174	-32	-174
-25	3	9	1057	1095	36
-23	3	9	701	-677	38
-21	3	9	1175	-1263	35
-19	3	9	1718	1801	32
-17	3	9	88	-239	-88
-15	3	9	849	-816	32
-13	3	9	81	170	-81
-11	3	9	787	757	31
-9	3	9	360	-367	44
-7	3	9	1225	-1212	26
-5	3	9	704	716	29
-3	3	9	2138	2095	25
-1	3	9	781	-787	28
1	3	9	1264	-1278	25
3	3	9	532	527	29

h	k	l	10Fo	10Fc	10s
5	3	9	308	-293	38
7	3	9	1050	-1065	27
9	3	9	804	-838	27
11	3	9	1622	1633	26
13	3	9	157	-93	-91
15	3	9	1758	-1799	27
17	3	9	250	249	56
19	3	9	73	97	-73
21	3	9	327	-251	41
23	3	9	598	-561	35
25	3	9	737	734	34
27	3	9	1352	1315	30
29	3	9	624	-657	34
31	3	9	572	-525	33
33	3	9	744	743	30
-32	4	9	586	532	39
-30	4	9	574	-553	42
-28	4	9	268	-339	-78
-26	4	9	1322	1302	36
-24	4	9	305	-420	74
-22	4	9	1470	-1590	35
-20	4	9	342	350	60
-18	4	9	1799	1793	33
-16	4	9	530	-499	43
-14	4	9	1542	-1527	31
-12	4	9	1833	1770	30
-10	4	9	407	427	42
-8	4	9	2134	-2124	28
-6	4	9	892	-842	30
-4	4	9	2223	2195	27
-2	4	9	579	583	33
0	4	9	866	-805	47
2	4	9	439	-472	34
4	4	9	1238	1228	27
6	4	9	626	-630	30
8	4	9	1735	-1786	27
10	4	9	506	492	33
12	4	9	1780	1819	28
14	4	9	489	-473	36
16	4	9	1070	-1063	31
18	4	9	1263	1247	30
20	4	9	182	184	-94
22	4	9	1740	-1720	30
24	4	9	208	-111	-77
26	4	9	1217	1174	30
28	4	9	440	477	40
30	4	9	950	-887	30
32	4	9	70	116	-70
-31	5	9	682	653	39
-29	5	9	211	82	-93
-27	5	9	349	-380	67
-25	5	9	237	-169	-91
-23	5	9	268	-225	-74
-21	5	9	628	664	44
-19	5	9	240	-155	-84
-17	5	9	367	-374	53

Observed and calculated structure factors for {[Ru(bipy)$_2$]$_2$L}(PF$_6$)$_4$

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
-15	5	9	972	981	36	-19	7	9	721	-736	47	-1	9	9	134	176	-134	30	0	10	316	-343	42	10	2	10	387	-361	39
-13	5	9	280	-322	-72	-17	7	9	480	518	52	1	9	9	694	-593	44	32	0	10	736	743	29	12	2	10	694	737	31
-11	5	9	88	-102	-88	-15	7	9	455	-538	57	3	9	9	860	824	40	-33	1	10	236	-224	-61	14	2	10	854	849	30
-9	5	9	372	-393	55	-13	7	9	95	199	-95	5	9	9	1103	1040	40	-31	1	10	625	-632	38	16	2	10	869	-817	29
-7	5	9	173	189	-133	-11	7	9	214	262	-106	7	9	9	1511	-1525	38	-29	1	10	83	39	-83	18	2	10	1254	-1237	29
-5	5	9	424	-420	44	-9	7	9	211	-2	-106	9	9	9	567	-467	42	-27	1	10	88	91	-88	20	2	10	280	288	52
-3	5	9	408	-363	45	-7	7	9	803	785	39	11	9	9	92	92	-92	-25	1	10	480	-361	44	22	2	10	908	912	32
-1	5	9	443	381	37	-5	7	9	91	133	-91	13	9	9	168	275	-168	-23	1	10	82	243	-82	24	2	10	577	-521	35
1	5	9	1357	1347	28	-3	7	9	869	-852	36	15	9	9	1115	-1104	38	-21	1	10	355	320	51	26	2	10	793	-771	32
3	5	9	127	-150	-127	-1	7	9	351	-416	61	17	9	9	244	275	-67	-19	1	10	213	320	-98	28	2	10	1016	984	29
5	5	9	340	-334	48	1	7	9	583	-580	40	19	9	9	1179	1172	34	-17	1	10	1043	-980	32	30	2	10	699	658	30
7	5	9	79	109	-79	3	7	9	86	-145	-86	-14	10	9	423	380	76	-15	1	10	1128	-1035	30	-31	3	10	1202	1185	34
9	5	9	262	-274	60	5	7	9	79	94	-79	-12	10	9	243	-136	-134	-13	1	10	876	869	32	-29	3	10	345	-379	56
11	5	9	283	212	56	7	7	9	764	811	37	-10	10	9	381	-361	85	-11	1	10	490	470	36	-27	3	10	806	-811	37
13	5	9	294	383	54	9	7	9	1439	1389	33	-8	10	9	586	476	52	-9	1	10	76	159	-76	-25	3	10	721	727	39
15	5	9	934	903	31	11	7	9	219	-217	-80	-6	10	9	104	-100	-104	-7	1	10	316	311	43	-23	3	10	192	277	-120
17	5	9	148	-120	-148	13	7	9	83	-162	-83	-4	10	9	329	-489	-102	-5	1	10	439	487	35	-21	3	10	1032	-1091	35
19	5	9	225	-165	-77	15	7	9	623	671	42	-2	10	9	367	523	92	-3	1	10	361	376	33	-19	3	10	349	-316	52
21	5	9	76	8	-76	17	7	9	147	-297	-147	0	10	9	422	394	44	-1	1	10	1328	-1389	25	-17	3	10	1868	1882	32
23	5	9	178	42	-84	19	7	9	167	-174	-163	2	10	9	355	395	69	1	1	10	65	142	-65	-15	3	10	794	789	34
25	5	9	72	1	-72	21	7	9	194	260	-85	4	10	9	87	41	-87	3	1	10	1226	1240	25	-13	3	10	1475	-1472	30
27	5	9	409	-421	44	23	7	9	242	299	-75	6	10	9	619	-657	49	5	1	10	1385	-1389	25	-11	3	10	595	-545	37
29	5	9	210	130	-65	25	7	9	411	-370	40	8	10	9	88	2	-88	7	1	10	615	628	28	-9	3	10	269	156	55
-28	6	9	194	51	-107	-24	8	9	431	435	57	10	10	9	323	-338	69	9	1	10	68	145	-68	-7	3	10	199	164	-81
-26	6	9	1776	-1774	36	-22	8	9	1174	-1152	40	12	10	9	537	-438	44	11	1	10	963	-951	28	-5	3	10	1460	-1473	28
-24	6	9	549	531	52	-20	8	9	101	80	-101	-32	0	10	1369	-1369	33	13	1	10	416	-383	34	-3	3	10	210	253	-65
-22	6	9	797	748	39	-18	8	9	701	643	46	-30	0	10	723	-711	39	15	1	10	544	-559	31	-1	3	10	2085	2051	26
-20	6	9	489	-519	45	-16	8	9	444	-391	65	-28	0	10	834	770	38	17	1	10	700	663	31	1	3	10	904	-900	27
-18	6	9	676	-599	42	-14	8	9	416	-404	61	-26	0	10	744	712	36	19	1	10	458	-405	36	3	3	10	892	-899	27
-16	6	9	92	246	-92	-12	8	9	589	595	46	-24	0	10	528	-439	40	21	1	10	74	-44	-74	5	3	10	743	720	29
-14	6	9	1373	1378	36	-10	8	9	619	614	48	-22	0	10	1151	1107	33	23	1	10	846	874	31	7	3	10	351	322	42
-12	6	9	1685	-1694	35	-8	8	9	1032	-1027	40	-20	0	10	738	671	36	25	1	10	341	393	43	9	3	10	590	-638	32
-10	6	9	900	-886	36	-6	8	9	98	-186	-98	-18	0	10	1839	-1815	30	27	1	10	139	-17	-139	11	3	10	178	-207	-69
-8	6	9	1813	1780	33	-4	8	9	1353	1379	39	-16	0	10	2120	-2070	29	29	1	10	602	-604	32	13	3	10	1574	1642	28
-6	6	9	323	312	59	-2	8	9	589	-664	49	-14	0	10	460	-397	37	31	1	10	64	-174	-64	15	3	10	834	868	32
-4	6	9	1843	-1852	32	0	8	9	1706	-1636	54	-12	0	10	2861	2667	27	-32	2	10	755	768	36	17	3	10	1334	-1267	29
-2	6	9	774	-687	36	2	8	9	575	571	44	-10	0	10	331	-226	43	-30	2	10	499	448	41	19	3	10	426	-429	38
0	6	9	1065	1101	24	4	8	9	1261	1226	38	-8	0	10	1044	-1072	28	-28	2	10	1241	-1240	35	21	3	10	474	547	38
2	6	9	78	-79	-78	6	8	9	603	570	44	-6	0	10	1680	1608	25	-26	2	10	309	-216	59	23	3	10	632	-664	32
4	6	9	1880	-1912	30	8	8	9	1196	-1092	36	-4	0	10	1177	1177	26	-24	2	10	805	873	39	25	3	10	651	-660	33
6	6	9	872	839	34	10	8	9	229	94	-100	-2	0	10	2212	-2158	24	-22	2	10	390	-361	51	27	3	10	519	536	35
8	6	9	1762	1700	30	12	8	9	606	645	46	0	0	10	367	-397	35	-20	2	10	1273	-1266	33	29	3	10	922	965	30
10	6	9	644	-633	37	14	8	9	1049	-1076	36	2	0	10	1189	1210	24	-18	2	10	753	759	36	-30	4	10	82	137	-82
12	6	9	557	-510	37	16	8	9	80	-97	-80	4	0	10	955	965	25	-16	2	10	1974	1886	30	-28	4	10	979	1003	37
14	6	9	163	175	-134	18	8	9	633	656	41	6	0	10	2823	-2959	24	-14	2	10	447	-394	43	-26	4	10	245	285	-86
16	6	9	1365	1381	33	20	8	9	534	491	38	8	0	10	1010	1092	26	-12	2	10	1733	-1665	29	-24	4	10	667	-650	40
18	6	9	630	-565	39	22	8	9	287	-343	57	10	0	10	2169	2194	25	-10	2	10	899	889	31	-22	4	10	608	-613	42
20	6	9	861	-820	33	-19	9	9	312	388	-94	12	0	10	1952	-1881	26	-8	2	10	424	383	40	-20	4	10	960	960	37
22	6	9	1296	1286	32	-17	9	9	263	331	-112	14	0	10	1313	-1327	27	-6	2	10	871	-885	29	-18	4	10	276	182	61
24	6	9	188	187	-95	-15	9	9	899	-963	44	16	0	10	227	10	55	-4	2	10	185	-102	-60	-16	4	10	1133	-1032	34
26	6	9	957	-949	32	-13	9	9	285	-51	-80	18	0	10	1587	1585	28	-2	2	10	932	916	27	-14	4	10	904	934	35
28	6	9	382	-367	41	-11	9	9	1040	1088	45	20	0	10	1192	1153	29	0	2	10	768	778	22	-12	4	10	751	728	35
-27	7	9	212	-120	-111	-9	9	9	170	44	-170	22	0	10	515	-511	36	2	2	10	1609	-1676	25	-10	4	10	1208	-1161	32
-25	7	9	254	-319	-98	-7	9	9	1356	-1450	42	24	0	10	176	54	-85	4	2	10	1044	-1031	26	-8	4	10	659	-624	36
-23	7	9	366	296	58	-5	9	9	96	-92	-96	26	0	10	614	595	32	6	2	10	1874	1952	25	-6	4	10	315	285	57
-21	7	9	286	263	-86	-3	9	9	693	754	49	28	0	10	1128	-973	29	8	2	10	70	-41	-70	-4	4	10	305	326	58

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
-2	4	10	248	-170	60
0	4	10	96	69	-62
2	4	10	1320	1314	28
4	4	10	599	-541	30
6	4	10	827	-791	30
8	4	10	228	106	-61
10	4	10	167	126	-88
12	4	10	345	-284	40
14	4	10	478	-416	37
16	4	10	808	837	33
18	4	10	480	444	38
20	4	10	698	-670	33
22	4	10	455	-441	39
24	4	10	163	85	-114
26	4	10	68	2	-68
28	4	10	575	-560	31
-29	5	10	116	118	-116
-27	5	10	1137	1196	37
-25	5	10	520	-586	50
-23	5	10	1143	-1220	37
-21	5	10	2032	2122	35
-19	5	10	263	-26	66
-17	5	10	1299	-1354	35
-15	5	10	242	-273	-81
-13	5	10	1181	1141	34
-11	5	10	803	858	38
-9	5	10	1781	-1873	33
-7	5	10	170	-114	-123
-5	5	10	1599	1566	31
-3	5	10	1289	-1302	31
-1	5	10	1097	-1123	31
1	5	10	195	202	-70
3	5	10	1692	1653	29
5	5	10	109	-149	-109
7	5	10	1497	-1472	30
9	5	10	1923	1870	30
11	5	10	801	736	32
13	5	10	1469	-1517	30
15	5	10	77	264	-77
17	5	10	1275	1280	32
19	5	10	407	419	43
21	5	10	1404	-1374	31
23	5	10	80	-147	-80
25	5	10	718	728	33
27	5	10	483	-459	35
-26	6	10	278	224	69
-24	6	10	152	-23	-152
-22	6	10	593	-580	40
-20	6	10	429	439	53
-18	6	10	155	142	-155
-16	6	10	434	336	53
-14	6	10	94	-169	-94
-12	6	10	265	-350	-89
-10	6	10	463	453	51
-8	6	10	87	-22	-87
-6	6	10	90	129	-90

h	k	l	10Fo	10Fc	10s
-4	6	10	286	-257	63
-2	6	10	629	-678	40
0	6	10	887	-875	46
2	6	10	578	564	38
4	6	10	484	532	40
6	6	10	190	176	-92
8	6	10	129	-190	-129
10	6	10	363	-336	44
12	6	10	374	310	52
14	6	10	704	-747	35
16	6	10	311	256	53
18	6	10	190	-185	-88
20	6	10	81	104	-81
22	6	10	283	209	52
24	6	10	73	29	-73
26	6	10	105	23	-105
-23	7	10	736	738	41
-21	7	10	675	-739	46
-19	7	10	592	-553	44
-17	7	10	867	841	40
-15	7	10	92	125	-92
-13	7	10	976	-1048	41
-11	7	10	461	369	44
-9	7	10	718	782	44
-7	7	10	377	434	56
-5	7	10	1251	-1217	35
-3	7	10	313	219	60
-1	7	10	982	974	37
1	7	10	257	-153	-72
3	7	10	1307	-1207	33
5	7	10	885	872	34
7	7	10	816	794	38
9	7	10	1569	-1563	34
11	7	10	918	-911	35
13	7	10	1110	1124	35
15	7	10	572	564	38
17	7	10	999	-931	34
19	7	10	151	-71	-147
21	7	10	779	711	34
23	7	10	292	271	55
-20	8	10	507	-545	51
-18	8	10	233	113	-93
-16	8	10	691	575	43
-14	8	10	228	-115	-119
-12	8	10	1038	-1045	43
-10	8	10	99	212	-99
-8	8	10	897	824	41
-6	8	10	172	-128	-147
-4	8	10	865	-869	40
-2	8	10	1030	1006	40
0	8	10	878	813	60
2	8	10	749	-738	40
4	8	10	275	-355	64
6	8	10	508	421	39
8	8	10	621	-651	43
10	8	10	571	-609	41

h	k	l	10Fo	10Fc	10s
12	8	10	276	326	-72
14	8	10	756	675	36
16	8	10	81	12	-81
18	8	10	588	-571	40
20	8	10	714	757	38
-15	9	10	404	-368	55
-13	9	10	838	877	45
-11	9	10	213	16	-147
-9	9	10	633	-587	47
-7	9	10	94	-24	-94
-5	9	10	650	614	48
-3	9	10	316	340	78
-1	9	10	449	-439	58
1	9	10	641	577	44
3	9	10	241	70	-82
5	9	10	1169	-1054	38
7	9	10	86	-10	-86
9	9	10	218	-143	-84
11	9	10	611	599	45
13	9	10	545	-475	44
15	9	10	814	-771	38
-8	10	10	835	-849	47
-6	10	10	714	751	50
-4	10	10	894	983	46
-2	10	10	956	-1072	45
0	10	10	298	-268	-105
2	10	10	756	712	45
4	10	10	311	211	60
6	10	10	701	-732	47
-29	1	11	769	861	38
-27	1	11	658	-635	38
-25	1	11	1598	-1503	32
-23	1	11	443	359	44
-21	1	11	1476	1610	33
-19	1	11	85	168	-85
-17	1	11	81	29	-81
-15	1	11	1092	1048	31
-13	1	11	122	137	-122
-11	1	11	2428	-2358	29
-9	1	11	1045	-1006	31
-7	1	11	1747	1687	27
-5	1	11	969	885	29
-3	1	11	1394	-1389	27
-1	1	11	213	150	-59
1	1	11	667	652	29
3	1	11	1201	-1209	27
5	1	11	1672	-1676	26
7	1	11	222	167	55
9	1	11	2194	2280	26
11	1	11	568	-609	34
13	1	11	341	-350	43
15	1	11	478	457	38
17	1	11	257	283	64
19	1	11	1399	-1405	29
21	1	11	513	-526	36
23	1	11	1669	1610	29

h	k	l	10Fo	10Fc	10s
25	1	11	926	910	30
27	1	11	1052	-1014	29
29	1	11	283	284	40
-30	2	11	914	922	34
-28	2	11	216	-22	-62
-26	2	11	911	-976	37
-24	2	11	445	-528	47
-22	2	11	1135	1125	34
-20	2	11	471	448	42
-18	2	11	722	617	36
-16	2	11	574	532	39
-14	2	11	618	602	35
-12	2	11	657	-641	35
-10	2	11	1883	-1809	29
-8	2	11	486	472	38
-6	2	11	1022	1043	29
-4	2	11	209	127	-59
-2	2	11	225	-104	54
0	2	11	870	-883	20
2	2	11	286	256	42
4	2	11	1547	-1577	27
6	2	11	872	-861	30
8	2	11	875	808	29
10	2	11	771	-791	30
12	2	11	505	537	35
14	2	11	228	154	55
16	2	11	396	-363	39
18	2	11	848	-765	30
20	2	11	652	-609	32
22	2	11	779	765	31
24	2	11	716	662	31
26	2	11	336	-280	40
28	2	11	452	397	34
-29	3	11	658	-604	34
-27	3	11	194	300	-89
-25	3	11	1117	1056	34
-23	3	11	546	-493	40
-21	3	11	675	-628	38
-19	3	11	576	642	40
-17	3	11	507	516	40
-15	3	11	715	-687	37
-13	3	11	647	-639	36
-11	3	11	1366	1272	32
-9	3	11	291	348	60
-7	3	11	1440	-1408	29
-5	3	11	364	468	52
-3	3	11	562	498	34
-1	3	11	319	-383	54
1	3	11	493	-526	32
3	3	11	899	-944	29
5	3	11	744	754	30
7	3	11	989	-1050	29
9	3	11	436	-466	39
11	3	11	491	473	37
13	3	11	751	689	31
15	3	11	185	-31	-77

h	k	l	10Fo	10Fc	10s
17	3	11	162	-82	-109
19	3	11	837	802	33
21	3	11	283	-301	49
23	3	11	838	-805	31
25	3	11	71	-98	-71
27	3	11	1356	1352	28
-28	4	11	81	-42	-81
-26	4	11	831	853	37
-24	4	11	445	550	51
-22	4	11	1235	-1231	34
-20	4	11	191	-100	-117
-18	4	11	1007	1043	36
-16	4	11	383	-354	54
-14	4	11	1031	-1027	35
-12	4	11	487	448	40
-10	4	11	1529	1475	32
-8	4	11	219	-132	-88
-6	4	11	1768	-1712	30
-4	4	11	609	545	36
-2	4	11	693	667	33
0	4	11	1053	-1048	21
2	4	11	245	219	53
4	4	11	1815	1903	28
6	4	11	268	-229	51
8	4	11	943	-970	32
10	4	11	487	-497	35
12	4	11	476	449	38
14	4	11	109	-5	-109
16	4	11	666	-636	33
18	4	11	692	701	32
20	4	11	650	629	32
22	4	11	750	-701	32
24	4	11	894	-853	31
26	4	11	769	721	30
-25	5	11	145	118	-145
-23	5	11	181	234	-135
-21	5	11	161	198	-161
-19	5	11	584	-602	42
-17	5	11	88	-7	-88
-15	5	11	88	58	-88
-13	5	11	89	-218	-89
-11	5	11	181	145	-118
-9	5	11	454	555	50
-7	5	11	225	-253	-83
-5	5	11	528	-498	42
-3	5	11	375	-348	53
-1	5	11	148	95	-148
1	5	11	988	1011	32
3	5	11	721	763	34
5	5	11	296	307	46
7	5	11	295	235	47
9	5	11	281	-387	60
11	5	11	441	-381	37
13	5	11	125	-3	-125
15	5	11	77	144	-77
17	5	11	377	-345	42

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
19	5	11	75	-54	-75
21	5	11	314	-228	45
23	5	11	268	254	48
25	5	11	190	-142	-63
-24	6	11	132	-145	-132
-22	6	11	362	332	53
-20	6	11	123	-35	-123
-18	6	11	919	-925	38
-16	6	11	427	-493	53
-14	6	11	1227	1167	35
-12	6	11	639	-663	44
-10	6	11	857	-809	39
-8	6	11	361	287	52
-6	6	11	1402	1403	35
-4	6	11	793	-757	38
-2	6	11	1197	-1150	34
0	6	11	2049	2051	29
2	6	11	601	630	39
4	6	11	804	-785	34
6	6	11	75	104	-75
8	6	11	1182	1109	32
10	6	11	501	423	38
12	6	11	1091	-1060	33
14	6	11	369	269	43
16	6	11	1261	1227	31
18	6	11	277	-214	52
20	6	11	1070	-1107	31
22	6	11	441	413	38
-21	7	11	86	145	-86
-19	7	11	261	-326	-70
-17	7	11	375	-374	54
-15	7	11	218	-161	-96
-13	7	11	535	618	47
-11	7	11	191	-136	-133
-9	7	11	810	-857	40
-7	7	11	763	766	38
-5	7	11	523	541	44
-3	7	11	83	-26	-83
-1	7	11	192	216	-130
1	7	11	79	238	-79
3	7	11	170	27	-99
5	7	11	781	-731	36
7	7	11	523	543	41
9	7	11	297	336	54
11	7	11	157	145	-157
13	7	11	225	218	-70
15	7	11	312	-314	53
17	7	11	217	223	-68
19	7	11	428	-386	40
-16	8	11	242	385	-100
-14	8	11	687	-770	44
-12	8	11	181	-25	-158
-10	8	11	819	783	45
-8	8	11	946	-943	41
-6	8	11	425	-429	55
-4	8	11	1385	1281	37

h	k	l	10Fo	10Fc	10s
-2	8	11	496	470	51
0	8	11	982	-999	30
2	8	11	1486	-1423	35
4	8	11	649	592	40
6	8	11	832	783	37
8	8	11	909	-932	37
10	8	11	761	779	38
12	8	11	627	636	41
14	8	11	370	-382	44
-9	9	11	292	354	-81
-7	9	11	848	-830	41
-5	9	11	449	-408	49
-3	9	11	673	799	49
-1	9	11	87	-59	-87
1	9	11	1478	-1430	37
3	9	11	370	452	61
5	9	11	429	357	50
7	9	11	644	-669	42
-26	0	12	241	155	-63
-24	0	12	657	-610	36
-22	0	12	130	93	-130
-20	0	12	1499	1373	32
-18	0	12	384	380	49
-16	0	12	1670	-1592	31
-14	0	12	1659	-1574	31
-12	0	12	1212	1173	31
-10	0	12	618	-583	35
-8	0	12	1096	-1034	30
-6	0	12	1380	1371	29
-4	0	12	570	542	34
-2	0	12	1073	1024	28
0	0	12	261	202	45
2	0	12	2508	2574	27
4	0	12	1161	1127	28
6	0	12	2164	-2201	27
8	0	12	840	786	29
10	0	12	2454	2438	28
12	0	12	77	127	-77
14	0	12	2098	-2023	28
16	0	12	930	-932	32
18	0	12	577	530	32
20	0	12	822	-813	29
22	0	12	773	-782	30
24	0	12	878	856	29
26	0	12	1161	1078	27
-27	1	12	210	-161	-78
-25	1	12	77	-66	-77
-23	1	12	81	-43	-81
-21	1	12	240	147	-72
-19	1	12	363	327	51
-17	1	12	216	-149	-66
-15	1	12	987	-957	33
-13	1	12	232	-284	-69
-11	1	12	230	263	-64
-9	1	12	109	-38	-109
-7	1	12	221	-189	-70

h	k	l	10Fo	10Fc	10s
-5	1	12	591	553	36
-3	1	12	423	442	38
-1	1	12	473	-478	37
1	1	12	846	786	28
3	1	12	618	684	32
5	1	12	172	-188	-76
7	1	12	457	423	38
9	1	12	234	-287	-68
11	1	12	294	213	46
13	1	12	198	359	-88
15	1	12	72	-55	-72
17	1	12	211	-238	-59
19	1	12	831	-850	30
21	1	12	731	-782	31
23	1	12	67	139	-67
25	1	12	557	540	32
-26	2	12	160	-154	-140
-24	2	12	478	504	42
-22	2	12	267	290	-67
-20	2	12	1363	-1310	32
-18	2	12	298	-351	66
-16	2	12	1154	1118	33
-14	2	12	297	259	59
-12	2	12	682	-581	35
-10	2	12	395	459	47
-8	2	12	695	655	35
-6	2	12	515	-504	36
-4	2	12	1048	-1072	30
-2	2	12	749	765	32
0	2	12	328	316	36
2	2	12	602	-576	32
4	2	12	304	-285	42
6	2	12	547	519	31
8	2	12	1010	982	29
10	2	12	1452	-1443	28
12	2	12	177	-184	-76
14	2	12	1113	1114	30
16	2	12	206	172	-63
18	2	12	1194	-1148	29
20	2	12	515	545	33
22	2	12	763	746	31
24	2	12	904	-881	29
-25	3	12	81	-149	-81
-23	3	12	571	595	39
-21	3	12	356	-294	53
-19	3	12	773	-770	36
-17	3	12	716	709	37
-15	3	12	1170	1162	33
-13	3	12	370	-408	53
-11	3	12	403	-435	51
-9	3	12	240	208	-67
-7	3	12	917	866	31
-5	3	12	927	-902	33
-3	3	12	108	-110	-108
-1	3	12	481	-441	38
1	3	12	169	-968	-51

h	k	l	10Fo	10Fc	10s
3	3	12	71	82	-71
5	3	12	68	9	-68
7	3	12	642	586	32
9	3	12	726	-656	32
11	3	12	937	-820	30
13	3	12	228	183	-61
15	3	12	834	800	30
17	3	12	311	255	45
19	3	12	288	-206	49
21	3	12	1201	1252	29
23	3	12	71	100	-71
-24	4	12	308	-310	60
-22	4	12	240	-314	-79
-20	4	12	1033	971	35
-18	4	12	419	376	43
-16	4	12	394	-352	47
-14	4	12	289	331	68
-12	4	12	410	336	49
-10	4	12	82	-129	-82
-8	4	12	512	-501	39
-6	4	12	139	-62	-139
-4	4	12	403	436	47
-2	4	12	967	-930	31
0	4	12	739	-1072	-439
2	4	12	226	-1146	-58
4	4	12	538	-518	33
6	4	12	333	-331	44
8	4	12	734	-696	33
10	4	12	727	665	33
12	4	12	68	-161	-68
14	4	12	779	-792	32
16	4	12	396	472	42
18	4	12	1132	1095	30
20	4	12	345	323	40
22	4	12	227	227	54
-21	5	12	650	680	38
-19	5	12	735	812	41
-17	5	12	83	-74	-83
-15	5	12	1031	-1009	35
-13	5	12	1001	1052	35
-11	5	12	760	750	39
-9	5	12	1304	-1286	34
-7	5	12	336	221	53
-5	5	12	743	797	37
-3	5	12	451	-479	42
-1	5	12	700	-714	35
1	5	12	400	-449	39
3	5	12	683	605	33
5	5	12	973	-983	31
7	5	12	1238	-1213	30
9	5	12	1075	1022	31
11	5	12	642	665	34
13	5	12	586	-543	35
15	5	12	957	-944	32
17	5	12	1144	1148	30
19	5	12	705	788	33

h	k	l	10Fo	10Fc	10s
21	5	12	754	-716	32
-20	6	12	372	330	52
-18	6	12	578	-538	41
-16	6	12	82	145	-82
-14	6	12	84	17	-84
-12	6	12	391	476	55
-10	6	12	477	447	44
-8	6	12	763	-721	39
-6	6	12	246	13	-66
-4	6	12	84	230	-84
-2	6	12	574	-576	41
0	6	12	659	614	25
2	6	12	67	19	-67
4	6	12	858	-825	33
6	6	12	314	163	47
8	6	12	243	-255	-62
10	6	12	403	378	44
12	6	12	211	234	-77
14	6	12	233	155	57
16	6	12	216	149	-63
18	6	12	69	57	-69
-15	7	12	480	517	51
-13	7	12	242	-246	-82
-11	7	12	572	-671	51
-9	7	12	964	915	37
-7	7	12	88	-45	-88
-5	7	12	1152	-1263	37
-3	7	12	247	337	-81
-1	7	12	1740	1697	33
1	7	12	271	210	63
3	7	12	490	-423	37
5	7	12	434	492	43
7	7	12	1025	966	33
9	7	12	927	-877	33
11	7	12	1010	-1030	33
13	7	12	895	913	33
-10	8	12	272	-252	-70
-8	8	12	375	374	52
-6	8	12	284	-195	61
-4	8	12	191	-213	-126
-2	8	12	903	980	37
0	8	12	1096	1100	33
2	8	12	697	702	37
4	8	12	485	461	40
6	8	12	545	588	41
8	8	12	78	138	-78
-23	1	13	337	-439	56
-21	1	13	218	2	-72
-19	1	13	848	-841	33
-17	1	13	357	-337	50
-15	1	13	1330	1310	31
-13	1	13	1495	1375	31
-11	1	13	758	-688	33
-9	1	13	862	-849	31
-7	1	13	857	803	32
-5	1	13	262	-303	58

Observed and calculated structure factors for $\{[Ru(bipy)_2]_2L\}(PF_6)_4$

h	k	l	10Fo	10Fc	10s
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3	1	13	259	253	50
5	1	13	1921	-1953	28
7	1	13	496	-544	35
9	1	13	1729	1726	29
11	1	13	1171	-1168	30
13	1	13	540	-448	33
15	1	13	1341	1363	29
17	1	13	753	741	30
19	1	13	1340	-1323	28
21	1	13	1007	-987	28
-22	2	13	427	-412	43
-20	2	13	240	-227	60
-18	2	13	832	-790	34
-16	2	13	656	619	38
-14	2	13	1295	1248	32
-12	2	13	324	231	51
-10	2	13	787	-725	33
-8	2	13	177	-77	-95
-6	2	13	77	135	-77
-4	2	13	851	872	32
-2	2	13	324	368	44
0	2	13	406	470	-109
2	2	13	403	1327	-36
4	2	13	1172	-1364	29
6	2	13	1217	-1300	30
8	2	13	141	161	-141
10	2	13	131	-99	-131
12	2	13	207	190	-58
14	2	13	292	325	44
16	2	13	1029	983	29
18	2	13	125	-223	-125
20	2	13	989	-1039	29
-21	3	13	736	-728	35
-19	3	13	73	13	-73
-17	3	13	761	683	35
-15	3	13	480	-546	42
-13	3	13	604	-621	39
-11	3	13	939	866	34
-9	3	13	399	325	46
-7	3	13	615	-591	35
-5	3	13	344	261	44
-3	3	13	1250	1307	31
-1	3	13	1593	1640	30
1	3	13	38	-1363	-38
3	3	13	48	-171	-48
5	3	13	57	449	-57
7	3	13	399	-506	37
9	3	13	496	-447	35
11	3	13	300	305	45
13	3	13	579	584	33
15	3	13	624	-623	32
17	3	13	549	-532	33
19	3	13	773	841	29
-20	4	13	209	-253	-83
-18	4	13	1092	1060	32
-16	4	13	152	-14	-152
-14	4	13	1017	-993	34
-12	4	13	202	-257	-105
-10	4	13	1003	899	34
-8	4	13	115	-55	-115
-6	4	13	254	-206	-67
-4	4	13	847	813	33
-2	4	13	320	341	49
0	4	13	1588	-1586	30
2	4	13	41	-553	-41
4	4	13	45	363	-45
6	4	13	154	1248	-38
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12	4	13	1042	1001	31
14	4	13	223	-113	47
16	4	13	1279	-1253	28
18	4	13	226	318	-65
-17	5	13	85	-211	-85
-15	5	13	445	-409	43
-13	5	13	405	386	44
-11	5	13	234	-224	-67
-9	5	13	253	-297	-81
-7	5	13	276	263	60
-5	5	13	75	97	-75
-3	5	13	631	-595	36
-1	5	13	1581	-1591	32
1	5	13	40	-109	-40
3	5	13	44	618	-44
5	5	13	47	122	-47
7	5	13	53	581	-53
9	5	13	268	195	40
11	5	13	243	-254	58
13	5	13	285	-234	48
15	5	13	220	-198	55
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-10	6	13	800	-735	36
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-6	6	13	717	743	38
-4	6	13	1018	-1098	35
-2	6	13	1303	-1322	33
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4	6	13	44	-75	-44
6	6	13	96	-414	-96
8	6	13	321	1279	-43
10	6	13	369	285	39
12	6	13	1523	-1563	30
-7	7	13	207	-94	-89
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3	7	13	54	-248	-54
5	7	13	78	-638	-78
-18	0	14	638	579	33
-16	0	14	156	-86	-111
-14	0	14	166	-137	-133
-12	0	14	1016	959	32
-10	0	14	192	-150	-74
-8	0	14	1549	-1533	30
-6	0	14	267	217	56
-4	0	14	1276	1205	30
-2	0	14	161	34	-102
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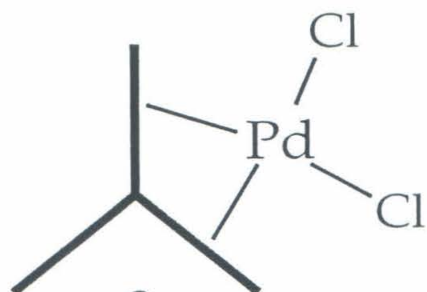
2	0	14	1544	1486	29
4	0	14	149	113	-116
6	0	14	1669	-1632	28
8	0	14	1139	-1135	30
10	0	14	1379	1360	29
12	0	14	873	818	29
14	0	14	964	-1001	29
16	0	14	204	-230	-55
-17	1	14	245	213	57
-15	1	14	330	-278	44
-13	1	14	175	142	-99
-11	1	14	75	84	-75
-9	1	14	613	-572	35
-7	1	14	531	-497	38
-5	1	14	852	844	32
-3	1	14	215	225	-68
-1	1	14	410	-420	38
1	1	14	92	-395	-92
3	1	14	242	284	43
5	1	14	445	500	34
7	1	14	1106	-1122	29
9	1	14	500	506	34
11	1	14	208	44	-65
13	1	14	102	-7	-102
15	1	14	149	179	-104
17	1	14	146	136	-99
-18	2	14	688	-609	34
-16	2	14	771	682	34
-14	2	14	287	-152	54
-12	2	14	792	-725	34
-10	2	14	147	124	-147
-8	2	14	1373	1325	31
-6	2	14	182	-167	-94
-4	2	14	811	-797	32
-2	2	14	565	564	35
0	2	14	277	495	-224
2	2	14	43	-848	-43
4	2	14	44	-987	-44
6	2	14	51	546	-51
8	2	14	606	1538	-32
10	2	14	894	-929	30
12	2	14	788	-726	29
14	2	14	966	915	28
16	2	14	72	126	-72
-15	3	14	553	578	39
-13	3	14	620	-606	36
-11	3	14	663	-611	36
-9	3	14	989	874	32
-7	3	14	1013	1009	32
-5	3	14	702	-641	33
-3	3	14	760	-821	33
-1	3	14	618	640	35
1	3	14	54	346	-54
5	3	14	40	-132	-40
7	3	14	46	1629	-46
9	3	14	52	-400	-52
11	3	14	483	-813	32
13	3	14	113	-26	-113
-14	4	14	279	-290	69
-12	4	14	814	794	35
-10	4	14	381	326	46
-8	4	14	1329	-1304	32
-6	4	14	81	14	-81
-4	4	14	416	353	40
-2	4	14	368	-344	47
0	4	14	270	295	51
2	4	14	54	-44	-54
4	4	14	32	1312	-32
6	4	14	92	-249	-60
8	4	14	37	-421	-37
10	4	14	48	792	-48
12	4	14	88	-184	-88
-9	5	14	535	-496	41
-7	5	14	527	-516	39
-5	5	14	516	539	39
-3	5	14	801	793	34
-1	5	14	1389	-1330	31
1	5	14	32	53	-32
3	5	14	32	1563	-32
7	5	14	44	-1280	-44
-11	1	15	304	320	54
-9	1	15	840	-848	33
-7	1	15	905	915	31
-5	1	15	631	587	34
-3	1	15	809	-760	31
-1	1	15	773	-794	32
1	1	15	50	622	-50
3	1	15	44	642	-44
5	1	15	72	-1205	-72
7	1	15	50	-276	-50
9	1	15	591	1374	-28
-8	2	15	257	-297	58
-6	2	15	611	529	34
-4	2	15	208	222	-63
-2	2	15	1078	-1002	29
0	2	15	352	355	-195
2	2	15	51	497	-51
4	2	15	51	24	-51
-5	3	15	1132	-1099	31
-3	3	15	1113	1177	30
-1	3	15	838	835	30
1	3	15	72	-579	-33
3	3	15	87	-6	-43



2

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
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4	0	0	149	209	-38
5	0	0	1075	1100	17
6	0	0	286	325	26
7	0	0	379	408	24
8	0	0	977	-989	23
9	0	0	57	-42	-57
10	0	0	87	-125	-87
11	0	0	592	555	19
12	0	0	141	92	-49
13	0	0	223	212	27
-13	1	0	187	168	27
-12	1	0	126	93	-57
-11	1	0	47	-22	-47
-10	1	0	62	-49	-62
-9	1	0	484	-535	29
-8	1	0	484	464	26
-7	1	0	86	26	-86
-6	1	0	1429	1458	18
-5	1	0	892	-905	17
-4	1	0	679	705	16
-3	1	0	3417	-3439	13
-2	1	0	597	653	12
-1	1	0	1365	1399	8
1	1	0	291	338	11
2	1	0	1749	-1703	11
3	1	0	2455	2387	13
4	1	0	737	-733	16
5	1	0	1446	1506	17
6	1	0	373	-432	23
7	1	0	365	-365	25
8	1	0	257	-286	34
9	1	0	157	-135	-53
10	1	0	499	492	29
11	1	0	86	49	-86
12	1	0	52	-40	-52
13	1	0	404	-408	22
-13	2	0	68	-107	-47
-12	2	0	279	301	26
-11	2	0	460	-468	20
-10	2	0	112	49	-112
-9	2	0	153	-131	-52
-8	2	0	427	423	27
-7	2	0	560	655	22
-6	2	0	107	-39	-59
-5	2	0	468	-494	20
-4	2	0	891	-860	15
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-2	2	0	663	-634	13
-1	2	0	124	-188	-35
0	2	0	1750	-1766	9
1	2	0	550	-492	12
2	2	0	393	396	16
3	2	0	428	440	17
4	2	0	1109	1097	16
5	2	0	690	-748	18
6	2	0	547	488	20
7	2	0	1202	-1229	21
8	2	0	359	396	31
9	2	0	58	-106	-58
10	2	0	517	551	31
11	2	0	394	-375	20
12	2	0	219	-210	33
13	2	0	302	-285	21
-12	3	0	333	-327	24
-11	3	0	264	251	24
-10	3	0	165	-297	-71
-9	3	0	774	802	25
-8	3	0	308	-298	30
-7	3	0	586	624	22
-6	3	0	848	-799	20
-5	3	0	94	-111	-94
-4	3	0	288	277	20
-3	3	0	199	-156	25
-2	3	0	400	414	16
-1	3	0	688	-741	13
0	3	0	273	-311	18
1	3	0	2260	-2213	12
2	3	0	1527	1492	13
3	3	0	349	-383	20
4	3	0	559	497	18
5	3	0	1147	-1208	18
6	3	0	395	-371	25
7	3	0	125	22	-48
8	3	0	111	-30	-111
9	3	0	653	697	28
10	3	0	422	-429	32
11	3	0	50	8	-50
12	3	0	502	-521	24

h	k	l	10Fo	10Fc	10s
13	3	0	365	331	20
-12	4	0	348	-354	24
-11	4	0	281	270	24
-10	4	0	159	169	-53
-9	4	0	132	-70	-53
-8	4	0	51	46	-51
-7	4	0	975	-964	21
-6	4	0	48	8	-48
-5	4	0	650	-660	19
-4	4	0	1394	1423	16
-3	4	0	1076	-1079	15
-2	4	0	145	-134	-38
-1	4	0	500	-527	15
0	4	0	1011	-1028	13
1	4	0	239	248	23
2	4	0	327	354	22
3	4	0	353	347	21
4	4	0	1016	-1057	17
5	4	0	320	267	22
6	4	0	837	-880	21
7	4	0	437	462	27
8	4	0	61	58	-61
9	4	0	523	558	30
10	4	0	476	-385	35
11	4	0	240	-283	32
12	4	0	176	159	-48
-12	5	0	344	372	24
-11	5	0	48	10	-48
-10	5	0	433	404	30
-9	5	0	502	-508	28
-8	5	0	53	4	-53
-7	5	0	708	-706	22
-6	5	0	351	329	23
-5	5	0	1273	1312	18
-4	5	0	539	-552	18
-3	5	0	309	309	22
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1	5	0	753	781	16
2	5	0	296	-317	22
3	5	0	112	-174	-66
4	5	0	410	-392	22
5	5	0	113	-143	-74
6	5	0	142	192	-45
7	5	0	549	443	26
8	5	0	254	305	44
9	5	0	524	-492	30
10	5	0	69	97	-69
11	5	0	284	-307	29
12	5	0	397	404	27
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-11	6	0	177	208	32
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-1	6	0	257	-249	22
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2	6	0	674	674	19
3	6	0	1621	-1509	18
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6	6	0	714	721	24
7	6	0	225	-119	39
8	6	0	141	104	-76
9	6	0	66	-152	-66
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11	6	0	438	415	24
12	6	0	59	-6	-59
-11	7	0	49	59	-49
-10	7	0	623	-592	17
-9	7	0	454	-437	28
-8	7	0	398	418	28
-7	7	0	48	53	-48
-6	7	0	773	764	22
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-4	7	0	44	70	-44
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0	7	0	460	465	20
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2	7	0	240	-278	29

h	k	l	10Fo	10Fc	10s
3	7	0	985	1020	19
4	7	0	441	427	24
5	7	0	1240	1186	22
6	7	0	997	-915	24
7	7	0	57	69	-57
8	7	0	475	-430	32
9	7	0	235	271	46
10	7	0	111	115	-111
11	7	0	269	266	34
12	7	0	94	-85	-94
-11	8	0	629	-630	18
-10	8	0	101	102	-56
-9	8	0	76	109	-76
-8	8	0	433	439	27
-7	8	0	258	243	32
-6	8	0	245	-241	30
-5	8	0	309	-348	29
-4	8	0	454	-446	23
-3	8	0	855	889	20
-2	8	0	394	384	22
-1	8	0	567	499	19
0	8	0	1232	-1164	19
1	8	0	406	380	22
2	8	0	280	-327	28
3	8	0	1088	1077	20
4	8	0	442	447	24
5	8	0	223	-164	45
6	8	0	186	-199	-52
7	8	0	441	-435	31
8	8	0	366	364	35
9	8	0	63	-48	-63
10	8	0	384	397	26
11	8	0	291	-256	29
-10	9	0	135	-101	-40
-9	9	0	674	668	17
-8	9	0	207	-220	41
-7	9	0	369	350	29
-6	9	0	603	-555	24
-5	9	0	54	-27	-54
-4	9	0	197	149	36
-3	9	0	895	864	21
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1	9	0	265	-272	31
2	9	0	705	730	22
3	9	0	54	-108	-54
4	9	0	489	454	24
5	9	0	955	-939	24
6	9	0	57	26	-57
7	9	0	126	-91	-72
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9	9	0	125	99	-61
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1	10	0	335	348	28
2	10	0	489	479	24
3	10	0	190	-119	41
4	10	0	564	-553	24
5	10	0	271	-246	34
6	10	0	152	-245	-75
7	10	0	672	652	30
8	10	0	281	-231	27
9	10	0	140	187	-62
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-7	11	0	407	-391	16
-6	11	0	319	322	32
-5	11	0	235	201	38
-4	11	0	54	-34	-54
-3	11	0	49	6	-49
-2	11	0	990	-985	22
-1	11	0	111	-94	-81
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1	11	0	639	604	25
2	11	0	589	-589	25
3	11	0	92	12	-92
4	11	0	598	-592	27
5	11	0	173	29	-51

h	k	l	10Fo	10Fc	10s
6	11	0	61	30	-61
7	11	0	128	151	-57
8	11	0	232	-188	32
9	11	0	344	-358	28
-8	12	0	139	-78	33
-7	12	0	289	295	20
-6	12	0	259	-251	20
-5	12	0	131	89	-33
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-3	12	0	100	110	-83
-2	12	0	167	-170	-55
-1	12	0	705	728	24
0	12	0	460	418	26
1	12	0	254	-226	34
2	12	0	53	31	-53
3	12	0	386	-444	34
4	12	0	313	350	37
5	12	0	61	99	-61
6	12	0	448	434	20
7	12	0	399	-392	23
8	12	0	181	-138	37
9	12	0	411	-416	26
-7	13	0	205	242	25
-6	13	0	91	-49	-53
-5	13	0	90	92	-52
-4	13	0	101	115	-44
-3	13	0	405	-350	17
-2	13	0	436	442	26
-1	13	0	745	-693	25
0	13	0	789	775	26
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2	13	0	83	18	-83
3	13	0	123	-104	-97
4	13	0	230	205	24
5	13	0	352	333	21
6	13	0	82	105	-82
7	13	0	48	73	-48
8	13	0	56	-115	-56
-5	14	0	495	-526	17
-4	14	0	317	315	19
-3	14	0	308	-322	19
-2	14	0	291	280	19
-1	14	0	175	201	28
0	14	0	370	-380	18
1	14	0	134	-8	33
2	14	0	247	-268	24
3	14	0	518	500	17
4	14	0	135	-143	-39
5	14	0	189	210	32
6	14	0	231	-249	30
-4	15	0	158	115	28
-3	15	0	235	231	21
-2	15	0	93	-86	-55
-1	15	0	43	27	-43
0	15	0	301	-312	20
1	15	0	210	204	27
2	15	0	70	132	-70
3	15	0	106	123	-61
4	15	0	147	148	-40
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-2	-13	1	45	-39	-45
-1	-13	1	155	151	-47
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2	-13	1	380	374	17
3	-13	1	347	-382	19
4	-13	1	674	699	16
5	-13	1	814	-874	15
6	-13	1	155	-232	34

h	k	l	10Fo	10Fc	10s
-8	-12	1	282	236	28
-7	-12	1	52	13	-52
-6	-12	1	80	-95	-80
-5	-12	1	172	-219	29
-4	-12	1	163	182	-62
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0	-12	1	80	121	-80
1	-12	1	681	-658	25
2	-12	1	627	637	25
3	-12	1	514	521	27
4	-12	1	167	-279	-50
5	-12	1	554	572	16
6	-12	1	185	-181	26
7	-12	1	208	232	25
8	-12	1	301	-299	21
-9	-11	1	192	-186	40
-8	-11	1	101	51	-101
-7	-11	1	608	-608	19
-6	-11	1	66	87	-66
-5	-11	1	171	213	-68
-4	-11	1	256	311	45
-3	-11	1	177	-169	-55
-2	-11	1	317	-257	29
-1	-11	1	253	-283	40
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7	-11	1	41	10	-41
8	-11	1	416	386	17
9	-11	1	107	-146	-58
-10	-10	1	57	96	-57
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-6	-10	1	181	-185	-47
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8	-10	1	402	380	18
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-9	-9	1	179	153	39
-8	-9	1	608	-547	32
-7	-9	1	393	395	35
-6	-9	1	368	401	33
-5	-9	1	237	218	37
-4	-9	1	120	147	-93
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-2	-9	1	512	529	24
-1	-9	1	140	-61	-49
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1	-9	1	192	-170	32
2	-9	1	163	-139	41
3	-9	1	851	-887	21
4	-9	1	470	503	24
5	-9	1	450	406	24
6	-9	1	186	130	37
7	-9	1	160	157	-43
8	-9	1	435	-445	17
9	-9	1	210	215	23
10	-9	1	207	-217	29
-11	-8	1	57	-129	-57
-10	-8	1	113	-121	-113
-9	-8	1	423	-408	23
-8	-8	1	388	421	36
-7	-8	1	144	3	-57
-6	-8	1	660	696	28
-5	-8	1	692	-708	25
-4	-8	1	53	15	-53
-3	-8	1	458	-434	24
-2	-8	1	657	624	21
-1	-8	1	757	727	21
0	-8	1	411	-382	22
1	-8	1	143	124	-44

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
2	-8	1	1050	-1054	20
3	-8	1	490	457	22
4	-8	1	157	154	-41
5	-8	1	686	713	22
6	-8	1	490	-491	25
7	-8	1	133	-97	-43
8	-8	1	264	-252	32
9	-8	1	42	-6	-42
10	-8	1	304	305	20
11	-8	1	46	100	-46
-11	-7	1	59	-115	-59
-10	-7	1	217	210	39
-9	-7	1	115	108	-115
-8	-7	1	326	338	37
-7	-7	1	417	356	29
-6	-7	1	58	-181	-58
-5	-7	1	54	-92	-54
-4	-7	1	980	-950	22
-3	-7	1	1514	1494	20
-2	-7	1	97	61	-97
-1	-7	1	420	508	21
0	-7	1	735	-768	19
1	-7	1	180	-170	32
2	-7	1	80	-113	-80
3	-7	1	494	482	21
4	-7	1	1074	1104	20
5	-7	1	816	-822	21
6	-7	1	269	-267	29
7	-7	1	687	-689	24
8	-7	1	338	340	31
9	-7	1	174	227	-57
10	-7	1	585	588	17
11	-7	1	422	-403	21
-12	-6	1	583	-535	27
-11	-6	1	182	230	44
-10	-6	1	153	-79	-41
-9	-6	1	632	624	30
-8	-6	1	249	-172	38
-7	-6	1	83	8	-83
-6	-6	1	963	-913	24
-5	-6	1	52	93	-52
-4	-6	1	1166	1056	20
-3	-6	1	767	750	19
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2	-6	1	1295	1281	17
3	-6	1	83	-111	-83
4	-6	1	128	84	-37
5	-6	1	773	-805	20
6	-6	1	986	-985	21
7	-6	1	245	252	32
8	-6	1	134	-109	-57
9	-6	1	219	168	40
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11	-6	1	47	25	-47
12	-6	1	223	-233	30
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-2	-4	1	564	-605	17
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6	-4	1	1323	1320	19
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9	3	1	167	-214	-51
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12	3	1	117	-78	-117
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6	5	1	169	-203	40
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9	5	1	65	138	-65
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11	5	1	227	-225	36
12	5	1	56	-28	-56
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-6	6	1	147	-134	-43
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1	6	1	530	487	18
2	6	1	797	799	17
3	6	1	110	153	-57
4	6	1	81	59	-81
5	6	1	301	-317	26
6	6	1	56	123	-56
7	6	1	78	44	-78
8	6	1	145	141	-53
9	6	1	165	-143	-56
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3	7	1	471	-426	21
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5	7	1	202	-123	34
6	7	1	173	123	-47
7	7	1	382	405	29
8	7	1	382	269	30
9	7	1	67	52	-67
10	7	1	505	-461	35
11	7	1	106	44	-106
12	7	1	62	-178	-62
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-10	8	1	198	225	26
-9	8	1	596	-583	16
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3	8	1	510	510	22
4	8	1	440	-474	24
5	8	1	581	566	23
6	8	1	111	-13	-111
7	8	1	320	339	40
8	8	1	329	-326	35
9	8	1	225	-207	46
10	8	1	101	-4	-101
11	8	1	57	64	-57
12	8	1	274	226	36
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3	9	1	114	-31	-64
4	9	1	203	221	38
5	9	1	52	-40	-52
6	9	1	327	340	34
7	9	1	681	-721	28
8	9	1	60	46	-60
9	9	1	184	-259	-74
10	9	1	315	326	29
11	9	1	89	-56	-89
-10	10	1	642	-611	17
-9	10	1	336	349	20
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-7	10	1	448	444	28
-6	10	1	252	-312	35
-5	10	1	279	-300	32
-4	10	1	266	-302	28
-3	10	1	203	-195	32
-2	10	1	776	771	21
-1	10	1	125	126	-52
0	10	1	287	-289	29
1	10	1	703	-762	22
2	10	1	148	182	-49
3	10	1	84	4	-84
4	10	1	625	628	25

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
5	10	1	518	-444	28
6	10	1	204	-204	-51
7	10	1	314	-418	37
8	10	1	169	-85	-56
9	10	1	540	489	20
10	10	1	57	-35	-57
11	10	1	62	167	-62
-9	11	1	150	152	33
-8	11	1	482	470	17
-7	11	1	484	-469	16
-6	11	1	145	-80	-48
-5	11	1	579	-510	25
-4	11	1	178	240	-50
-3	11	1	421	442	24
-2	11	1	51	103	-51
-1	11	1	432	-460	26
0	11	1	1050	-1066	22
1	11	1	198	189	37
2	11	1	193	192	33
3	11	1	458	383	26
4	11	1	81	-2	-81
5	11	1	207	193	43
6	11	1	829	-797	28
7	11	1	403	356	34
8	11	1	52	-121	-52
9	11	1	418	431	23
10	11	1	60	-138	-60
-8	12	1	99	122	-54
-7	12	1	350	-374	18
-6	12	1	256	-259	19
-5	12	1	367	345	27
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-3	12	1	470	400	26
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2	12	1	151	-55	-49
3	12	1	678	670	25
4	12	1	556	-524	29
5	12	1	124	-46	-124
6	12	1	185	-101	-55
7	12	1	134	175	-55
8	12	1	393	423	24
9	12	1	324	-292	28
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2	13	1	213	217	35
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3	14	1	266	-284	23
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6	14	1	112	112	-64
7	14	1	224	291	31
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6	15	1	49	-4	-49
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h	k	l	10Fo	10Fc	10s
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3	16	1	80	-63	-80
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-3	-14	2	209	-169	28
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7	-11	2	187	188	25
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-7	-10	2	53	-162	-53
-6	-10	2	299	-367	39
-5	-10	2	59	-23	-59
-4	-10	2	120	137	-120
-3	-10	2	730	684	25
-2	-10	2	135	-167	-73
-1	-10	2	58	170	-58
0	-10	2	605	-603	25
1	-10	2	443	440	25
2	-10	2	324	-326	27
3	-10	2	749	745	23
4	-10	2	159	157	37
5	-10	2	51	-21	-51
6	-10	2	92	15	-92
7	-10	2	404	-409	17
8	-10	2	213	220	23
9	-10	2	68	-84	-68
-10	-9	2	57	-5	-57
-9	-9	2	438	450	24
-8	-9	2	383	-388	24
-7	-9	2	245	216	42
-6	-9	2	819	-803	27
-5	-9	2	497	490	27
-4	-9	2	268	268	33
-3	-9	2	235	294	40
-2	-9	2	177	-29	38
-1	-9	2	261	-316	31
0	-9	2	101	98	-101
1	-9	2	128	-6	-50
2	-9	2	811	836	22
3	-9	2	288	-301	30
4	-9	2	53	66	-53

h	k	l	10Fo	10Fc	10s
5	-9	2	793	-783	23
6	-9	2	427	424	25
7	-9	2	139	-73	-45
8	-9	2	208	181	21
9	-9	2	42	94	-42
10	-9	2	321	-320	21
-10	-8	2	138	-91	-62
-9	-8	2	216	152	33
-8	-8	2	395	-345	36
-7	-8	2	190	-286	-58
-6	-8	2	375	375	31
-5	-8	2	57	-31	-57
-4	-8	2	1081	1060	24
-3	-8	2	953	-967	23
-2	-8	2	54	108	-54
-1	-8	2	465	-480	23
0	-8	2	468	492	23
1	-8	2	262	298	31
2	-8	2	117	66	-53
3	-8	2	97	-105	-97
4	-8	2	794	-805	21
5	-8	2	375	320	24
6	-8	2	86	97	-86
7	-8	2	494	515	26
8	-8	2	450	-455	28
9	-8	2	42	99	-42
10	-8	2	387	-374	20
11	-8	2	47	34	-47
-11	-7	2	61	-15	-61
-10	-7	2	165	189	-47
-9	-7	2	592	-582	20
-8	-7	2	66	176	-66
-7	-7	2	522	-476	30
-6	-7	2	566	644	27
-5	-7	2	142	193	-64
-4	-7	2	229	-212	32
-3	-7	2	476	-485	24
-2	-7	2	624	-689	21
-1	-7	2	722	749	20
0	-7	2	859	-849	20
1	-7	2	570	566	21
2	-7	2	1118	-1118	19
3	-7	2	476	-478	22
4	-7	2	302	-337	24
5	-7	2	528	554	23
6	-7	2	348	311	26
7	-7	2	116	-146	-65
8	-7	2	284	-267	29
9	-7	2	390	-371	27
10	-7	2	166	173	34
11	-7	2	85	-16	-85
-11	-6	2	444	355	26
-10	-6	2	55	-90	-55
-9	-6	2	64	-8	-64
-8	-6	2	196	-236	-57
-7	-6	2	519	522	30
-6	-6	2	237	-230	40
-5	-6	2	597	601	24
-4	-6	2	1599	-1636	21
-3	-6	2	51	63	-51
-2	-6	2	576	-593	21
-1	-6	2	1056	1067	18
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2	-6	2	168	-149	29
3	-6	2	1192	-1189	18
4	-6	2	1101	1061	19
5	-6	2	318	276	25
6	-6	2	402	390	25
7	-6	2	860	-909	23
8	-6	2	54	-21	-54
9	-6	2	55	83	-55
10	-6	2	430	421	18
11	-6	2	106	106	-60
12	-6	2	76	-59	-76
-11	-5	2	55	21	-55
-10	-5	2	320	-301	25
-9	-5	2	429	352	33
-8	-5	2	63	86	-63
-7	-5	2	57	128	-57
-6	-5	2	139	185	-71
-5	-5	2	717	-737	23
-4	-5	2	411	316	25
-3	-5	2	1451	-1344	18
-2	-5	2	2284	2229	17
-1	-5	2	1036	-1019	17
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1	-5	2	1411	-1423	16
2	-5	2	119	-3	-47
3	-5	2	100	77	-64

h	k	l	10Fo	10Fc	10s
4	-5	2	208	226	30
5	-5	2	790	786	20
6	-5	2	1242	-1180	20
7	-5	2	52	-33	-52
8	-5	2	444	-433	26
9	-5	2	382	406	34
10	-5	2	112	-73	-112
11	-5	2	326	289	22
12	-5	2	253	-269	28
-12	-4	2	233	-189	37
-11	-4	2	494	-420	23
-10	-4	2	231	279	46
-9	-4	2	282	-244	41
-8	-4	2	678	687	26
-7	-4	2	863	-841	25
-6	-4	2	231	243	34
-5	-4	2	792	-771	21
-4	-4	2	127	229	-58
-3	-4	2	785	736	19
-2	-4	2	95	-14	-95
-1	-4	2	298	-243	22
0	-4	2	1513	-1500	15
1	-4	2	1263	1283	15
2	-4	2	823	-782	16
3	-4	2	1244	1239	16
4	-4	2	93	-59	-75
5	-4	2	260	193	23
6	-4	2	539	-576	21
7	-4	2	52	-45	-52
8	-4	2	805	793	24
9	-4	2	140	79	-63
10	-4	2	505	493	29
11	-4	2	514	-544	18
12	-4	2	100	93	-100
-12	-3	2	182	119	45
-11	-3	2	281	-248	28
-10	-3	2	377	351	36
-9	-3	2	137	88	-66
-8	-3	2	229	-367	48
-7	-3	2	146	165	-67
-6	-3	2	587	-636	23
-5	-3	2	946	953	20
-4	-3	2	99	-26	-99
-3	-3	2	1031	1044	17
-2	-3	2	519	-480	17
-1	-3	2	183	-130	28
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1	-3	2	606	645	15
2	-3	2	422	463	17
3	-3	2	158	-48	29
4	-3	2	529	534	17
5	-3	2	1198	-1201	18
6	-3	2	989	976	19
7	-3	2	204	-185	35
8	-3	2	1062	1070	23
9	-3	2	63	-177	-63
10	-3	2	110	-162	-110
11	-3	2	238	-220	24
12	-3	2	51	-69	-51
13	-3	2	325	351	27
-12	-2	2	84	-149	-84
-11	-2	2	527	503	21
-10	-2	2	300	-327	45
-9	-2	2	372	425	36
-8	-2	2	799	-783	25
-7	-2	2	351	345	28
-6	-2	2	158	265	-49
-5	-2	2	114	93	-51
-4	-2	2	655	690	19
-3	-2	2	772	-787	16
-2	-2	2	945	952	15
-1	-2	2	953	-958	13
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2	-2	2	167	228	29
3	-2	2	668	-699	15
4	-2	2	421	417	19
5	-2	2	98	-83	-72
6	-2	2	138	60	34
7	-2	2	377	428	26
8	-2	2	245	-257	31
9	-2	2	237	200	33
10	-2	2	847	-888	27
11	-2	2	416	408	19
12	-2	2	135	-71	-46
13	-2	2	384	349	30
-12	-1	2	197	160	38
-11	-1	2	326	268	24
-10	-1	2	263	207	40
-9	-1	2	670	-722	29

h	k	l	10Fo	10Fc	10s
-8	-1	2	329	325	27
-7	-1	2	272	-322	34
-6	-1	2	1511	1519	20
-5	-1	2	593	-531	20
-4	-1	2	48	87	-48
-3	-1	2	272	-262	23
-2	-1	2	152	210	35
-1	-1	2	1178	1187	12
0	-1	2	332	300	15
1	-1	2	269	-248	18
2	-1	2	741	-688	13
3	-1	2	1812	1888	13
4	-1	2	255	185	23
5	-1	2	48	6	-48
6	-1	2	282	-279	25
7	-1	2	1401	1363	20
8	-1	2	768	-727	22
9	-1	2	295	-303	31
10	-1	2	131	-110	-103
11	-1	2	117	64	-54
12	-1	2	446	411	21
13	-1	2	265	-259	23
-12	0	2	425	424	24
-11	0	2	122	-149	-63
-10	0	2	274	-282	41
-9	0	2	386	-358	33
-8	0	2	56	25	-56
-7	0	2	429	445	25
-6	0	2	206	-139	30
-5	0	2	83	-97	-83
-4	0	2	1176	-1216	16
-3	0	2	1312	1291	14
-2	0	2	821	-834	13
-1	0	2	1563	1519	11
0	0	2	1044	-1071	9
1	0	2	40	0	-40
2	0	2	1348	-1429	11
3	0	2	230	-252	21
4	0	2	4013	-3859	14
5	0	2	214	181	30
6	0	2	240	269	26
7	0	2	615	-630	22
8	0	2	221	-233	35
9	0	2	485	-514	28
10	0	2	506	525	31
11	0	2	47	-103	-47
12	0	2	132	10	-49
13	0	2	99	-136	-52
-12	1	2	350	-361	25
-11	1	2	217	-172	30
-10	1	2	180	-182	-57
-9	1	2	708	683	28
-8	1	2	557	556	25
-7	1	2	787	786	22
-6	1	2	799	-831	20
-5	1	2	961	-1019	18
-4	1	2	383	-393	20
-3	1	2	264	286	23
-2	1	2	648	679	13
-1	1	2	414	-360	13
0	1	2	204	-200	16
1	1	2	1829	-1737	9
2	1	2	403	365	14
3	1	2	528	-569	15
4	1	2	3394	3181	14
5	1	2	70	68	-70
6	1	2	1070	-1076	19
7	1	2	715	-657	21
8	1	2	93	-71	-93
9	1	2	665	620	26
10	1	2	133	-29	-76
11	1	2	50	-13	-50
12	1	2	671	-665	20
13	1	2	54	64	-38
-12	2	2	347	-298	24
-11	2	2	50	-60	-50
-10	2	2	63	-35	-63
-9	2	2	56	-12	-56
-8	2	2	764	746	25
-7	2	2	418	-446	24
-6	2	2	182	-209	33
-5	2	2	1152	-1226	18
-4	2	2	1232	1243	16
-3	2	2	365	352	18
-2	2	2	46	4	-46
-1	2	2	42	-174	-42
0	2	2	668	-698	10
1	2	2	79	-98	-79
2	2	2	305	178	16
3	2	2	3475	3366	13

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
4	2	2	2295	-2317	15
5	2	2	49	-136	-49
6	2	2	1259	-1224	19
7	2	2	702	733	21
8	2	2	181	226	-48
9	2	2	478	448	27
10	2	2	152	-143	-63
11	2	2	254	-302	30
12	2	2	54	12	-54
13	2	2	222	165	27
-12	3	2	288	329	26
-11	3	2	472	-503	20
-10	3	2	507	456	30
-9	3	2	178	-194	-59
-8	3	2	146	-29	-51
-7	3	2	606	-588	22
-6	3	2	935	-999	20
-5	3	2	438	430	20
-4	3	2	212	202	26
-3	3	2	197	137	26
-2	3	2	1054	-1082	13
-1	3	2	338	-337	16
0	3	2	1633	-1581	11
1	3	2	1704	1759	11
2	3	2	1117	1106	13
3	3	2	301	-291	20
4	3	2	730	-703	16
5	3	2	580	-499	19
6	3	2	761	779	20
7	3	2	186	171	38
8	3	2	833	829	23
9	3	2	425	-474	29
10	3	2	66	-128	-66
11	3	2	267	-271	25
12	3	2	319	355	30
13	3	2	145	184	-66
-12	4	2	99	-45	-99
-11	4	2	297	286	22
-10	4	2	161	-155	-62
-9	4	2	184	213	41
-8	4	2	659	-674	24
-7	4	2	248	282	32
-6	4	2	74	-189	-74
-5	4	2	761	768	19
-4	4	2	406	433	20
-3	4	2	1039	-1081	15
-2	4	2	307	320	21
-1	4	2	46	44	-46
0	4	2	370	393	17
1	4	2	735	740	14
2	4	2	527	494	16
3	4	2	1081	-1032	15
4	4	2	50	-2	-50
5	4	2	226	-203	26
6	4	2	1444	1494	19
7	4	2	300	319	28
8	4	2	117	-60	-117
9	4	2	333	-251	32
10	4	2	396	-391	37
11	4	2	586	571	20
12	4	2	116	-9	-84
13	4	2	183	248	42
-12	5	2	49	-40	-49
-11	5	2	155	179	-40
-10	5	2	319	-350	20
-9	5	2	106	-162	-106
-8	5	2	147	78	-47
-7	5	2	351	-338	24
-6	5	2	1076	1131	20
-5	5	2	381	-366	21
-4	5	2	81	34	-81
-3	5	2	1325	-1283	16
-2	5	2	475	-445	17
-1	5	2	141	-144	-36
0	5	2	743	756	15
1	5	2	955	949	14
2	5	2	421	-450	19
3	5	2	671	-633	17
4	5	2	52	-97	-52
5	5	2	1043	1052	18
6	5	2	257	295	30
7	5	2	369	383	27
8	5	2	824	-815	24
9	5	2	278	301	43
10	5	2	65	-63	-65
11	5	2	53	171	-53
12	5	2	242	179	38
13	5	2	228	-193	29
-11	6	2	216	-245	29
-10	6	2	45	16	-45

h	k	l	10Fo	10Fc	10s
-9	6	2	236	-265	33
-8	6	2	685	695	25
-7	6	2	52	66	-52
-6	6	2	355	344	25
-5	6	2	153	184	-41
-4	6	2	483	-540	20
-3	6	2	86	107	-86
-2	6	2	271	-231	21
-1	6	2	1490	1512	15
0	6	2	499	-420	17
1	6	2	158	214	38
2	6	2	194	-140	29
3	6	2	224	-192	29
4	6	2	228	227	28
5	6	2	772	834	21
6	6	2	373	-348	25
7	6	2	57	-171	-57
8	6	2	355	279	33
9	6	2	126	-137	-126
10	6	2	541	516	35
11	6	2	54	-60	-54
12	6	2	56	76	-56
13	6	2	502	-469	27
-11	7	2	145	-158	-38
-10	7	2	42	-29	-42
-9	7	2	351	359	33
-8	7	2	164	-146	40
-7	7	2	254	247	34
-6	7	2	146	-133	-38
-5	7	2	821	813	20
-4	7	2	562	-589	20
-3	7	2	1251	1217	18
-2	7	2	492	485	19
-1	7	2	453	-459	19
0	7	2	145	-148	34
1	7	2	805	-812	17
2	7	2	144	117	-40
3	7	2	315	-287	24
4	7	2	689	689	20
5	7	2	620	-574	22
6	7	2	338	-323	27
7	7	2	996	-939	24
8	7	2	156	-96	-61
9	7	2	130	-76	-130
10	7	2	612	564	32
11	7	2	55	-59	-55
12	7	2	340	-349	30
-11	8	2	47	79	-47
-10	8	2	137	106	-35
-9	8	2	373	372	18
-8	8	2	154	-101	-51
-7	8	2	192	-269	44
-6	8	2	204	-178	33
-5	8	2	673	-676	22
-4	8	2	1006	1035	20
-3	8	2	211	-184	27
-2	8	2	1048	998	18
-1	8	2	1324	-1302	18
0	8	2	140	102	-40
1	8	2	307	-317	23
2	8	2	177	167	38
3	8	2	152	122	-38
4	8	2	199	-248	36
5	8	2	245	-276	32
6	8	2	768	-842	24
7	8	2	226	236	39
8	8	2	114	35	-114
9	8	2	488	456	33
10	8	2	440	-451	35
11	8	2	99	17	-99
12	8	2	304	-341	36
-10	9	2	540	550	18
-9	9	2	147	-177	35
-8	9	2	82	-25	-82
-7	9	2	648	-655	26
-6	9	2	192	152	36
-5	9	2	110	158	-64
-4	9	2	446	457	24
-3	9	2	166	-111	33
-2	9	2	846	-846	20
-1	9	2	109	-155	-66
0	9	2	195	-151	31
1	9	2	977	944	19
2	9	2	601	-600	21
3	9	2	338	282	25
4	9	2	517	-550	25
5	9	2	57	-39	-57
6	9	2	55	36	-55
7	9	2	109	154	-109
8	9	2	242	235	45

h	k	l	10Fo	10Fc	10s
9	9	2	272	-275	44
10	9	2	53	11	-53
11	9	2	332	-314	31
12	9	2	335	294	33
-9	10	2	203	-157	25
-8	10	2	629	-588	16
-7	10	2	50	17	-50
-6	10	2	77	105	-77
-5	10	2	380	408	26
-4	10	2	266	-271	30
-3	10	2	362	-360	25
-2	10	2	687	-671	21
-1	10	2	168	196	35
0	10	2	449	420	22
1	10	2	537	558	23
2	10	2	432	-407	25
3	10	2	506	-560	23
4	10	2	429	429	27
5	10	2	574	-548	27
6	10	2	764	831	27
7	10	2	338	-311	36
8	10	2	164	133	-71
9	10	2	536	-489	20
10	10	2	58	56	-58
11	10	2	61	106	-61
-9	11	2	244	-260	24
-8	11	2	226	-201	22
-7	11	2	292	293	19
-6	11	2	401	410	28
-5	11	2	217	-231	38
-4	11	2	154	-151	-46
-3	11	2	703	-686	23
-2	11	2	53	52	-53
-1	11	2	223	246	33
0	11	2	1130	1086	21
1	11	2	493	-518	24
2	11	2	266	231	30
3	11	2	439	-420	27
4	11	2	383	335	28
5	11	2	134	212	-76
6	11	2	512	500	30
7	11	2	63	-45	-63
8	11	2	511	-494	34
9	11	2	326	313	27
10	11	2	110	-125	-110
-8	12	2	275	267	21
-7	12	2	143	124	34
-6	12	2	318	332	18
-5	12	2	442	-433	28
-4	12	2	344	-349	27
-3	12	2	50	-37	-50
-2	12	2	314	281	29
-1	12	2	587	617	24
0	12	2	270	-279	32
1	12	2	335	-366	32
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3	12	2	262	244	36
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3	13	2	852	874	26
4	13	2	61	27	-61
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6	13	2	185	-194	32
7	13	2	151	-254	-49
8	13	2	509	463	22
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6	14	2	115	-95	-59
7	14	2	54	37	-54
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3	15	2	216	236	26
4	15	2	558	-564	18
5	15	2	153	94	34
6	15	2	233	-176	27
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-2	16	2	269	-268	20
-1	16	2	136	169	-38
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2	16	2	223	-186	24
3	16	2	135	-91	-37
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6	-10	3	106	111	-81
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8	-10	3	103	102	-45

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-9	-9	3	178	-143	43
-8	-9	3	154	131	-45
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-6	-9	3	273	-248	41
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-4	-9	3	615	-659	28
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2	-9	3	227	-259	35
3	-9	3	47	-48	-47
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6	-9	3	102	121	-102
7	-9	3	540	-510	26
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-9	-8	3	515	501	21
-8	-8	3	137	41	-43
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-4	-8	3	92	151	-92
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2	-8	3	183	214	37
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8	-8	3	158	-107	-46
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-10	-6	3	403	372	24
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-7	-6	3	484	-431	31
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5	-6	3	687	-680	21
6	-6	3	754	727	22
7	-6	3	262	258	35
8	-6	3	416	398	28
9	-6	3	413	-424	29
10	-6	3	131	100	-35
11	-6	3	181	-181	27
12	-6	3	276	272	28
-11	-5	3	594	568	22
-10	-5	3	107	-139	-107

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
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-4	-5	3	238	-187	31
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7	-5	3	278	273	31
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9	-5	3	54	-21	-54
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-7	-4	3	60	-137	-60
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6	-4	3	138	-107	-49
7	-4	3	207	-181	34
8	-4	3	811	-805	23
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-9	8	3	42	-2	-42
-8	8	3	52	65	-52
-7	8	3	520	500	26
-6	8	3	278	-271	30
-5	8	3	331	311	26
-4	8	3	521	-540	21
-3	8	3	184	203	32
-2	8	3	354	-314	22
-1	8	3	107	112	-77
0	8	3	328	373	22
1	8	3	654	-701	19
2	8	3	69	81	-69
3	8	3	854	-848	19
4	8	3	380	385	24
5	8	3	186	-149	41
6	8	3	60	46	-60
7	8	3	833	-780	25
8	8	3	440	-464	34
9	8	3	120	127	-120
10	8	3	193	207	-75
11	8	3	426	386	24
12	8	3	284	-226	33
-10	9	3	45	-62	-45
-9	9	3	41	35	-41
-8	9	3	361	355	28
-7	9	3	169	-139	-44
-6	9	3	325	-339	27
-5	9	3	478	-378	23
-4	9	3	111	117	-62
-3	9	3	685	-674	21
-2	9	3	842	855	20
-1	9	3	257	-274	29
0	9	3	107	-168	-76
1	9	3	539	-538	20
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3	9	3	599	590	21
4	9	3	80	-76	-80
5	9	3	529	575	24
6	9	3	644	-631	24
7	9	3	144	-82	-74
8	9	3	330	-325	35
9	9	3	594	523	33
10	9	3	53	38	-53
11	9	3	133	143	-61
12	9	3	201	-163	48
-9	10	3	282	268	21
-8	10	3	166	191	30
-7	10	3	282	-283	38
-6	10	3	307	-310	29
-5	10	3	113	-20	-70
-4	10	3	82	45	-82
-3	10	3	319	346	27
-2	10	3	103	108	-73
-1	10	3	215	-173	31
0	10	3	899	-933	20
1	10	3	485	508	23
2	10	3	77	-95	-77
3	10	3	659	725	23
4	10	3	48	21	-48
5	10	3	166	-130	-46
6	10	3	141	76	-65
7	10	3	228	-222	51
8	10	3	690	671	30
9	10	3	67	-32	-67
10	10	3	213	234	35
11	10	3	304	-358	31
-9	11	3	390	341	18
-8	11	3	257	-265	21
-7	11	3	282	-275	18
-6	11	3	55	-144	-55
-5	11	3	502	490	26
-4	11	3	229	261	32
-3	11	3	215	176	33
-2	11	3	338	-333	25
-1	11	3	527	-510	23
0	11	3	50	-59	-50
1	11	3	226	184	30
2	11	3	855	912	22
3	11	3	289	-273	31
4	11	3	270	256	34
5	11	3	867	-883	25
6	11	3	578	561	29
7	11	3	165	128	-61
8	11	3	315	349	44
9	11	3	189	-89	41
10	11	3	233	-192	35
11	11	3	62	33	-62
-8	12	3	279	-267	21
-7	12	3	286	-307	20
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-5	12	3	219	221	36
-4	12	3	468	448	26
-3	12	3	280	-325	33
-2	12	3	134	-153	-57
-1	12	3	364	-376	27
0	12	3	588	601	24
1	12	3	687	718	25
2	12	3	298	312	31
3	12	3	340	-388	33
4	12	3	384	-395	29
5	12	3	534	591	28
6	12	3	319	271	39
7	12	3	62	130	-62
8	12	3	89	-230	-89
9	12	3	54	89	-54
10	12	3	59	-188	-59
-7	13	3	149	-140	31
-6	13	3	569	562	16
-5	13	3	178	185	24
-4	13	3	204	-279	43
-3	13	3	119	-115	-62
-2	13	3	321	-297	27
-1	13	3	741	710	24
0	13	3	621	598	24
1	13	3	210	-177	40
2	13	3	907	-935	24
3	13	3	1013	-1015	25
4	13	3	666	610	27
5	13	3	55	125	-55
6	13	3	60	-16	-60
7	13	3	192	-172	35

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
8	13	3	140	-203	-57
9	13	3	344	-341	25
-6	14	3	81	-56	-81
-5	14	3	42	41	-42
-4	14	3	603	-589	15
-3	14	3	131	131	31
-2	14	3	103	29	-86
-1	14	3	183	185	34
0	14	3	52	1	-52
1	14	3	734	-729	25
2	14	3	95	126	-95
3	14	3	339	360	34
4	14	3	135	144	-76
5	14	3	92	-25	-92
6	14	3	79	13	-79
7	14	3	385	-384	21
8	14	3	125	-6	-56
-5	15	3	279	-287	20
-4	15	3	119	54	-34
-3	15	3	41	2	-41
-2	15	3	609	629	16
-1	15	3	364	-350	18
0	15	3	75	146	-75
1	15	3	313	-328	19
2	15	3	172	116	29
3	15	3	103	-14	-48
4	15	3	237	266	26
5	15	3	95	76	-95
6	15	3	305	-323	22
7	15	3	50	0	-50
-3	16	3	147	86	27
-2	16	3	39	-37	-39
-1	16	3	42	-1	-42
0	16	3	382	-398	19
1	16	3	208	211	25
2	16	3	214	-288	26
3	16	3	582	597	18
4	16	3	303	-304	23
5	16	3	137	-93	-42
1	17	3	200	141	23
2	17	3	186	194	29
-3	-13	4	326	-345	24
-2	-13	4	341	360	22
-1	-13	4	133	152	-39
0	-13	4	46	83	-46
1	-13	4	45	49	-45
2	-13	4	474	-498	18
3	-13	4	181	175	28
4	-13	4	41	47	-41
-5	-12	4	49	-36	-49
-4	-12	4	194	-150	30
-3	-12	4	545	595	18
-2	-12	4	69	-118	-69
-1	-12	4	691	647	16
0	-12	4	486	-509	17
1	-12	4	43	-52	-43
2	-12	4	335	-327	19
3	-12	4	281	284	21
4	-12	4	419	415	18
5	-12	4	125	-144	-36
6	-12	4	46	-106	-46
-6	-11	4	197	-233	33
-5	-11	4	80	29	-80
-4	-11	4	195	-268	28
-3	-11	4	228	166	26
-2	-11	4	46	-87	-46
-1	-11	4	53	99	-53
0	-11	4	56	88	-56
1	-11	4	431	-431	29
2	-11	4	595	591	26
3	-11	4	134	-65	-45
4	-11	4	409	377	17
5	-11	4	483	-492	16
6	-11	4	300	-289	20
7	-11	4	283	-283	20
-7	-10	4	178	-165	37
-6	-10	4	100	-64	-80
-5	-10	4	105	-17	-57
-4	-10	4	498	470	31
-3	-10	4	223	-193	35
-2	-10	4	55	58	-55
-1	-10	4	534	-515	26
0	-10	4	138	79	-47
1	-10	4	111	-3	-111
2	-10	4	320	277	28
3	-10	4	348	319	29
4	-10	4	505	-513	26
5	-10	4	82	-69	-82
6	-10	4	351	-373	18
7	-10	4	461	431	17

h	k	l	10Fo	10Fc	10s
8	-10	4	272	-299	22
9	-10	4	113	132	-49
-8	-9	4	126	-16	-56
-7	-9	4	301	-299	26
-6	-9	4	196	187	30
-5	-9	4	547	466	29
-4	-9	4	58	10	-58
-3	-9	4	52	-49	-52
-2	-9	4	533	-561	27
-1	-9	4	271	226	33
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1	-9	4	564	536	25
2	-9	4	247	-258	34
3	-9	4	131	72	-52
4	-9	4	583	-549	24
5	-9	4	151	118	-47
6	-9	4	388	369	27
7	-9	4	43	-7	-43
8	-9	4	390	369	16
9	-9	4	369	-362	20
-9	-8	4	238	-104	31
-8	-8	4	396	-358	23
-7	-8	4	628	659	19
-6	-8	4	184	-188	-62
-5	-8	4	387	393	34
-4	-8	4	537	-542	29
-3	-8	4	259	-273	37
-2	-8	4	54	-75	-54
-1	-8	4	53	-7	-53
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3	-8	4	622	-614	23
4	-8	4	148	113	-42
5	-8	4	54	-130	-54
6	-8	4	632	686	26
7	-8	4	350	-330	29
8	-8	4	43	0	-43
9	-8	4	263	-205	21
10	-8	4	104	-134	-56
-9	-7	4	51	38	-51
-8	-7	4	156	150	-45
-7	-7	4	109	189	-109
-6	-7	4	332	333	32
-5	-7	4	496	-529	28
-4	-7	4	52	-1	-52
-3	-7	4	537	-577	26
-2	-7	4	1078	1059	22
-1	-7	4	101	-81	-101
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3	-7	4	262	263	30
4	-7	4	405	403	24
5	-7	4	381	400	27
6	-7	4	195	-238	37
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8	-7	4	246	-289	38
9	-7	4	367	343	18
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11	-7	4	282	297	24
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-9	-6	4	435	-427	23
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-7	-6	4	600	-607	30
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4	-6	4	169	-135	32
5	-6	4	166	160	-45
6	-6	4	454	-468	25
7	-6	4	171	-181	-46
8	-6	4	261	230	31
9	-6	4	328	356	31
10	-6	4	187	145	27
11	-6	4	80	-70	-80
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-9	-5	4	835	783	18
-8	-5	4	162	155	-80
-7	-5	4	58	-18	-58
-6	-5	4	774	-818	25
-5	-5	4	167	160	-51
-4	-5	4	54	-102	-54

h	k	l	10Fo	10Fc	10s
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2	-5	4	232	305	28
3	-5	4	139	196	-39
4	-5	4	780	829	20
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6	-5	4	215	-197	35
7	-5	4	75	194	-75
8	-5	4	609	652	26
9	-5	4	58	45	-58
10	-5	4	62	130	-62
11	-5	4	204	-213	26
12	-5	4	173	138	35
-11	-4	4	358	330	28
-10	-4	4	108	120	-78
-9	-4	4	344	319	22
-8	-4	4	59	2	-59
-7	-4	4	240	-242	44
-6	-4	4	57	-30	-57
-5	-4	4	306	299	33
-4	-4	4	534	539	23
-3	-4	4	463	451	23
-2	-4	4	45	140	-45
-1	-4	4	742	-775	18
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4	-4	4	572	-617	20
5	-4	4	252	-279	27
6	-4	4	179	-115	33
7	-4	4	910	929	22
8	-4	4	165	-110	-41
9	-4	4	156	-147	-59
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11	-4	4	119	200	-58
12	-4	4	113	-50	-57
-11	-3	4	57	-89	-57
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4	-2	4	132	96	-38
5	-2	4	240	212	25
6	-2	4	741	766	20
7	-2	4	391	-444	25
8	-2	4	340	-419	29
9	-2	4	555	-578	26
10	-2	4	416	448	32
11	-2	4	434	434	19
12	-2	4	51	-51	-51
13	-2	4	211	-181	24

h	k	l	10Fo	10Fc	10s
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-9	-1	4	174	285	-70
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-7	-1	4	419	459	27
-6	-1	4	52	-117	-52
-5	-1	4	522	-533	21
-4	-1	4	107	-84	-75
-3	-1	4	222	-239	27
-2	-1	4	109	34	-57
-1	-1	4	47	-10	-47
0	-1	4	684	630	15
1	-1	4	1372	-1405	14
2	-1	4	1241	-1244	14
3	-1	4	625	-643	16
4	-1	4	564	543	17
5	-1	4	339	316	22
6	-1	4	48	-47	-48
7	-1	4	1038	-1111	21
8	-1	4	683	-687	24
9	-1	4	707	738	25
10	-1	4	178	188	-57
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12	-1	4	276	-335	30
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-7	0	4	489	-474	25
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-5	0	4	986	-983	20
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-3	0	4	556	507	18
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7	0	4	365	357	24
8	0	4	1030	887	23
9	0	4	227	238	35
10	0	4	58	75	-58
11	0	4	84	34	-84
12	0	4	169	-84	39
13	0	4	192	-161	29
-11	1	4	273	-274	27
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-8	1	4	139	130	-65
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-6	1	4	1378	-1364	21
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3	1	4	1108	1164	14
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5	1	4	49	-20	-49
6	1	4	356	326	22
7	1	4	49	63	-49
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9	1	4	57	-102	-57
10	1	4	495	527	30
11	1	4	492	-498	19
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-9	2	4	389	368	30
-8	2	4	627	-656	25
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-5	2	4	901	882	19
-4	2	4	46	118	-46
-3	2	4	563	-538	17
-2	2	4	1216	-1214	15
-1	2	4	146	149	35
0	2	4	352	372	16
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3	2	4	1879	-1774	14

h	k	l	10Fo	10Fc	10s
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5	2	4	697	-666	18
6	2	4	838	878	20
7	2	4	267	-201	29
8	2	4	1267	1191	23
9	2	4	91	4	-91
10	2	4	240	-297	46
11	2	4	214	-221	30
12	2	4	139	-106	-62
13	2	4	414	428	23
-11	3	4	328	357	23
-10	3	4	223	235	27
-9	3	4	559	-584	29
-8	3	4	204	-220	43
-7	3	4	371	357	26
-6	3	4	590	592	22
-5	3	4	921	978	19
-4	3	4	48	105	-48
-3	3	4	1110	-1150	16
-2	3	4	189	190	31
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2	3	4	45	-65	-45
3	3	4	429	-444	18
4	3	4	564	-506	17
5	3	4	1151	1230	17
6	3	4	196	-184	33
7	3	4	1169	1169	21
8	3	4	685	-623	24
9	3	4	59	123	-59
10	3	4	424	-389	35
11	3	4	269	283	25
12	3	4	58	111	-58
13	3	4	57	66	-40
-11	4	4	48	-91	-48
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-6	4	4	373	363	24
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9	4	4	335	-341	35
10	4	4	459	456	34
11	4	4	49	-91	-49
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13	4	4	352	-355	20
-11	5	4	49	65	-49
-10	5	4	343	-336	21
-9	5	4	381	415	31
-8	5	4	52	17	-52
-7	5	4	689	704	23
-6	5	4	51	-149	-51
-5	5	4	242	-192	27
-4	5	4	758	-787	19
-3	5	4	388	415	19
-2	5	4	1075	1066	16
-1	5	4	951	954	15
0	5	4	210	-140	26
1	5	4	562	-551	16
2	5	4	194	190	29
3	5	4	48	-64	-48
4	5	4	1106	1117	17
5	5	4	479	-475	22
6	5	4	51	-22	-51
7	5	4	1198	-1199	21
8	5	4	213	157	35
9	5	4	146	74	-58
10	5	4	190	208	-63
11	5	4	266	242	25
12	5	4	453	-434	24
13	5	4	71	-53	-53
-11	6	4	175	-135	33
-10	6	4	198	-244	30
-9	6	4	184	218	-58
-8	6	4	315	320	32
-7	6	4	114	-67	-53

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
-6	6	4	49	-22	-49
-5	6	4	883	-830	20
-4	6	4	118	-103	-50
-3	6	4	82	-24	-82
-2	6	4	954	931	16
-1	6	4	1001	-1043	16
0	6	4	656	-664	16
1	6	4	310	-384	21
2	6	4	521	466	18
3	6	4	492	-489	18
4	6	4	484	410	21
5	6	4	368	-366	23
6	6	4	1059	-1125	21
7	6	4	307	308	30
8	6	4	243	-246	37
9	6	4	937	828	27
10	6	4	484	-471	33
11	6	4	76	-15	-76
12	6	4	588	-516	23
13	6	4	70	86	-52
-11	7	4	322	-277	21
-10	7	4	158	225	36
-9	7	4	42	62	-42
-8	7	4	58	152	-58
-7	7	4	580	-584	24
-6	7	4	124	107	-54
-5	7	4	210	-183	32
-4	7	4	525	520	20
-3	7	4	544	608	19
-2	7	4	1045	-1017	18
-1	7	4	1319	-1242	16
0	7	4	949	-900	16
1	7	4	344	328	19
2	7	4	228	-212	25
3	7	4	791	779	18
4	7	4	827	-825	19
5	7	4	409	-438	24
6	7	4	609	-667	23
7	7	4	753	725	24
8	7	4	300	378	36
9	7	4	64	-13	-64
10	7	4	66	-40	-66
11	7	4	399	-476	24
12	7	4	704	600	22
13	7	4	61	-78	-43
-10	8	4	103	109	-46
-9	8	4	45	-113	-45
-8	8	4	339	-372	31
-7	8	4	126	-153	-71
-6	8	4	188	-125	38
-5	8	4	430	438	25
-4	8	4	323	-342	24
-3	8	4	494	464	21
-2	8	4	536	-593	20
-1	8	4	583	502	18
0	8	4	772	-712	18
1	8	4	562	541	19
2	8	4	328	353	23
3	8	4	155	-183	-39
4	8	4	150	-159	-42
5	8	4	799	-794	21
6	8	4	495	496	24
7	8	4	342	307	32
8	8	4	741	737	27
9	8	4	552	-510	32
10	8	4	65	-45	-65
11	8	4	223	-173	33
12	8	4	56	47	-56
-10	9	4	45	6	-45
-9	9	4	178	-193	27
-8	9	4	366	-366	18
-7	9	4	281	300	30
-6	9	4	129	107	-50
-5	9	4	149	152	-40
-4	9	4	246	-304	32
-3	9	4	48	-95	-48
-2	9	4	165	88	28
-1	9	4	675	-655	19
0	9	4	1189	1238	18
1	9	4	256	-282	27
2	9	4	539	581	20
3	9	4	444	-405	23
4	9	4	177	-118	41
5	9	4	53	45	-53
6	9	4	207	213	43
7	9	4	449	562	30
8	9	4	710	-617	28
9	9	4	65	83	-65
10	9	4	462	-450	22
11	9	4	490	510	24

h	k	l	10Fo	10Fc	10s
12	9	4	62	-88	-62
-9	10	4	386	-337	18
-8	10	4	174	201	30
-7	10	4	250	213	30
-6	10	4	239	190	34
-5	10	4	181	-201	38
-4	10	4	47	35	-47
-3	10	4	138	-174	-53
-2	10	4	102	156	-102
-1	10	4	387	399	22
0	10	4	319	310	24
1	10	4	445	410	23
2	10	4	1147	-1134	20
3	10	4	758	783	22
4	10	4	620	-544	23
5	10	4	795	831	24
6	10	4	202	-106	40
7	10	4	56	68	-56
8	10	4	344	-363	38
9	10	4	70	74	-70
10	10	4	241	303	31
11	10	4	130	99	-74
12	10	4	62	137	-62
-9	11	4	69	51	-69
-8	11	4	113	139	-45
-7	11	4	423	456	16
-6	11	4	440	-422	26
-5	11	4	88	-117	-88
-4	11	4	146	-120	-43
-3	11	4	564	547	23
-2	11	4	51	-30	-51
-1	11	4	638	590	22
0	11	4	481	-463	22
1	11	4	52	160	-52
2	11	4	212	-212	36
3	11	4	324	331	30
4	11	4	144	169	-65
5	11	4	151	-185	-63
6	11	4	96	143	-96
7	11	4	687	-777	29
8	11	4	393	373	36
9	11	4	52	43	-52
10	11	4	53	143	-53
11	11	4	98	108	-98
-8	12	4	223	200	24
-7	12	4	75	33	-75
-6	12	4	398	-393	16
-5	12	4	111	-203	-111
-4	12	4	411	388	25
-3	12	4	371	367	26
-2	12	4	163	182	-45
-1	12	4	353	-339	24
0	12	4	102	78	-102
1	12	4	481	-481	25
2	12	4	907	886	23
3	12	4	54	-28	-54
4	12	4	717	651	25
5	12	4	539	-527	28
6	12	4	321	-329	36
7	12	4	388	264	34
8	12	4	476	-473	35
9	12	4	619	533	20
10	12	4	281	-258	31
-7	13	4	485	-471	17
-6	13	4	69	-87	-69
-5	13	4	185	-184	23
-4	13	4	532	497	24
-3	13	4	118	-41	-57
-2	13	4	197	-147	36
-1	13	4	394	-349	26
0	13	4	498	-516	26
1	13	4	212	253	41
2	13	4	479	502	26
3	13	4	1025	1016	24
4	13	4	582	-653	27
5	13	4	631	511	28
6	13	4	584	-533	31
7	13	4	137	229	-47
8	13	4	146	91	-46
9	13	4	57	-54	-57
10	13	4	143	-95	-60
-6	14	4	41	51	-41
-5	14	4	483	503	17
-4	14	4	39	-10	-39
-3	14	4	39	-1	-39
-2	14	4	706	-656	25
-1	14	4	163	163	40
0	14	4	253	-240	36
1	14	4	270	212	32
2	14	4	443	-422	28

h	k	l	10Fo	10Fc	10s
3	14	4	886	-883	26
4	14	4	100	-214	-100
5	14	4	298	-287	36
6	14	4	701	656	17
7	14	4	48	54	-48
8	14	4	185	197	41
9	14	4	521	-481	23
-5	15	4	449	445	17
-4	15	4	275	-289	20
-3	15	4	338	-300	18
-2	15	4	84	-97	-84
-1	15	4	112	-67	-39
0	15	4	582	595	16
1	15	4	317	-313	19
2	15	4	164	211	31
3	15	4	752	-760	16
4	15	4	154	141	31
5	15	4	48	80	-48
6	15	4	262	299	27
7	15	4	98	-98	-98
8	15	4	192	-178	39
-3	16	4	477	-445	17
-2	16	4	409	421	16
-1	16	4	41	-52	-41
0	16	4	258	308	21
1	16	4	140	-51	29
2	16	4	388	-370	19
3	16	4	205	192	25
4	16	4	76	-142	-76
5	16	4	595	599	18
6	16	4	330	-264	22
-1	17	4	341	347	18
0	17	4	360	-407	20
1	17	4	254	260	23
2	17	4	342	-327	18
3	17	4	190	240	33
4	17	4	249	198	25
0	-13	5	303	295	22
1	-13	5	189	95	23
2	-13	5	160	216	36
-4	-12	5	186	171	35
-3	-12	5	300	-326	22
-2	-12	5	227	-251	25
-1	-12	5	396	399	18
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1	-12	5	553	567	17
2	-12	5	294	-291	21
3	-12	5	143	-121	33
4	-12	5	253	-251	23
5	-12	5	244	279	23
-5	-11	5	202	226	31
-4	-11	5	364	-393	21
-3	-11	5	122	-31	-36
-2	-11	5	155	-69	36
-1	-11	5	357	360	20
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1	-11	5	90	-133	-65
2	-11	5	157	-165	31
3	-11	5	423	-410	17
4	-11	5	483	509	17
5	-11	5	77	-4	-77
6	-11	5	281	309	20
7	-11	5	312	-327	20
-6	-10	5	48	63	-48
-5	-10	5	265	-284	25
-4	-10	5	248	-242	26
-3	-10	5	43	-3	-43
-2	-10	5	53	86	-53
-1	-10	5	219	-238	46
0	-10	5	117	136	-117
1	-10	5	519	-495	28
2	-10	5	48	-34	-48
3	-10	5	263	-294	34
4	-10	5	462	444	28
5	-10	5	189	176	24
6	-10	5	567	-555	16
7	-10	5	74	-104	-74
8	-10	5	373	-419	20
-7	-9	5	294	-277	26
-6	-9	5	149	-105	-40
-5	-9	5	257	-255	23
-4	-9	5	254	205	37
-3	-9	5	122	99	-80
-2	-9	5	152	201	-59
-1	-9	5	93	-114	-93
0	-9	5	262	-329	35
1	-9	5	51	-65	-51
2	-9	5	271	-264	35
3	-9	5	542	567	27
4	-9	5	137	-126	-51

h	k	l	10Fo	10Fc	10s
5	-9	5	51	122	-51
6	-9	5	612	-567	26
7	-9	5	40	-48	-40
8	-9	5	104	58	-49
9	-9	5	44	81	-44
-8	-8	5	233	-190	32
-7	-8	5	54	-92	-54
-6	-8	5	349	-337	21
-5	-8	5	418	403	33
-4	-8	5	373	-346	33
-3	-8	5	530	560	27
-2	-8	5	305	-306	32
-1	-8	5	127	-138	-64
0	-8	5	131	-151	-61
1	-8	5	244	179	28
2	-8	5	51	-88	-51
3	-8	5	297	299	30
4	-8	5	51	-68	-51
5	-8	5	570	-563	25
6	-8	5	190	187	41
7	-8	5	56	-20	-56
8	-8	5	450	464	17
9	-8	5	44	-104	-44
10	-8	5	45	101	-45
-9	-7	5	281	216	29
-8	-7	5	461	-475	22
-7	-7	5	335	299	22
-6	-7	5	199	-74	46
-5	-7	5	435	399	32
-4	-7	5	310	288	33
-3	-7	5	302	-286	32
-2	-7	5	132	-43	-59
-1	-7	5	328	-354	29
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1	-7	5	47	36	-47
2	-7	5	431	425	24
3	-7	5	284	-233	29
4	-7	5	215	186	34
5	-7	5	294	-257	30
6	-7	5	455	435	26
7	-7	5	59	-49	-59
8	-7	5	255	208	30
9	-7	5	107	-34	-50
10	-7	5	341	-316	20
11	-7	5	123	154	-51
-9	-6	5	232	-223	28
-8	-6	5	49	-3	-49
-7	-6	5	62	17	-62
-6	-6	5	862	840	27
-5	-6	5	247	-225	38
-4	-6	5	322	389	34
-3	-6	5	659	-670	24
-2	-6	5	173	-68	41
-1	-6	5	437	415	26
0	-6	5	416	441	24
1	-6	5	117	13	-50
2	-6	5	448	-466	24
3	-6	5	299	289	26
4	-6	5	491	488	24
5	-6	5	232	262	34
6	-6	5	193	213	36
7	-6	5	354	384	28
8	-6	5	448	-453	28
9	-6	5	48	110	-48
10	-6	5	228	-235	24
11	-6	5	51	125	-51
-10	-5	5	237	-222	35
-9	-5	5	755	-715	20
-8	-5	5	49	-16	-49
-7	-5	5	188	-160	46
-6	-5	5	177	132	-47
-5	-5	5	132	101	-71
-4	-5	5	471	-505	27
-3	-5	5	371	349	26
-2	-5	5	51	-95	-51
-1	-5	5	1322	1321	20
0	-5	5	91	43	-91
1	-5	5	357	-286	22
2	-5	5	140	-45	-38
3	-5	5	306	-311	24
4	-5	5	301	-304	27
5	-5	5	80	114	-80
6	-5	5	297	265	30
7	-5	5	200	-206	42
8	-5	5	324	-326	30
9	-5	5	188	-214	45
10	-5	5	341	377	19
11	-5	5	115	-125	-44
12	-5	5	205	240	35
-10	-4	5	55	-32	-55

h	k	l	10Fo	10Fc	10s
-9	-4	5	562	561	20
-8	-4	5	236	177	49
-7	-4	5	546	523	30
-6	-4	5	647	-646	27
-5	-4	5	261	-231	33
-4	-4	5	453	-471	25
-3	-4	5	321	311	25
-2	-4	5	524	529	22
-1	-4	5	45	29	-45
0	-4	5	293	-306	25
1	-4	5	918	-984	18
2	-4	5	327	349	22
3	-4	5	182	-193	33
4	-4	5	791	795	20
5	-4	5	163	-133	40
6	-4	5	120	-71	-66
7	-4	5	740	-742	23
8	-4	5	101	26	-101
9	-4	5	347	322	31
10	-4	5	210	181	37
11	-4	5	47	21	-47
12	-4	5	195	-187	32
-10	-3	5	148	-124	-50
-9	-3	5	291	306	25
-8	-3	5	298	324	42
-7	-3	5	55	-81	-55
-6	-3	5	55	-121	-55
-5	-3	5	558	-600	25
-4	-3	5	377	413	26
-3	-3	5	270	233	25
-2	-3	5	653	668	20
-1	-3	5	688	-719	19
0	-3	5	781	-780	18
1	-3	5	575	-566	18
2	-3	5	641	645	18
3	-3	5	1004	984	18
4	-3	5	487	-473	21
5	-3	5	143	-167	-39
6	-3	5	1110	-1134	21
7	-3	5	335	354	30
8	-3	5	107	45	-107
9	-3	5	527	532	28
10	-3	5	301	-350	38
11	-3	5	285	-265	24
12	-3	5	193	-235	36
-11	-2	5	268	-291	31
-10	-2	5	414	412	22
-9	-2	5	255	-249	27
-8	-2	5	572	533	28
-7	-2	5	475	-522	30
-6	-2	5	357	-366	28
-5	-2	5	271	275	34
-4	-2	5	47	16	-47
-3	-2	5	447	462	21
-2	-2	5	507	-524	20
-1	-2	5	785	-811	18
0	-2	5	1019	-1018	17
1	-2	5	542	531	18
2	-2	5	444	405	19
3	-2	5	249	248	24
4	-2	5	1337	-1322	18
5	-2	5	267	-289	25
6	-2	5	49	52	-49
7	-2	5	145	181	-47
8	-2	5	708	742	24
9	-2	5	318	-334	30
10	-2	5	358	-392	33
11	-2	5	404	-397	20
12	-2	5	321	302	23
13	-2	5	166	194	31
-11	-1	5	55	-10	-55
-10	-1	5	50	71	-50
-9	-1	5	201	181	48
-8	-1	5	597	-599	28
-7	-1	5	58	31	-58
-6	-1	5	260	-251	33
-5	-1	5	520	488	24
-4	-1	5	160	-157	38
-3	-1	5	176	-169	31
-2	-1	5	461	-499	20
-1	-1	5	472	-482	19
0	-1	5	48	6	-48
1	-1	5	567	551	17
2	-1	5	457	463	18
3	-1	5	710	-680	17
4	-1	5	512	-464	19
5	-1	5	692	-701	20
6	-1	5	709	718	20
7	-1	5	44	-33	-44
8	-1	5	385	429	26

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
9	-1	5	722	-703	26
10	-1	5	472	-491	30
11	-1	5	691	688	18
12	-1	5	100	-55	-100
13	-1	5	442	417	25
-11	0	5	144	150	-52
-10	0	5	221	-291	32
-9	0	5	61	44	-61
-8	0	5	321	-360	38
-7	0	5	121	-83	-70
-6	0	5	250	315	34
-5	0	5	52	48	-52
-4	0	5	142	221	-48
-3	0	5	797	-788	18
-2	0	5	100	-27	-63
-1	0	5	295	-280	20
0	0	5	867	872	16
1	0	5	251	203	23
2	0	5	409	410	18
3	0	5	794	-788	16
4	0	5	391	447	20
5	0	5	961	978	18
6	0	5	125	98	-55
7	0	5	783	843	21
8	0	5	1616	-1484	22
9	0	5	285	311	35
10	0	5	506	-500	30
11	0	5	496	543	19
12	0	5	215	126	29
13	0	5	121	-31	-56
-11	1	5	341	-335	24
-10	1	5	114	86	-51
-9	1	5	347	-309	34
-8	1	5	414	400	29
-7	1	5	334	-292	29
-6	1	5	958	953	22
-5	1	5	508	-513	21
-4	1	5	342	317	24
-3	1	5	219	192	24
-2	1	5	581	548	17
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1	1	5	75	-117	-75
2	1	5	756	-768	15
3	1	5	46	13	-46
4	1	5	494	553	19
5	1	5	1171	1235	18
6	1	5	286	263	26
7	1	5	626	591	22
8	1	5	1055	898	23
9	1	5	158	-34	-49
10	1	5	531	526	28
11	1	5	160	-21	31
12	1	5	52	108	-52
13	1	5	426	-421	32
-11	2	5	341	-339	23
-10	2	5	132	-98	-41
-9	2	5	307	239	34
-8	2	5	268	295	36
-7	2	5	616	588	24
-6	2	5	786	-763	22
-5	2	5	603	-602	21
-4	2	5	625	-637	19
-3	2	5	1162	1162	17
-2	2	5	460	533	19
-1	2	5	624	640	16
0	2	5	46	-20	-46
1	2	5	125	-65	-44
2	2	5	209	-152	24
3	2	5	362	-322	18
4	2	5	1341	1398	16
5	2	5	335	-325	21
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7	2	5	628	-601	22
8	2	5	650	-478	24
9	2	5	56	64	-56
10	2	5	721	712	29
11	2	5	49	-60	-49
12	2	5	53	-99	-53
13	2	5	185	-193	30
-11	3	5	49	62	-49
-10	3	5	77	32	-77
-9	3	5	446	469	31
-8	3	5	60	138	-60
-7	3	5	224	-184	31
-6	3	5	178	-239	40
-5	3	5	182	-107	33
-4	3	5	506	540	20
-3	3	5	322	354	22
-2	3	5	493	522	18

h	k	l	10Fo	10Fc	10s
-1	3	5	974	-973	15
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2	3	5	890	874	15
3	3	5	710	-719	16
4	3	5	47	-18	-47
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6	3	5	950	-995	19
7	3	5	162	-72	-41
8	3	5	148	-129	-47
9	3	5	616	556	25
10	3	5	342	-332	32
11	3	5	108	52	-65
12	3	5	585	-590	22
13	3	5	352	294	19
-11	4	5	52	-61	-52
-10	4	5	629	599	18
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-8	4	5	55	54	-55
-7	4	5	383	-382	28
-6	4	5	129	55	-48
-5	4	5	178	169	36
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-2	4	5	176	-136	30
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2	4	5	515	-506	17
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5	4	5	323	356	23
6	4	5	254	-293	29
7	4	5	824	715	22
8	4	5	136	-117	-59
9	4	5	156	-164	-65
10	4	5	136	-174	-107
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-7	5	5	53	13	-53
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9	5	5	959	-999	26
10	5	5	61	121	-61
11	5	5	170	-170	41
12	5	5	163	181	-53
13	5	5	60	110	-43
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-8	6	5	461	-449	29
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3	6	5	1215	-1228	16
4	6	5	429	406	21
5	6	5	48	-113	-48
6	6	5	1061	1029	21
7	6	5	316	-314	29
8	6	5	566	-632	28
9	6	5	319	284	36
10	6	5	457	-404	33
11	6	5	691	689	19
12	6	5	233	-254	36
13	6	5	225	250	29
-10	7	5	582	-564	18

h	k	l	10Fo	10Fc	10s
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-7	7	5	126	-70	-62
-6	7	5	518	559	24
-5	7	5	689	-697	22
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-2	7	5	588	637	19
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2	7	5	738	-703	17
3	7	5	47	102	-47
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5	7	5	751	794	21
6	7	5	802	-750	22
7	7	5	162	103	-41
8	7	5	754	-753	25
9	7	5	534	568	30
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11	7	5	243	-147	30
12	7	5	58	-2	-58
13	7	5	608	-555	18
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-9	8	5	195	-236	28
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-6	8	5	149	-199	-52
-5	8	5	163	-110	36
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-3	8	5	368	360	22
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3	8	5	864	845	19
4	8	5	509	538	21
5	8	5	105	27	-78
6	8	5	218	-173	35
7	8	5	347	-361	30
8	8	5	784	743	26
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11	8	5	272	-312	31
12	8	5	204	163	45
13	8	5	153	-240	-60
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-7	9	5	62	172	-62
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5	9	5	562	-515	23
6	9	5	131	96	-61
7	9	5	123	-29	-63
8	9	5	534	547	31
9	9	5	280	358	45
10	9	5	221	-132	31
11	9	5	59	-122	-59
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-9	10	5	151	136	31
-8	10	5	40	-4	-40
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-6	10	5	219	202	36
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-4	10	5	618	603	22
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3	10	5	51	160	-51
4	10	5	753	-782	22
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6	10	5	533	-522	25
7	10	5	526	534	27
8	10	5	103	-132	-103
9	10	5	60	71	-60
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h	k	l	10Fo	10Fc	10s
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-5	11	5	192	225	40
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-2	11	5	323	-331	24
-1	11	5	373	349	27
0	11	5	137	-184	-56
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2	11	5	563	-603	22
3	11	5	170	193	-43
4	11	5	554	-588	25
5	11	5	90	52	-90
6	11	5	251	276	35
7	11	5	63	-201	-63
8	11	5	356	358	36
9	11	5	549	-560	36
10	11	5	136	52	-63
11	11	5	202	-221	42
-8	12	5	288	-290	20
-7	12	5	478	458	16
-6	12	5	143	140	27
-5	12	5	187	160	32
-4	12	5	688	-687	24
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-2	12	5	72	-123	-72
-1	12	5	248	273	31
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2	12	5	152	55	-43
3	12	5	800	-764	23
4	12	5	361	384	28
5	12	5	774	-761	26
6	12	5	382	415	34
7	12	5	58	-157	-58
8	12	5	148	-16	-65
9	12	5	445	-398	22
10	12	5	353	-313	27
11	12	5	752	633	23
-7	13	5	343	365	19
-6	13	5	193	196	24
-5	13	5	479	-443	16
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-3	13	5	263	-242	33
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2	13	5	56	-2	-56
3	13	5	119	-55	-65
4	13	5	194	-93	42
5	13	5	623	622	28
6	13	5	391	-390	34
7	13	5	677	550	30
8	13	5	1058	-1005	18
9	13	5	763	744	20
10	13	5	86	-16	-86
-6	14	5	40	41	-40
-5	14	5	678	-665	15
-4	14	5	158	129	24
-3	14	5	478	481	16
-2	14	5	48	-19	-48
-1	14	5	78	91	-78
0	14	5	669	-711	24
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2	14	5	50	-85	-50
3	14	5	964	955	25
4	14	5	414	369	30
5	14	5	64	128	-64
6	14	5	754	-744	17
7	14	5	575	-522	19
8	14	5	545	492	21
9	14	5	53	14	-53
-5	15	5	164	174	29
-4	15	5	43	16	-43
-3	15	5	542	538	16
-2	15	5	285	-271	18
-1	15	5	279	-270	19
0	15	5	178	-231	27
1	15	5	228	-214	39
2	15	5	256	262	36
3	15	5	83	-116	-83
4	15	5	103	-35	-47
5	15	5	507	-567	19
6	15	5	149	184	-43
7	15	5	325	285	25
8	15	5	54	209	-54
-3	16	5	193	-233	24

h	k	l	10Fo	10Fc	10s
-2	16	5	64	66	-64
-1	16	5	522	-541	17
0	16	5	534	511	16
1	16	5	71	-1	-71
2	16	5	396	440	18
3	16	5	188	-218	30
4	16	5	308	-302	22
5	16	5	47	-1	-47
6	16	5	202	170	32
7	16	5	310	275	25
-1	17	5	60	65	-60
0	17	5	119	42	-37
1	17	5	394	387	18
2	17	5	310	-295	21
3	17	5	150	200	-38
4	17	5	425	-423	19
5	17	5	413	377	20
-1	-12	6	363	-366	20
0	-12	6	272	-315	23
1	-12	6	46	18	-46
2	-12	6	130	103	-39
3	-12	6	223	255	25
-4	-11	6	168	145	36
-3	-11	6	319	321	22
-2	-11	6	661	-679	17
-1	-11	6	154	194	35
0	-11	6	203	-115	25
1	-11	6	502	578	18
2	-11	6	205	255	28
3	-11	6	156	-171	32
4	-11	6	260	-295	22
5	-11	6	348	-389	20
6	-11	6	212	188	25
-5	-10	6	348	369	23
-4	-10	6	163	-88	32
-3	-10	6	237	-261	26
-2	-10	6	155	-91	32
-1	-10	6	251	-264	24
0	-10	6	257	269	23
1	-10	6	179	-142	25
2	-10	6	364	381	18
3	-10	6	506	-468	16
4	-10	6	43	12	-43
5	-10	6	145	-75	29
6	-10	6	407	402	18
7	-10	6	136	106	-34
-6	-9	6	303	300	24
-5	-9	6	218	-174	27
-4	-9	6	136	153	-41
-3	-9	6	464	-434	18
-2	-9	6	52	-10	-52
-1	-9	6	182	-168	-51
0	-9	6	448	392	28
1	-9	6	155	-187	-52
2	-9	6	81	-97	-81
3	-9	6	285	-293	35
4	-9	6	115	-117	-72
5	-9	6	515	494	16
6	-9	6	44	38	-44
7	-9	6	42	25	-42
8	-9	6	512	-490	17
9	-9	6	71	37	-71
-7	-8	6	122	-134	-54
-6	-8	6	50	40	-50
-5	-8	6	105	-26	-61
-4	-8	6	279	-328	44
-3	-8	6	59	-35	-59
-2	-8	6	135	193	-82
-1	-8	6	526	495	26
0	-8	6	112	-32	-67
1	-8	6	127	68	-67
2	-8	6	360	-380	29
3	-8	6	308	301	32
4	-8	6	151	54	-46
5	-8	6	597	617	26
6	-8	6	157	-202	-51
7	-8	6	245	-240	22
8	-8	6	126	-118	-39
9	-8	6	45	34	-45
-8	-7	6	115	-43	-74
-7	-7	6	270	247	28
-6	-7	6	429	-461	19
-5	-7	6	116	128	-116
-4	-7	6	411	-415	32
-3	-7	6	417	404	28
-2	-7	6	247	259	37
-1	-7	6	51	19	-51
0	-7	6	138	-136	-51
1	-7	6	250	-255	36
2	-7	6	54	27	-54

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
3	-7	6	255	208	33
4	-7	6	358	318	28
5	-7	6	53	-33	-53
6	-7	6	57	-85	-57
7	-7	6	625	-596	26
8	-7	6	313	320	20
9	-7	6	105	85	-46
10	-7	6	215	248	27
-9	-6	6	496	470	24
-8	-6	6	258	-192	28
-7	-6	6	75	31	-75
-6	-6	6	63	36	-63
-5	-6	6	167	91	-51
-4	-6	6	700	708	27
-3	-6	6	55	37	-55
-2	-6	6	510	473	25
-1	-6	6	487	-516	24
0	-6	6	167	-42	39
1	-6	6	49	30	-49
2	-6	6	447	473	25
3	-6	6	101	196	-101
4	-6	6	157	202	-41
5	-6	6	224	-214	38
6	-6	6	314	-279	30
7	-6	6	56	-1	-56
8	-6	6	311	309	29
9	-6	6	282	285	21
10	-6	6	374	-351	20
11	-6	6	48	63	-48
-9	-5	6	52	-103	-52
-8	-5	6	434	359	22
-7	-5	6	405	-405	21
-6	-5	6	431	479	32
-5	-5	6	57	-73	-57
-4	-5	6	374	332	31
-3	-5	6	215	-172	30
-2	-5	6	352	-360	28
-1	-5	6	177	-174	41
0	-5	6	221	-216	33
1	-5	6	596	605	21
2	-5	6	52	-109	-52
3	-5	6	51	-52	-51
4	-5	6	228	216	30
5	-5	6	72	-35	-72
6	-5	6	105	114	-105
7	-5	6	341	373	29
8	-5	6	187	-194	42
9	-5	6	55	-38	-55
10	-5	6	212	-211	25
11	-5	6	145	-222	-42
-9	-4	6	55	-116	-55
-8	-4	6	898	-889	18
-7	-4	6	63	-45	-63
-6	-4	6	121	132	-121
-5	-4	6	681	674	26
-4	-4	6	399	-358	28
-3	-4	6	111	69	-84
-2	-4	6	885	-919	21
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2	-4	6	478	-525	22
3	-4	6	1012	-1050	20
4	-4	6	318	-334	24
5	-4	6	49	-24	-49
6	-4	6	242	231	34
7	-4	6	168	-49	33
8	-4	6	165	130	-48
9	-4	6	520	-503	28
10	-4	6	224	190	40
11	-4	6	107	-108	-80
12	-4	6	315	339	23
-10	-3	6	51	-75	-51
-9	-3	6	373	-337	22
-8	-3	6	49	-69	-49
-7	-3	6	375	381	35
-6	-3	6	254	210	41
-5	-3	6	128	-180	-95
-4	-3	6	570	-527	24
-3	-3	6	337	-329	26
-2	-3	6	311	283	25
-1	-3	6	97	10	-71
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1	-3	6	1042	-1025	19
2	-3	6	263	-247	26
3	-3	6	957	-963	19
4	-3	6	818	806	20
5	-3	6	255	-244	27
6	-3	6	371	335	25
7	-3	6	189	-145	40

h	k	l	10Fo	10Fc	10s
8	-3	6	418	-432	28
9	-3	6	56	37	-56
10	-3	6	62	122	-62
11	-3	6	518	482	19
12	-3	6	49	-62	-49
-10	-2	6	397	-358	21
-9	-2	6	50	-68	-50
-8	-2	6	224	219	48
-7	-2	6	192	234	-50
-6	-2	6	113	40	-56
-5	-2	6	582	-574	25
-4	-2	6	558	-504	24
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3	-2	6	1075	1048	18
4	-2	6	106	-137	-54
5	-2	6	730	748	20
6	-2	6	1171	-1185	21
7	-2	6	83	63	-83
8	-2	6	224	-241	39
9	-2	6	312	311	34
10	-2	6	402	384	31
11	-2	6	130	-106	-40
12	-2	6	51	116	-51
13	-2	6	350	-373	18
-10	-1	6	171	169	35
-9	-1	6	219	152	27
-8	-1	6	64	145	-64
-7	-1	6	128	180	-84
-6	-1	6	568	-593	26
-5	-1	6	323	-321	29
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-3	-1	6	921	921	19
-2	-1	6	47	44	-47
-1	-1	6	475	474	20
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2	-1	6	182	151	31
3	-1	6	1735	1799	17
4	-1	6	275	280	25
5	-1	6	349	-341	23
6	-1	6	194	-186	33
7	-1	6	631	-642	22
8	-1	6	816	834	24
9	-1	6	114	-122	-114
10	-1	6	661	685	30
11	-1	6	435	-452	21
12	-1	6	51	-47	-51
13	-1	6	142	-137	-57
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-9	0	6	493	506	19
-8	0	6	277	-243	35
-7	0	6	157	82	-49
-6	0	6	715	-734	24
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-4	0	6	481	474	23
-3	0	6	102	52	-65
-2	0	6	46	-15	-46
-1	0	6	556	-546	18
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3	0	6	269	248	23
4	0	6	474	513	20
5	0	6	886	-861	19
6	0	6	162	214	35
7	0	6	332	-292	27
8	0	6	371	389	27
9	0	6	288	274	32
10	0	6	553	-492	30
11	0	6	83	-69	-83
12	0	6	780	-711	19
13	0	6	875	856	15
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-10	1	6	107	-19	-58
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-8	1	6	56	-18	-56
-7	1	6	103	-135	-103
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-3	1	6	501	-541	19
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-1	1	6	88	-82	-88
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h	k	l	10Fo	10Fc	10s
2	1	6	820	846	16
3	1	6	431	-443	19
4	1	6	974	-972	17
5	1	6	220	288	30
6	1	6	450	478	21
7	1	6	997	1035	21
8	1	6	848	-802	23
9	1	6	104	-68	-104
10	1	6	1122	-1137	27
11	1	6	48	38	-48
12	1	6	1033	917	19
13	1	6	114	-1	-54
-11	2	6	79	-74	-79
-10	2	6	141	98	-39
-9	2	6	386	-408	20
-8	2	6	195	255	-53
-7	2	6	112	-57	-85
-6	2	6	467	405	24
-5	2	6	508	519	23
-4	2	6	193	227	32
-3	2	6	756	681	19
-2	2	6	1301	-1309	17
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3	2	6	675	-699	16
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6	2	6	826	809	20
7	2	6	1434	1351	21
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9	2	6	525	-542	27
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12	2	6	141	179	-51
13	2	6	284	-286	28
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-10	3	6	335	-342	22
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9	3	6	283	-311	35
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11	3	6	141	70	-40
12	3	6	181	81	41
13	3	6	65	22	-47
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8	4	6	887	-864	24
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3	5	6	1093	1029	17
4	5	6	853	-863	18
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6	5	6	1024	-1007	20
7	5	6	268	-302	33
8	5	6	916	909	24
9	5	6	117	-100	-117
10	5	6	528	524	32
11	5	6	538	-503	19
12	5	6	141	75	-52
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-6	6	6	619	-607	23
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5	6	6	1474	-1488	19
6	6	6	726	770	21
7	6	6	213	175	32
8	6	6	555	590	26
9	6	6	264	-211	38
10	6	6	286	-197	38
11	6	6	52	-13	-52
12	6	6	59	-85	-59
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-5	7	6	157	150	-41
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13	7	6	225	260	39
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-9	8	6	782	-783	17
-8	8	6	324	-313	19
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3	8	6	529	-479	21
4	8	6	91	-85	-91
5	8	6	930	949	21
6	8	6	286	276	31
7	8	6	58	115	-58
8	8	6	457	-435	29
9	8	6	365	-309	36
10	8	6	370	330	35
11	8	6	252	-209	32

h	k	l	10Fo	10Fc	10s
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13	8	6	412	-417	21
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-8	9	6	44	-76	-44
-7	9	6	336	314	29
-6	9	6	77	89	-77
-5	9	6	339	305	25
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-3	9	6	447	389	23
-2	9	6	488	-475	22
-1	9	6	1134	1118	19
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1	9	6	685	-665	20
2	9	6	445	-407	22
3	9	6	48	-147	-48
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5	9	6	197	-193	34
6	9	6	347	400	29
7	9	6	770	-778	25
8	9	6	87	20	-87
9	9	6	65	-126	-65
10	9	6	697	674	19
11	9	6	51	63	-51
12	9	6	60	21	-60
-9	10	6	141	139	-35
-8	10	6	71	142	-71
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-1	10	6	367	-351	24
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1	10	6	1388	-1420	20
2	10	6	557	566	22
3	10	6	77	-62	-77
4	10	6	519	518	24
5	10	6	51	38	-51
6	10	6	388	-389	28
7	10	6	330	-326	33
8	10	6	285	-256	38
9	10	6	475	417	34
10	10	6	52	-53	-52
11	10	6	226	225	34
12	10	6	440	-421	28
-8	11	6	211	186	24
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-5	11	6	517	-475	25
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3	11	6	1197	1229	21
4	11	6	728	-681	23
5	11	6	218	165	41
6	11	6	697	-741	26
7	11	6	178	118	39
8	11	6	205	211	-63
9	11	6	64	-13	-64
10	11	6	144	142	-56
11	11	6	526	-470	24
12	11	6	62	-23	-62
-8	12	6	42	-69	-42
-7	12	6	77	-86	-77
-6	12	6	371	-361	16
-5	12	6	414	392	27
-4	12	6	108	-112	-91
-3	12	6	261	271	31
-2	12	6	774	-770	23
-1	12	6	82	114	-82
0	12	6	682	-655	23
1	12	6	418	430	25
2	12	6	262	259	32
3	12	6	51	28	-51
4	12	6	290	-291	33
5	12	6	547	-601	27
6	12	6	361	368	31
7	12	6	352	-344	35
8	12	6	629	604	32
9	12	6	268	-278	30
10	12	6	55	155	-55
11	12	6	549	-532	25
-7	13	6	42	38	-42
-6	13	6	43	30	-43
-5	13	6	271	271	18

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
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0	13	6	349	379	29
1	13	6	179	-117	37
2	13	6	454	454	25
3	13	6	680	-713	25
4	13	6	267	232	33
5	13	6	328	-399	35
6	13	6	253	227	39
7	13	6	219	-247	49
8	13	6	183	80	34
9	13	6	246	-125	32
10	13	6	417	-390	25
-6	14	6	587	572	16
-5	14	6	40	13	-40
-4	14	6	176	173	25
-3	14	6	573	-574	15
-2	14	6	136	88	-43
-1	14	6	210	203	33
0	14	6	56	-7	-56
1	14	6	181	242	-51
2	14	6	372	-429	32
3	14	6	60	-23	-60
4	14	6	168	-214	-56
5	14	6	782	781	28
6	14	6	204	135	48
7	14	6	877	882	18
8	14	6	587	-598	20
9	14	6	270	252	33
10	14	6	56	-123	-56
-5	15	6	41	-96	-41
-4	15	6	566	-579	16
-3	15	6	366	398	18
-2	15	6	73	-2	-73
-1	15	6	665	674	15
0	15	6	320	-344	18
1	15	6	52	16	-52
2	15	6	126	-167	-83
3	15	6	195	188	37
4	15	6	348	388	19
5	15	6	188	214	28
6	15	6	197	-101	29
7	15	6	511	-502	20
8	15	6	262	212	28
-3	16	6	349	326	18
-2	16	6	465	442	16
-1	16	6	252	-226	21
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2	16	6	297	297	20
3	16	6	119	11	-39
4	16	6	310	351	21
5	16	6	251	-263	27
6	16	6	187	-148	35
7	16	6	191	-184	33
-1	17	6	543	-538	17
0	17	6	107	-62	-41
1	17	6	79	12	-79
2	17	6	160	126	31
3	17	6	366	364	20
4	17	6	241	-246	26
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-2	-11	7	209	245	31
-1	-11	7	143	104	34
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3	-11	7	394	420	19
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-4	-10	7	76	-88	-76
-3	-10	7	507	519	18
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3	-10	7	102	120	-53
4	-10	7	156	142	32
5	-10	7	498	-520	17
6	-10	7	44	-39	-44
-5	-9	7	136	111	-45
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-3	-9	7	212	184	27
-2	-9	7	96	21	-78
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2	-9	7	634	626	26
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4	-9	7	81	-18	-81
5	-9	7	429	-444	18
6	-9	7	42	45	-42
7	-9	7	344	363	20
8	-9	7	83	91	-83
-6	-8	7	331	319	23
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-4	-8	7	421	395	19
-3	-8	7	109	-107	-47
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3	-8	7	56	103	-56
4	-8	7	640	-606	25
5	-8	7	239	228	37
6	-8	7	44	27	-44
7	-8	7	602	629	17
8	-8	7	264	-257	23
9	-8	7	232	-234	23
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6	-7	7	404	353	28
7	-7	7	114	-54	-41
8	-7	7	119	-102	-45
9	-7	7	571	-562	17
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-7	-6	7	363	368	25
-6	-6	7	78	-164	-78
-5	-6	7	63	103	-63
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3	-6	7	276	-261	29
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5	-6	7	57	-60	-57
6	-6	7	330	303	32
7	-6	7	728	-683	25
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11	-6	7	203	183	30
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-6	-5	7	141	246	-89
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9	-4	7	55	17	-55
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5	-3	7	508	-487	23
6	-3	7	393	384	25
7	-3	7	107	-127	-107
8	-3	7	498	466	26
9	-3	7	175	-94	-48
10	-3	7	89	-63	-89
11	-3	7	188	-134	29
12	-3	7	84	38	-84
-9	-2	7	494	-415	21
-8	-2	7	360	-422	22
-7	-2	7	115	-50	-115
-6	-2	7	428	438	29
-5	-2	7	431	433	26
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3	-2	7	628	-652	20
4	-2	7	409	-437	22
5	-2	7	862	903	21
6	-2	7	52	-81	-52
7	-2	7	747	783	23
8	-2	7	400	-384	27
9	-2	7	127	119	-81
10	-2	7	548	-544	29
11	-2	7	412	457	21
12	-2	7	102	53	-74
-10	-1	7	130	-46	-63
-9	-1	7	380	-425	22
-8	-1	7	175	137	35
-7	-1	7	62	34	-62
-6	-1	7	725	663	26
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Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

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-3	0	8	121	-102	-66
-2	0	8	949	-986	20
-1	0	8	467	444	21
0	0	8	50	-73	-50
1	0	8	1424	1432	18
2	0	8	497	-494	22
3	0	8	152	-150	-44
4	0	8	760	-745	20
5	0	8	49	-127	-49
6	0	8	737	692	21
7	0	8	403	-454	27
8	0	8	548	539	26
9	0	8	868	-836	26
10	0	8	318	373	43
11	0	8	106	-167	-66
12	0	8	386	352	22
13	0	8	54	8	-38
-9	1	8	178	178	32
-8	1	8	394	-430	20
-7	1	8	454	466	30
-6	1	8	54	-94	-54
-5	1	8	719	703	25
-4	1	8	346	-322	28
-3	1	8	701	-716	22
-2	1	8	290	-337	28
-1	1	8	345	411	26
0	1	8	891	859	19
1	1	8	622	-566	19
2	1	8	114	-64	-49
3	1	8	1370	-1403	18
4	1	8	818	767	20
5	1	8	475	-500	23
6	1	8	842	836	22
7	1	8	723	-784	23
8	1	8	467	-532	26
9	1	8	273	-215	32
10	1	8	243	-258	41
11	1	8	577	546	19
12	1	8	83	35	-83
13	1	8	323	287	20
-9	2	8	44	-32	-44
-8	2	8	45	52	-45
-7	2	8	155	140	-46
-6	2	8	221	271	40
-5	2	8	679	-641	23
-4	2	8	101	-61	-101
-3	2	8	1234	-1247	20
-2	2	8	1189	1152	19
-1	2	8	522	-499	19
0	2	8	371	-365	21
1	2	8	1178	-1167	18
2	2	8	158	-199	35
3	2	8	77	107	-77
4	2	8	363	393	23
5	2	8	1216	1236	20
6	2	8	613	-575	21
7	2	8	55	-152	-55
8	2	8	1070	-1111	24
9	2	8	328	353	37
10	2	8	152	-258	-67
11	2	8	190	-96	33
12	2	8	558	-457	20
13	2	8	439	-382	20
-9	3	8	216	-229	27
-8	3	8	535	555	17
-7	3	8	317	-316	31
-6	3	8	302	293	26
-5	3	8	572	-540	25
-4	3	8	303	-361	27
-3	3	8	374	315	22
-2	3	8	306	322	24
-1	3	8	967	969	18
0	3	8	1283	-1295	18
1	3	8	1031	963	17
2	3	8	1771	-1745	17
3	3	8	600	616	19
4	3	8	112	118	-57
5	3	8	596	535	21
6	3	8	178	-115	38
7	3	8	604	-569	23
8	3	8	299	373	35
9	3	8	273	359	35
10	3	8	532	561	33
11	3	8	108	-144	-78
12	3	8	242	155	30
13	3	8	431	-410	20
-9	4	8	206	267	29
-8	4	8	166	-161	33
-7	4	8	50	58	-50
-6	4	8	515	-510	26
-5	4	8	320	322	30
-4	4	8	765	-691	21
-3	4	8	993	976	20

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
-2	4	8	446	-407	21
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0	4	8	48	-95	-48
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2	4	8	843	842	18
3	4	8	469	-451	20
4	4	8	1060	1063	19
5	4	8	869	-839	20
6	4	8	47	95	-47
7	4	8	166	-183	-48
8	4	8	865	853	24
9	4	8	313	306	29
10	4	8	272	273	36
11	4	8	190	-156	33
12	4	8	169	-158	-43
13	4	8	142	144	-47
-9	5	8	213	194	28
-8	5	8	210	-206	26
-7	5	8	251	-227	30
-6	5	8	143	112	-57
-5	5	8	212	221	37
-4	5	8	398	380	25
-3	5	8	209	-232	31
-2	5	8	666	694	20
-1	5	8	1035	-1049	18
0	5	8	599	581	18
1	5	8	221	-254	27
2	5	8	827	795	18
3	5	8	152	-58	36
4	5	8	138	-96	-42
5	5	8	370	403	23
6	5	8	611	-588	23
7	5	8	936	976	22
8	5	8	58	-26	-58
9	5	8	236	260	40
10	5	8	433	-442	31
11	5	8	46	45	-46
12	5	8	190	-177	40
13	5	8	333	331	27
-9	6	8	278	-317	23
-8	6	8	45	63	-45
-7	6	8	308	-367	34
-6	6	8	657	649	25
-5	6	8	86	-43	-86
-4	6	8	140	114	-52
-3	6	8	49	-87	-49
-2	6	8	516	-509	20
-1	6	8	199	188	29
0	6	8	460	449	20
1	6	8	1345	1353	18
2	6	8	880	-839	18
3	6	8	647	695	19
4	6	8	1022	-1004	19
5	6	8	458	451	23
6	6	8	330	318	26
7	6	8	105	222	-105
8	6	8	380	417	31
9	6	8	675	-652	28
10	6	8	231	129	45
11	6	8	533	-490	20
12	6	8	701	637	21
13	6	8	57	-13	-40
-9	7	8	182	-195	30
-8	7	8	415	-431	18
-7	7	8	648	649	27
-6	7	8	55	-37	-55
-5	7	8	265	223	32
-4	7	8	872	-949	22
-3	7	8	46	74	-46
-2	7	8	417	-439	24
-1	7	8	729	709	19
0	7	8	374	358	20
1	7	8	98	65	-81
2	7	8	426	-450	21
3	7	8	708	-733	19
4	7	8	663	661	20
5	7	8	915	-881	21
6	7	8	652	690	22
7	7	8	582	-630	24
8	7	8	544	504	27
9	7	8	820	-825	28
10	7	8	64	32	-64
11	7	8	427	366	22
12	7	8	106	-34	-106
13	7	8	170	130	-44
-9	8	8	46	-91	-46
-8	8	8	46	102	-46
-7	8	8	800	772	15
-6	8	8	298	296	31
-5	8	8	52	-169	-52

h	k	l	10Fo	10Fc	10s
-4	8	8	350	383	28
-3	8	8	472	-468	23
-2	8	8	833	761	20
-1	8	8	139	-2	-36
0	8	8	534	541	20
1	8	8	986	-979	19
2	8	8	50	-56	-50
3	8	8	565	-466	20
4	8	8	320	340	27
5	8	8	545	-526	22
6	8	8	291	223	31
7	8	8	54	-10	-54
8	8	8	922	-950	25
9	8	8	559	571	31
10	8	8	228	-234	42
11	8	8	431	462	24
12	8	8	281	-324	32
13	8	8	125	-50	-58
-8	9	8	464	452	19
-7	9	8	463	-488	17
-6	9	8	220	202	35
-5	9	8	867	-814	24
-4	9	8	53	122	-53
-3	9	8	414	430	23
-2	9	8	124	155	-64
-1	9	8	161	186	34
0	9	8	755	-783	20
1	9	8	47	-60	-47
2	9	8	53	-125	-53
3	9	8	1221	1171	20
4	9	8	51	-3	-51
5	9	8	460	411	25
6	9	8	1030	-1036	23
7	9	8	263	-239	33
8	9	8	156	-58	-61
9	9	8	446	337	32
10	9	8	138	173	-117
11	9	8	436	-437	24
12	9	8	59	-86	-59
13	9	8	444	-389	24
-8	10	8	137	101	33
-7	10	8	198	252	27
-6	10	8	793	-785	15
-5	10	8	127	116	-42
-4	10	8	201	-193	34
-3	10	8	875	859	22
-2	10	8	575	-602	23
-1	10	8	111	-72	-60
0	10	8	788	-801	21
1	10	8	145	-198	-45
2	10	8	640	622	21
3	10	8	254	239	31
4	10	8	52	-97	-52
5	10	8	753	-741	24
6	10	8	57	88	-57
7	10	8	49	-60	-49
8	10	8	598	591	29
9	10	8	108	-153	-108
10	10	8	49	30	-49
11	10	8	425	-401	25
12	10	8	121	-15	-88
-7	11	8	211	-230	23
-6	11	8	406	-399	17
-5	11	8	79	123	-79
-4	11	8	514	537	25
-3	11	8	127	-93	-50
-2	11	8	166	-96	39
-1	11	8	916	-856	22
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1	11	8	197	-196	38
2	11	8	1015	1021	21
3	11	8	542	-521	24
4	11	8	391	-358	25
5	11	8	266	-342	35
6	11	8	282	284	35
7	11	8	455	432	30
8	11	8	128	112	-78
9	11	8	60	2	-60
10	11	8	337	-289	24
11	11	8	193	134	43
12	11	8	94	4	-94
-7	12	8	395	-417	17
-6	12	8	357	372	16
-5	12	8	38	-51	-38
-4	12	8	411	406	26
-3	12	8	610	-610	24
-2	12	8	49	38	-49
-1	12	8	52	-103	-52
0	12	8	239	281	37
1	12	8	497	495	25

h	k	l	10Fo	10Fc	10s
2	12	8	52	-57	-52
3	12	8	57	27	-57
4	12	8	709	-764	24
5	12	8	553	567	26
6	12	8	55	28	-55
7	12	8	529	580	30
8	12	8	208	-93	52
9	12	8	299	-250	27
10	12	8	199	-218	42
11	12	8	313	258	32
-6	13	8	99	88	-50
-5	13	8	336	347	18
-4	13	8	335	-327	18
-3	13	8	46	-57	-46
-2	13	8	407	-376	27
-1	13	8	744	712	23
0	13	8	85	29	-85
1	13	8	449	468	27
2	13	8	350	-325	30
3	13	8	231	-216	34
4	13	8	153	119	-60
5	13	8	95	185	-95
6	13	8	577	589	29
7	13	8	256	-258	48
8	13	8	103	57	-68
9	13	8	86	-183	-86
10	13	8	385	342	24
11	13	8	202	127	44
-5	14	8	70	53	-70
-4	14	8	215	-211	21
-3	14	8	336	-372	17
-2	14	8	435	408	16
-1	14	8	246	-213	29
0	14	8	53	84	-53
1	14	8	275	-296	34
2	14	8	228	181	30
3	14	8	285	-295	37
4	14	8	723	713	26
5	14	8	242	-204	36
6	14	8	213	181	39
7	14	8	373	-445	21
8	14	8	172	26	35
9	14	8	160	66	36
10	14	8	53	-37	-53
-4	15	8	265	252	19
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-2	15	8	414	360	16
-1	15	8	137	-93	32
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1	15	8	247	-266	38
2	15	8	55	12	-55
3	15	8	186	116	41
4	15	8	248	138	31
5	15	8	44	36	-44
6	15	8	680	-635	17
7	15	8	144	-137	-44
8	15	8	410	-441	23
9	15	8	512	483	21
-3	16	8	322	282	19
-2	16	8	153	-93	29
-1	16	8	94	-116	-50
0	16	8	319	-328	19
1	16	8	242	254	20
2	16	8	40	2	-40
3	16	8	211	230	24
4	16	8	46	-59	-46
5	16	8	45	-20	-45
6	16	8	107	-55	-54
7	16	8	149	127	37
8	16	8	283	272	26
-1	17	8	242	-242	22
0	17	8	143	129	31
1	17	8	43	81	-43
2	17	8	188	214	28
3	17	8	254	-266	22
4	17	8	143	-73	33
5	17	8	229	-283	27
6	17	8	227	190	28
-2	-9	9	427	-451	20
-1	-9	9	312	313	23
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1	-9	9	434	419	18
2	-9	9	409	-397	18
3	-9	9	101	61	-48
4	-9	9	110	-42	-49
5	-9	9	199	-154	24
-4	-8	9	49	38	-49
-3	-8	9	47	-84	-47
-2	-8	9	144	-157	-40
-1	-8	9	240	235	24

h	k	l	10Fo	10Fc	10s
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1	-8	9	407	-358	19
2	-8	9	216	216	23
3	-8	9	487	-450	17
4	-8	9	302	361	21
5	-8	9	79	-62	-79
6	-8	9	272	249	22
7	-8	9	222	-224	27
-5	-7	9	350	-353	22
-4	-7	9	46	7	-46
-3	-7	9	301	-279	23
-2	-7	9	443	444	18
-1	-7	9	45	73	-45
0	-7	9	266	273	20
1	-7	9	506	-563	31
2	-7	9	200	-246	-54
3	-7	9	83	66	-83
4	-7	9	43	25	-43
5	-7	9	451	452	17
6	-7	9	526	-532	17
7	-7	9	44	63	-44
8	-7	9	466	-459	18
-6	-6	9	125	-23	-44
-5	-6	9	255	-211	25
-4	-6	9	234	-202	27
-3	-6	9	355	371	18
-2	-6	9	56	29	-56
-1	-6	9	300	337	34
0	-6	9	508	-508	29
1	-6	9	93	-4	-93
2	-6	9	398	-325	28
3	-6	9	711	723	26
4	-6	9	141	-111	-54
5	-6	9	117	123	-86
6	-6	9	307	-280	18
7	-6	9	367	-354	18
8	-6	9	430	456	19
9	-6	9	46	-73	-46
-6	-5	9	521	-537	19
-5	-5	9	209	264	30
-4	-5	9	115	52	-44
-3	-5	9	53	69	-53
-2	-5	9	335	-363	32
-1	-5	9	148	-221	-63
0	-5	9	332	-381	32
1	-5	9	356	-381	29
2	-5	9	531	498	26
3	-5	9	51	79	-51
4	-5	9	347	319	27
5	-5	9	703	-687	25
6	-5	9	242	218	31
7	-5	9	412	-440	33
8	-5	9	640	649	17
9	-5	9	47	71	-47
10	-5	9	48	-24	-48
-7	-4	9	48	-9	-48
-6	-4	9	48	51	-48
-5	-4	9	47	39	-47
-4	-4	9	59	-107	-59
-3	-4	9	592	-610	27
-2	-4	9	679	670	26
-1	-4	9	330	-265	30
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1	-4	9	243	260	33
2	-4	9	517	543	25
3	-4	9	88	83	-88
4	-4	9	440	-380	25
5	-4	9	52	2	-52
6	-4	9	221	-188	38
7	-4	9	453	422	28
8	-4	9	373	-353	30
9	-4	9	288	282	22
10	-4	9	795	-803	18
11	-4	9	164	178	37
-7	-3	9	276	-255	24
-6	-3	9	604	621	18
-5	-3	9	185	-200	-57
-4	-3	9	559	591	27
-3	-3	9	523	468	27
-2	-3	9	551	-558	25
-1	-3	9	190	119	38
0	-3	9	637	-664	23
1	-3	9	1294	1286	22
2	-3	9	387	-360	25
3	-3	9	291	312	31
4	-3	9	579	-551	24
5	-3	9	423	445	28
6	-3	9	317	311	29
7	-3	9	325	385	32
8	-3	9	286	274	33

h	k	l	10Fo	10Fc	10s
9	-3	9	520	-505	30
10	-3	9	48	99	-48
11	-3	9	111	-135	-60
-8	-2	9	49	-123	-49
-7	-2	9	336	354	22
-6	-2	9	348	-376	21
-5	-2	9	1007	930	27
-4	-2	9	755	-776	26
-3	-2	9	286	258	31
-2	-2	9	488	-525	25
-1	-2	9	919	913	23
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1	-2	9	210	-198	35
2	-2	9	48	73	-48
3	-2	9	879	-833	22
4	-2	9	755	785	22
5	-2	9	271	-265	32
6	-2	9	583	570	25
7	-2	9	385	-384	27
8	-2	9	164	143	-45
9	-2	9	274	-312	35
10	-2	9	88	-2	-88
11	-2	9	131	150	-50
12	-2	9	47	45	-47
-8	-1	9	158	-112	-40
-7	-1	9	361	384	20
-6	-1	9	177	207	-59
-5	-1	9	356	-379	35
-4	-1	9	281	-291	35
-3	-1	9	108	-63	-90
-2	-1	9	988	967	22
-1	-1	9	406	-378	25
0	-1	9	440	421	23
1	-1	9	1063	-1052	21
2	-1	9	135	154	-54
3	-1	9	337	-401	27
4	-1	9	565	583	23
5	-1	9	401	409	24
6	-1	9	774	-774	24
7	-1	9	199	291	48
8	-1	9	616	-639	27
9	-1	9	475	455	29
10	-1	9	63	-106	-63
11	-1	9	392	378	22
12	-1	9	307	-302	26
-8	0	9	571	533	19
-7	0	9	446	-465	19
-6	0	9	132	-83	-73
-5	0	9	822	-812	25
-4	0	9	508	500	25
-3	0	9	406	348	26
-2	0	9	351	400	26
-1	0	9	345	-317	26
0	0	9	785	-769	21
1	0	9	197	186	34
2	0	9	611	-574	21
3	0	9	1184	1203	20
4	0	9	539	-535	22
5	0	9	107	189	-107
6	0	9	1096	-1120	22
7	0	9	51	-1	-51
8	0	9	210	130	40
9	0	9	138	-110	-57
10	0	9	439	449	35
11	0	9	386	-406	21
12	0	9	52	65	-52
13	0	9	273	-311	26
-9	1	9	50	48	-50
-8	1	9	45	16	-45
-7	1	9	195	-133	28
-6	1	9	697	-700	27
-5	1	9	131	185	-47
-4	1	9	87	-116	-87
-3	1	9	860	919	22
-2	1	9	708	-678	22
-1	1	9	541	-484	21
0	1	9	667	-686	21
1	1	9	558	498	21
2	1	9	677	645	20
3	1	9	105	-26	-61
4	1	9	46	-90	-46
5	1	9	939	-972	21
6	1	9	789	798	23
7	1	9	330	-370	30
8	1	9	720	686	25
9	1	9	516	-554	29
10	1	9	379	329	31
11	1	9	171	-198	36
12	1	9	53	72	-53
13	1	9	214	249	27

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
-9	2	9	398	446	22
-8	2	9	349	-341	21
-7	2	9	79	118	-79
-6	2	9	240	-271	39
-5	2	9	315	315	30
-4	2	9	426	421	25
-3	2	9	430	-449	25
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9	2	9	128	47	-66
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11	4	9	52	65	-52
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6	10	9	54	-23	-54
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5	15	9	112	-169	-51
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8	15	9	442	-455	21
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-2	16	9	164	185	26
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3	16	9	77	3	-77
4	16	9	74	59	-74
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3	17	9	117	171	-43
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-5	-4	10	71	9	-71

h	k	l	10Fo	10Fc	10s
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7	-4	10	318	-276	32
8	-4	10	158	-82	25
9	-4	10	483	488	18
10	-4	10	47	19	-47
-7	-3	10	213	-243	30
-6	-3	10	227	186	28
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5	-3	10	52	70	-52
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7	-3	10	84	82	-84
8	-3	10	111	-89	-111
9	-3	10	375	344	18
10	-3	10	192	-145	32
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4	-2	10	256	-268	37
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6	-2	10	217	193	32
7	-2	10	53	-7	-53
8	-2	10	368	372	31
9	-2	10	114	-159	-114
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7	-1	10	138	179	-69
8	-1	10	204	-190	43
9	-1	10	100	-193	-100
10	-1	10	276	-263	23
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1	0	10	317	-251	25
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3	0	10	47	-41	-47
4	0	10	696	-660	23
5	0	10	871	884	22
6	0	10	233	-200	29
7	0	10	477	438	28
8	0	10	761	-812	27

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
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13	1	10	274	-251	22
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Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

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8	12	11	363	349	35
9	12	11	294	-338	24
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6	13	11	287	275	34
7	13	11	61	119	-61
8	13	11	268	-248	27
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11	13	11	157	149	-54
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7	14	11	118	49	-46
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9	14	11	126	-64	-55
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4	15	11	221	209	24
5	15	11	73	-52	-73
6	15	11	221	230	25
7	15	11	617	-605	18
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9	15	11	102	-15	-102
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4	-5	12	222	-237	25
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6	-5	12	624	-617	17
7	-5	12	310	288	21
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7	-4	12	43	23	-43
8	-4	12	323	304	20
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7	-3	12	91	80	-91
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9	-3	12	158	-131	37
-5	-2	12	146	-103	-40
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-3	-2	12	623	-588	17
-2	-2	12	83	-120	-83
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5	-2	12	118	117	-118
6	-2	12	176	131	-47
7	-2	12	267	216	21
8	-2	12	349	-354	19
9	-2	12	89	-26	-89
10	-2	12	312	-285	24
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-4	-1	12	48	-149	-48
-3	-1	12	72	-39	-72
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6	-1	12	286	323	39
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9	-1	12	99	-112	-81
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11	-1	12	50	43	-50
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3	0	12	575	-558	25
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6	0	12	59	188	-59
7	0	12	401	-432	29
8	0	12	54	-79	-54
9	0	12	218	160	24
10	0	12	233	273	30
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3	1	12	300	281	27
4	1	12	108	131	-108
5	1	12	224	210	34
6	1	12	480	-453	26
7	1	12	125	86	-73
8	1	12	252	-211	37
9	1	12	406	406	34
10	1	12	49	81	-49
11	1	12	84	87	-84
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-5	2	12	78	117	-78
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6	2	12	471	-475	28
7	2	12	95	-61	-95
8	2	12	219	228	46
9	2	12	186	-228	-62
10	2	12	169	166	35
11	2	12	459	-450	21
12	2	12	50	107	-50
-6	3	12	249	-324	25
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-3	3	12	191	134	33
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-1	3	12	246	-236	32
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1	3	12	312	317	28
2	3	12	205	165	38
3	3	12	157	-121	-50
4	3	12	53	2	-53
5	3	12	378	-344	27
6	3	12	551	594	28
7	3	12	93	-146	-93
8	3	12	732	705	27
9	3	12	290	-331	42
10	3	12	377	-356	22
11	3	12	118	-152	-77
12	3	12	52	-45	-52

Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

h	k	l	10Fo	10Fc	10s
-7	4	12	84	89	-84
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2	4	12	349	-359	28
3	4	12	665	-597	23
4	4	12	207	228	39
5	4	12	150	156	-56
6	4	12	53	18	-53
7	4	12	173	147	-44
8	4	12	329	-363	36
9	4	12	58	-75	-58
10	4	12	149	-245	-49
11	4	12	522	516	21
12	4	12	55	-60	-55
-7	5	12	44	42	-44
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-5	5	12	564	-573	16
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-3	5	12	253	-241	31
-2	5	12	54	7	-54
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2	5	12	1014	-976	22
3	5	12	93	-16	-93
4	5	12	202	-174	39
5	5	12	504	491	25
6	5	12	57	-174	-57
7	5	12	80	-19	-80
8	5	12	655	-660	27
9	5	12	136	169	-88
10	5	12	180	167	44
11	5	12	51	74	-51
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-5	6	12	156	-77	26
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2	6	12	338	-340	28
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3	7	12	215	233	35
4	7	12	535	532	24
5	7	12	432	-383	25
6	7	12	304	-265	32
7	7	12	93	-1	-93
8	7	12	130	111	-66
9	7	12	317	402	41
10	7	12	147	-146	-111
11	7	12	126	-55	-56
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2	8	12	125	76	-62
3	8	12	951	927	22
4	8	12	547	-514	24

h	k	l	10Fo	10Fc	10s
5	8	12	55	23	-55
6	8	12	579	-512	27
7	8	12	681	717	26
8	8	12	87	66	-87
9	8	12	298	286	38
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-3	9	12	308	287	31
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3	9	12	120	170	-64
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5	9	12	89	94	-89
6	9	12	359	340	29
7	9	12	179	164	-48
8	9	12	466	430	30
9	9	12	519	-519	32
10	9	12	133	176	-54
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-2	10	12	410	-475	27
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3	10	12	478	-470	24
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6	10	12	762	741	25
7	10	12	58	-121	-58
8	10	12	65	-119	-65
9	10	12	408	-371	33
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4	11	12	149	197	-57
5	11	12	373	418	31
6	11	12	244	-239	39
7	11	12	54	66	-54
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9	11	12	231	278	30
10	11	12	155	-191	-48
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9	12	12	48	-39	-48
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3	13	12	57	-78	-57
4	13	12	251	312	37
5	13	12	647	-629	26

h	k	l	10Fo	10Fc	10s
6	13	12	52	11	-52
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9	13	12	49	65	-49
10	13	12	51	-7	-51
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3	14	12	78	-145	-78
4	14	12	405	-375	17
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6	14	12	67	-102	-67
7	14	12	513	482	18
8	14	12	105	-112	-62
9	14	12	192	221	34
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2	15	12	414	-448	18
3	15	12	128	156	-42
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6	15	12	69	96	-69
7	15	12	249	258	24
8	15	12	238	301	29
9	15	12	459	-468	24
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2	16	12	139	34	30
3	16	12	197	-223	27
4	16	12	351	345	19
5	16	12	374	-412	20
6	16	12	624	655	18
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3	17	12	154	-191	32
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6	-3	13	633	-624	17
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8	-2	13	334	362	22
9	-2	13	93	123	-93
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-2	-1	13	149	-124	30
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h	k	l	10Fo	10Fc	10s
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7	-1	13	524	518	17
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9	-1	13	49	129	-49
10	-1	13	348	-339	22
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2	0	13	53	-141	-53
3	0	13	123	-47	-64
4	0	13	156	-170	-58
5	0	13	196	-208	45
6	0	13	373	405	30
7	0	13	132	213	-77
8	0	13	102	31	-49
9	0	13	450	-447	20
10	0	13	115	111	-49
11	0	13	91	-50	-91
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-3	1	13	190	-208	27
-2	1	13	91	-62	-65
-1	1	13	54	-32	-54
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2	1	13	102	157	-102
3	1	13	543	-496	26
4	1	13	57	92	-57
5	1	13	148	-63	-44
6	1	13	408	414	31
7	1	13	58	40	-58
8	1	13	431	-417	18
9	1	13	76	-111	-76
10	1	13	109	-84	-55
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1	2	13	394	-390	26
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3	2	13	240	198	36
4	2	13	203	-203	45
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7	2	13	118	39	-69
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5	3	13	79	30	-79
6	3	13	213	-251	40
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8	3	13	100	57	-100
9	3	13	310	-301	22
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9	4	13	223	238	51
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7	5	13	459	504	29
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9	5	13	64	89	-64
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11	5	13	91	216	-91
12	5	13	53	6	-53
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7	6	13	143	173	-61
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9	6	13	189	-229	43
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11	6	13	155	-118	-47
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11	8	13	198	185	35
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h	k	l	10Fo	10Fc	10s
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8	9	13	277	266	40
9	9	13	152	168	-42
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11	9	13	513	-514	23
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3	10	13	183	-198	37
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9	10	13	121	-63	-49
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5	11	13	466	-461	27
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8	11	13	158	-146	33
9	11	13	174	133	34
10	11	13	629	-635	20
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-1	12	13	130	214	-34
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2	12	13	136	-143	-65
3	12	13	138	-13	-55
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6	12	13	54	6	-54
7	12	13	445	446	19
8	12	13	370	-355	21
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8	13	13	126	-55	-51
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5	14	13	202	165	26
6	14	13	101	-131	-64
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9	14	13	356	394	24
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h	k	l	10Fo	10Fc	10s
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6	16	13	238	263	27
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6	-3	14	418	412	20
7	-3	14	92	-52	-92
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3	-2	14	139	24	33
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6	-2	14	46	-69	-46
7	-2	14	466	-485	19
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-2	-1	14	521	509	17
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7	1	14	143	-163	-39
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6	2	14	54	-2	-54
7	2	14	482	501	18
8	2	14	137	-116	-38

h	k	l	10Fo	10Fc	10s
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3	3	14	121	16	-53
4	3	14	488	-523	29
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6	3	14	289	-305	31
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7	5	14	177	-113	-51
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9	7	14	334	-341	21
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h	k	l	10Fo	10Fc	10s
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3	8	14	1037	-1031	24
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5	8	14	124	-126	-76
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7	8	14	56	4	-56
8	8	14	243	-215	38
9	8	14	45	-35	-45
10	8	14	219	-287	34
11	8	14	160	149	-43
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3	9	14	551	-573	26
4	9	14	298	-288	31
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6	9	14	473	-478	29
7	9	14	308	264	35
8	9	14	280	-315	23
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4	10	14	255	-157	33
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6	10	14	388	396	32
7	10	14	756	-757	28
8	10	14	245	256	25
9	10	14	376	-420	22
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4	12	14	107	9	-89
5	12	14	43	32	-43
6	12	14	650	-600	16
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8	12	14	124	-71	-45
9	12	14	474	523	21
10	12	14	226	-238	33
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5	13	14	134	-30	30
6	13	14	86	37	-67
7	13	14	114	140	-46
8	13	14	352	375	24
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10	13	14	96	12	-96
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h	k	l	10Fo	10Fc	10s
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6	15	14	47	-53	-47
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8	15	14	427	-413	22
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6	16	14	427	-451	20
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2	-2	15	61	56	-61
3	-2	15	44	-59	-44
4	-2	15	125	-96	-40
5	-2	15	288	-282	21
6	-2	15	392	452	20
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1	-1	15	114	35	-46
2	-1	15	46	97	-46
3	-1	15	266	-247	21
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5	-1	15	45	-4	-45
6	-1	15	82	93	-82
7	-1	15	178	189	33
-1	0	15	123	108	-35
0	0	15	194	227	-61
1	0	15	104	-102	-48
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3	0	15	43	73	-43
4	0	15	44	-76	-44
5	0	15	215	205	24
6	0	15	111	88	-51
7	0	15	83	-154	-83
8	0	15	457	-445	20
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2	1	15	444	-428	17
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5	1	15	67	82	-67
6	1	15	43	-73	-43
7	1	15	350	-361	21
8	1	15	111	64	-47
9	1	15	94	-39	-94
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3	2	15	204	-220	24
4	2	15	509	546	17
5	2	15	432	-432	17
6	2	15	45	15	-45
7	2	15	317	-337	21
8	2	15	167	151	34
9	2	15	284	324	26
10	2	15	49	-40	-49
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6	3	15	595	-598	17
7	3	15	528	524	18
8	3	15	147	-97	35
9	3	15	448	458	20
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-3	4	15	74	61	-74
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Observed and calculated structure factors for MN364 in P-1; Vince's PdCl2L

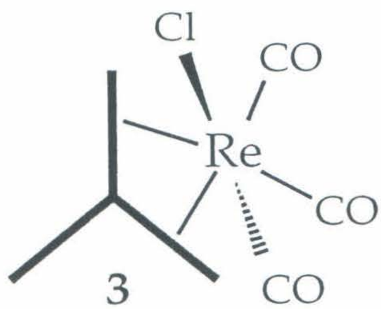
h	k	l	10Fo	10Fc	10s
0	4	15	248	-239	22
1	4	15	413	376	18
2	4	15	53	70	-53
3	4	15	390	351	28
4	4	15	585	-605	27
5	4	15	54	152	-54
6	4	15	44	-76	-44
7	4	15	80	22	-80
8	4	15	435	453	20
9	4	15	462	-488	20
10	4	15	50	83	-50
-3	5	15	42	-38	-42
-2	5	15	82	-111	-82
-1	5	15	94	-174	-56
0	5	15	222	235	23
1	5	15	323	313	31
2	5	15	297	236	32
3	5	15	532	-481	28
4	5	15	150	153	-57
5	5	15	231	-217	38
6	5	15	679	661	27
7	5	15	202	-191	26
8	5	15	88	73	-88
9	5	15	322	-286	22
10	5	15	102	-166	-102
11	5	15	301	290	27
-3	6	15	286	-320	21
-2	6	15	370	254	17
-1	6	15	43	145	-43
0	6	15	198	194	26
1	6	15	114	-20	-60
2	6	15	54	-192	-54
3	6	15	197	-228	44
4	6	15	81	150	-81
5	6	15	421	425	28
6	6	15	57	-33	-57
7	6	15	204	230	27
8	6	15	457	-461	19
9	6	15	274	265	23
10	6	15	192	-235	33
11	6	15	451	452	22
-3	7	15	125	98	-37
-2	7	15	194	230	26
-1	7	15	182	187	24
0	7	15	453	-447	16
1	7	15	123	45	-52
2	7	15	445	-430	27
3	7	15	469	473	26
4	7	15	57	-36	-57
5	7	15	284	286	33
6	7	15	344	-387	34
7	7	15	160	-192	32
8	7	15	112	-63	-49
9	7	15	86	48	-86
10	7	15	202	169	30
11	7	15	188	-174	40
-3	8	15	613	639	16
-2	8	15	230	-184	21
-1	8	15	128	78	31
0	8	15	494	-491	16
1	8	15	55	4	-55
2	8	15	186	204	45
3	8	15	114	73	-75
4	8	15	710	694	27
5	8	15	585	-560	27
6	8	15	58	-27	-58
7	8	15	149	-154	-38
8	8	15	258	277	26
9	8	15	49	-65	-49
10	8	15	97	50	-97
11	8	15	51	2	-51
-3	9	15	146	106	30
-2	9	15	143	86	28
-1	9	15	735	-680	15
0	9	15	145	160	31
1	9	15	469	-421	16
2	9	15	485	521	27
3	9	15	58	-98	-58
4	9	15	391	-371	28
5	9	15	216	-184	44
6	9	15	297	-272	33
7	9	15	491	525	18
8	9	15	405	-376	20
9	9	15	428	428	22
10	9	15	495	-519	21
11	9	15	143	130	-51
-3	10	15	160	-184	31
-2	10	15	279	-281	21

h	k	l	10Fo	10Fc	10s
-1	10	15	245	-216	19
0	10	15	82	90	-82
1	10	15	513	488	16
2	10	15	629	-657	15
3	10	15	156	-236	-51
4	10	15	943	-951	26
5	10	15	533	520	28
6	10	15	125	-86	-36
7	10	15	711	770	17
8	10	15	47	28	-47
9	10	15	471	-456	21
10	10	15	136	126	-49
-2	11	15	516	-479	16
-1	11	15	403	391	16
0	11	15	256	273	21
1	11	15	477	496	16
2	11	15	41	66	-41
3	11	15	101	-4	-46
4	11	15	44	66	-44
5	11	15	427	-472	18
6	11	15	766	817	16
7	11	15	591	-574	18
8	11	15	347	322	22
9	11	15	421	-452	22
10	11	15	236	228	28
-2	12	15	185	204	26
-1	12	15	40	-51	-40
0	12	15	505	465	16
1	12	15	324	-318	18
2	12	15	74	94	-74
3	12	15	371	-375	17
4	12	15	376	406	18
5	12	15	269	284	21
6	12	15	135	112	-37
7	12	15	44	-19	-44
8	12	15	461	-475	20
9	12	15	303	346	27
-1	13	15	254	218	20
0	13	15	41	-26	-41
1	13	15	142	-186	33
2	13	15	291	-306	19
3	13	15	316	332	18
4	13	15	97	84	-58
5	13	15	230	245	23
6	13	15	170	-226	33
7	13	15	45	-74	-45
8	13	15	87	-137	-87
9	13	15	262	240	27
0	14	15	472	-452	16
1	14	15	41	67	-41
2	14	15	42	41	-42
3	14	15	276	258	19
4	14	15	83	46	-83
5	14	15	184	-209	28
6	14	15	77	-26	-77
7	14	15	254	-294	24
8	14	15	264	259	24
1	15	15	181	-200	27
2	15	15	560	591	17
3	15	15	223	-298	23
4	15	15	99	81	-57
5	15	15	339	-296	19
6	15	15	47	-34	-47
7	15	15	196	153	29
1	0	16	45	7	-45
2	0	16	288	307	22
3	0	16	148	-195	-38
4	0	16	43	-23	-43
5	0	16	197	-188	28
6	0	16	43	68	-43
0	1	16	92	-6	-68
1	1	16	458	487	19
2	1	16	301	-293	21
3	1	16	154	58	30
4	1	16	490	-483	18
5	1	16	359	353	20
6	1	16	43	-47	-43
7	1	16	267	256	22
-1	2	16	421	436	19
0	2	16	80	45	-80
1	2	16	220	222	26
2	2	16	204	-195	26
3	2	16	321	-310	19
4	2	16	276	326	22
5	2	16	154	-133	32
6	2	16	608	513	17
7	2	16	331	-364	21
8	2	16	92	160	-92

h	k	l	10Fo	10Fc	10s
-1	3	16	81	-59	-81
0	3	16	440	396	18
1	3	16	563	-586	17
2	3	16	44	68	-44
3	3	16	428	-472	17
4	3	16	581	588	17
5	3	16	210	215	23
6	3	16	166	-182	30
7	3	16	45	49	-45
8	3	16	406	-391	19
9	3	16	358	362	22
-2	4	16	235	221	23
-1	4	16	103	-150	-49
0	4	16	43	-94	-43
1	4	16	136	-192	-35
2	4	16	193	-147	24
3	4	16	691	712	16
4	4	16	120	-81	-37
5	4	16	397	369	19
6	4	16	498	-490	18
7	4	16	128	108	-46
8	4	16	102	-83	-70
9	4	16	299	274	24
-2	5	16	75	-143	-75
-1	5	16	201	289	28
0	5	16	357	-378	20
1	5	16	182	115	27
2	5	16	45	-15	-45
3	5	16	171	82	27
4	5	16	153	155	33
5	5	16	372	-373	17
6	5	16	79	64	-79
7	5	16	362	-370	20
8	5	16	514	472	19
9	5	16	284	-297	26
10	5	16	216	228	34
-2	6	16	45	116	-45
-1	6	16	430	-446	17
0	6	16	383	459	19
1	6	16	333	-365	19
2	6	16	497	498	16
3	6	16	168	-165	28
4	6	16	128	82	-37
5	6	16	533	-514	18
6	6	16	118	65	-40
7	6	16	115	91	-48
8	6	16	89	72	-89
9	6	16	151	155	-42
10	6	16	467	-490	23
-2	7	16	43	107	-43
-1	7	16	86	-75	-86
0	7	16	114	128	-42
1	7	16	155	169	28
2	7	16	236	-217	20
3	7	16	127	119	-38
4	7	16	527	-536	16
5	7	16	122	151	-44
6	7	16	146	-122	34
7	7	16	361	358	20
8	7	16	152	-219	-41
9	7	16	133	38	-41
10	7	16	202	-242	34
-2	8	16	308	-282	20
-1	8	16	654	635	16
0	8	16	339	-348	19
1	8	16	120	194	-35
2	8	16	473	-426	16
3	8	16	42	-18	-42
4	8	16	41	17	-41
5	8	16	44	95	-44
6	8	16	368	347	19
7	8	16	265	-273	23
8	8	16	70	17	-70
9	8	16	443	-464	21
10	8	16	275	284	26
-2	9	16	179	203	27
-1	9	16	43	120	-43
0	9	16	45	89	-45
1	9	16	567	-550	16
2	9	16	299	320	20
3	9	16	368	-363	17
4	9	16	664	671	16
5	9	16	139	104	-37
6	9	16	312	282	20
7	9	16	241	-263	24
8	9	16	260	-268	27
9	9	16	310	291	23
10	9	16	251	179	26

h	k	l	10Fo	10Fc	10s
-2	10	16	528	549	17
-1	10	16	256	-250	21
0	10	16	42	-76	-42
1	10	16	312	-377	18
2	10	16	165	181	32
3	10	16	263	324	22
4	10	16	44	47	-44
5	10	16	140	127	-38
6	10	16	901	-914	16
7	10	16	48	-5	-48
8	10	16	111	-65	-52
9	10	16	728	701	19
-1	11	16	83	-68	-83
0	11	16	481	-485	17
1	11	16	416	398	17
2	11	16	187	-208	25
3	11	16	373	382	19
4	11	16	571	-571	16
5	11	16	129	160	-40
6	11	16	177	-153	29
7	11	16	692	708	18
8	11	16	253	279	27
9	11	16	469	-436	21
-1	12	16	190	-247	28
0	12	16	185	214	27
1	12	16	293	254	20
2	12	16	470	477	17
3	12	16	273	-275	19
4	12	16	42	7	-42
5	12	16	473	-502	18
6	12	16	690	696	17
7	12	16	282	-301	24
8	12	16	320	354	25
9	12	16	54	-118	-54
0	13	16	373	392	19
1	13	16	191	185	25
2	13	16	77	-24	-77
3	13	16	203	-216	25
4	13	16	210	-199	26
5	13	16	135	168	-37
6	13	16	121	-148	-49
7	13	16	433	418	20
8	13	16	292	-325	24
2	14	16	454	-434	17
3	14	16	111	-31	-45
4	14	16	73	-68	-73
5	14	16	176	232	32
6	14	16	155	108	32
7	14	16	46	-88	-46
2	2	17	44	51	-44
3	2	17	312	322	22
4	2	17	263	-256	23
5	2	17	162	-139	35
6	2	17	159	166	35
1	3	17	45	50	-45
2	3	17	517	526	18
3	3	17	519	-496	18
4	3	17	134	144	-38
5	3	17	239	-207	24
6	3	17	470	475	18
7	3	17	46	-44	-46
0	4	17	407	439	18
1	4	17	132	-128	-40
2	4	17	158	-191	34
3	4	17	424	-475	18
4	4	17	138	-184	-40
5	4	17	582	589	17
6	4	17	314	-308	21
7	4	17	366	391	20
8	4	17	388	-450	21
0	5	17	184	-181	27
1	5	17	244	274	23
2	5	17	570	-514	17
3	5	17	360	405	18
4	5	17	221	-195	23
5	5	17	311	296	20
6	5	17	45	-81	-45
7	5	17	149	-215	37
8	5	17	118	15	-52
0	6	17	48	-118	-48
1	6	17	265	-240	21
2	6	17	102	154	-56
3	6	17	369	-399	19
4	6	17	469	533	18
5	6	17	238	-249	24
6	6	17	210	204	27
7	6	17	572	-575	18

h	k	l	10Fo	10Fc	10s
8	6	17	72	93	-72
0	7	17	181	203	25
1	7	17	263	-255	20
2	7	17	110	52	-43
3	7	17	219	241	25
4	7	17	97	69	-51
5	7	17	45	36	-45
6	7	17	413	-413	19
7	7	17	109	131	-55
8	7	17	47	-91	-47
9	7	17	328	344	24
0	8	17	219	-215	25
1	8	17	394	359	18
2	8	17	208	-164	25
3	8	17	259	248	20
4	8	17	250	-246	24
5	8	17	171	-136	28
6	8	17	46	-87	-46
7	8	17	100	115	-68
8	8	17	173	128	30
9	8	17	50	11	-50
0	9	17	43	6	-43
1	9	17	202	190	25
2	9	17	91	19	-62
3	9	17	241	-241	24
4	9	17	232	227	24
5	9	17	153	-176	36
6	9	17	438	432	18
7	9	17	45	-38	-45
8	9	17	295	311	25
9	9	17	246	-298	29
0	10	17	547	508	17
1	10	17	291	-299	21
2	10	17	114	100	-42
3	10	17	326	-300	19
4	10	17	175	181	29
5	10	17	256	267	21
6	10	17	321	325	21
7	10	17	479	489	19
8	10	17	279	-273	24
1	11	17	171	-183	30
2	11	17	416	-417	18
3	11	17	317	303	19
4	11	17	188	-237	29
5	11	17	157	187	34
6	11	17	411	-473	19
7	11	17	400	-372	20
8	11	17	49	-89	-49
1	12	17	43	-88	-43
2	12	17	159	-107	28
3	12	17	233	295	24
4	12	17	212	184	24
5	12	17	289	-244	20
6	12	17	69	-46	-69
7	12	17	162	-198	36
3	13	17	43	59	-43
4	13	17	45	28	-45
5	13	17	138	-146	-36
6	13	17	167	-86	31
4	5	18	584	-581	17
5	5	18	99	194	-75
3	6	18	42	90	-42
4	6	18	438	-439	18
5	6	18	145	127	-37
6	6	18	336	350	22
2	7	18	68	78	-68
3	7	18	343	-371	19
4	7	18	193	238	28
5	7	18	45	-24	-45
6	7	18	341	322	21
2	8	18	195	-155	23
3	8	18	145	177	30
4	8	18	41	16	-41
5	8	18	360	368	19
6	8	18	191	-232	31
7	8	18	47	-79	-47
2	9	18	124	-112	-38
3	9	18	306	289	21
4	9	18	86	61	-86
5	9	18	45	-59	-45
6	9	18	144	-150	33
3	10	18	220	-202	24
4	10	18	185	236	28
5	10	18	198	-173	25
6	10	18	94	94	-69
4	11	18	123	-149	-42
5	11	18	158	131	32



3

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
2	0	0	3719	3556	12
4	0	0	902	899	18
6	0	0	1222	-1210	23
8	0	0	1459	-1393	28
10	0	0	1664	-1513	35
12	0	0	983	-968	48
1	1	0	2166	2285	8
2	1	0	1588	-1569	12
3	1	0	514	-462	16
4	1	0	1843	-1820	17
5	1	0	238	177	31
6	1	0	962	-921	23
7	1	0	619	-629	28
8	1	0	620	-517	31
9	1	0	966	-947	33
10	1	0	283	176	69
11	1	0	808	-801	43
12	1	0	475	439	65
0	2	0	489	-445	7
1	2	0	1061	-1117	9
2	2	0	420	421	15
3	2	0	1944	-1960	15
4	2	0	306	209	23
5	2	0	2329	-2401	20
6	2	0	209	-93	37
7	2	0	1345	-1324	25
8	2	0	505	-439	32
9	2	0	818	-822	34
10	2	0	298	-327	52
11	2	0	370	345	56
12	2	0	185	-318	-185
1	3	0	1956	-1991	9
2	3	0	2104	-2224	12
3	3	0	162	-82	31
4	3	0	2437	-2548	17
5	3	0	418	370	24
6	3	0	1613	-1609	22
7	3	0	168	88	-53
8	3	0	1025	-1003	29
9	3	0	665	697	36
10	3	0	283	110	53
11	3	0	196	134	-91
12	3	0	436	473	60
0	4	0	2942	-2826	9
1	4	0	946	-887	10
2	4	0	798	-798	13
3	4	0	1343	-1441	15
4	4	0	839	-925	18
5	4	0	1046	-1095	20
6	4	0	575	586	24
7	4	0	793	-824	26
8	4	0	847	853	29
9	4	0	268	-326	59
10	4	0	1179	1135	36
11	4	0	266	70	57
12	4	0	443	571	62

h	k	l	10Fo	10Fc	10s
1	5	0	2633	-2576	11
2	5	0	186	224	21
3	5	0	1395	-1490	15
4	5	0	91	100	-91
5	5	0	165	200	-41
6	5	0	116	115	-74
7	5	0	944	927	26
8	5	0	216	-82	-56
9	5	0	1138	1150	32
10	5	0	148	-138	-148
11	5	0	1043	1007	41
12	5	0	105	130	-105
0	6	0	951	-913	11
1	6	0	1156	1095	12
2	6	0	1840	-1851	13
3	6	0	531	489	17
4	6	0	50	116	-50
5	6	0	1650	1809	20
6	6	0	292	215	32
7	6	0	735	689	25
8	6	0	670	671	31
9	6	0	317	213	40
10	6	0	755	736	38
11	6	0	321	-177	64
12	6	0	710	659	47
1	7	0	1121	-1079	13
2	7	0	746	744	14
3	7	0	88	36	-88
4	7	0	1924	2023	18
5	7	0	125	-32	-56
6	7	0	1451	1500	23
7	7	0	219	58	46
8	7	0	842	860	30
9	7	0	68	-104	-68
10	7	0	73	6	-73
11	7	0	303	391	62
12	7	0	317	-195	73
0	8	0	907	908	13
1	8	0	241	-189	17
2	8	0	710	686	15
3	8	0	2203	2251	16
4	8	0	347	374	22
5	8	0	1289	1365	20
6	8	0	507	-485	25
7	8	0	1199	1270	25
8	8	0	297	-334	41
9	8	0	328	294	46
10	8	0	530	-546	44
11	8	0	294	-163	71
12	8	0	245	-241	-102
1	9	0	1799	1760	14
2	9	0	401	369	17
3	9	0	935	979	17
4	9	0	645	638	19
5	9	0	80	-79	-80
6	9	0	504	508	25

h	k	l	10Fo	10Fc	10s
7	9	0	801	-804	27
8	9	0	531	538	31
9	9	0	805	-803	32
10	9	0	148	235	-148
11	9	0	880	-917	41
12	9	0	336	-238	71
0	10	0	1165	1116	14
1	10	0	1191	-1166	15
2	10	0	1841	1831	15
3	10	0	326	-316	20
4	10	0	816	812	19
5	10	0	923	-906	21
6	10	0	149	0	-50
7	10	0	148	-75	-61
8	10	0	868	-830	29
9	10	0	74	56	-74
10	10	0	793	-749	36
11	10	0	127	-51	-127
12	10	0	776	-728	46
1	11	0	1215	1156	15
2	11	0	1244	-1199	16
3	11	0	1214	1171	18
4	11	0	1485	-1469	19
5	11	0	174	20	35
6	11	0	1490	-1524	23
7	11	0	718	-691	28
8	11	0	913	-943	29
9	11	0	701	-691	33
10	11	0	175	-206	-96
11	11	0	710	-673	45
12	11	0	414	415	63
0	12	0	245	-230	19
1	12	0	266	-250	21
2	12	0	247	260	23
3	12	0	1762	-1777	18
4	12	0	582	-553	21
5	12	0	852	-858	22
6	12	0	543	-475	25
7	12	0	1132	-1190	26
8	12	0	206	-221	-56
9	12	0	386	-397	37
10	12	0	71	126	-71
11	12	0	81	-76	-81
12	12	0	98	106	-98
1	13	0	1280	-1244	16
2	13	0	1365	-1305	17
3	13	0	499	-505	20
4	13	0	1207	-1187	20
5	13	0	210	166	33
6	13	0	1304	-1350	24
7	13	0	707	737	29
8	13	0	221	-246	-56
9	13	0	691	699	33
10	13	0	115	-42	-115
11	13	0	556	601	47
0	14	0	2194	-2143	17

h	k	l	10Fo	10Fc	10s
1	14	0	223	-200	24
2	14	0	2121	-2129	18
3	14	0	169	-169	33
4	14	0	475	-407	22
5	14	0	774	-740	22
6	14	0	430	416	27
7	14	0	417	-400	30
8	14	0	1092	1086	29
9	14	0	171	130	-78
10	14	0	876	888	37
11	14	0	163	-23	-163
1	15	0	1775	-1714	17
2	15	0	749	743	19
3	15	0	1243	-1207	19
4	15	0	630	633	21
5	15	0	114	97	-86
6	15	0	316	272	33
7	15	0	823	814	27
8	15	0	424	384	38
9	15	0	828	800	34
10	15	0	258	187	61
11	15	0	785	827	40
0	16	0	1148	-1095	18
1	16	0	200	107	26
2	16	0	1076	-1079	19
3	16	0	1865	1866	20
4	16	0	409	-392	25
5	16	0	984	992	23
6	16	0	380	388	30
7	16	0	1087	1093	27
8	16	0	522	554	31
9	16	0	286	287	43
10	16	0	512	524	41
11	16	0	273	-189	62
1	17	0	312	297	23
2	17	0	1286	1300	19
3	17	0	212	170	35
4	17	0	1694	1702	21
5	17	0	281	-192	31
6	17	0	1165	1205	25
7	17	0	200	-78	47
8	17	0	727	728	30
9	17	0	65	-111	-65
10	17	0	163	71	-100
11	17	0	218	-226	-73
0	18	0	849	825	19
1	18	0	580	574	20
2	18	0	1416	1410	20
3	18	0	1218	1214	21
4	18	0	216	112	31
5	18	0	1068	1060	23
6	18	0	275	-239	38
7	18	0	622	643	29
8	18	0	686	-712	32
9	18	0	330	342	44
10	18	0	518	-526	44

h	k	l	10Fo	10Fc	10s
1	19	0	2063	2002	20
2	19	0	451	457	23
3	19	0	1180	1144	21
4	19	0	569	586	24
5	19	0	137	193	-59
6	19	0	54	-2	-54
7	19	0	765	-870	29
8	19	0	213	194	49
9	19	0	924	-925	33
10	19	0	251	-38	51
0	20	0	1843	1807	20
1	20	0	216	-93	27
2	20	0	854	847	21
3	20	0	931	-907	22
4	20	0	499	454	26
5	20	0	407	-438	29
6	20	0	179	-91	38
7	20	0	589	-599	28
8	20	0	664	-645	32
9	20	0	223	-116	-58
10	20	0	822	-868	36
1	21	0	966	973	21
2	21	0	1309	-1279	21
3	21	0	55	-39	-55
4	21	0	1510	-1509	23
5	21	0	115	-153	-115
6	21	0	781	-776	26
7	21	0	214	-155	45
8	21	0	553	-548	33
9	21	0	501	-559	37
10	21	0	70	-65	-70
0	22	0	858	-846	22
1	22	0	908	-877	22
2	22	0	1082	-1054	22
3	22	0	1703	-1717	22
4	22	0	240	-246	42
5	22	0	1489	-1562	25
6	22	0	197	144	45
7	22	0	747	-781	29
8	22	0	461	435	37
9	22	0	442	-487	39
1	23	0	857	-829	22
2	23	0	55	-67	-55
3	23	0	148	-32	-49
4	23	0	372	-312	31
5	23	0	58	24	-58
6	23	0	405	-433	31
7	23	0	529	531	31
8	23	0	567	-573	33
9	23	0	544	551	37
0	24	0	2017	-1949	22
1	24	0	114	-101	-86
2	24	0	709	-705	24
3	24	0	297	300	30
4	24	0	435	-411	27
5	24	0	110	90	-110

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
6	24	0	316	313	37
7	24	0	58	92	-58
8	24	0	656	683	35
9	24	0	73	-1	-73
1	25	0	1187	-1194	23
2	25	0	368	342	26
3	25	0	642	-661	25
4	25	0	697	692	27
5	25	0	132	-151	-64
6	25	0	631	621	29
7	25	0	357	381	38
8	25	0	222	240	-56
0	26	0	402	-377	29
1	26	0	478	448	25
2	26	0	158	-59	-41
3	26	0	715	660	25
4	26	0	352	-325	30
5	26	0	1284	1249	26
6	26	0	151	140	-63
7	26	0	719	759	30
8	26	0	158	99	-91
1	27	0	470	463	26
2	27	0	626	634	25
3	27	0	290	263	32
4	27	0	1007	1030	26
5	27	0	191	-158	-51
6	27	0	890	882	29
7	27	0	241	-179	50
8	27	0	500	487	36
0	28	0	1112	1077	25
1	28	0	191	197	43
2	28	0	748	699	25
3	28	0	414	429	29
4	28	0	493	492	28
5	28	0	527	534	29
6	28	0	380	-355	34
7	28	0	303	286	41
1	29	0	1257	1211	25
2	29	0	83	-36	-83
3	29	0	782	779	27
4	29	0	55	-1	-55
5	29	0	105	-50	-105
6	29	0	123	-98	-98
7	29	0	417	-390	33
0	30	0	964	906	25
1	30	0	336	-302	30
2	30	0	720	680	26
3	30	0	480	-433	28
4	30	0	271	257	38
5	30	0	774	-765	29
6	30	0	288	-245	36
1	31	0	195	63	35
2	31	0	440	-392	29
3	31	0	214	116	37
4	31	0	921	-913	28
5	31	0	54	43	-54

h	k	l	10Fo	10Fc	10s
6	31	0	793	-783	30
0	32	0	840	-842	26
1	32	0	179	-163	-50
2	32	0	219	-185	39
3	32	0	699	-641	29
4	32	0	197	-147	-49
5	32	0	751	-749	30
1	33	0	888	-826	27
2	33	0	357	-335	35
3	33	0	392	-370	32
4	33	0	419	-392	33
0	34	0	785	-760	27
1	34	0	102	96	-102
2	34	0	578	-586	31
3	34	0	58	-133	-58
1	35	0	613	-602	28
-13	0	1	1083	-1073	51
-11	0	1	1333	-1249	39
-9	0	1	716	-718	35
-7	0	1	654	611	27
-5	0	1	2732	2650	19
-3	0	1	5205	4875	14
-1	0	1	3571	3511	9
1	0	1	458	395	12
3	0	1	520	463	17
5	0	1	1895	-1807	21
7	0	1	1411	-1315	26
9	0	1	1316	-1248	34
11	0	1	92	-31	-92
-13	1	1	115	172	-115
-12	1	1	593	-637	55
-11	1	1	386	344	59
-10	1	1	688	-600	36
-9	1	1	1120	1115	31
-8	1	1	217	152	44
-7	1	1	1129	1085	25
-6	1	1	827	767	23
-5	1	1	577	578	21
-4	1	1	2072	2042	17
-3	1	1	4651	-4449	14
-2	1	1	2220	2210	11
-1	1	1	2656	-2688	9
0	1	1	1562	1429	20
1	1	1	1634	-1738	10
2	1	1	236	203	20
3	1	1	1283	-1254	16
4	1	1	834	-817	19
5	1	1	515	-490	22
6	1	1	1806	-1690	23
7	1	1	175	86	-54
8	1	1	1362	-1302	29
9	1	1	647	675	41
10	1	1	719	-676	38
11	1	1	770	815	46
12	1	1	259	-145	-90
-13	2	1	324	-207	70

h	k	l	10Fo	10Fc	10s
-12	2	1	240	279	-96
-11	2	1	278	-302	-71
-10	2	1	1041	954	35
-9	2	1	254	-152	60
-8	2	1	1468	1426	27
-7	2	1	201	62	50
-6	2	1	2682	2672	22
-5	2	1	376	335	22
-4	2	1	590	537	18
-3	2	1	802	-719	15
-2	2	1	705	-759	13
-1	2	1	159	100	17
0	2	1	1519	-1375	26
1	2	1	621	633	11
2	2	1	1453	-1530	13
3	2	1	299	250	19
4	2	1	2228	-2265	18
5	2	1	285	-234	28
6	2	1	689	-639	25
7	2	1	502	-525	31
8	2	1	62	-10	-62
9	2	1	435	-352	40
10	2	1	945	919	38
11	2	1	352	-239	59
12	2	1	898	904	49
-13	3	1	323	137	-96
-12	3	1	89	184	-89
-11	3	1	538	547	47
-10	3	1	440	312	42
-9	3	1	1416	1368	31
-8	3	1	299	-229	43
-7	3	1	1602	1559	25
-6	3	1	213	-63	34
-5	3	1	1572	1514	19
-4	3	1	1578	-1638	17
-3	3	1	347	343	18
-2	3	1	1221	-1301	12
-1	3	1	1658	-1643	10
0	3	1	311	-248	8
1	3	1	2845	-2799	11
2	3	1	807	844	14
3	3	1	1941	-2072	16
4	3	1	434	424	22
5	3	1	1407	-1435	21
6	3	1	750	726	25
7	3	1	101	-10	-101
8	3	1	355	357	37
9	3	1	711	680	36
10	3	1	359	280	50
11	3	1	838	764	46
12	3	1	107	133	-107
-12	4	1	94	94	-94
-11	4	1	868	892	40
-10	4	1	355	366	55
-9	4	1	185	188	-87
-8	4	1	1130	1105	28

h	k	l	10Fo	10Fc	10s
-7	4	1	716	-667	27
-6	4	1	355	358	25
-5	4	1	1961	-1984	19
-4	4	1	1468	1454	17
-3	4	1	1601	-1620	15
-2	4	1	304	363	16
-1	4	1	1303	-1289	10
0	4	1	1343	-1308	8
1	4	1	389	-363	13
2	4	1	929	-961	14
3	4	1	448	449	18
4	4	1	970	-1024	18
5	4	1	1588	1698	21
6	4	1	739	-757	24
7	4	1	1077	1104	26
8	4	1	231	162	-65
9	4	1	1063	1030	33
10	4	1	352	291	58
11	4	1	316	272	65
12	4	1	297	320	-81
-12	5	1	868	869	46
-11	5	1	227	-52	-92
-10	5	1	787	817	35
-9	5	1	414	-385	40
-8	5	1	286	-264	38
-7	5	1	151	198	-58
-6	5	1	1162	-1214	23
-5	5	1	672	-659	21
-4	5	1	2286	-2365	17
-3	5	1	1549	1565	15
-2	5	1	1427	-1433	13
-1	5	1	450	-436	13
0	5	1	1653	-1635	18
1	5	1	431	461	14
2	5	1	77	-31	-77
3	5	1	504	526	18
4	5	1	1293	1412	19
5	5	1	569	-514	23
6	5	1	1431	1495	24
7	5	1	242	-143	46
8	5	1	1496	1520	29
9	5	1	346	-235	46
10	5	1	720	670	39
11	5	1	153	-5	-153
12	5	1	92	60	-92
-12	6	1	288	-262	-73
-11	6	1	471	544	53
-10	6	1	801	-859	35
-9	6	1	337	241	44
-8	6	1	962	-938	28
-7	6	1	335	-353	32
-6	6	1	1041	-1059	23
-5	6	1	1203	-1242	20
-4	6	1	167	-112	32
-3	6	1	1585	-1661	15
-2	6	1	877	839	13

h	k	l	10Fo	10Fc	10s
-1	6	1	1612	-1580	12
0	6	1	1168	1153	14
1	6	1	812	-803	13
2	6	1	1925	1972	14
3	6	1	757	774	17
4	6	1	966	1041	19
5	6	1	836	855	22
6	6	1	214	-120	44
7	6	1	1268	1334	26
8	6	1	217	-145	48
9	6	1	677	766	35
10	6	1	664	-680	41
11	6	1	254	209	-90
12	6	1	308	-356	-80
-12	7	1	319	234	65
-11	7	1	538	-539	49
-10	7	1	225	-110	-68
-9	7	1	1367	-1337	31
-8	7	1	329	253	35
-7	7	1	1640	-1656	25
-6	7	1	451	-498	26
-5	7	1	1270	-1324	20
-4	7	1	151	-85	34
-3	7	1	657	668	17
-2	7	1	605	-584	14
-1	7	1	1374	1393	12
0	7	1	382	404	10
1	7	1	2467	2436	13
2	7	1	832	-846	15
3	7	1	1508	1586	17
4	7	1	116	91	-65
5	7	1	957	1013	21
6	7	1	57	173	-57
7	7	1	57	125	-57
8	7	1	327	349	40
9	7	1	671	-628	35
10	7	1	169	51	-118
11	7	1	679	-705	46
12	7	1	307	-95	75
-12	8	1	101	-274	-101
-11	8	1	437	-396	49
-10	8	1	855	-822	35
-9	8	1	77	-116	-77
-8	8	1	1285	-1290	28
-7	8	1	302	219	34
-6	8	1	1120	-1122	23
-5	8	1	992	1044	20
-4	8	1	452	-490	20
-3	8	1	730	738	17
-2	8	1	1283	1250	14
-1	8	1	1598	1571	13
0	8	1	1164	1077	9
1	8	1	1020	-962	14
2	8	1	2644	2643	15
3	8	1	368	-343	20
4	8	1	1173	1185	19

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
5	8	1	770	-788	22
6	8	1	921	976	24
7	8	1	436	-393	32
8	8	1	621	-640	33
9	8	1	618	-607	36
10	8	1	783	-754	38
11	8	1	88	-133	-88
12	8	1	891	-824	50
-12	9	1	680	-630	49
-11	9	1	437	-404	49
-10	9	1	517	-478	39
-9	9	1	339	-327	40
-8	9	1	142	76	-51
-7	9	1	633	-672	27
-6	9	1	1312	1367	23
-5	9	1	481	-473	23
-4	9	1	1447	1476	18
-3	9	1	194	-138	24
-2	9	1	2180	2117	15
-1	9	1	1253	1186	14
0	9	1	291	261	12
1	9	1	1080	1058	14
2	9	1	143	-65	30
3	9	1	676	690	18
4	9	1	920	-979	19
5	9	1	356	284	25
6	9	1	1219	-1277	24
7	9	1	334	297	33
8	9	1	1054	-1085	29
9	9	1	317	-243	47
10	9	1	700	-702	38
11	9	1	285	-330	60
-12	10	1	89	-73	-89
-11	10	1	337	-264	63
-10	10	1	261	202	55
-9	10	1	369	-324	39
-8	10	1	644	688	30
-7	10	1	973	1002	26
-6	10	1	799	771	24
-5	10	1	1541	1554	20
-4	10	1	215	177	26
-3	10	1	2244	2262	17
-2	10	1	228	-175	18
-1	10	1	1295	1266	15
0	10	1	95	-147	-30
1	10	1	397	378	17
2	10	1	186	-186	25
3	10	1	453	-480	20
4	10	1	675	-647	20
5	10	1	1534	-1592	22
6	10	1	264	78	37
7	10	1	1457	-1575	27
8	10	1	113	-5	-113
9	10	1	753	-711	34
10	10	1	299	161	52
11	10	1	348	-337	62
-12	11	1	470	-467	54
-11	11	1	482	473	47
-10	11	1	216	-163	-69
-9	11	1	592	551	35
-8	11	1	443	-451	35
-7	11	1	810	833	27
-6	11	1	1055	1070	23
-5	11	1	595	584	22
-4	11	1	683	670	20
-3	11	1	257	237	23
-2	11	1	1617	1677	16
-1	11	1	588	-594	16
0	11	1	706	668	11
1	11	1	2173	-2147	15
2	11	1	646	611	17
3	11	1	2458	-2396	18
4	11	1	665	-648	21
5	11	1	1640	-1665	22
6	11	1	1488	-1532	24
7	11	1	295	-277	39
8	11	1	729	-658	31
9	11	1	545	596	38
10	11	1	513	-479	42
11	11	1	828	819	42
-12	12	1	389	443	59
-11	12	1	278	-236	64
-10	12	1	1133	1074	34
-9	12	1	356	-331	42
-8	12	1	1502	1480	28
-7	12	1	226	32	39
-6	12	1	1218	1264	24
-5	12	1	170	153	41
-4	12	1	388	414	23
-3	12	1	209	192	27
-2	12	1	966	-1006	17
-1	12	1	255	-269	21
0	12	1	1564	-1530	11
1	12	1	206	-218	26
2	12	1	1597	-1633	17
3	12	1	317	-291	22
4	12	1	718	-729	21
5	12	1	201	113	37
6	12	1	557	-584	28
7	12	1	89	90	-89
8	12	1	565	619	33
9	12	1	233	232	57
10	12	1	614	585	39
11	12	1	303	-84	67
-12	13	1	434	434	61
-11	13	1	527	559	51
-10	13	1	424	372	47
-9	13	1	900	852	32
-8	13	1	450	488	37
-7	13	1	1236	1286	26
-6	13	1	638	-599	25
-5	13	1	359	313	25
-4	13	1	950	-967	20
-3	13	1	101	57	-50
-2	13	1	1438	-1414	17
-1	13	1	1492	-1421	16
0	13	1	518	-515	25
1	13	1	1255	-1217	17
2	13	1	639	-616	18
3	13	1	1261	-1318	19
4	13	1	298	317	25
5	13	1	557	-503	24
6	13	1	971	1004	25
7	13	1	90	-12	-90
8	13	1	797	826	31
9	13	1	540	513	38
10	13	1	471	513	47
11	13	1	633	652	45
-12	14	1	94	7	-94
-11	14	1	654	572	42
-10	14	1	285	181	52
-9	14	1	573	570	35
-8	14	1	456	476	33
-7	14	1	521	-502	30
-6	14	1	364	355	29
-5	14	1	1341	-1299	22
-4	14	1	111	45	-66
-3	14	1	2292	-2290	19
-2	14	1	491	-464	19
-1	14	1	1244	-1216	17
0	14	1	776	-789	14
1	14	1	768	-767	18
2	14	1	701	-673	19
3	14	1	600	575	20
4	14	1	207	-253	35
5	14	1	1031	1019	23
6	14	1	230	12	40
7	14	1	1471	1511	27
8	14	1	140	84	-99
9	14	1	737	728	34
10	14	1	97	187	-97
11	14	1	239	250	-78
-11	15	1	249	-183	-65
-10	15	1	353	370	46
-9	15	1	360	-410	40
-8	15	1	270	221	41
-7	15	1	687	-652	28
-6	15	1	1156	-1178	25
-5	15	1	330	-255	25
-4	15	1	1481	-1476	20
-3	15	1	229	-194	27
-2	15	1	2095	-2105	18
-1	15	1	709	675	18
0	15	1	869	-839	13
1	15	1	423	405	18
2	15	1	226	159	26
3	15	1	544	563	21
4	15	1	810	816	22
5	15	1	422	396	27
6	15	1	1190	1186	25
7	15	1	229	190	42
8	15	1	916	961	32
9	15	1	250	-288	56
10	15	1	673	680	39
11	15	1	261	-270	-66
-11	16	1	387	353	49
-10	16	1	690	-742	38
-9	16	1	225	188	-62
-8	16	1	1321	-1322	29
-7	16	1	420	-348	30
-6	16	1	772	-743	25
-5	16	1	788	-765	23
-4	16	1	485	-535	22
-3	16	1	789	-753	20
-2	16	1	574	634	22
-1	16	1	1031	-1018	18
0	16	1	1252	1218	14
1	16	1	124	-98	-35
2	16	1	1702	1726	19
3	16	1	208	155	29
4	16	1	1034	1036	22
5	16	1	725	720	25
6	16	1	665	765	26
7	16	1	484	573	31
8	16	1	597	-573	32
9	16	1	412	390	43
10	16	1	546	-563	42
11	16	1	185	148	-141
-11	17	1	588	-589	44
-10	17	1	264	81	54
-9	17	1	1199	-1214	32
-8	17	1	209	-206	-56
-7	17	1	1360	-1396	26
-6	17	1	179	87	-46
-5	17	1	570	-575	24
-4	17	1	176	138	42
-3	17	1	46	-4	-46
-2	17	1	240	220	23
-1	17	1	1179	1177	19
0	17	1	230	206	18
1	17	1	1627	1584	19
2	17	1	152	-76	-40
3	17	1	1521	1511	20
4	17	1	154	-107	-40
5	17	1	927	902	24
6	17	1	99	-51	-99
7	17	1	64	32	-64
8	17	1	253	-221	46
9	17	1	614	-617	36
10	17	1	182	-112	-105
-11	18	1	542	-505	42
-10	18	1	680	-652	36
-9	18	1	265	-273	53
-8	18	1	699	-680	30
-7	18	1	323	311	38
-6	18	1	843	-790	26
-5	18	1	850	858	24
-4	18	1	257	-251	35
-3	18	1	1444	1406	21
-2	18	1	653	635	21
-1	18	1	885	841	20
0	18	1	1070	1014	18
1	18	1	855	846	20
2	18	1	1569	1535	20
3	18	1	747	-765	22
4	18	1	899	898	23
5	18	1	552	-543	26
6	18	1	377	334	33
7	18	1	986	-1025	28
8	18	1	247	-210	58
9	18	1	494	-502	40
10	18	1	521	-542	45
-11	19	1	84	-4	-84
-10	19	1	526	-529	41
-9	19	1	70	-58	-70
-8	19	1	113	-16	-113
-7	19	1	202	-96	48
-6	19	1	1102	1101	26
-5	19	1	757	-765	25
-4	19	1	1752	1753	22
-3	19	1	508	471	24
-2	19	1	1757	1732	20
-1	19	1	244	-235	27
0	19	1	814	791	20
1	19	1	394	374	22
2	19	1	155	113	-39
3	19	1	316	316	26
4	19	1	951	-926	23
5	19	1	155	113	-63
6	19	1	1068	-1065	26
7	19	1	187	32	-58
8	19	1	1090	-1122	32
9	19	1	110	-112	-110
10	19	1	503	-490	42
-10	20	1	376	371	48
-9	20	1	137	-207	-137
-8	20	1	633	693	32
-7	20	1	483	469	33
-6	20	1	242	165	37
-5	20	1	1361	1420	24
-4	20	1	381	401	30
-3	20	1	1612	1582	22
-2	20	1	390	-374	24
-1	20	1	931	902	21
0	20	1	910	-905	21
1	20	1	105	25	-71
2	20	1	851	-839	22
3	20	1	135	-142	-56
4	20	1	290	-265	31
5	20	1	805	-847	26

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
6	20	1	404	-397	34
7	20	1	1024	-1032	29
8	20	1	236	264	-61
9	20	1	810	-866	34
10	20	1	240	205	53
-10	21	1	298	-308	56
-9	21	1	779	822	34
-8	21	1	262	244	48
-7	21	1	1097	1131	28
-6	21	1	142	47	-77
-5	21	1	576	615	27
-4	21	1	910	884	24
-3	21	1	320	-363	34
-2	21	1	359	342	26
-1	21	1	1418	-1406	21
0	21	1	128	-30	-36
1	21	1	1807	-1808	21
2	21	1	433	-407	24
3	21	1	1282	-1285	23
4	21	1	232	-192	35
5	21	1	793	-813	26
6	21	1	371	-393	33
7	21	1	252	173	40
8	21	1	393	-435	41
9	21	1	561	554	38
-10	22	1	684	758	37
-9	22	1	367	282	40
-8	22	1	1200	1234	30
-7	22	1	459	-451	34
-6	22	1	1525	1533	26
-5	22	1	737	-794	25
-4	22	1	357	320	29
-3	22	1	624	-610	24
-2	22	1	637	-653	23
-1	22	1	203	-86	33
0	22	1	1128	-1115	15
1	22	1	191	40	36
2	22	1	1242	-1228	22
3	22	1	166	51	39
4	22	1	1211	-1212	24
5	22	1	169	117	-51
6	22	1	316	-283	32
7	22	1	228	271	54
8	22	1	74	142	-74
9	22	1	75	108	-75
-9	23	1	581	580	35
-8	23	1	100	-105	-100
-7	23	1	479	467	33
-6	23	1	869	-908	27
-5	23	1	649	640	28
-4	23	1	1117	-1127	24
-3	23	1	50	-24	-50
-2	23	1	1008	-1017	23
-1	23	1	189	180	32
0	23	1	241	144	30
1	23	1	366	-338	25
2	23	1	342	363	28
3	23	1	857	-824	24
4	23	1	710	698	26
5	23	1	691	-673	26
6	23	1	952	1004	28
7	23	1	70	-132	-70
8	23	1	747	791	33
9	23	1	144	188	-144
-9	24	1	188	295	-90
-8	24	1	55	-76	-55
-7	24	1	182	-11	-50
-6	24	1	302	-412	43
-5	24	1	784	-771	27
-4	24	1	529	-526	28
-3	24	1	1287	-1229	23
-2	24	1	175	-160	42
-1	24	1	1342	-1377	22
0	24	1	360	-347	18
1	24	1	391	-345	25
2	24	1	140	86	-48
3	24	1	51	6	-51
4	24	1	224	-219	41
5	24	1	959	956	26
6	24	1	231	140	40
7	24	1	858	832	30
8	24	1	234	163	57
-9	25	1	393	-402	39
-8	25	1	236	-187	55
-7	25	1	577	-633	33
-6	25	1	377	-435	35
-5	25	1	473	-471	28
-4	25	1	1159	-1136	25
-3	25	1	430	399	27
-2	25	1	1050	-1000	24
-1	25	1	480	478	25
0	25	1	955	-935	17
1	25	1	659	665	23
2	25	1	90	81	-90
3	25	1	775	771	25
4	25	1	589	575	27
5	25	1	304	330	37
6	25	1	884	862	28
7	25	1	99	94	-99
8	25	1	523	539	33
-8	26	1	831	-804	32
-7	26	1	61	-86	-61
-6	26	1	941	-920	28
-5	26	1	266	-303	38
-4	26	1	181	-135	40
-3	26	1	277	-250	31
-2	26	1	353	338	29
-1	26	1	356	-372	27
0	26	1	931	910	22
1	26	1	101	-52	-101
2	26	1	1086	1050	24
3	26	1	55	41	-55
4	26	1	1067	1092	26
5	26	1	235	243	47
6	26	1	210	206	47
7	26	1	199	139	-54
8	26	1	67	-46	-67
-8	27	1	69	73	-69
-7	27	1	690	-669	31
-6	27	1	161	150	-72
-5	27	1	743	-713	27
-4	27	1	457	420	28
-3	27	1	165	129	-45
-2	27	1	301	282	29
-1	27	1	552	560	25
0	27	1	396	373	19
1	27	1	1213	1160	24
2	27	1	45	21	-45
3	27	1	1096	1031	25
4	27	1	273	-265	36
5	27	1	645	653	30
6	27	1	414	-428	34
7	27	1	58	49	-58
-8	28	1	489	-451	37
-7	28	1	213	215	50
-6	28	1	338	-403	35
-5	28	1	811	773	28
-4	28	1	111	-42	-111
-3	28	1	802	796	26
-2	28	1	170	179	41
-1	28	1	875	893	25
0	28	1	596	582	19
1	28	1	415	391	30
2	28	1	583	573	26
3	28	1	130	-132	-92
4	28	1	552	534	29
5	28	1	769	-771	29
6	28	1	175	184	-80
7	28	1	568	-544	33
-7	29	1	64	-23	-64
-6	29	1	533	535	34
-5	29	1	267	224	42
-4	29	1	1173	1129	26
-3	29	1	85	-18	-85
-2	29	1	1042	1005	25
-1	29	1	55	-75	-55
0	29	1	797	787	18
1	29	1	178	-142	43
2	29	1	153	58	-39
3	29	1	54	-31	-54
4	29	1	505	-505	29
5	29	1	93	70	-93
6	29	1	771	-743	30
-6	30	1	510	522	33
-5	30	1	504	517	31
-4	30	1	162	-1	-42
-3	30	1	796	774	27
-2	30	1	348	-320	31
-1	30	1	786	753	26
0	30	1	732	-695	19
1	30	1	324	277	31
2	30	1	647	-645	27
3	30	1	133	-160	-81
4	30	1	606	-597	29
5	30	1	605	-606	31
6	30	1	240	-189	49
-6	31	1	63	108	-63
-5	31	1	656	660	30
-4	31	1	137	129	-67
-3	31	1	350	-335	31
-2	31	1	216	222	45
-1	31	1	494	-447	28
0	31	1	165	1	37
1	31	1	924	-933	26
2	31	1	141	57	-77
3	31	1	829	-786	27
4	31	1	149	-129	-53
5	31	1	502	-506	32
-5	32	1	360	-361	34
-4	32	1	311	246	34
-3	32	1	397	-421	32
-2	32	1	337	-298	32
-1	32	1	584	-543	28
0	32	1	607	-540	32
1	32	1	150	61	-55
2	32	1	980	-946	27
3	32	1	63	67	-63
4	32	1	672	-673	30
-4	33	1	645	-586	29
-3	33	1	147	164	-67
-2	33	1	727	-734	28
-1	33	1	252	-238	36
0	33	1	570	-546	20
1	33	1	316	-297	33
2	33	1	126	-114	-97
3	33	1	216	-324	48
4	33	1	397	363	32
-3	34	1	750	-778	29
-2	34	1	50	-1	-50
-1	34	1	469	-455	29
0	34	1	202	144	43
1	34	1	61	-68	-61
2	34	1	90	-26	-90
-1	35	1	473	447	31
0	35	1	172	-216	-68
-12	0	2	93	-122	-93
-10	0	2	618	617	38
-8	0	2	1518	1500	27
-6	0	2	332	-67	27
-4	0	2	397	296	21
-2	0	2	135	67	31
0	0	2	2061	-2110	11
2	0	2	378	-261	18
4	0	2	1761	-1657	20
6	0	2	692	-632	26
8	0	2	337	-363	45
10	0	2	685	680	43
-13	1	2	300	-332	-99
-12	1	2	739	717	44
-11	1	2	251	-180	-70
-10	1	2	938	897	35
-9	1	2	1165	1116	31
-8	1	2	163	9	-56
-7	1	2	1357	1272	24
-6	1	2	1758	-1663	22
-5	1	2	1782	1739	19
-4	1	2	2812	-2706	17
-3	1	2	3439	3302	14
-2	1	2	847	-880	13
-1	1	2	524	587	13
0	1	2	2681	-2597	82
1	1	2	986	-921	13
2	1	2	113	3	-43
3	1	2	1918	-1809	17
4	1	2	311	-300	26
5	1	2	1924	-1864	22
6	1	2	716	697	26
7	1	2	883	-834	29
8	1	2	739	659	32
9	1	2	400	-257	47
10	1	2	739	718	43
11	1	2	521	521	55
-13	2	2	884	755	50
-12	2	2	98	19	-98
-11	2	2	1033	1021	38
-10	2	2	85	41	-85
-9	2	2	1273	1280	30
-8	2	2	537	460	31
-7	2	2	140	143	-73
-6	2	2	439	393	25
-5	2	2	947	-969	19
-4	2	2	436	398	19
-3	2	2	734	-699	15
-2	2	2	283	-265	18
-1	2	2	2380	-2388	11
0	2	2	639	-595	9
1	2	2	1912	-1939	13
2	2	2	362	328	17
3	2	2	855	-910	18
4	2	2	507	-509	22
5	2	2	724	717	23
6	2	2	301	-239	33
7	2	2	1180	1122	28
8	2	2	742	-551	32
9	2	2	1663	1602	34
10	2	2	270	-190	-82
11	2	2	647	565	50
-13	3	2	194	31	-194
-12	3	2	1057	985	42
-11	3	2	252	86	-74

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

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
-10	3	2	1110	1065	35	-4	5	2	962	987	17	2	7	2	2006	2026	16	10	9	2	429	-400	54	-6	12	2	421	421	27
-9	3	2	1124	-1053	30	-3	5	2	979	-1002	15	3	7	2	647	668	19	11	9	2	381	314	54	-5	12	2	622	-592	22
-8	3	2	555	545	31	-2	5	2	315	332	17	4	7	2	123	60	-53	-12	10	2	309	-247	67	-4	12	2	176	-114	32
-7	3	2	489	-516	28	-1	5	2	72	62	-72	5	7	2	49	-117	-49	-11	10	2	185	153	-101	-3	12	2	1835	-1831	18
-6	3	2	717	726	23	0	5	2	958	929	14	6	7	2	1174	-1235	25	-10	10	2	436	427	38	-2	12	2	41	6	-41
-5	3	2	561	-615	21	1	5	2	1846	1727	13	7	7	2	334	268	38	-9	10	2	408	423	37	-1	12	2	2455	-2426	16
-4	3	2	567	-604	18	2	5	2	351	-353	18	8	7	2	1283	-1310	31	-8	10	2	1259	1287	27	0	12	2	581	506	14
-3	3	2	210	230	21	3	5	2	1741	1807	17	9	7	2	159	-111	-159	-7	10	2	291	202	36	1	12	2	1735	-1717	17
-2	3	2	1851	-1842	13	4	5	2	265	144	27	10	7	2	962	-972	39	-6	10	2	1982	2051	22	2	12	2	588	531	19
-1	3	2	271	-317	17	5	5	2	1784	1920	22	11	7	2	225	4	-103	-5	10	2	194	-154	34	3	12	2	351	-346	22
0	3	2	3340	-3167	44	6	5	2	530	-545	27	-12	8	2	219	6	-87	-4	10	2	1332	1346	18	4	12	2	371	387	26
1	3	2	622	605	14	7	5	2	980	1029	28	-11	8	2	1108	-1088	38	-3	10	2	110	-77	-46	5	12	2	616	662	24
2	3	2	1019	-1082	15	8	5	2	211	-267	-59	-10	8	2	85	237	-85	-2	10	2	107	63	-38	6	12	2	260	-135	38
3	3	2	801	824	18	9	5	2	224	252	-72	-9	8	2	791	-720	32	-1	10	2	416	-449	16	7	12	2	1302	1385	28
4	3	2	194	-188	32	10	5	2	329	-363	53	-8	8	2	824	824	28	0	10	2	269	-272	14	8	12	2	72	-60	-72
5	3	2	832	878	23	11	5	2	609	-583	46	-7	8	2	469	-470	29	1	10	2	127	-108	30	9	12	2	1081	1174	35
6	3	2	783	756	25	-13	6	2	675	-657	53	-6	8	2	745	765	23	2	10	2	3002	-2933	17	10	12	2	319	-238	55
7	3	2	384	353	33	-12	6	2	190	164	-190	-5	8	2	782	847	20	3	10	2	1094	-1076	19	11	12	2	1060	1094	43
8	3	2	1136	1097	31	-11	6	2	782	-696	39	-4	8	2	694	672	18	4	10	2	2318	-2361	20	-12	13	2	981	918	43
9	3	2	343	-192	54	-10	6	2	439	-346	42	-3	8	2	1356	1378	16	5	10	2	124	162	-108	-11	13	2	82	-72	-82
10	3	2	1013	905	39	-9	6	2	843	-800	31	-2	8	2	284	288	19	6	10	2	1398	-1491	25	-10	13	2	780	816	35
11	3	2	376	-257	62	-8	6	2	909	-884	28	-1	8	2	2429	2377	14	7	10	2	286	243	33	-9	13	2	488	-439	35
-13	4	2	312	332	-79	-7	6	2	286	-238	38	0	8	2	611	-593	11	8	10	2	186	-163	-66	-8	13	2	588	550	30
-12	4	2	155	153	-155	-6	6	2	1430	-1443	22	1	8	2	2533	2450	15	9	10	2	423	471	45	-7	13	2	870	-913	26
-11	4	2	730	682	39	-5	6	2	689	683	20	2	8	2	836	-842	17	10	10	2	404	346	44	-6	13	2	664	-649	24
-10	4	2	424	-415	41	-4	6	2	1699	-1753	17	3	8	2	433	427	20	11	10	2	263	267	-84	-5	13	2	718	-723	22
-9	4	2	249	85	51	-3	6	2	1746	1764	15	4	8	2	1189	-1316	20	-12	11	2	500	424	53	-4	13	2	806	-806	20
-8	4	2	1400	-1391	27	-2	6	2	446	-440	15	5	8	2	424	-404	26	-11	11	2	91	39	-91	-3	13	2	1146	-1161	18
-7	4	2	649	651	27	-1	6	2	1579	1556	13	6	8	2	540	-545	28	-10	11	2	463	484	42	-2	13	2	1726	-1770	17
-6	4	2	1593	-1626	22	0	6	2	116	-48	26	7	8	2	1139	-1281	28	-9	11	2	232	144	50	-1	13	2	602	-552	19
-5	4	2	567	548	21	1	6	2	999	941	14	8	8	2	366	-338	41	-8	11	2	560	523	30	0	13	2	925	-925	12
-4	4	2	1495	-1529	17	2	6	2	1475	1513	15	9	8	2	671	-706	39	-7	11	2	1156	1207	25	1	13	2	179	-96	26
-3	4	2	662	-664	16	3	6	2	576	615	18	10	8	2	435	388	52	-6	11	2	369	-333	26	2	13	2	886	-881	18
-2	4	2	988	-1016	13	4	6	2	1377	1529	20	11	8	2	799	-774	46	-5	11	2	931	885	21	3	13	2	1335	1359	20
-1	4	2	1816	-1789	12	5	6	2	664	-716	23	-12	9	2	489	-509	47	-4	11	2	594	-576	20	4	13	2	305	240	25
0	4	2	1423	1354	13	6	6	2	1210	1290	25	-11	9	2	185	331	-138	-3	11	2	807	828	18	5	13	2	659	677	24
1	4	2	1521	-1452	13	7	6	2	778	-821	29	-10	9	2	269	-228	52	-2	11	2	1943	-1971	16	6	13	2	712	662	26
2	4	2	1734	1811	15	8	6	2	374	404	44	-9	9	2	984	970	31	-1	11	2	133	-68	31	7	13	2	623	605	30
3	4	2	173	-93	28	9	6	2	884	-841	35	-8	9	2	473	-485	33	0	11	2	1781	-1718	11	8	13	2	637	668	32
4	4	2	1725	1821	19	10	6	2	215	-215	-93	-7	9	2	1626	1662	25	1	11	2	127	-2	-38	9	13	2	130	148	-130
5	4	2	171	15	-45	11	6	2	485	-415	53	-6	9	2	271	228	32	2	11	2	1314	-1241	17	10	13	2	601	622	44
6	4	2	923	922	25	-13	7	2	345	145	83	-5	9	2	1705	1776	20	3	11	2	1894	-1952	19	11	13	2	157	-110	-157
7	4	2	649	637	29	-12	7	2	923	-906	43	-4	9	2	270	256	23	4	11	2	146	-13	-43	-12	14	2	298	203	71
8	4	2	619	664	34	-11	7	2	262	-82	-75	-3	9	2	843	866	17	5	11	2	772	-777	24	-11	14	2	121	214	-121
9	4	2	388	289	47	-10	7	2	1357	-1305	34	-2	9	2	1026	1070	15	6	11	2	766	838	27	-10	14	2	508	-503	39
10	4	2	367	-292	50	-9	7	2	191	132	-73	-1	9	2	40	-75	-40	7	11	2	606	-571	30	-9	14	2	379	287	38
11	4	2	549	540	52	-8	7	2	800	-755	28	0	9	2	1851	1731	16	8	11	2	760	787	33	-8	14	2	950	-901	29
-13	5	2	541	458	60	-7	7	2	291	-302	31	1	9	2	1455	-1443	15	9	11	2	282	235	54	-7	14	2	197	-137	-50
-12	5	2	134	70	-134	-6	7	2	53	121	-53	2	9	2	819	813	17	10	11	2	530	552	49	-6	14	2	1504	-1516	23
-11	5	2	198	-163	-75	-5	7	2	199	-126	31	3	9	2	2052	-2052	18	11	11	2	262	322	-101	-5	14	2	268	-294	31
-10	5	2	352	-308	42	-4	7	2	1539	1583	18	4	9	2	293	-188	25	-12	12	2	278	-30	-78	-4	14	2	933	-957	20
-9	5	2	1003	-961	30	-3	7	2	439	-466	18	5	9	2	1278	-1382	22	-11	12	2	1125	1242	38	-3	14	2	601	-564	20
-8	5	2	226	-32	52	-2	7	2	1863	1829	14	6	9	2	290	-256	33	-10	12	2	73	86	-73	-2	14	2	478	-487	19
-7	5	2	1742	-1704	24	-1	7	2	584	544	14	7	9	2	656	-702	30	-9	12	2	1043	1085	31	-1	14	2	235	-251	24
-6	5	2	169	-115	42	0	7	2	2117	2039	30	8	9	2	631	-661	33	-8	12	2	141	33	-73	0	14	2	198	211	16
-5	5	2	2017	-2136	19	1	7	2	212	-171	18	9	9	2	158	-32	-79	-7	12	2	291	277	33	1	14	2	382	-396	20

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
2	14	2	1784	1730	19
3	14	2	589	-534	22
4	14	2	1531	1549	22
5	14	2	347	350	28
6	14	2	1087	1136	26
7	14	2	416	433	34
8	14	2	119	106	-119
9	14	2	283	287	53
10	14	2	79	-236	-79
-12	15	2	428	-458	56
-11	15	2	396	-366	49
-10	15	2	287	-319	51
-9	15	2	584	-595	35
-8	15	2	342	-304	38
-7	15	2	1443	-1471	26
-6	15	2	166	46	40
-5	15	2	1133	-1081	22
-4	15	2	359	352	24
-3	15	2	998	-1002	19
-2	15	2	515	552	19
-1	15	2	221	195	23
0	15	2	800	766	15
1	15	2	715	684	19
2	15	2	300	308	24
3	15	2	1785	1797	20
4	15	2	95	-4	-95
5	15	2	1181	1132	24
6	15	2	174	-91	-62
7	15	2	786	762	30
8	15	2	525	-575	34
9	15	2	74	-106	-74
10	15	2	160	-246	-160
-11	16	2	1115	-1058	37
-10	16	2	422	-286	42
-9	16	2	514	-551	35
-8	16	2	541	-527	31
-7	16	2	255	-297	43
-6	16	2	643	-602	25
-5	16	2	446	445	25
-4	16	2	607	-547	22
-3	16	2	1479	1437	20
-2	16	2	47	-49	-47
-1	16	2	1369	1326	18
0	16	2	439	443	14
1	16	2	1521	1492	19
2	16	2	760	739	20
3	16	2	195	157	36
4	16	2	645	641	23
5	16	2	54	-30	-54
6	16	2	408	363	30
7	16	2	1031	-1086	29
8	16	2	246	143	53
9	16	2	705	-777	36
10	16	2	160	-151	-160
-11	17	2	298	191	59
-10	17	2	798	-806	36

h	k	l	10Fo	10Fc	10s
-9	17	2	132	-111	-132
-8	17	2	493	-486	33
-7	17	2	231	178	34
-6	17	2	58	108	-58
-5	17	2	107	14	-70
-4	17	2	1095	1050	21
-3	17	2	383	384	24
-2	17	2	1859	1873	19
-1	17	2	282	-257	23
0	17	2	1533	1520	14
1	17	2	156	134	34
2	17	2	824	796	21
3	17	2	319	-339	25
4	17	2	152	-82	-43
5	17	2	54	61	-54
6	17	2	582	-569	28
7	17	2	206	-162	-55
8	17	2	1087	-1096	32
9	17	2	160	45	-79
10	17	2	863	-875	40
-11	18	2	570	-625	45
-10	18	2	348	328	45
-9	18	2	357	-309	42
-8	18	2	448	426	33
-7	18	2	169	-152	-54
-6	18	2	976	1049	25
-5	18	2	624	605	25
-4	18	2	1187	1191	22
-3	18	2	921	908	21
-2	18	2	632	625	23
-1	18	2	1438	1476	19
0	18	2	261	-239	34
1	18	2	907	892	20
2	18	2	1301	-1260	21
3	18	2	244	191	31
4	18	2	906	-930	24
5	18	2	239	-185	39
6	18	2	836	-860	28
7	18	2	630	-638	32
8	18	2	301	-146	38
9	18	2	658	-615	37
10	18	2	143	32	-106
-11	19	2	81	206	-81
-10	19	2	112	-113	-112
-9	19	2	792	830	33
-8	19	2	124	96	-98
-7	19	2	1241	1255	27
-6	19	2	118	90	-118
-5	19	2	1070	1071	23
-4	19	2	186	202	42
-3	19	2	768	764	22
-2	19	2	274	-355	28
-1	19	2	191	-198	32
0	19	2	508	476	16
1	19	2	910	-893	21
2	19	2	142	-55	-42

h	k	l	10Fo	10Fc	10s
3	19	2	1522	-1510	22
4	19	2	151	132	-46
5	19	2	1200	-1192	25
6	19	2	238	-231	45
7	19	2	697	-661	31
8	19	2	210	-203	-59
9	19	2	74	52	-74
-11	20	2	513	528	41
-10	20	2	412	455	41
-9	20	2	170	63	-96
-8	20	2	1180	1236	29
-7	20	2	156	48	-77
-6	20	2	940	921	26
-5	20	2	321	-345	33
-4	20	2	1030	1049	23
-3	20	2	937	-875	22
-2	20	2	331	341	26
-1	20	2	917	-917	21
0	20	2	528	-513	16
1	20	2	690	-651	22
2	20	2	1207	-1170	22
3	20	2	158	-110	-44
4	20	2	1343	-1320	24
5	20	2	138	55	-69
6	20	2	814	-809	28
7	20	2	603	598	33
8	20	2	228	-280	-66
9	20	2	309	345	57
-10	21	2	636	679	39
-9	21	2	809	794	32
-8	21	2	343	389	39
-7	21	2	128	177	-128
-6	21	2	252	-297	37
-5	21	2	287	247	32
-4	21	2	857	-833	24
-3	21	2	53	-29	-53
-2	21	2	1664	-1604	21
-1	21	2	129	-138	-42
0	21	2	1820	-1783	15
1	21	2	802	-808	22
2	21	2	936	-952	22
3	21	2	293	-258	30
4	21	2	57	70	-57
5	21	2	464	-471	29
6	21	2	694	690	29
7	21	2	188	-184	-51
8	21	2	981	983	32
9	21	2	229	-123	-62
-10	22	2	285	-199	51
-9	22	2	734	756	34
-8	22	2	429	-418	34
-7	22	2	191	191	-59
-6	22	2	229	-212	41
-5	22	2	564	-576	27
-4	22	2	358	374	28
-3	22	2	613	-558	24

h	k	l	10Fo	10Fc	10s
-2	22	2	827	843	23
-1	22	2	1156	-1125	22
0	22	2	191	143	26
1	22	2	953	-935	22
2	22	2	238	154	30
3	22	2	287	-254	31
4	22	2	116	46	-76
5	22	2	274	264	39
6	22	2	234	134	40
7	22	2	646	679	33
8	22	2	204	-156	-58
9	22	2	841	891	37
-10	23	2	761	750	36
-9	23	2	816	-901	34
-8	23	2	540	620	34
-7	23	2	1273	-1259	28
-6	23	2	445	456	32
-5	23	2	1040	-1041	25
-4	23	2	614	-576	25
-3	23	2	802	-779	24
-2	23	2	664	-637	24
-1	23	2	160	105	38
0	23	2	1343	-1335	16
1	23	2	610	594	24
2	23	2	384	-355	28
3	23	2	1183	1148	24
4	23	2	289	-249	32
5	23	2	1234	1214	26
6	23	2	401	348	32
7	23	2	630	660	32
8	23	2	622	585	35
-9	24	2	213	-73	-62
-8	24	2	812	-855	32
-7	24	2	237	-138	52
-6	24	2	880	-802	28
-5	24	2	119	-126	-119
-4	24	2	1058	-1101	24
-3	24	2	595	-571	25
-2	24	2	799	-790	23
-1	24	2	222	-312	40
0	24	2	590	536	19
1	24	2	182	154	35
2	24	2	975	928	24
3	24	2	169	-14	-46
4	24	2	1458	1471	25
5	24	2	185	-117	42
6	24	2	838	839	30
7	24	2	240	-198	43
8	24	2	462	475	39
-9	25	2	382	-422	43
-8	25	2	407	-391	38
-7	25	2	493	-469	33
-6	25	2	214	230	49
-5	25	2	908	-839	26
-4	25	2	462	462	29
-3	25	2	909	-892	24

h	k	l	10Fo	10Fc	10s
-2	25	2	466	435	27
-1	25	2	222	-153	36
0	25	2	868	842	18
1	25	2	913	882	24
2	25	2	576	568	26
3	25	2	963	937	25
4	25	2	131	84	-88
5	25	2	760	791	28
6	25	2	206	-179	50
7	25	2	203	219	-61
8	25	2	376	-373	39
-9	26	2	636	-663	34
-8	26	2	380	-340	38
-7	26	2	271	-224	37
-6	26	2	267	-277	38
-5	26	2	316	377	38
-4	26	2	363	-361	28
-3	26	2	1004	977	24
-2	26	2	194	-236	42
-1	26	2	1285	1253	23
0	26	2	197	189	27
1	26	2	964	930	24
2	26	2	273	229	32
3	26	2	414	354	31
4	26	2	429	438	31
5	26	2	368	-336	34
6	26	2	96	11	-96
7	26	2	542	-507	36
-8	27	2	354	-370	37
-7	27	2	268	327	43
-6	27	2	150	-126	-72
-5	27	2	420	405	30
-4	27	2	832	816	26
-3	27	2	196	149	45
-2	27	2	1006	952	24
-1	27	2	190	123	36
0	27	2	1204	1186	36
1	27	2	357	-331	30
2	27	2	583	573	27
3	27	2	291	-274	32
4	27	2	260	229	37
5	27	2	435	-410	32
6	27	2	636	-575	31
7	27	2	292	-268	40
-8	28	2	542	609	36
-7	28	2	62	-171	-62
-6	28	2	842	853	29
-5	28	2	178	246	-56
-4	28	2	660	592	27
-3	28	2	530	532	27
-2	28	2	367	350	30
-1	28	2	702	707	25
0	28	2	275	-257	25
1	28	2	525	516	26
2	28	2	680	-653	26
3	28	2	421	364	30

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
4	28	2	821	-843	28
5	28	2	306	-280	35
6	28	2	550	-538	34
-7	29	2	677	689	33
-6	29	2	94	117	-94
-5	29	2	969	935	27
-4	29	2	230	-85	33
-3	29	2	360	373	32
-2	29	2	118	-53	-77
-1	29	2	196	161	40
0	29	2	268	-239	25
1	29	2	691	-638	26
2	29	2	139	-56	-44
3	29	2	911	-919	27
4	29	2	203	-149	45
5	29	2	967	-907	28
6	29	2	56	84	-56
-7	30	2	56	-20	-56
-6	30	2	652	573	29
-5	30	2	321	-325	39
-4	30	2	658	623	28
-3	30	2	647	-605	27
-2	30	2	196	220	44
-1	30	2	761	-755	27
0	30	2	162	-129	-42
1	30	2	501	-534	29
2	30	2	682	-674	27
3	30	2	324	-337	36
4	30	2	685	-682	29
5	30	2	322	367	39
-6	31	2	59	-99	-59
-5	31	2	207	108	40
-4	31	2	710	-724	29
-3	31	2	62	111	-62
-2	31	2	744	-743	27
-1	31	2	57	35	-57
0	31	2	1064	-1027	18
1	31	2	55	32	-55
2	31	2	499	-524	31
3	31	2	249	-258	37
4	31	2	59	-1	-59
5	31	2	60	-30	-60
-5	32	2	286	-295	40
-4	32	2	469	-446	32
-3	32	2	535	-542	29
-2	32	2	202	-183	50
-1	32	2	823	-796	27
0	32	2	253	263	26
1	32	2	710	-739	28
2	32	2	363	317	32
3	32	2	217	-221	51
4	32	2	554	544	33
-4	33	2	62	-19	-62
-3	33	2	490	-470	30
-2	33	2	191	-297	-59
-1	33	2	113	18	-113

h	k	l	10Fo	10Fc	10s
0	33	2	274	-271	28
1	33	2	620	614	28
2	33	2	260	-272	40
3	33	2	780	716	28
-3	34	2	158	133	-60
-2	34	2	232	-149	40
-1	34	2	356	370	37
0	34	2	280	239	34
1	34	2	172	179	-53
2	34	2	622	599	30
-13	0	3	770	794	53
-11	0	3	778	744	39
-9	0	3	327	146	37
-7	0	3	606	-476	26
-5	0	3	503	495	22
-3	0	3	1710	-1624	15
-1	0	3	1519	-1486	13
1	0	3	2250	-2005	15
3	0	3	1849	-1713	19
5	0	3	102	-112	-102
7	0	3	775	718	30
9	0	3	922	902	37
11	0	3	748	670	47
-13	1	3	505	395	57
-12	1	3	627	616	49
-11	1	3	167	220	-167
-10	1	3	996	940	34
-9	1	3	177	-154	-65
-8	1	3	922	845	27
-7	1	3	647	-620	26
-6	1	3	1621	1539	21
-5	1	3	1114	-1132	19
-4	1	3	95	22	-74
-3	1	3	775	-738	16
-2	1	3	1048	-1048	14
-1	1	3	786	-784	14
0	1	3	2120	-2122	72
1	1	3	373	-325	17
2	1	3	1049	-922	17
3	1	3	173	103	30
4	1	3	857	-827	22
5	1	3	857	862	24
6	1	3	355	363	35
7	1	3	454	368	34
8	1	3	623	523	36
9	1	3	499	391	43
10	1	3	784	684	42
11	1	3	98	-54	-98
-13	2	3	104	55	-104
-12	2	3	400	353	59
-11	2	3	282	299	66
-10	2	3	232	194	-66
-9	2	3	1059	987	30
-8	2	3	763	-772	28
-7	2	3	1059	1018	24
-6	2	3	2134	-2028	21

h	k	l	10Fo	10Fc	10s
-5	2	3	119	100	-53
-4	2	3	3061	-3034	17
-3	2	3	442	-425	18
-2	2	3	1792	-1831	14
-1	2	3	908	-921	14
0	2	3	173	-122	18
1	2	3	720	-690	16
2	2	3	858	905	17
3	2	3	330	-336	23
4	2	3	1867	1859	21
5	2	3	515	-403	26
6	2	3	1853	1738	26
7	2	3	254	-90	43
8	2	3	985	978	34
9	2	3	296	236	63
10	2	3	213	183	-93
11	2	3	238	70	-109
-13	3	3	724	616	51
-12	3	3	472	-506	51
-11	3	3	525	518	41
-10	3	3	632	-552	36
-9	3	3	126	142	-126
-8	3	3	184	80	-58
-7	3	3	496	-434	26
-6	3	3	1228	-1215	22
-5	3	3	1870	-1917	19
-4	3	3	244	146	24
-3	3	3	1377	-1393	15
-2	3	3	308	-299	19
-1	3	3	925	-895	14
0	3	3	2527	2370	43
1	3	3	89	22	-49
2	3	3	572	581	18
3	3	3	401	375	22
4	3	3	750	783	22
5	3	3	1950	1973	23
6	3	3	614	-654	29
7	3	3	1365	1313	29
8	3	3	194	-87	-76
9	3	3	657	646	39
10	3	3	458	-374	50
11	3	3	99	-220	-99
-13	4	3	429	-417	70
-12	4	3	414	434	53
-11	4	3	831	-797	37
-10	4	3	206	175	-71
-9	4	3	1441	-1416	30
-8	4	3	422	-380	35
-7	4	3	1179	-1080	24
-6	4	3	735	-714	22
-5	4	3	613	-607	20
-4	4	3	1361	-1334	17
-3	4	3	1136	1140	16
-2	4	3	408	-380	16
-1	4	3	1573	1541	14
0	4	3	141	34	19

h	k	l	10Fo	10Fc	10s
1	4	3	2392	2218	15
2	4	3	391	-395	20
3	4	3	1210	1291	19
4	4	3	884	950	22
5	4	3	427	423	26
6	4	3	861	862	27
7	4	3	235	-300	50
8	4	3	619	581	35
9	4	3	854	-790	39
10	4	3	91	-3	-91
11	4	3	736	-775	51
-13	5	3	206	-106	-135
-12	5	3	545	-537	46
-11	5	3	76	36	-76
-10	5	3	1310	-1267	33
-9	5	3	74	-18	-74
-8	5	3	1723	-1714	26
-7	5	3	202	7	41
-6	5	3	1130	-1133	22
-5	5	3	762	795	20
-4	5	3	137	-35	33
-3	5	3	348	-388	19
-2	5	3	1300	1300	14
-1	5	3	1488	1480	14
0	5	3	2767	2604	40
1	5	3	398	-355	18
2	5	3	2193	2220	17
3	5	3	257	288	26
4	5	3	1058	1166	21
5	5	3	592	-690	25
6	5	3	329	287	34
7	5	3	221	-216	53
8	5	3	695	-759	36
9	5	3	310	-279	58
10	5	3	986	-906	42
11	5	3	237	19	-109
-13	6	3	99	-230	-99
-12	6	3	311	-347	60
-11	6	3	694	-637	39
-10	6	3	340	-316	44
-9	6	3	868	-834	30
-8	6	3	267	228	45
-7	6	3	1378	-1393	24
-6	6	3	1332	1312	22
-5	6	3	537	-514	21
-4	6	3	1529	1563	18
-3	6	3	151	112	30
-2	6	3	1566	1567	15
-1	6	3	1876	1852	14
0	6	3	709	693	29
1	6	3	2277	2169	15
2	6	3	1041	-1064	17
3	6	3	805	823	20
4	6	3	1073	-1180	22
5	6	3	651	722	25
6	6	3	1224	-1258	26

h	k	l	10Fo	10Fc	10s
7	6	3	453	-338	35
8	6	3	636	-662	34
9	6	3	656	-613	39
10	6	3	291	-166	58
11	6	3	647	-554	50
-13	7	3	839	-772	50
-12	7	3	87	-149	-87
-11	7	3	521	-452	41
-10	7	3	76	82	-76
-9	7	3	68	56	-68
-8	7	3	300	-293	40
-7	7	3	1138	1115	25
-6	7	3	142	-24	-53
-5	7	3	2220	2250	20
-4	7	3	178	-171	29
-3	7	3	1829	1848	16
-2	7	3	562	586	16
-1	7	3	2663	2614	14
0	7	3	291	242	16
1	7	3	497	-476	18
2	7	3	467	457	19
3	7	3	1248	-1229	19
4	7	3	258	-167	27
5	7	3	1813	-1935	23
6	7	3	378	286	33
7	7	3	1180	-1289	29
8	7	3	411	-327	37
9	7	3	627	-669	39
10	7	3	93	177	-93
11	7	3	93	-12	-93
-13	8	3	356	266	73
-12	8	3	759	-742	46
-11	8	3	469	409	45
-10	8	3	305	-250	55
-9	8	3	934	878	31
-8	8	3	350	349	36
-7	8	3	488	487	26
-6	8	3	1448	1439	22
-5	8	3	579	611	21
-4	8	3	1559	1601	18
-3	8	3	264	-256	20
-2	8	3	2070	2074	15
-1	8	3	999	-985	15
0	8	3	419	422	12
1	8	3	1542	-1502	16
2	8	3	458	-410	19
3	8	3	910	-957	20
4	8	3	1146	-1185	21
5	8	3	224	-170	37
6	8	3	1286	-1422	26
7	8	3	235	109	48
8	8	3	844	-886	34
9	8	3	473	450	43
10	8	3	389	-364	61
11	8	3	333	362	70
-13	9	3	251	-302	-92

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-12	9	3	649	642	47
-11	9	3	205	-71	-88
-10	9	3	1361	1313	33
-9	9	3	204	1	-60
-8	9	3	1438	1429	27
-7	9	3	570	573	27
-6	9	3	932	927	23
-5	9	3	351	364	25
-4	9	3	88	29	-68
-3	9	3	1805	1754	17
-2	9	3	2013	-2028	16
-1	9	3	86	90	-86
0	9	3	2338	-2271	51
1	9	3	426	413	18
2	9	3	2397	-2361	18
3	9	3	568	-570	20
4	9	3	722	-724	22
5	9	3	388	-438	29
6	9	3	63	-19	-63
7	9	3	880	-874	29
8	9	3	610	697	36
9	9	3	203	-124	-84
10	9	3	960	953	41
11	9	3	332	-38	72
-12	10	3	94	-184	-94
-11	10	3	885	848	38
-10	10	3	125	-12	-125
-9	10	3	1287	1257	30
-8	10	3	426	-447	33
-7	10	3	1295	1364	25
-6	10	3	137	-49	-58
-5	10	3	637	639	22
-4	10	3	352	-336	21
-3	10	3	1189	-1170	17
-2	10	3	395	-369	19
-1	10	3	2581	-2475	16
0	10	3	855	-811	13
1	10	3	2841	-2723	17
2	10	3	265	-231	27
3	10	3	1702	-1738	20
4	10	3	570	610	24
5	10	3	367	-345	27
6	10	3	360	391	32
7	10	3	295	277	44
8	10	3	528	568	37
9	10	3	804	824	39
10	10	3	236	75	-84
-12	11	3	250	304	-113
-11	11	3	400	377	46
-10	11	3	622	640	38
-9	11	3	180	47	-52
-8	11	3	996	970	27
-7	11	3	858	-885	25
-6	11	3	431	448	27
-5	11	3	1346	-1401	21
-4	11	3	129	175	-52

h	k	l	10Fo	10Fc	10s
-3	11	3	1993	-2034	18
-2	11	3	1105	-1115	17
-1	11	3	219	128	24
0	11	3	811	-798	13
1	11	3	1253	1145	18
2	11	3	1543	-1534	18
3	11	3	1456	1512	20
4	11	3	234	-161	30
5	11	3	948	1001	24
6	11	3	240	-85	39
7	11	3	677	658	31
8	11	3	567	604	37
9	11	3	84	4	-84
10	11	3	606	561	44
-12	12	3	839	773	42
-11	12	3	72	56	-72
-10	12	3	73	-10	-73
-9	12	3	62	-7	-62
-8	12	3	496	-499	31
-7	12	3	215	-185	44
-6	12	3	1638	-1650	23
-5	12	3	215	173	31
-4	12	3	2248	-2247	19
-3	12	3	824	760	18
-2	12	3	2690	-2664	17
-1	12	3	649	645	18
0	12	3	333	-302	14
1	12	3	252	201	23
2	12	3	635	656	20
3	12	3	353	-280	23
4	12	3	1415	1448	22
5	12	3	156	-23	-46
6	12	3	1579	1630	26
7	12	3	251	-106	50
8	12	3	1025	1059	33
9	12	3	202	117	-64
10	12	3	460	639	54
-12	13	3	516	-477	49
-11	13	3	388	384	51
-10	13	3	761	-698	36
-9	13	3	115	-75	-115
-8	13	3	918	-870	28
-7	13	3	1064	-1095	25
-6	13	3	511	-447	25
-5	13	3	1158	-1100	21
-4	13	3	188	150	34
-3	13	3	2028	-2018	18
-2	13	3	725	763	18
-1	13	3	564	-540	18
0	13	3	780	748	17
1	13	3	101	-63	-55
2	13	3	1068	1039	20
3	13	3	1293	1281	21
4	13	3	557	534	23
5	13	3	937	943	25
6	13	3	164	59	-60

h	k	l	10Fo	10Fc	10s
7	13	3	964	1032	30
8	13	3	743	-756	33
9	13	3	581	578	41
10	13	3	726	-719	41
-12	14	3	85	109	-85
-11	14	3	837	-770	37
-10	14	3	80	-4	-80
-9	14	3	1116	-1087	31
-8	14	3	249	-177	42
-7	14	3	989	-1040	26
-6	14	3	397	-374	25
-5	14	3	335	-318	27
-4	14	3	88	-102	-88
-3	14	3	767	735	20
-2	14	3	344	-364	21
-1	14	3	1488	1490	18
0	14	3	420	-399	14
1	14	3	1571	1573	19
2	14	3	264	222	27
3	14	3	1347	1383	21
4	14	3	431	447	25
5	14	3	455	424	27
6	14	3	244	270	43
7	14	3	252	-333	54
8	14	3	223	208	-60
9	14	3	725	-772	37
10	14	3	236	37	-80
-12	15	3	532	-520	49
-11	15	3	153	-98	-153
-10	15	3	887	-879	33
-9	15	3	67	98	-67
-8	15	3	1159	-1182	28
-7	15	3	278	272	37
-6	15	3	444	-448	26
-5	15	3	356	320	26
-4	15	3	133	7	-39
-3	15	3	1155	1123	20
-2	15	3	1648	1670	19
-1	15	3	153	63	32
0	15	3	1397	1400	14
1	15	3	84	17	-84
2	15	3	1784	1770	20
3	15	3	597	-592	24
4	15	3	469	402	26
5	15	3	341	-373	30
6	15	3	157	-6	-68
7	15	3	436	-431	35
8	15	3	924	-989	34
9	15	3	244	-59	52
10	15	3	586	-615	45
-12	16	3	810	-707	43
-11	16	3	376	-384	48
-10	16	3	73	-18	-73
-9	16	3	707	-657	33
-8	16	3	228	214	54
-7	16	3	481	-461	28

h	k	l	10Fo	10Fc	10s
-6	16	3	1253	1239	24
-5	16	3	96	-32	-96
-4	16	3	1416	1432	21
-3	16	3	593	587	21
-2	16	3	1358	1411	19
-1	16	3	736	721	19
0	16	3	187	184	25
1	16	3	873	863	20
2	16	3	583	-561	21
3	16	3	709	658	23
4	16	3	1014	-1008	24
5	16	3	109	126	-109
6	16	3	1133	-1155	28
7	16	3	255	-229	43
8	16	3	664	-641	35
9	16	3	480	-474	42
10	16	3	434	-411	51
-11	17	3	275	-315	56
-10	17	3	142	-45	-91
-9	17	3	143	134	-87
-8	17	3	329	366	34
-7	17	3	1004	1026	27
-6	17	3	62	69	-62
-5	17	3	1572	1511	22
-4	17	3	262	249	28
-3	17	3	1670	1663	20
-2	17	3	46	-121	-46
-1	17	3	742	757	20
0	17	3	156	-188	34
1	17	3	47	-13	-47
2	17	3	212	-193	32
3	17	3	1010	-991	23
4	17	3	145	-1	-51
5	17	3	1231	-1214	26
6	17	3	199	-170	-61
7	17	3	1203	-1192	30
8	17	3	250	354	58
9	17	3	526	-501	39
-11	18	3	447	413	42
-10	18	3	110	-5	-110
-9	18	3	710	682	32
-8	18	3	313	333	41
-7	18	3	906	917	27
-6	18	3	821	847	25
-5	18	3	89	-28	-89
-4	18	3	1189	1205	22
-3	18	3	187	-218	45
-2	18	3	867	865	21
-1	18	3	881	-906	21
0	18	3	46	45	-32
1	18	3	1005	-1011	21
2	18	3	583	-562	23
3	18	3	798	-780	24
4	18	3	816	-806	25
5	18	3	559	-585	28
6	18	3	737	-788	29

h	k	l	10Fo	10Fc	10s
7	18	3	382	416	39
8	18	3	550	-491	36
9	18	3	582	654	41
-11	19	3	301	237	53
-10	19	3	737	735	36
-9	19	3	283	171	47
-8	19	3	1054	1083	29
-7	19	3	153	-41	-51
-6	19	3	648	644	27
-5	19	3	319	277	28
-4	19	3	250	-231	32
-3	19	3	93	-66	-93
-2	19	3	1060	-1092	21
-1	19	3	523	521	22
0	19	3	1417	-1385	15
1	19	3	458	-426	23
2	19	3	1505	-1486	22
3	19	3	134	-46	-64
4	19	3	840	-800	25
5	19	3	425	-441	32
6	19	3	153	-133	-67
7	19	3	116	-16	-116
8	19	3	747	804	36
9	19	3	81	24	-81
-11	20	3	729	702	37
-10	20	3	203	-82	-64
-9	20	3	725	702	32
-8	20	3	207	-264	-55
-7	20	3	827	818	28
-6	20	3	608	-579	26
-5	20	3	199	209	42
-4	20	3	983	-997	23
-3	20	3	919	-920	22
-2	20	3	934	-935	21
-1	20	3	1156	-1159	21
0	20	3	154	-134	28
1	20	3	1351	-1305	22
2	20	3	259	171	27
3	20	3	847	-804	24
4	20	3	609	659	28
5	20	3	325	-350	34
6	20	3	449	454	33
7	20	3	509	491	36
8	20	3	334	340	43
9	20	3	507	518	42
-10	21	3	515	503	36
-9	21	3	146	-109	-90
-8	21	3	137	164	-137
-7	21	3	436	-395	31
-6	21	3	631	664	27
-5	21	3	835	-805	25
-4	21	3	227	-242	35
-3	21	3	1433	-1431	22
-2	21	3	259	-191	29
-1	21	3	833	-811	22
0	21	3	728	-707	25

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
1	21	3	148	-162	-52
2	21	3	298	-325	31
3	21	3	737	747	24
4	21	3	808	-791	25
5	21	3	952	950	27
6	21	3	155	96	-87
7	21	3	665	720	34
8	21	3	229	71	52
-10	22	3	194	29	-68
-9	22	3	69	27	-69
-8	22	3	287	-310	43
-7	22	3	58	49	-58
-6	22	3	535	-551	28
-5	22	3	406	377	28
-4	22	3	1120	-1054	24
-3	22	3	211	203	37
-2	22	3	1016	-981	22
-1	22	3	345	334	26
0	22	3	383	-366	23
1	22	3	354	347	27
2	22	3	456	423	25
3	22	3	181	133	38
4	22	3	1146	1167	26
5	22	3	194	-71	-53
6	22	3	1073	1077	29
7	22	3	102	-55	-102
8	22	3	660	708	38
-10	23	3	713	-711	36
-9	23	3	68	112	-68
-8	23	3	739	-760	31
-7	23	3	387	-447	36
-6	23	3	909	-895	27
-5	23	3	1369	-1462	25
-4	23	3	335	-373	29
-3	23	3	960	-966	23
-2	23	3	648	632	24
-1	23	3	658	-613	23
0	23	3	896	811	23
1	23	3	349	315	25
2	23	3	1107	1076	24
3	23	3	326	324	32
4	23	3	519	513	29
5	23	3	951	962	28
6	23	3	62	20	-62
7	23	3	539	498	36
8	23	3	279	-223	43
-9	24	3	921	-983	32
-8	24	3	99	136	-99
-7	24	3	830	-882	29
-6	24	3	89	-68	-89
-5	24	3	743	-765	28
-4	24	3	260	-247	35
-3	24	3	702	721	25
-2	24	3	172	141	43
-1	24	3	1282	1267	23
0	24	3	94	-49	-66

h	k	l	10Fo	10Fc	10s
1	24	3	1572	1524	23
2	24	3	350	-343	28
3	24	3	1290	1299	25
4	24	3	231	-265	36
5	24	3	304	350	38
6	24	3	59	4	-59
7	24	3	335	-306	38
-9	25	3	184	-130	-97
-8	25	3	457	-502	36
-7	25	3	298	295	37
-6	25	3	552	-490	30
-5	25	3	613	608	27
-4	25	3	251	218	35
-3	25	3	519	557	27
-2	25	3	423	418	28
-1	25	3	526	555	25
0	25	3	966	945	18
1	25	3	145	-79	-47
2	25	3	748	723	26
3	25	3	433	-438	30
4	25	3	731	765	28
5	25	3	567	-568	31
6	25	3	61	9	-61
7	25	3	407	-378	37
-9	26	3	470	-451	39
-8	26	3	285	317	48
-7	26	3	240	-238	49
-6	26	3	1049	1090	28
-5	26	3	60	-45	-60
-4	26	3	1259	1228	25
-3	26	3	56	95	-56
-2	26	3	775	782	25
-1	26	3	210	208	37
0	26	3	327	315	31
1	26	3	302	285	35
2	26	3	349	-329	32
3	26	3	186	168	-53
4	26	3	784	-738	28
5	26	3	153	127	-79
6	26	3	859	-909	30
7	26	3	72	-14	-72
-8	27	3	203	214	-60
-7	27	3	462	465	33
-6	27	3	265	285	46
-5	27	3	1118	1160	26
-4	27	3	120	9	-68
-3	27	3	908	909	25
-2	27	3	235	-210	35
-1	27	3	808	770	25
0	27	3	518	-477	19
1	27	3	164	-130	-53
2	27	3	443	-466	30
3	27	3	510	-427	29
4	27	3	216	-254	51
5	27	3	937	-973	29
6	27	3	183	173	-62

h	k	l	10Fo	10Fc	10s
-8	28	3	205	186	-58
-7	28	3	463	479	33
-6	28	3	359	340	36
-5	28	3	263	258	40
-4	28	3	585	579	29
-3	28	3	490	-416	28
-2	28	3	631	539	26
-1	28	3	877	-835	25
0	28	3	235	206	31
1	28	3	1106	-1099	25
2	28	3	178	-146	-51
3	28	3	599	-595	30
4	28	3	421	-430	36
5	28	3	53	-83	-53
6	28	3	330	-314	44
-7	29	3	63	-6	-63
-6	29	3	433	450	32
-5	29	3	313	-297	37
-4	29	3	208	-227	46
-3	29	3	85	-24	-85
-2	29	3	532	-499	28
-1	29	3	281	-225	32
0	29	3	1349	-1313	18
1	29	3	57	-7	-57
2	29	3	828	-807	26
3	29	3	137	-25	-60
4	29	3	512	-513	32
5	29	3	269	242	40
-7	30	3	421	445	34
-6	30	3	572	-630	31
-5	30	3	129	148	-92
-4	30	3	724	-729	29
-3	30	3	340	-274	31
-2	30	3	563	-477	26
-1	30	3	626	-599	28
0	30	3	248	-223	29
1	30	3	704	-674	26
2	30	3	404	350	31
3	30	3	323	-280	35
4	30	3	577	581	31
5	30	3	179	-146	-51
-6	31	3	63	43	-63
-5	31	3	1025	-1025	28
-4	31	3	61	83	-61
-3	31	3	802	-734	27
-2	31	3	174	-116	40
-1	31	3	695	-631	27
0	31	3	61	15	-46
1	31	3	290	234	29
2	31	3	237	-175	36
3	31	3	501	480	29
4	31	3	62	76	-62
-5	32	3	281	-261	37
-4	32	3	698	-734	29
-3	32	3	200	162	43
-2	32	3	681	-617	27

h	k	l	10Fo	10Fc	10s
-1	32	3	503	437	29
0	32	3	53	-50	-37
1	32	3	557	538	30
2	32	3	327	316	36
3	32	3	356	362	37
-4	33	3	61	102	-61
-3	33	3	286	-310	40
-2	33	3	750	690	28
-1	33	3	235	-208	43
0	33	3	970	949	19
1	33	3	208	-137	45
2	33	3	500	532	31
-3	34	3	280	244	40
-2	34	3	166	196	-61
-1	34	3	674	659	28
0	34	3	164	113	36
1	34	3	902	847	28
-12	0	4	653	580	47
-10	0	4	771	714	34
-8	0	4	160	177	-64
-6	0	4	333	289	28
-4	0	4	2664	-2592	18
-2	0	4	2175	-2183	16
0	0	4	3269	-3313	16
2	0	4	661	-551	19
4	0	4	566	522	24
6	0	4	1149	1080	28
8	0	4	1301	1221	34
10	0	4	740	649	47
-13	1	4	765	673	51
-12	1	4	479	494	47
-11	1	4	862	820	38
-10	1	4	244	151	55
-9	1	4	201	-2	-61
-8	1	4	695	-648	29
-7	1	4	762	-643	25
-6	1	4	1071	-1054	22
-5	1	4	1645	-1615	20
-4	1	4	699	-716	19
-3	1	4	1767	-1771	17
-2	1	4	404	-408	18
-1	1	4	853	-853	16
0	1	4	1436	1450	60
1	1	4	550	-527	19
2	1	4	373	366	23
3	1	4	884	792	21
4	1	4	526	485	25
5	1	4	1082	1039	25
6	1	4	405	364	37
7	1	4	984	885	31
8	1	4	79	109	-79
9	1	4	1001	876	38
10	1	4	488	-320	49
-13	2	4	90	-131	-90
-12	2	4	649	686	45
-11	2	4	233	-127	-68

h	k	l	10Fo	10Fc	10s
-10	2	4	786	735	34
-9	2	4	2033	-1946	29
-8	2	4	222	196	52
-7	2	4	1948	-1875	24
-6	2	4	199	162	41
-5	2	4	1896	-1901	20
-4	2	4	726	-723	18
-3	2	4	74	-78	-74
-2	2	4	680	-673	16
-1	2	4	1131	1114	16
0	2	4	830	-779	12
1	2	4	2047	2174	17
2	2	4	200	-224	30
3	2	4	1413	1360	20
4	2	4	596	581	25
5	2	4	1197	1168	25
6	2	4	353	303	35
7	2	4	475	410	35
8	2	4	273	291	61
9	2	4	349	-356	62
10	2	4	91	45	-91
-13	3	4	105	-216	-105
-12	3	4	370	-315	55
-11	3	4	315	-189	48
-10	3	4	848	-784	33
-9	3	4	424	-371	38
-8	3	4	1438	-1440	27
-7	3	4	202	27	46
-6	3	4	1371	-1340	22
-5	3	4	334	334	24
-4	3	4	1034	-1024	18
-3	3	4	364	390	21
-2	3	4	426	406	18
-1	3	4	1117	1080	16
0	3	4	1682	1621	16
1	3	4	226	133	25
2	3	4	1782	1916	19
3	3	4	263	96	28
4	3	4	1987	2006	22
5	3	4	598	-580	27
6	3	4	637	661	30
7	3	4	297	-235	43
8	3	4	144	55	-144
9	3	4	608	-587	41
10	3	4	507	-501	52
-13	4	4	104	104	-104
-12	4	4	933	-978	41
-11	4	4	658	-662	40
-10	4	4	1236	-1197	32
-9	4	4	374	-415	40
-8	4	4	61	71	-61
-7	4	4	988	-987	24
-6	4	4	558	520	24
-5	4	4	608	-601	21
-4	4	4	1852	1901	18
-3	4	4	467	-503	19

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn) \cdot MeOH$

h	k	l	10Fo	10Fc	10s
-2	4	4	1538	1577	16
-1	4	4	1264	1228	16
0	4	4	2324	2200	27
1	4	4	1088	1029	17
2	4	4	237	-164	27
3	4	4	1175	1246	21
4	4	4	431	-421	28
5	4	4	505	508	27
6	4	4	1066	-1163	28
7	4	4	254	-49	46
8	4	4	835	-867	36
9	4	4	246	-128	-72
10	4	4	746	-669	46
-13	5	4	888	-846	47
-12	5	4	95	-139	-95
-11	5	4	1331	-1292	35
-10	5	4	73	4	-73
-9	5	4	682	-643	31
-8	5	4	61	150	-61
-7	5	4	139	44	-51
-6	5	4	165	284	-54
-5	5	4	1293	1316	20
-4	5	4	138	-129	-42
-3	5	4	1694	1737	17
-2	5	4	667	642	17
-1	5	4	2634	2590	16
0	5	4	177	-91	18
1	5	4	1099	1025	17
2	5	4	64	17	-64
3	5	4	114	81	-50
4	5	4	411	-418	26
5	5	4	949	-1000	26
6	5	4	271	-43	37
7	5	4	1153	-1169	31
8	5	4	265	-62	48
9	5	4	867	-817	40
10	5	4	97	83	-97
-13	6	4	164	-63	-164
-12	6	4	901	-794	40
-11	6	4	330	175	55
-10	6	4	566	-556	38
-9	6	4	1070	1083	31
-8	6	4	303	-323	39
-7	6	4	1182	1149	24
-6	6	4	848	829	23
-5	6	4	1222	1269	20
-4	6	4	1112	1123	19
-3	6	4	270	240	24
-2	6	4	1624	1622	16
-1	6	4	100	95	-65
0	6	4	895	832	16
1	6	4	1496	-1405	17
2	6	4	710	691	20
3	6	4	1537	-1581	20
4	6	4	423	-437	26
5	6	4	998	-1102	25
6	6	4	839	-862	29
7	6	4	280	-278	46
8	6	4	737	-778	36
9	6	4	123	218	-123
10	6	4	569	-501	49
-13	7	4	100	-111	-100
-12	7	4	89	160	-89
-11	7	4	150	19	-150
-10	7	4	963	893	34
-9	7	4	285	-206	47
-8	7	4	1766	1763	27
-7	7	4	155	-39	-61
-6	7	4	1629	1676	22
-5	7	4	248	266	28
-4	7	4	1076	1070	19
-3	7	4	449	449	20
-2	7	4	441	-452	19
-1	7	4	192	157	25
0	7	4	1345	-1298	49
1	7	4	465	405	20
2	7	4	2189	-2147	19
3	7	4	296	-229	27
4	7	4	1566	-1618	23
5	7	4	181	-54	-47
6	7	4	544	-592	30
7	7	4	261	-307	50
8	7	4	144	-153	-144
9	7	4	142	91	-142
10	7	4	600	625	45
-13	8	4	200	-242	-167
-12	8	4	444	434	52
-11	8	4	567	515	42
-10	8	4	770	752	34
-9	8	4	840	796	30
-8	8	4	136	8	-96
-7	8	4	1666	1627	24
-6	8	4	248	230	36
-5	8	4	866	861	21
-4	8	4	1117	-1127	19
-3	8	4	597	632	18
-2	8	4	1098	-1070	17
-1	8	4	747	-754	17
0	8	4	918	-912	12
1	8	4	1107	-1078	18
2	8	4	206	-56	26
3	8	4	1649	-1638	21
4	8	4	172	127	-43
5	8	4	1026	-1113	25
6	8	4	469	489	32
7	8	4	554	-546	36
8	8	4	441	468	42
9	8	4	188	131	-120
10	8	4	533	506	49
-13	9	4	784	710	49
-12	9	4	256	89	-80
-11	9	4	1011	978	36
-10	9	4	369	309	44
-9	9	4	860	844	31
-8	9	4	481	541	33
-7	9	4	206	-104	41
-6	9	4	481	479	25
-5	9	4	1510	-1531	21
-4	9	4	105	147	-56
-3	9	4	2263	-2275	18
-2	9	4	423	-370	19
-1	9	4	2728	-2650	17
0	9	4	693	-633	29
1	9	4	1225	-1162	18
2	9	4	718	-674	20
3	9	4	92	19	-92
4	9	4	377	-355	25
5	9	4	907	983	26
6	9	4	273	-233	39
7	9	4	1158	1275	31
8	9	4	273	300	59
9	9	4	891	947	39
10	9	4	82	190	-82
-13	10	4	90	-111	-90
-12	10	4	1092	977	39
-11	10	4	309	-183	51
-10	10	4	865	842	34
-9	10	4	647	-581	31
-8	10	4	546	587	31
-7	10	4	293	-265	31
-6	10	4	1538	-1514	23
-5	10	4	486	-504	23
-4	10	4	1131	-1117	19
-3	10	4	481	465	21
-2	10	4	1740	-1810	17
-1	10	4	40	-47	-40
0	10	4	1353	-1319	19
1	10	4	921	855	19
2	10	4	700	-651	20
3	10	4	573	607	23
4	10	4	487	497	25
5	10	4	318	347	31
6	10	4	819	853	29
7	10	4	241	-45	51
8	10	4	825	843	35
9	10	4	480	-420	45
10	10	4	543	445	47
-12	11	4	92	59	-92
-11	11	4	685	620	40
-10	11	4	790	-811	35
-9	11	4	571	571	33
-8	11	4	1332	-1304	27
-7	11	4	528	-536	27
-6	11	4	995	-1007	23
-5	11	4	838	-817	22
-4	11	4	191	-170	30
-3	11	4	648	-663	20
-2	11	4	1087	1016	18
-1	11	4	683	-663	18
0	11	4	725	690	28
1	11	4	1170	-1075	19
2	11	4	1961	1895	20
3	11	4	215	114	36
4	11	4	1323	1344	23
5	11	4	378	355	32
6	11	4	697	729	30
7	11	4	928	992	31
8	11	4	204	-90	-64
9	11	4	690	689	40
10	11	4	501	-526	52
-12	12	4	196	-87	-75
-11	12	4	660	-639	40
-10	12	4	247	-166	58
-9	12	4	1235	-1214	30
-8	12	4	256	131	36
-7	12	4	1912	-1928	25
-6	12	4	173	79	-46
-5	12	4	1468	-1477	21
-4	12	4	216	168	27
-3	12	4	628	-622	20
-2	12	4	236	-164	23
-1	12	4	915	944	18
0	12	4	224	-212	19
1	12	4	1392	1347	19
2	12	4	221	-92	35
3	12	4	2156	2151	22
4	12	4	251	105	33
5	12	4	627	595	28
6	12	4	456	475	32
7	12	4	333	254	42
8	12	4	204	243	-75
9	12	4	347	-386	60
10	12	4	259	244	-92
-12	13	4	286	22	55
-11	13	4	535	-529	43
-10	13	4	632	-627	37
-9	13	4	444	-413	34
-8	13	4	1171	-1143	28
-7	13	4	378	405	33
-6	13	4	1457	-1479	23
-5	13	4	1163	1129	22
-4	13	4	1237	-1254	20
-3	13	4	1474	1486	19
-2	13	4	45	7	-45
-1	13	4	1204	1194	18
0	13	4	642	596	15
1	13	4	689	673	20
2	13	4	2008	1972	20
3	13	4	560	-508	24
4	13	4	1213	1185	24
5	13	4	667	-697	29
6	13	4	872	903	29
7	13	4	1084	-1159	31
8	13	4	348	389	46
9	13	4	939	-1019	39
10	13	4	206	-152	-102
-12	14	4	952	-938	41
-11	14	4	214	-121	-73
-10	14	4	658	-663	35
-9	14	4	323	-278	40
-8	14	4	648	-606	29
-7	14	4	285	-264	37
-6	14	4	976	978	24
-5	14	4	199	-171	33
-4	14	4	1265	1263	20
-3	14	4	45	-5	-45
-2	14	4	1762	1853	19
-1	14	4	48	83	-48
0	14	4	1277	1273	20
1	14	4	304	286	25
2	14	4	436	438	23
3	14	4	472	466	25
4	14	4	409	-374	28
5	14	4	59	-44	-59
6	14	4	889	-972	29
7	14	4	345	246	40
8	14	4	1059	-1060	35
9	14	4	235	86	-70
-12	15	4	305	117	61
-11	15	4	864	-847	39
-10	15	4	292	252	44
-9	15	4	550	-539	33
-8	15	4	560	569	31
-7	15	4	274	256	34
-6	15	4	611	620	25
-5	15	4	1129	1150	22
-4	15	4	308	340	26
-3	15	4	1980	2007	20
-2	15	4	120	-106	-52
-1	15	4	1618	1575	19
0	15	4	684	-666	22
1	15	4	880	826	21
2	15	4	607	-570	22
3	15	4	348	-350	28
4	15	4	543	-509	27
5	15	4	821	-819	28
6	15	4	285	-246	43
7	15	4	1157	-1180	31
8	15	4	184	-48	-70
9	15	4	425	-430	46
-12	16	4	450	-442	49
-11	16	4	594	594	40
-10	16	4	545	-490	36
-9	16	4	745	714	30
-8	16	4	64	-63	-64
-7	16	4	1482	1500	26
-6	16	4	223	245	34
-5	16	4	606	567	24
-4	16	4	757	752	22
-3	16	4	731	727	22

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-2	16	4	1121	1127	20
-1	16	4	976	-946	20
0	16	4	922	871	19
1	16	4	933	-883	21
2	16	4	283	267	27
3	16	4	1491	-1522	23
4	16	4	340	-323	33
5	16	4	681	-715	28
6	16	4	686	-672	30
7	16	4	316	-394	45
8	16	4	385	-379	46
9	16	4	123	-75	-123
-11	17	4	72	59	-72
-10	17	4	766	768	34
-9	17	4	246	101	41
-8	17	4	1318	1330	28
-7	17	4	246	135	37
-6	17	4	1262	1285	24
-5	17	4	159	73	-46
-4	17	4	943	963	22
-3	17	4	329	-335	25
-2	17	4	206	-163	30
-1	17	4	79	15	-79
0	17	4	1103	-1072	15
1	17	4	270	-219	29
2	17	4	1676	-1654	22
3	17	4	193	152	-52
4	17	4	1321	-1281	25
5	17	4	199	3	50
6	17	4	488	-497	33
7	17	4	287	247	51
8	17	4	76	70	-76
9	17	4	71	-2	-71
-11	18	4	225	294	-77
-10	18	4	75	217	-75
-9	18	4	805	782	32
-8	18	4	172	184	-67
-7	18	4	895	886	27
-6	18	4	413	-613	49
-5	18	4	656	684	24
-4	18	4	801	-783	23
-3	18	4	171	195	39
-2	18	4	1253	-1282	21
-1	18	4	531	-508	23
0	18	4	655	-606	19
1	18	4	1152	-1132	22
2	18	4	299	-305	29
3	18	4	1054	-1073	24
4	18	4	344	399	34
5	18	4	887	-875	28
6	18	4	732	749	30
7	18	4	233	81	50
8	18	4	472	516	41
9	18	4	275	338	57
-11	19	4	789	700	38
-10	19	4	179	38	-64

h	k	l	10Fo	10Fc	10s
-9	19	4	454	441	35
-8	19	4	219	219	47
-7	19	4	59	-69	-59
-6	19	4	167	149	-54
-5	19	4	945	-936	23
-4	19	4	98	109	-98
-3	19	4	1447	-1406	22
-2	19	4	101	122	-101
-1	19	4	1463	-1449	21
0	19	4	396	-400	23
1	19	4	770	-738	23
2	19	4	159	-92	-46
3	19	4	51	21	-51
4	19	4	322	-339	33
5	19	4	608	600	29
6	19	4	169	-28	-70
7	19	4	856	868	33
8	19	4	197	98	-66
-11	20	4	404	-340	42
-10	20	4	625	582	35
-9	20	4	270	-210	47
-8	20	4	63	152	-63
-7	20	4	763	-746	28
-6	20	4	565	-586	27
-5	20	4	443	-459	26
-4	20	4	1500	-1482	23
-3	20	4	393	-410	31
-2	20	4	1394	-1388	22
-1	20	4	394	359	25
0	20	4	859	-832	17
1	20	4	307	278	26
2	20	4	149	19	-42
3	20	4	678	632	26
4	20	4	362	336	30
5	20	4	313	237	36
6	20	4	614	543	31
7	20	4	64	-15	-64
8	20	4	697	669	35
-10	21	4	331	-346	48
-9	21	4	489	468	34
-8	21	4	655	-644	31
-7	21	4	544	598	29
-6	21	4	604	-572	27
-5	21	4	162	-115	-52
-4	21	4	563	-553	26
-3	21	4	524	-500	24
-2	21	4	254	223	31
-1	21	4	892	-887	23
0	21	4	693	667	17
1	21	4	269	-260	27
2	21	4	1011	945	24
3	21	4	144	-95	-64
4	21	4	760	772	27
5	21	4	316	274	36
6	21	4	482	489	34
7	21	4	259	224	51

h	k	l	10Fo	10Fc	10s
8	21	4	68	-97	-68
-10	22	4	279	-184	46
-9	22	4	981	-942	32
-8	22	4	465	-492	33
-7	22	4	983	-1010	28
-6	22	4	60	55	-60
-5	22	4	1013	-1023	25
-4	22	4	138	74	-66
-3	22	4	488	-490	26
-2	22	4	489	501	24
-1	22	4	428	435	26
0	22	4	196	130	37
1	22	4	1316	1341	23
2	22	4	278	319	31
3	22	4	1257	1212	25
4	22	4	102	-72	-102
5	22	4	1005	1040	29
6	22	4	64	61	-64
7	22	4	308	317	43
8	22	4	73	-85	-73
-10	23	4	595	-634	39
-9	23	4	454	-487	38
-8	23	4	1042	-1109	30
-7	23	4	150	-98	-57
-6	23	4	727	-704	28
-5	23	4	733	735	27
-4	23	4	93	-112	-93
-3	23	4	954	906	24
-2	23	4	50	84	-50
-1	23	4	653	631	24
0	23	4	813	831	23
1	23	4	352	320	30
2	23	4	622	629	25
3	23	4	237	-249	36
4	23	4	829	801	27
5	23	4	425	-393	35
6	23	4	247	166	48
7	23	4	560	-541	36
-9	24	4	121	121	-121
-8	24	4	139	-108	-99
-7	24	4	194	213	47
-6	24	4	298	237	34
-5	24	4	60	-84	-60
-4	24	4	1291	1306	24
-3	24	4	54	-15	-54
-2	24	4	1148	1106	24
-1	24	4	208	-248	36
0	24	4	1297	1288	17
1	24	4	80	-110	-80
2	24	4	185	223	-49
3	24	4	56	115	-56
4	24	4	354	-355	33
5	24	4	165	49	-55
6	24	4	804	-727	32
7	24	4	67	-84	-67
-9	25	4	161	-24	-104

h	k	l	10Fo	10Fc	10s
-8	25	4	632	715	32
-7	25	4	218	168	51
-6	25	4	534	496	30
-5	25	4	483	515	28
-4	25	4	192	271	-54
-3	25	4	921	834	25
-2	25	4	222	-164	34
-1	25	4	1027	1012	24
0	25	4	751	-776	37
1	25	4	658	634	25
2	25	4	800	-768	26
3	25	4	168	-26	-50
4	25	4	451	-476	33
5	25	4	467	-474	38
6	25	4	344	-328	44
-9	26	4	947	955	33
-8	26	4	239	193	49
-7	26	4	918	977	29
-6	26	4	157	-119	-68
-5	26	4	899	817	26
-4	26	4	309	313	34
-3	26	4	60	140	-60
-2	26	4	210	192	39
-1	26	4	341	-358	29
0	26	4	267	274	27
1	26	4	1060	-1003	25
2	26	4	58	-83	-58
3	26	4	934	-913	27
4	26	4	278	-138	31
5	26	4	648	-618	30
6	26	4	157	-142	-86
-8	27	4	822	823	31
-7	27	4	61	-124	-61
-6	27	4	842	881	28
-5	27	4	294	-276	42
-4	27	4	451	426	29
-3	27	4	300	-299	32
-2	27	4	55	20	-55
-1	27	4	559	-556	26
0	27	4	651	-606	32
1	27	4	284	-229	31
2	27	4	920	-883	27
3	27	4	202	67	39
4	27	4	985	-966	28
5	27	4	375	396	38
6	27	4	349	-354	38
-8	28	4	156	-119	-81
-7	28	4	327	309	37
-6	28	4	339	-406	42
-5	28	4	366	361	33
-4	28	4	930	-902	26
-3	28	4	53	-41	-53
-2	28	4	882	-895	26
-1	28	4	54	-83	-54
0	28	4	952	-943	30
1	28	4	377	-374	30

h	k	l	10Fo	10Fc	10s
2	28	4	88	-84	-88
3	28	4	508	-480	30
4	28	4	273	228	36
5	28	4	172	-288	-80
-7	29	4	316	-212	36
-6	29	4	224	-218	46
-5	29	4	740	-734	28
-4	29	4	58	-38	-58
-3	29	4	979	-965	26
-2	29	4	49	20	-49
-1	29	4	1080	-1081	26
0	29	4	317	288	27
1	29	4	366	-328	31
2	29	4	62	76	-62
3	29	4	141	-2	-58
4	29	4	61	113	-61
5	29	4	599	610	32
-7	30	4	506	-526	33
-6	30	4	360	-324	33
-5	30	4	649	-680	30
-4	30	4	539	-513	29
-3	30	4	58	-12	-58
-2	30	4	558	-577	28
-1	30	4	229	277	42
0	30	4	502	-485	20
1	30	4	794	747	28
2	30	4	209	-153	47
3	30	4	525	553	31
4	30	4	250	182	46
-6	31	4	880	-867	30
-5	31	4	63	-93	-63
-4	31	4	402	-373	31
-3	31	4	103	-12	-103
-2	31	4	134	144	-78
-1	31	4	57	-102	-57
0	31	4	678	671	20
1	31	4	61	-55	-61
2	31	4	919	832	28
3	31	4	272	210	45
-5	32	4	415	-451	34
-4	32	4	506	516	30
-3	32	4	128	-106	-97
-2	32	4	361	306	34
-1	32	4	257	244	36
0	32	4	298	289	37
1	32	4	494	488	30
2	32	4	107	22	-107
-4	33	4	152	-198	-70
-3	33	4	674	666	29
-2	33	4	62	10	-62
-1	33	4	810	725	28
0	33	4	94	102	-53
1	33	4	352	358	38
-13	0	5	873	816	45
-11	0	5	601	557	40
-9	0	5	491	-448	35

Observed and calculated structure factors for Re(CO)$_3$Cl(hhtn)·MeOH

h	k	l	10Fo	10Fc	10s
-7	0	5	1320	-1271	24
-5	0	5	2693	-2658	20
-3	0	5	1226	-1175	18
-1	0	5	1026	-1004	18
1	0	5	245	-149	28
3	0	5	1311	1187	22
5	0	5	2037	1933	27
7	0	5	1177	1051	33
9	0	5	457	453	53
-13	1	5	180	-2	-180
-12	1	5	193	-6	-85
-11	1	5	506	-460	42
-10	1	5	421	-395	43
-9	1	5	968	-984	30
-8	1	5	1093	-1054	27
-7	1	5	476	-449	28
-6	1	5	1865	-1783	22
-5	1	5	48	-16	-48
-4	1	5	1647	-1653	19
-3	1	5	1300	1310	18
-2	1	5	503	-566	20
-1	1	5	1068	1109	18
0	1	5	138	124	29
1	1	5	918	877	20
2	1	5	797	759	21
3	1	5	1125	982	23
4	1	5	1596	1516	24
5	1	5	317	-239	36
6	1	5	1199	1100	30
7	1	5	462	-428	39
8	1	5	582	531	41
9	1	5	487	-539	59
10	1	5	323	-188	67
-13	2	5	161	99	-161
-12	2	5	635	-686	47
-11	2	5	133	42	-133
-10	2	5	1245	-1252	33
-9	2	5	222	-2	52
-8	2	5	905	-814	27
-7	2	5	438	-374	28
-6	2	5	782	-770	23
-5	2	5	700	-704	22
-4	2	5	1368	1329	19
-3	2	5	350	-373	21
-2	2	5	1107	1120	18
-1	2	5	620	576	19
0	2	5	1570	1720	43
1	2	5	968	942	19
2	2	5	1017	944	21
3	2	5	482	423	24
4	2	5	746	746	26
5	2	5	457	460	30
6	2	5	748	-718	32
7	2	5	349	260	41
8	2	5	758	-752	38
9	2	5	150	143	-150
10	2	5	917	-848	48
-13	3	5	1059	-1036	45
-12	3	5	84	105	-84
-11	3	5	1182	-1123	36
-10	3	5	243	248	-63
-9	3	5	1315	-1256	29
-8	3	5	517	544	31
-7	3	5	915	-860	25
-6	3	5	658	623	24
-5	3	5	318	335	26
-4	3	5	409	408	22
-3	3	5	1711	1747	18
-2	3	5	195	219	27
-1	3	5	1774	1772	18
0	3	5	302	-259	16
1	3	5	2304	2255	19
2	3	5	458	-416	22
3	3	5	1021	1003	23
4	3	5	665	-697	26
5	3	5	126	-49	-126
6	3	5	365	-314	39
7	3	5	802	-748	34
8	3	5	535	-502	47
9	3	5	887	-870	43
10	3	5	102	-38	-102
-13	4	5	715	-641	49
-12	4	5	536	-512	48
-11	4	5	249	-172	-64
-10	4	5	426	-439	40
-9	4	5	563	601	34
-8	4	5	577	-538	30
-7	4	5	1069	1055	25
-6	4	5	131	-57	-46
-5	4	5	1764	1786	20
-4	4	5	626	653	21
-3	4	5	1402	1400	18
-2	4	5	935	988	18
-1	4	5	524	569	19
0	4	5	1499	1346	13
1	4	5	1155	-1063	19
2	4	5	1187	1164	21
3	4	5	1080	-1122	23
4	4	5	254	-174	34
5	4	5	1418	-1441	27
6	4	5	187	-109	-64
7	4	5	675	-663	34
8	4	5	807	-867	39
9	4	5	585	-544	48
10	4	5	372	-338	66
-13	5	5	255	155	-104
-12	5	5	437	-305	48
-11	5	5	78	-112	-78
-10	5	5	121	160	-121
-9	5	5	334	334	40
-8	5	5	1181	1152	27
-7	5	5	349	-377	31
-6	5	5	1721	1728	22
-5	5	5	287	224	28
-4	5	5	1736	1766	19
-3	5	5	139	-188	-37
-2	5	5	948	954	18
-1	5	5	200	-180	28
0	5	5	998	-965	31
1	5	5	370	317	22
2	5	5	967	-877	21
3	5	5	335	-416	30
4	5	5	1485	-1588	24
5	5	5	374	253	31
6	5	5	1085	-1139	30
7	5	5	314	-225	45
8	5	5	890	-878	37
9	5	5	130	56	-130
10	5	5	87	-8	-87
-13	6	5	341	-299	67
-12	6	5	536	500	48
-11	6	5	133	0	-133
-10	6	5	1027	1079	33
-9	6	5	301	280	45
-8	6	5	758	692	28
-7	6	5	1300	1265	25
-6	6	5	330	361	28
-5	6	5	1190	1190	21
-4	6	5	388	-401	23
-3	6	5	1157	1169	18
-2	6	5	1232	-1272	18
-1	6	5	297	-245	23
0	6	5	1664	-1567	22
1	6	5	410	-411	22
2	6	5	1002	-931	21
3	6	5	752	-781	23
4	6	5	459	-446	29
5	6	5	1133	-1195	27
6	6	5	320	293	39
7	6	5	585	-595	37
8	6	5	644	557	39
9	6	5	326	5	54
10	6	5	690	723	55
-13	7	5	733	688	49
-12	7	5	90	-155	-90
-11	7	5	1256	1108	35
-10	7	5	74	-20	-74
-9	7	5	1419	1361	29
-8	7	5	178	167	-67
-7	7	5	631	583	26
-6	7	5	301	313	28
-5	7	5	335	-375	26
-4	7	5	170	194	39
-3	7	5	1332	-1385	19
-2	7	5	87	-7	-67
-1	7	5	2329	-2315	18
0	7	5	144	-49	30
1	7	5	1754	-1661	19
2	7	5	152	-4	-43
3	7	5	779	-796	23
4	7	5	277	-296	32
5	7	5	56	-2	-56
6	7	5	445	-497	35
7	7	5	672	710	35
8	7	5	390	375	45
9	7	5	1226	1199	40
10	7	5	185	115	-185
-13	8	5	520	406	53
-12	8	5	1039	1004	40
-11	8	5	149	68	-149
-10	8	5	996	984	32
-9	8	5	350	-379	44
-8	8	5	723	681	29
-7	8	5	610	-551	26
-6	8	5	353	-354	27
-5	8	5	1213	-1286	21
-4	8	5	344	-313	22
-3	8	5	396	-365	21
-2	8	5	1744	-1798	18
-1	8	5	704	-709	19
0	8	5	1447	-1341	17
1	8	5	852	789	20
2	8	5	1491	-1425	21
3	8	5	609	579	25
4	8	5	171	-167	-54
5	8	5	792	858	28
6	8	5	367	319	38
7	8	5	505	543	37
8	8	5	940	969	37
9	8	5	593	538	47
10	8	5	762	842	48
-13	9	5	94	129	-94
-12	9	5	484	422	48
-11	9	5	533	498	43
-10	9	5	173	-235	-93
-9	9	5	67	24	-67
-8	9	5	949	-875	27
-7	9	5	55	26	-55
-6	9	5	1478	-1489	23
-5	9	5	48	-125	-48
-4	9	5	1749	-1752	20
-3	9	5	744	-705	19
-2	9	5	1370	-1353	18
-1	9	5	933	-956	19
0	9	5	56	12	-42
1	9	5	612	-561	21
2	9	5	1414	1361	21
3	9	5	154	-78	-48
4	9	5	1361	1336	25
5	9	5	264	279	40
6	9	5	972	1046	29
7	9	5	195	309	-90
8	9	5	378	294	44
9	9	5	198	-19	-114
-13	10	5	735	675	48
-12	10	5	126	-126	-126
-11	10	5	116	14	-116
-10	10	5	551	-547	38
-9	10	5	562	-554	32
-8	10	5	172	-226	-74
-7	10	5	1207	-1224	25
-6	10	5	56	136	-56
-5	10	5	1051	-1051	21
-4	10	5	916	930	21
-3	10	5	1391	-1424	19
-2	10	5	681	692	20
-1	10	5	195	-144	25
0	10	5	768	728	14
1	10	5	912	839	20
2	10	5	306	227	28
3	10	5	1315	1299	23
4	10	5	136	107	-83
5	10	5	847	852	28
6	10	5	284	-253	46
7	10	5	774	835	34
8	10	5	435	-499	46
9	10	5	84	-214	-84
-12	11	5	357	377	59
-11	11	5	1002	-971	37
-10	11	5	562	-480	38
-9	11	5	682	-634	32
-8	11	5	552	-574	32
-7	11	5	522	-541	29
-6	11	5	962	-1040	24
-5	11	5	111	-55	-58
-4	11	5	585	-633	22
-3	11	5	875	833	20
-2	11	5	867	-827	20
-1	11	5	1432	1372	19
0	11	5	155	60	26
1	11	5	1753	1621	20
2	11	5	680	650	22
3	11	5	1191	1181	24
4	11	5	522	494	29
5	11	5	473	491	29
6	11	5	1140	1246	30
7	11	5	231	-293	-66
8	11	5	503	478	42
9	11	5	447	-443	49
-12	12	5	978	-984	41
-11	12	5	200	-31	-102
-10	12	5	1041	-1045	33
-9	12	5	126	-24	-126
-8	12	5	967	-983	28
-7	12	5	412	-434	30
-6	12	5	301	-342	33
-5	12	5	244	-250	32
-4	12	5	655	649	22
-3	12	5	146	-129	-36
-2	12	5	2178	2150	19

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-1	12	5	228	209	29
0	12	5	1820	1736	17
1	12	5	252	70	28
2	12	5	1239	1224	22
3	12	5	187	191	47
4	12	5	283	-226	34
5	12	5	216	179	40
6	12	5	709	-770	32
7	12	5	340	366	46
8	12	5	1066	-1136	36
9	12	5	182	132	-182
-12	13	5	334	-280	54
-11	13	5	993	-975	37
-10	13	5	302	364	52
-9	13	5	963	-916	31
-8	13	5	829	831	29
-7	13	5	646	-701	27
-6	13	5	1081	1136	24
-5	13	5	369	-378	27
-4	13	5	1014	1036	21
-3	13	5	889	861	20
-2	13	5	871	871	20
-1	13	5	1418	1383	20
0	13	5	108	-34	-43
1	13	5	1721	1604	21
2	13	5	733	-726	23
3	13	5	543	491	26
4	13	5	916	-946	26
5	13	5	284	268	38
6	13	5	929	-952	30
7	13	5	505	-529	39
8	13	5	180	-153	-115
9	13	5	744	-754	40
-12	14	5	219	-117	-83
-11	14	5	69	-61	-69
-10	14	5	366	-396	39
-9	14	5	520	480	33
-8	14	5	314	-278	33
-7	14	5	1479	1496	25
-6	14	5	202	-64	40
-5	14	5	1335	1349	23
-4	14	5	93	56	-93
-3	14	5	1614	1631	20
-2	14	5	408	445	23
-1	14	5	245	147	28
0	14	5	577	555	16
1	14	5	465	-405	24
2	14	5	234	216	34
3	14	5	1602	-1558	24
4	14	5	191	161	-50
5	14	5	1648	-1686	27
6	14	5	666	637	33
7	14	5	1194	-1335	33
8	14	5	152	-69	-152
9	14	5	82	-169	-82
-12	15	5	526	-490	47

h	k	l	10Fo	10Fc	10s
-11	15	5	396	403	42
-10	15	5	68	173	-68
-9	15	5	358	405	40
-8	15	5	567	562	31
-7	15	5	541	480	27
-6	15	5	1600	1643	24
-5	15	5	170	15	37
-4	15	5	1538	1518	22
-3	15	5	621	-643	23
-2	15	5	1100	1088	20
-1	15	5	546	-547	22
0	15	5	68	21	-41
1	15	5	659	-606	23
2	15	5	924	-885	23
3	15	5	568	-477	25
4	15	5	1140	-1131	26
5	15	5	233	-106	42
6	15	5	1226	-1225	30
7	15	5	353	391	47
8	15	5	379	-420	50
9	15	5	235	258	-77
-12	16	5	826	749	40
-11	16	5	251	-26	-65
-10	16	5	738	781	35
-9	16	5	251	190	50
-8	16	5	936	957	28
-7	16	5	532	550	28
-6	16	5	164	97	-48
-5	16	5	1024	994	23
-4	16	5	463	-471	25
-3	16	5	690	714	22
-2	16	5	1416	-1404	21
-1	16	5	543	524	23
0	16	5	1134	-1085	25
1	16	5	460	-433	25
2	16	5	1069	-1059	23
3	16	5	630	-610	26
4	16	5	284	-283	37
5	16	5	579	-534	30
6	16	5	201	-110	-61
7	16	5	456	-449	36
8	16	5	775	859	38
-11	17	5	880	863	38
-10	17	5	140	-132	-112
-9	17	5	977	997	31
-8	17	5	121	-114	-78
-7	17	5	770	790	27
-6	17	5	179	-270	-53
-5	17	5	163	-233	-50
-4	17	5	53	-8	-53
-3	17	5	1218	-1167	22
-2	17	5	131	-49	-41
-1	17	5	1557	-1535	21
0	17	5	236	184	37
1	17	5	1415	-1404	22
2	17	5	157	-48	-53

h	k	l	10Fo	10Fc	10s
3	17	5	658	-574	26
4	17	5	392	410	30
5	17	5	195	-233	-61
6	17	5	456	455	35
7	17	5	625	590	36
8	17	5	205	-131	-65
-11	18	5	243	-101	-64
-10	18	5	730	695	34
-9	18	5	329	-268	37
-8	18	5	655	664	31
-7	18	5	989	-985	27
-6	18	5	368	348	33
-5	18	5	701	-669	24
-4	18	5	391	-405	28
-3	18	5	1018	-1065	23
-2	18	5	1068	-1046	22
-1	18	5	52	90	-52
0	18	5	1197	-1141	16
1	18	5	52	86	-52
2	18	5	914	-953	25
3	18	5	916	931	25
4	18	5	389	-391	31
5	18	5	910	914	29
6	18	5	327	312	42
7	18	5	553	515	36
8	18	5	455	503	44
-11	19	5	117	47	-117
-10	19	5	259	-193	45
-9	19	5	203	227	47
-8	19	5	819	-844	29
-7	19	5	115	21	-115
-6	19	5	1304	-1279	25
-5	19	5	131	25	-52
-4	19	5	1272	-1250	23
-3	19	5	138	-204	-60
-2	19	5	651	-634	24
-1	19	5	182	-165	42
0	19	5	228	214	21
1	19	5	49	11	-49
2	19	5	800	733	25
3	19	5	559	-524	28
4	19	5	1050	1056	28
5	19	5	233	87	43
6	19	5	886	841	32
7	19	5	168	50	-69
8	19	5	445	461	45
-11	20	5	279	231	45
-10	20	5	155	-91	-128
-9	20	5	306	-258	40
-8	20	5	322	-338	38
-7	20	5	890	-926	27
-6	20	5	55	74	-55
-5	20	5	1240	-1278	24
-4	20	5	236	211	36
-3	20	5	876	-832	24
-2	20	5	527	559	25

h	k	l	10Fo	10Fc	10s
-1	20	5	417	-417	25
0	20	5	478	414	18
1	20	5	361	278	28
2	20	5	402	380	29
3	20	5	763	732	27
4	20	5	227	-214	47
5	20	5	979	963	29
6	20	5	222	59	47
7	20	5	445	436	38
-10	21	5	297	241	45
-9	21	5	574	-511	34
-8	21	5	124	-143	-124
-7	21	5	352	-361	33
-6	21	5	418	-444	29
-5	21	5	393	410	30
-4	21	5	474	-487	27
-3	21	5	852	816	24
-2	21	5	89	-183	-89
-1	21	5	990	959	24
0	21	5	194	162	38
1	21	5	1155	1110	24
2	21	5	278	257	33
3	21	5	669	647	28
4	21	5	752	794	28
5	21	5	176	86	-63
6	21	5	261	234	48
7	21	5	626	-630	39
-10	22	5	1107	-1123	34
-9	22	5	215	-175	52
-8	22	5	764	-798	30
-7	22	5	212	255	51
-6	22	5	455	-441	30
-5	22	5	136	159	-74
-4	22	5	776	780	25
-3	22	5	215	229	40
-2	22	5	1055	1048	24
-1	22	5	51	47	-51
0	22	5	1202	1152	23
1	22	5	52	40	-52
2	22	5	860	886	26
3	22	5	183	-166	-61
4	22	5	519	511	30
5	22	5	64	-32	-64
6	22	5	346	-326	41
7	22	5	314	-313	49
-10	23	5	74	167	-74
-9	23	5	496	-507	36
-8	23	5	583	627	32
-7	23	5	185	-161	41
-6	23	5	1025	1021	27
-5	23	5	147	171	-61
-4	23	5	770	757	25
-3	23	5	855	911	25
-2	23	5	283	206	30
-1	23	5	717	668	25
0	23	5	131	-150	-50

h	k	l	10Fo	10Fc	10s
1	23	5	565	491	27
2	23	5	771	-739	26
3	23	5	341	307	32
4	23	5	810	-812	30
5	23	5	234	-152	45
6	23	5	680	-668	34
-9	24	5	554	512	35
-8	24	5	99	-115	-99
-7	24	5	721	695	29
-6	24	5	155	-191	-93
-5	24	5	1069	1090	26
-4	24	5	406	370	29
-3	24	5	488	458	28
-2	24	5	52	23	-52
-1	24	5	238	218	33
0	24	5	182	134	28
1	24	5	666	-602	26
2	24	5	193	-96	41
3	24	5	843	-783	28
4	24	5	144	57	-75
5	24	5	906	-968	31
6	24	5	136	-9	-136
-9	25	5	491	521	37
-8	25	5	512	503	33
-7	25	5	63	79	-63
-6	25	5	760	781	28
-5	25	5	62	-98	-62
-4	25	5	934	916	26
-3	25	5	702	-710	25
-2	25	5	665	663	25
-1	25	5	900	-916	25
0	25	5	189	-127	28
1	25	5	723	-697	27
2	25	5	557	-554	29
3	25	5	307	-298	32
4	25	5	913	-873	29
5	25	5	163	6	-96
6	25	5	498	-479	36
-9	26	5	267	252	48
-8	26	5	438	460	36
-7	26	5	156	154	-79
-6	26	5	270	307	42
-5	26	5	349	325	29
-4	26	5	546	-558	27
-3	26	5	195	211	41
-2	26	5	972	-928	26
-1	26	5	180	46	35
0	26	5	1258	-1206	19
1	26	5	262	-296	33
2	26	5	624	-578	29
3	26	5	219	-181	44
4	26	5	242	-194	44
5	26	5	273	-249	42
-8	27	5	262	-233	49
-7	27	5	395	346	34
-6	27	5	421	-426	33

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-5	27	5	59	-78	-59
-4	27	5	366	-354	33
-3	27	5	737	-744	27
-2	27	5	277	-251	30
-1	27	5	941	-941	26
0	27	5	153	86	-41
1	27	5	867	-809	27
2	27	5	269	234	33
3	27	5	428	-400	34
4	27	5	400	344	35
5	27	5	68	99	-68
-8	28	5	236	220	46
-7	28	5	556	-606	33
-6	28	5	62	47	-62
-5	28	5	938	-979	28
-4	28	5	279	-318	37
-3	28	5	658	-691	29
-2	28	5	421	-383	27
-1	28	5	293	-318	38
0	28	5	601	-569	20
1	28	5	510	502	29
2	28	5	229	-286	45
3	28	5	647	611	31
4	28	5	204	-92	-53
-7	29	5	62	15	-62
-6	29	5	821	-834	29
-5	29	5	130	25	-60
-4	29	5	854	-874	27
-3	29	5	216	180	43
-2	29	5	499	-513	29
-1	29	5	236	193	37
0	29	5	176	191	37
1	29	5	127	148	-73
2	29	5	547	531	30
3	29	5	63	86	-63
4	29	5	836	813	31
-6	30	5	136	-101	-95
-5	30	5	483	-484	32
-4	30	5	267	290	37
-3	30	5	590	-568	29
-2	30	5	482	441	29
-1	30	5	284	-243	38
0	30	5	838	837	24
1	30	5	335	305	32
2	30	5	478	463	34
3	30	5	538	465	32
-5	31	5	56	-3	-56
-4	31	5	159	-147	-53
-3	31	5	533	505	32
-2	31	5	274	-201	34
-1	31	5	976	982	28
0	31	5	219	200	30
1	31	5	798	785	28
2	31	5	243	230	48
-4	32	5	62	102	-62
-3	32	5	54	64	-54
-2	32	5	585	578	28
-1	32	5	58	63	-58
0	32	5	594	595	21
1	32	5	258	-245	37
-2	33	5	551	518	31
-1	33	5	457	423	32
-12	0	6	766	-681	41
-10	0	6	1308	-1281	32
-8	0	6	1624	-1572	27
-6	0	6	1415	-1363	23
-4	0	6	69	82	-69
-2	0	6	534	-507	21
0	0	6	2834	2921	20
2	0	6	1633	1416	23
4	0	6	1554	1430	26
6	0	6	288	241	46
8	0	6	144	-41	-144
-13	1	6	317	-264	66
-12	1	6	594	-611	45
-11	1	6	512	-429	44
-10	1	6	540	-557	40
-9	1	6	955	-947	30
-8	1	6	274	232	40
-7	1	6	1138	-1137	25
-6	1	6	738	693	24
-5	1	6	870	-872	22
-4	1	6	1778	1770	20
-3	1	6	715	-645	21
-2	1	6	1592	1598	19
-1	1	6	513	578	22
0	1	6	985	1001	15
1	1	6	1855	1826	21
2	1	6	367	-284	27
3	1	6	1234	1126	25
4	1	6	811	-715	27
5	1	6	775	698	30
6	1	6	881	-837	33
7	1	6	293	-142	52
8	1	6	498	-497	43
9	1	6	462	-515	62
-13	2	6	555	-486	51
-12	2	6	330	-352	67
-11	2	6	733	-636	39
-10	2	6	322	-331	52
-9	2	6	148	65	-100
-8	2	6	489	-461	31
-7	2	6	537	538	27
-6	2	6	341	-261	28
-5	2	6	1429	1441	22
-4	2	6	252	220	31
-3	2	6	1253	1310	20
-2	2	6	893	873	20
-1	2	6	1505	1522	19
0	2	6	642	602	15
1	2	6	351	371	28
2	2	6	598	576	24
3	2	6	407	-369	30
4	2	6	308	226	38
5	2	6	1565	-1508	28
6	2	6	207	119	-75
7	2	6	1087	-1008	34
8	2	6	321	-189	54
9	2	6	743	-673	43
-13	3	6	372	347	70
-12	3	6	887	-888	41
-11	3	6	402	361	46
-10	3	6	796	-725	34
-9	3	6	1063	1037	30
-8	3	6	340	348	37
-7	3	6	322	206	28
-6	3	6	1158	1146	23
-5	3	6	413	440	25
-4	3	6	1849	1923	20
-3	3	6	222	124	28
-2	3	6	1188	1252	19
-1	3	6	365	-342	22
0	3	6	1007	992	27
1	3	6	911	-897	21
2	3	6	132	-94	-58
3	3	6	741	-713	26
4	3	6	985	-973	27
5	3	6	502	-403	33
6	3	6	1413	-1387	31
7	3	6	131	-87	-131
8	3	6	797	-790	41
9	3	6	488	423	49
-13	4	6	469	-412	60
-12	4	6	315	346	69
-11	4	6	337	-397	59
-10	4	6	964	884	34
-9	4	6	137	-49	-137
-8	4	6	1200	1146	27
-7	4	6	422	386	30
-6	4	6	1211	1185	23
-5	4	6	1020	1080	22
-4	4	6	332	338	27
-3	4	6	929	941	20
-2	4	6	772	-768	20
-1	4	6	823	841	20
0	4	6	2060	-2010	16
1	4	6	519	461	23
2	4	6	1331	-1327	22
3	4	6	249	-279	38
4	4	6	1132	-1181	26
5	4	6	717	-697	30
6	4	6	247	-215	55
7	4	6	715	-668	36
8	4	6	215	115	-93
9	4	6	137	-193	-137
-13	5	6	177	242	-177
-12	5	6	86	-24	-86
-11	5	6	853	843	37
-10	5	6	228	224	-68
-9	5	6	1572	1480	29
-8	5	6	65	-123	-65
-7	5	6	1461	1439	25
-6	5	6	57	-98	-57
-5	5	6	865	849	22
-4	5	6	431	-424	24
-3	5	6	628	-601	21
-2	5	6	205	-177	29
-1	5	6	1697	-1679	20
0	5	6	173	-103	33
1	5	6	1955	-1818	21
2	5	6	206	121	40
3	5	6	1451	-1633	24
4	5	6	215	-162	46
5	5	6	548	-523	34
6	5	6	316	266	40
7	5	6	69	70	-69
8	5	6	215	19	-79
9	5	6	530	548	51
-13	6	6	654	561	49
-12	6	6	473	433	44
-11	6	6	710	692	38
-10	6	6	759	711	34
-9	6	6	178	60	-70
-8	6	6	1120	1075	28
-7	6	6	464	-459	31
-6	6	6	549	524	27
-5	6	6	1400	-1435	22
-4	6	6	336	377	25
-3	6	6	979	-988	20
-2	6	6	1029	-1059	20
-1	6	6	1514	-1528	20
0	6	6	933	-837	25
1	6	6	269	211	31
2	6	6	1815	-1731	22
3	6	6	216	112	35
4	6	6	473	-521	28
5	6	6	1176	1335	29
6	6	6	147	175	-147
7	6	6	815	864	36
8	6	6	304	377	69
9	6	6	395	326	58
-13	7	6	89	-16	-89
-12	7	6	1013	903	39
-11	7	6	248	132	-68
-10	7	6	542	576	40
-9	7	6	68	-73	-68
-8	7	6	475	-476	31
-7	7	6	450	407	29
-6	7	6	1107	-1111	24
-5	7	6	85	-14	-85
-4	7	6	1750	-1798	21
-3	7	6	161	203	-41
-2	7	6	1713	-1716	20
-1	7	6	407	-448	23
0	7	6	1105	-1014	15
1	7	6	304	-303	29
2	7	6	88	49	-88
3	7	6	314	-264	33
4	7	6	874	963	28
5	7	6	315	216	38
6	7	6	1313	1452	32
7	7	6	299	245	50
8	7	6	949	949	39
9	7	6	90	12	-90
-13	8	6	823	787	46
-12	8	6	315	-288	72
-11	8	6	643	590	37
-10	8	6	738	-734	35
-9	8	6	187	128	-55
-8	8	6	726	-731	29
-7	8	6	957	-963	26
-6	8	6	706	-702	25
-5	8	6	1592	-1646	22
-4	8	6	195	-162	33
-3	8	6	2059	-2070	20
-2	8	6	257	288	29
-1	8	6	940	-923	20
0	8	6	830	791	15
1	8	6	281	-263	28
2	8	6	1159	1068	23
3	8	6	1182	1164	24
4	8	6	849	904	28
5	8	6	674	778	31
6	8	6	104	-3	-104
7	8	6	843	963	35
8	8	6	258	-165	-65
9	8	6	439	487	54
-13	9	6	194	-76	-148
-12	9	6	375	271	56
-11	9	6	653	-584	40
-10	9	6	203	26	-69
-9	9	6	999	-959	30
-8	9	6	148	152	-83
-7	9	6	1143	-1154	26
-6	9	6	613	-697	25
-5	9	6	677	-690	23
-4	9	6	513	-511	22
-3	9	6	284	292	27
-2	9	6	569	-539	22
-1	9	6	1308	1288	20
0	9	6	429	-391	17
1	9	6	1671	1572	22
2	9	6	321	-259	29
3	9	6	1166	1126	25
4	9	6	265	238	39
5	9	6	156	53	-75
6	9	6	120	-187	-120
7	9	6	471	-513	38
8	9	6	248	264	-85
9	9	6	516	-505	53

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-13	10	6	296	-259	-75
-12	10	6	315	-257	60
-11	10	6	176	-212	-113
-10	10	6	889	-836	33
-9	10	6	113	95	-113
-8	10	6	1420	-1337	27
-7	10	6	189	169	-52
-6	10	6	824	-856	25
-5	10	6	681	662	23
-4	10	6	423	-476	24
-3	10	6	189	173	33
-2	10	6	1072	1051	20
-1	10	6	796	751	21
0	10	6	1432	1358	33
1	10	6	248	-195	29
2	10	6	1918	1825	23
3	10	6	501	492	29
4	10	6	990	942	27
5	10	6	166	3	-44
6	10	6	474	447	34
7	10	6	74	-94	-74
8	10	6	336	-296	55
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6	11	6	516	-445	34
7	11	6	227	189	-64
8	11	6	453	-519	46
-12	12	6	84	-81	-84
-11	12	6	461	-420	44
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-8	12	6	309	-264	33
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-6	12	6	140	47	-47
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-3	12	6	1784	1810	21
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2	12	6	182	102	43
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3	13	6	369	-244	30
4	13	6	1007	-996	28
5	13	6	125	-75	-125
6	13	6	1035	-1118	32
7	13	6	218	-10	-75
8	13	6	541	-531	42
-12	14	6	440	436	54
-11	14	6	365	-377	51
-10	14	6	1039	1044	33
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-7	14	6	194	158	-49
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2	14	6	2219	-2165	24
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4	14	6	1232	-1222	27
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6	14	6	399	-388	39
7	14	6	495	-535	40
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7	15	6	147	88	-147
8	15	6	287	241	69
-12	16	6	192	111	-94
-11	16	6	605	521	37
-10	16	6	435	452	39
-9	16	6	192	146	-52
-8	16	6	659	619	30
-7	16	6	495	-567	31
-6	16	6	601	601	28
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-1	16	6	821	-820	23
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2	16	6	747	-692	25
3	16	6	921	873	27
4	16	6	595	-583	30
5	16	6	669	648	31
6	16	6	173	-96	-90
7	16	6	796	797	37
8	16	6	124	115	-124
-11	17	6	328	-226	49
-10	17	6	374	374	43
-9	17	6	66	-165	-66
-8	17	6	67	-144	-67
-7	17	6	316	-308	35
-6	17	6	850	-884	26
-5	17	6	54	64	-54
-4	17	6	1514	-1463	23
-3	17	6	117	88	-67
-2	17	6	1501	-1484	22
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0	17	6	724	-691	17
1	17	6	220	237	42
2	17	6	159	8	-53
3	17	6	588	561	30
4	17	6	750	743	29
5	17	6	197	-91	-64
6	17	6	1056	980	32
7	17	6	310	-134	43
-11	18	6	608	494	38
-10	18	6	493	-481	39
-9	18	6	175	170	-72
-8	18	6	838	-899	30
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-5	18	6	703	-719	26
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-3	18	6	1089	-1021	23
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3	18	6	229	137	44
4	18	6	605	581	30
5	18	6	688	687	32
6	18	6	175	132	-87
7	18	6	593	575	38
-11	19	6	761	-723	38
-10	19	6	227	116	-63
-9	19	6	1080	-1091	31
-8	19	6	298	-246	38
-7	19	6	1222	-1253	27
-6	19	6	122	108	-75
-5	19	6	463	-475	26
-4	19	6	190	-146	39
-3	19	6	192	203	41
-2	19	6	109	-84	-83
-1	19	6	1011	978	24
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2	19	6	285	-237	32
3	19	6	1214	1191	27
4	19	6	163	-9	-62
5	19	6	592	563	34
6	19	6	70	56	-70
7	19	6	73	-99	-73
-11	20	6	165	-30	-88
-10	20	6	509	-450	40
-9	20	6	205	114	-56
-8	20	6	815	-832	31
-7	20	6	449	485	33
-6	20	6	745	-689	27
-5	20	6	538	519	28
-4	20	6	365	-372	28
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-2	20	6	213	193	34
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2	20	6	1091	1004	26
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4	20	6	803	776	30
5	20	6	415	-433	34
6	20	6	67	88	-67
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-7	21	6	344	-341	33
-6	21	6	732	659	27
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3	21	6	411	431	32
4	21	6	769	-800	30
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-10	22	6	255	232	55
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-7	22	6	445	488	34
-6	22	6	212	249	46
-5	22	6	1106	1100	26
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-3	22	6	1120	1092	24
-2	22	6	451	-442	27
-1	22	6	974	930	25
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1	22	6	98	36	-98
2	22	6	502	-453	28
3	22	6	516	-498	30
4	22	6	167	-79	-61
5	22	6	818	-852	31
6	22	6	167	-126	-73
-10	23	6	222	-228	-76
-9	23	6	714	711	33
-8	23	6	198	172	-58
-7	23	6	764	809	30
-6	23	6	299	340	36
-5	23	6	274	346	41
-4	23	6	817	811	26
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-2	23	6	548	566	26
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1	23	6	1174	-1171	26
2	23	6	211	-239	47
3	23	6	719	-731	30
4	23	6	417	-392	34
5	23	6	341	-320	38
6	23	6	487	-602	42
-9	24	6	69	-79	-69
-8	24	6	841	867	31
-7	24	6	145	96	-64
-6	24	6	493	458	31

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-5	24	6	365	383	30
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0	24	6	1175	-1210	24
1	24	6	219	-208	46
2	24	6	1021	-948	27
3	24	6	144	13	-74
4	24	6	786	-759	31
5	24	6	207	-96	50
-9	25	6	756	799	33
-8	25	6	71	-154	-71
-7	25	6	624	677	32
-6	25	6	447	-424	33
-5	25	6	452	400	30
-4	25	6	697	-681	27
-3	25	6	271	-261	35
-2	25	6	700	-660	26
-1	25	6	660	-620	27
0	25	6	342	-336	23
1	25	6	915	-912	27
2	25	6	59	87	-59
3	25	6	705	-648	31
4	25	6	297	316	44
5	25	6	371	-396	41
-8	26	6	261	334	44
-7	26	6	415	-394	36
-6	26	6	340	367	38
-5	26	6	1096	-1085	27
-4	26	6	113	-82	-113
-3	26	6	967	-965	27
-2	26	6	56	-35	-56
-1	26	6	945	-900	27
0	26	6	333	-331	24
1	26	6	103	8	-103
2	26	6	130	-135	-92
3	26	6	288	183	41
4	26	6	356	-284	38
-8	27	6	250	-288	54
-7	27	6	259	-216	46
-6	27	6	716	-664	30
-5	27	6	258	-269	45
-4	27	6	974	-990	28
-3	27	6	153	10	-46
-2	27	6	735	-719	28
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3	27	6	307	274	34
4	27	6	646	572	32
-7	28	6	189	-169	-49
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-5	28	6	436	-437	32
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-3	30	6	599	600	30
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-1	30	6	592	610	29
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2	30	6	614	565	31
-5	31	6	110	-65	-110
-4	31	6	772	796	30
-3	31	6	177	-102	-53
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-1	31	6	119	97	-119
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1	31	6	190	56	44
-3	32	6	527	559	29
-2	32	6	142	7	-55
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-13	0	7	1083	-1091	44
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-9	0	7	1027	-974	30
-7	0	7	156	75	-57
-5	0	7	1019	1006	23
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3	0	7	428	429	32
5	0	7	773	-717	32
7	0	7	741	-669	39
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-12	1	7	657	-544	42
-11	1	7	80	47	-80
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7	1	7	410	-410	52
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-3	2	7	144	173	-51
-2	2	7	341	351	25
-1	2	7	466	463	23
0	2	7	1075	-1110	53
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3	2	7	209	24	44
4	2	7	1617	-1501	28
5	2	7	274	-257	51
6	2	7	607	-612	37
7	2	7	398	-532	52
8	2	7	86	-100	-86
-13	3	7	272	-224	-95
-12	3	7	329	281	53
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-10	3	7	673	621	36
-9	3	7	985	902	30
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-7	3	7	1456	1449	26
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3	4	7	282	-247	41
4	4	7	687	-710	31
5	4	7	356	343	42
6	4	7	436	-439	43
7	4	7	749	706	37
8	4	7	228	-225	-84
-13	5	7	272	96	-80
-12	5	7	950	906	39
-11	5	7	88	118	-88
-10	5	7	1233	1168	33
-9	5	7	389	-407	37
-8	5	7	468	410	31
-7	5	7	140	194	-67
-6	5	7	140	-134	-67
-5	5	7	618	-638	24
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-3	5	7	280	286	28
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-1	5	7	506	-500	24
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6	5	7	569	565	35
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-12	6	7	83	37	-83
-11	6	7	824	836	36
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-9	6	7	577	625	35
-8	6	7	908	-866	28
-7	6	7	140	159	-77
-6	6	7	1067	-1082	25
-5	6	7	754	-716	24
-4	6	7	1019	-1062	23
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6	6	7	541	428	37
7	6	7	513	552	45
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-12	7	7	287	216	64
-11	7	7	369	-313	49
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-9	7	7	952	-927	30
-8	7	7	140	170	-123
-7	7	7	1394	-1357	26
-6	7	7	345	-348	31
-5	7	7	1725	-1752	23
-4	7	7	53	113	-53
-3	7	7	915	-951	22
-2	7	7	406	-379	26
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5	7	7	995	1042	31
6	7	7	263	297	63
7	7	7	599	635	40
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-13	8	7	613	-519	49
-12	8	7	296	212	53
-11	8	7	409	-378	46
-10	8	7	589	-614	37
-9	8	7	487	-438	33
-8	8	7	1278	-1226	28
-7	8	7	149	-224	-75
-6	8	7	1537	-1547	24
-5	8	7	261	300	34
-4	8	7	1261	-1317	22
-3	8	7	628	584	23
-2	8	7	50	5	-50
-1	8	7	1367	1302	22
0	8	7	829	783	24
1	8	7	330	289	30
2	8	7	1061	935	25
3	8	7	414	-388	31
4	8	7	539	533	31
5	8	7	384	-365	39
6	8	7	710	843	36
7	8	7	219	-253	-71
8	8	7	201	236	-104

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-13	9	7	207	298	-132
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-11	9	7	199	-79	-70
-10	9	7	808	-721	35
-9	9	7	140	-86	-106
-8	9	7	307	-299	40
-7	9	7	636	-612	29
-6	9	7	447	456	27
-5	9	7	357	-376	30
-4	9	7	992	1009	23
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-1	9	7	135	154	-56
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1	9	7	58	-9	-58
2	9	7	503	467	27
3	9	7	323	280	36
4	9	7	273	-262	42
5	9	7	263	240	37
6	9	7	578	-576	38
7	9	7	397	416	46
8	9	7	727	-733	44
-12	10	7	88	-60	-88
-11	10	7	1166	-1071	35
-10	10	7	151	80	-151
-9	10	7	936	-891	31
-8	10	7	161	204	-67
-7	10	7	256	-273	43
-6	10	7	143	87	-54
-5	10	7	307	351	31
-4	10	7	48	-18	-48
-3	10	7	1837	1925	22
-2	10	7	127	83	-61
-1	10	7	1844	1806	22
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1	10	7	1224	1098	24
2	10	7	482	513	28
3	10	7	916	844	27
4	10	7	145	140	-71
5	10	7	65	-57	-65
6	10	7	212	80	47
7	10	7	751	-834	38
8	10	7	151	-196	-151
-12	11	7	830	-835	42
-11	11	7	80	27	-80
-10	11	7	689	-631	35
-9	11	7	522	536	35
-8	11	7	601	-577	30
-7	11	7	1266	1258	26
-6	11	7	361	345	29
-5	11	7	1042	1060	24
-4	11	7	548	504	24
-3	11	7	563	545	25
-2	11	7	1497	1497	22
-1	11	7	378	-348	27
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h	k	l	10Fo	10Fc	10s
1	11	7	975	-907	24
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3	11	7	950	-882	27
4	11	7	165	47	-52
5	11	7	784	-832	32
6	11	7	457	-484	42
7	11	7	373	-401	49
8	11	7	490	-494	48
-12	12	7	124	-71	-124
-11	12	7	73	-46	-73
-10	12	7	605	597	38
-9	12	7	163	87	-65
-8	12	7	971	938	29
-7	12	7	263	156	37
-6	12	7	1274	1319	25
-5	12	7	159	-144	-47
-4	12	7	1117	1116	23
-3	12	7	200	-229	39
-2	12	7	718	726	23
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0	12	7	566	-541	18
1	12	7	139	-121	-61
2	12	7	1028	-987	26
3	12	7	303	-286	37
4	12	7	1037	-950	29
5	12	7	187	-32	-64
6	12	7	891	-933	35
7	12	7	170	-39	-84
8	12	7	82	-143	-82
-12	13	7	602	530	42
-11	13	7	621	547	41
-10	13	7	472	390	40
-9	13	7	605	597	34
-8	13	7	195	212	-61
-7	13	7	1210	1197	26
-6	13	7	397	-355	30
-5	13	7	774	804	25
-4	13	7	604	-574	24
-3	13	7	918	936	23
-2	13	7	785	-751	24
-1	13	7	986	-1012	23
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1	13	7	1346	-1276	25
2	13	7	214	-105	41
3	13	7	1266	-1187	27
4	13	7	68	-101	-68
5	13	7	721	-700	33
6	13	7	321	242	47
7	13	7	367	-372	44
-12	14	7	191	-7	-99
-11	14	7	1037	1033	35
-10	14	7	248	170	57
-9	14	7	828	853	32
-8	14	7	94	69	-94
-7	14	7	235	236	43
-6	14	7	239	302	43

h	k	l	10Fo	10Fc	10s
-5	14	7	538	-522	27
-4	14	7	533	533	26
-3	14	7	1603	-1582	23
-2	14	7	246	154	33
-1	14	7	1148	-1115	23
0	14	7	564	-556	19
1	14	7	724	-670	26
2	14	7	387	-400	31
3	14	7	129	-68	-90
4	14	7	243	-216	45
5	14	7	215	208	-54
6	14	7	182	-155	-80
7	14	7	635	655	41
-12	15	7	862	741	39
-11	15	7	259	-156	-65
-10	15	7	677	654	37
-9	15	7	202	-248	-59
-8	15	7	664	646	31
-7	15	7	640	-613	28
-6	15	7	303	-273	30
-5	15	7	210	-181	36
-4	15	7	795	-772	24
-3	15	7	263	-229	32
-2	15	7	1643	-1653	23
-1	15	7	592	592	25
0	15	7	1504	-1456	17
1	15	7	507	482	28
2	15	7	777	-759	27
3	15	7	707	699	29
4	15	7	112	145	-112
5	15	7	327	290	41
6	15	7	447	465	41
7	15	7	260	110	61
-11	16	7	177	268	-102
-10	16	7	476	-443	38
-9	16	7	298	316	46
-8	16	7	1037	-966	29
-7	16	7	63	81	-63
-6	16	7	1215	-1181	26
-5	16	7	178	-219	-46
-4	16	7	992	-967	24
-3	16	7	306	-284	29
-2	16	7	212	-145	33
-1	16	7	732	-771	25
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1	16	7	556	-489	27
2	16	7	1115	1021	26
3	16	7	160	37	-63
4	16	7	834	826	31
5	16	7	306	243	45
6	16	7	633	632	37
7	16	7	450	358	46
-11	17	7	322	-272	51
-10	17	7	251	-63	52
-9	17	7	754	-703	32
-8	17	7	214	-166	47

h	k	l	10Fo	10Fc	10s
-7	17	7	1304	-1324	27
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-5	17	7	932	-915	25
-4	17	7	168	149	39
-3	17	7	874	-868	24
-2	17	7	271	222	31
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1	17	7	825	781	26
2	17	7	325	249	33
3	17	7	1295	1222	28
4	17	7	259	-190	43
5	17	7	847	887	33
6	17	7	205	-141	-67
7	17	7	381	358	44
-11	18	7	736	-703	39
-10	18	7	339	-280	42
-9	18	7	508	-560	34
-8	18	7	655	-632	32
-7	18	7	140	-53	-89
-6	18	7	838	-853	28
-5	18	7	560	584	28
-4	18	7	573	-606	26
-3	18	7	974	958	25
-2	18	7	245	-215	33
-1	18	7	744	759	25
0	18	7	167	87	-77
1	18	7	1003	945	26
2	18	7	778	767	28
3	18	7	229	-33	41
4	18	7	809	780	31
5	18	7	331	-203	39
6	18	7	356	434	50
-11	19	7	83	68	-83
-10	19	7	804	-828	34
-9	19	7	70	-94	-70
-8	19	7	657	-702	31
-7	19	7	119	112	-119
-6	19	7	210	143	43
-5	19	7	491	-488	26
-4	19	7	1025	980	25
-3	19	7	171	165	42
-2	19	7	1432	1400	24
-1	19	7	421	-442	28
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1	19	7	211	59	38
2	19	7	701	670	29
3	19	7	154	55	-61
4	19	7	243	-260	46
5	19	7	122	80	-122
6	19	7	462	-467	44
-10	20	7	142	257	-142
-9	20	7	620	-626	34
-8	20	7	669	685	32
-7	20	7	240	-268	45
-6	20	7	742	703	27

h	k	l	10Fo	10Fc	10s
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-2	20	7	383	368	28
-1	20	7	1163	1181	25
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1	20	7	837	769	28
2	20	7	741	-704	29
3	20	7	155	145	-77
4	20	7	605	-593	32
5	20	7	323	-281	45
6	20	7	382	-448	43
-10	21	7	413	-464	43
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-8	21	7	161	-24	-61
-7	21	7	1224	1238	28
-6	21	7	56	-148	-56
-5	21	7	1063	1061	26
-4	21	7	583	584	27
-3	21	7	608	638	27
-2	21	7	272	307	35
-1	21	7	109	-93	-109
0	21	7	569	548	20
1	21	7	830	-804	27
2	21	7	129	140	-98
3	21	7	958	-908	29
4	21	7	69	-24	-69
5	21	7	816	-841	34
-10	22	7	394	455	41
-9	22	7	277	269	51
-8	22	7	850	855	31
-7	22	7	61	87	-61
-6	22	7	1172	1137	27
-5	22	7	176	-207	-63
-4	22	7	646	664	28
-3	22	7	451	-457	29
-2	22	7	56	59	-56
-1	22	7	539	-563	28
0	22	7	620	-612	20
1	22	7	247	-234	47
2	22	7	865	-848	29
3	22	7	66	-87	-66
4	22	7	1063	-1030	31
5	22	7	195	152	-72
-9	23	7	310	320	43
-8	23	7	436	437	35
-7	23	7	516	505	33
-6	23	7	61	-109	-61
-5	23	7	792	817	27
-4	23	7	648	-663	28
-3	23	7	239	196	35
-2	23	7	1116	-1158	26
-1	23	7	122	65	-122
0	23	7	800	-786	21
1	23	7	429	-442	30
2	23	7	372	-351	39

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
3	23	7	635	-554	31
4	23	7	71	114	-71
5	23	7	649	-598	36
-9	24	7	618	576	34
-8	24	7	193	156	-60
-7	24	7	148	128	-77
-6	24	7	57	-4	-57
-5	24	7	489	-507	32
-4	24	7	153	-155	-61
-3	24	7	1081	-1079	26
-2	24	7	218	146	39
-1	24	7	1245	-1233	26
0	24	7	76	54	-51
1	24	7	757	-765	30
2	24	7	121	-63	-95
3	24	7	127	-98	-127
4	24	7	376	-356	41
-8	25	7	67	46	-67
-7	25	7	323	-350	40
-6	25	7	65	-129	-65
-5	25	7	632	-632	28
-4	25	7	861	-858	27
-3	25	7	250	-251	44
-2	25	7	690	-663	28
-1	25	7	67	200	-67
0	25	7	928	-906	38
1	25	7	483	459	31
2	25	7	219	-231	49
3	25	7	559	532	33
4	25	7	72	-110	-72
-8	26	7	707	-769	33
-7	26	7	150	194	-70
-6	26	7	984	-995	29
-5	26	7	130	-39	-86
-4	26	7	655	-678	29
-3	26	7	237	-231	39
-2	26	7	136	-161	-67
-1	26	7	314	-331	34
0	26	7	477	502	23
1	26	7	208	-167	-56
2	26	7	699	643	31
3	26	7	67	-39	-67
-7	27	7	718	-741	32
-6	27	7	96	14	-96
-5	27	7	906	-896	28
-4	27	7	242	194	39
-3	27	7	323	-323	37
-2	27	7	215	193	41
-1	27	7	91	98	-91
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1	27	7	779	741	29
2	27	7	137	98	-68
3	27	7	660	705	34
-7	28	7	63	-24	-63
-6	28	7	450	-452	34
-5	28	7	336	340	36

h	k	l	10Fo	10Fc	10s
-4	28	7	342	-330	34
-3	28	7	768	729	28
-2	28	7	190	-163	47
-1	28	7	809	777	28
0	28	7	284	268	33
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2	28	7	344	359	40
-6	29	7	97	-1	-97
-5	29	7	66	136	-66
-4	29	7	655	683	30
-3	29	7	107	-73	-107
-2	29	7	845	808	29
-1	29	7	59	-20	-59
0	29	7	862	828	24
1	29	7	111	-61	-111
-5	30	7	229	211	44
-4	30	7	535	464	31
-3	30	7	671	654	29
-2	30	7	171	64	-54
-1	30	7	588	613	32
0	30	7	312	-320	36
-2	31	7	289	263	36
-12	0	8	591	-559	44
-10	0	8	338	-279	42
-8	0	8	1384	1360	29
-6	0	8	1455	1394	25
-4	0	8	1675	1701	23
-2	0	8	1027	1056	24
0	0	8	56	-8	-56
2	0	8	703	-712	28
4	0	8	1385	-1284	30
6	0	8	1077	-971	36
8	0	8	751	-717	47
-13	1	8	614	-621	52
-12	1	8	336	404	70
-11	1	8	630	-597	39
-10	1	8	825	744	33
-9	1	8	535	521	38
-8	1	8	892	883	29
-7	1	8	1270	1221	27
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-4	1	8	520	-490	26
-3	1	8	1302	1257	23
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-1	1	8	518	529	26
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2	1	8	858	-750	27
3	1	8	709	-579	30
4	1	8	850	-783	32
5	1	8	1004	-929	33
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7	1	8	606	-500	41
8	1	8	93	164	-93
-13	2	8	614	531	47

h	k	l	10Fo	10Fc	10s
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-11	2	8	899	920	37
-10	2	8	76	-131	-76
-9	2	8	1868	1791	30
-8	2	8	171	-74	-61
-7	2	8	1120	1089	27
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-5	2	8	260	220	36
-4	2	8	301	298	30
-3	2	8	859	-850	24
-2	2	8	456	454	26
-1	2	8	1522	-1586	23
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1	2	8	1655	-1683	25
2	2	8	135	-61	-96
3	2	8	1261	-1129	28
4	2	8	486	-466	36
5	2	8	165	129	-73
6	2	8	506	-439	37
7	2	8	422	384	50
8	2	8	267	-240	-86
-13	3	8	135	179	-135
-12	3	8	773	718	40
-11	3	8	461	392	46
-10	3	8	1231	1147	33
-9	3	8	251	-264	59
-8	3	8	953	918	29
-7	3	8	217	-132	45
-6	3	8	430	412	29
-5	3	8	618	-606	26
-4	3	8	401	-408	28
-3	3	8	366	-296	26
-2	3	8	995	-1058	23
-1	3	8	463	-468	27
0	3	8	1649	-1638	26
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2	3	8	1388	-1308	26
3	3	8	288	277	46
4	3	8	423	-412	37
5	3	8	418	383	42
6	3	8	383	367	46
7	3	8	232	157	-82
8	3	8	546	456	48
-13	4	8	271	149	-74
-12	4	8	551	579	48
-11	4	8	576	577	40
-10	4	8	303	264	54
-9	4	8	476	403	33
-8	4	8	651	-651	30
-7	4	8	431	420	33
-6	4	8	1112	-1090	26
-5	4	8	58	-58	-58
-4	4	8	1642	-1695	23
-3	4	8	358	-362	27
-2	4	8	1009	-1063	23
-1	4	8	761	-768	24

h	k	l	10Fo	10Fc	10s
0	4	8	215	-188	29
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3	4	8	530	-520	32
4	4	8	945	936	31
5	4	8	292	-221	50
6	4	8	1101	1130	38
7	4	8	294	81	56
-13	5	8	615	626	50
-12	5	8	85	87	-85
-11	5	8	394	381	49
-10	5	8	277	-217	47
-9	5	8	295	-269	38
-8	5	8	217	-69	47
-7	5	8	1022	-971	27
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-5	5	8	1827	-1859	24
-4	5	8	257	225	30
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-2	5	8	161	166	-47
-1	5	8	767	-796	25
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1	5	8	508	468	27
2	5	8	170	157	-62
3	5	8	657	670	31
4	5	8	285	254	47
5	5	8	1232	1248	33
6	5	8	400	-338	50
7	5	8	916	948	40
-13	6	8	420	-385	62
-12	6	8	566	553	46
-11	6	8	537	-551	43
-10	6	8	186	61	-68
-9	6	8	931	-911	31
-8	6	8	492	-458	34
-7	6	8	530	-476	28
-6	6	8	1168	-1153	25
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-4	6	8	1052	-1024	24
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-2	6	8	724	-672	24
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2	6	8	455	361	30
3	6	8	1006	1034	29
4	6	8	594	724	34
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6	6	8	840	851	37
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-11	7	8	79	-54	-79
-10	7	8	1285	-1181	33
-9	7	8	68	5	-68
-8	7	8	1199	-1183	29

h	k	l	10Fo	10Fc	10s
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-6	7	8	665	-646	26
-5	7	8	188	-135	39
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1	7	8	549	-514	29
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3	7	8	440	462	35
4	7	8	728	803	33
5	7	8	176	-34	-60
6	7	8	166	-68	-94
7	7	8	180	271	-149
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-11	8	8	840	-796	37
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-9	8	8	891	-856	31
-8	8	8	453	477	34
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-4	8	8	645	655	25
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3	8	8	693	615	30
4	8	8	570	-560	32
5	8	8	359	389	42
6	8	8	434	-483	40
7	8	8	127	-226	-127
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-6	9	8	99	-54	-99
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-2	9	8	376	355	25
-1	9	8	1219	1204	24
0	9	8	1189	1113	31
1	9	8	417	371	29
2	9	8	1038	1030	27
3	9	8	595	-581	33
4	9	8	291	117	40
5	9	8	946	-1015	33
6	9	8	82	21	-82
7	9	8	789	-909	43
-12	10	8	801	-763	41

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn) \cdot MeOH$

h	k	l	10Fo	10Fc	10s
-11	10	8	211	8	-75
-10	10	8	66	3	-66
-9	10	8	260	266	46
-8	10	8	425	348	33
-7	10	8	164	110	-68
-6	10	8	1471	1456	26
-5	10	8	106	-101	-106
-4	10	8	1368	1390	24
-3	10	8	470	-408	26
-2	10	8	1045	1020	24
-1	10	8	327	-294	29
0	10	8	908	908	19
1	10	8	256	240	34
2	10	8	417	-403	34
3	10	8	174	-235	-71
4	10	8	1034	-1001	31
5	10	8	217	-4	-57
6	10	8	950	-1021	37
7	10	8	274	118	-71
-12	11	8	602	597	45
-11	11	8	259	-189	-67
-10	11	8	908	905	33
-9	11	8	61	6	-61
-8	11	8	1032	1016	29
-7	11	8	764	793	29
-6	11	8	61	-86	-61
-5	11	8	963	989	25
-4	11	8	223	-209	34
-3	11	8	570	539	25
-2	11	8	908	-912	24
-1	11	8	139	-120	-67
0	11	8	1140	-1090	32
1	11	8	179	102	-53
2	11	8	1103	-1047	27
3	11	8	757	-724	30
4	11	8	619	-563	34
5	11	8	490	-464	38
6	11	8	192	128	-84
7	11	8	582	-594	45
-12	12	8	86	-16	-86
-11	12	8	795	794	36
-10	12	8	250	-49	44
-9	12	8	1116	1040	31
-8	12	8	253	-261	43
-7	12	8	864	840	28
-6	12	8	166	142	-59
-5	12	8	83	64	-83
-4	12	8	52	-109	-52
-3	12	8	154	-109	-53
-2	12	8	296	-227	32
-1	12	8	1184	-1184	24
0	12	8	251	-208	25
1	12	8	1419	-1349	26
2	12	8	239	57	39
3	12	8	1020	-982	30
4	12	8	305	195	41

h	k	l	10Fo	10Fc	10s
5	12	8	198	-158	-54
6	12	8	272	-138	60
7	12	8	344	442	58
-12	13	8	713	619	41
-11	13	8	164	122	-135
-10	13	8	782	705	35
-9	13	8	66	-180	-66
-8	13	8	1003	970	29
-7	13	8	685	-679	29
-6	13	8	262	245	39
-5	13	8	850	-832	26
-4	13	8	156	-23	39
-3	13	8	700	-705	25
-2	13	8	1039	-979	24
-1	13	8	378	-367	29
0	13	8	735	-661	21
1	13	8	261	-201	38
2	13	8	1015	-941	28
3	13	8	771	736	31
4	13	8	520	-496	36
5	13	8	556	488	38
6	13	8	77	-87	-77
7	13	8	626	502	43
-12	14	8	612	548	44
-11	14	8	212	271	-84
-10	14	8	75	-157	-75
-9	14	8	322	335	45
-8	14	8	409	-443	39
-7	14	8	279	253	42
-6	14	8	1298	-1335	26
-5	14	8	54	-42	-54
-4	14	8	645	-611	26
-3	14	8	923	-934	25
-2	14	8	308	-209	32
-1	14	8	917	-891	25
0	14	8	119	41	-73
1	14	8	189	-211	-51
2	14	8	688	699	30
3	14	8	345	-289	39
4	14	8	883	774	31
5	14	8	72	113	-72
6	14	8	782	686	37
-11	15	8	233	300	-73
-10	15	8	372	-378	41
-9	15	8	102	-139	-102
-8	15	8	433	-460	33
-7	15	8	1085	-1086	28
-6	15	8	60	79	-60
-5	15	8	1261	-1262	25
-4	15	8	307	317	30
-3	15	8	1154	-1132	25
-2	15	8	488	430	27
-1	15	8	576	-573	27
0	15	8	750	729	27
1	15	8	161	48	-61
2	15	8	646	614	31

h	k	l	10Fo	10Fc	10s
3	15	8	922	884	30
4	15	8	70	47	-70
5	15	8	956	859	34
6	15	8	327	148	49
-11	16	8	840	-808	36
-10	16	8	155	-33	-76
-9	16	8	816	-789	32
-8	16	8	313	-304	41
-7	16	8	777	-777	29
-6	16	8	558	-559	27
-5	16	8	56	87	-56
-4	16	8	731	-776	26
-3	16	8	820	838	26
-2	16	8	547	-499	26
-1	16	8	1041	1011	26
0	16	8	145	-7	-43
1	16	8	1109	1054	27
2	16	8	403	382	34
3	16	8	634	556	31
4	16	8	469	432	37
5	16	8	179	283	-101
6	16	8	488	479	46
-11	17	8	224	70	-61
-10	17	8	933	-887	34
-9	17	8	179	-25	-69
-8	17	8	983	-1007	30
-7	17	8	252	256	38
-6	17	8	538	-573	31
-5	17	8	55	-49	-55
-4	17	8	249	224	36
-3	17	8	57	51	-57
-2	17	8	1194	1184	25
-1	17	8	56	37	-56
0	17	8	1131	1058	52
1	17	8	186	216	-63
2	17	8	1089	1031	28
3	17	8	213	-233	-66
4	17	8	311	314	46
5	17	8	168	-54	-74
6	17	8	137	-15	-137
-11	18	8	695	-670	37
-10	18	8	72	19	-72
-9	18	8	795	-763	32
-8	18	8	197	270	-67
-7	18	8	490	-491	32
-6	18	8	916	918	28
-5	18	8	55	14	-55
-4	18	8	758	771	27
-3	18	8	380	359	30
-2	18	8	717	685	26
-1	18	8	777	721	26
0	18	8	231	249	30
1	18	8	893	821	28
2	18	8	531	-477	32
3	18	8	586	580	36
4	18	8	599	-600	34

h	k	l	10Fo	10Fc	10s
5	18	8	111	63	-111
-10	19	8	230	-169	56
-9	19	8	241	229	-62
-8	19	8	63	-125	-63
-7	19	8	801	784	29
-6	19	8	190	-48	43
-5	19	8	1176	1163	26
-4	19	8	254	205	36
-3	19	8	1166	1143	26
-2	19	8	110	-80	-110
-1	19	8	646	592	27
0	19	8	175	227	42
1	19	8	210	-143	46
2	19	8	134	-43	-82
3	19	8	886	-855	31
4	19	8	121	88	-121
5	19	8	811	-835	36
-10	20	8	248	-183	55
-9	20	8	428	417	35
-8	20	8	669	698	32
-7	20	8	538	590	31
-6	20	8	984	967	28
-5	20	8	178	226	-47
-4	20	8	1321	1328	26
-3	20	8	54	-43	-54
-2	20	8	787	808	27
-1	20	8	658	-610	28
0	20	8	367	320	27
1	20	8	745	-692	29
2	20	8	514	-473	32
3	20	8	426	-421	37
4	20	8	663	-708	35
5	20	8	288	-121	46
-10	21	8	819	883	35
-9	21	8	192	157	-60
-8	21	8	820	924	31
-7	21	8	147	26	-89
-6	21	8	208	228	52
-5	21	8	279	253	36
-4	21	8	198	-273	-49
-3	21	8	268	172	35
-2	21	8	851	-810	27
-1	21	8	418	439	31
0	21	8	1000	-976	19
1	21	8	169	-173	-69
2	21	8	916	-865	30
3	21	8	340	-257	40
4	21	8	396	-411	41
-9	22	8	884	934	33
-8	22	8	69	-17	-69
-7	22	8	653	672	31
-6	22	8	291	-343	40
-5	22	8	58	40	-58
-4	22	8	330	-364	36
-3	22	8	475	-498	28
-2	22	8	125	-118	-104

h	k	l	10Fo	10Fc	10s
-1	22	8	899	-840	27
0	22	8	146	-60	-57
1	22	8	977	-924	29
2	22	8	125	33	-101
3	22	8	690	-671	34
4	22	8	238	267	53
-9	23	8	174	-174	-73
-8	23	8	478	528	35
-7	23	8	651	-674	32
-6	23	8	408	405	34
-5	23	8	863	-838	28
-4	23	8	221	-209	37
-3	23	8	736	-749	29
-2	23	8	247	-264	46
-1	23	8	433	-431	32
0	23	8	649	-650	43
1	23	8	134	-37	-66
2	23	8	508	-466	34
3	23	8	499	471	37
4	23	8	415	-399	40
-8	24	8	509	-520	34
-7	24	8	66	-72	-66
-6	24	8	797	-746	29
-5	24	8	151	191	-67
-4	24	8	961	-979	28
-3	24	8	65	53	-65
-2	24	8	882	-885	28
-1	24	8	61	47	-61
0	24	8	226	-195	36
1	24	8	123	-106	-123
2	24	8	476	418	33
3	24	8	215	-209	-62
-8	25	8	363	-342	39
-7	25	8	510	-480	33
-6	25	8	229	-181	41
-5	25	8	784	-737	29
-4	25	8	64	144	-64
-3	25	8	701	-701	30
-2	25	8	469	450	32
-1	25	8	521	-501	30
0	25	8	598	527	23
1	25	8	222	200	53
2	25	8	452	477	36
3	25	8	248	269	55
-7	26	8	413	-504	37
-6	26	8	58	-84	-58
-5	26	8	231	-226	50
-4	26	8	252	-265	40
-3	26	8	604	559	30
-2	26	8	297	-278	37
-1	26	8	812	795	30
0	26	8	181	-86	43
1	26	8	975	917	30
2	26	8	70	-124	-70
-7	27	8	226	229	45
-6	27	8	362	-441	39

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn) \cdot MeOH$

h	k	l	10Fo	10Fc	10s
-5	27	8	421	395	34
-4	27	8	144	183	-67
-3	27	8	153	217	-64
-2	27	8	458	483	32
-1	27	8	154	130	-65
0	27	8	731	692	25
1	27	8	212	-168	47
-6	28	8	593	610	32
-5	28	8	97	-45	-97
-4	28	8	759	698	30
-3	28	8	173	210	-61
-2	28	8	390	364	33
-1	28	8	422	414	33
0	28	8	132	59	-52
-4	29	8	59	-85	-59
-3	29	8	641	607	31
-2	29	8	146	-60	-57
-1	29	8	314	354	39
-13	0	9	83	38	-83
-11	0	9	690	697	37
-9	0	9	1401	1371	31
-7	0	9	1221	1120	28
-5	0	9	1148	1106	26
-3	0	9	59	167	-59
-1	0	9	830	-828	26
1	0	9	1778	-1786	27
3	0	9	1182	-1086	31
5	0	9	878	-779	36
7	0	9	234	-190	-82
-13	1	9	598	521	46
-12	1	9	177	308	-123
-11	1	9	335	385	57
-10	1	9	901	834	34
-9	1	9	144	214	-144
-8	1	9	1142	1107	30
-7	1	9	184	-249	-60
-6	1	9	1205	1206	27
-5	1	9	548	-593	27
-4	1	9	527	500	28
-3	1	9	857	-859	26
-2	1	9	136	3	-62
-1	1	9	840	-852	26
0	1	9	1195	-1217	39
1	1	9	540	-528	31
2	1	9	1024	-928	29
3	1	9	67	-129	-67
4	1	9	926	-856	34
5	1	9	597	526	39
6	1	9	321	-279	66
7	1	9	517	475	51
-13	2	9	97	-40	-97
-12	2	9	936	803	40
-11	2	9	190	-92	-99
-10	2	9	991	954	35
-9	2	9	132	188	-132
-8	2	9	66	44	-66
-7	2	9	583	558	30
-6	2	9	666	-618	28
-5	2	9	287	277	36
-4	2	9	1639	-1644	25
-3	2	9	191	157	40
-2	2	9	1382	-1405	25
-1	2	9	297	-278	35
0	2	9	1183	-1214	66
1	2	9	282	-184	34
2	2	9	316	-261	35
3	2	9	291	-240	41
4	2	9	464	356	38
5	2	9	318	-101	52
6	2	9	800	683	40
7	2	9	291	-106	62
-13	3	9	843	785	43
-12	3	9	367	-318	53
-11	3	9	959	954	37
-10	3	9	635	-591	37
-9	3	9	511	554	38
-8	3	9	335	-339	43
-7	3	9	249	-257	40
-6	3	9	724	-686	28
-5	3	9	1159	-1134	26
-4	3	9	62	126	-62
-3	3	9	1395	-1375	25
-2	3	9	96	25	-96
-1	3	9	1361	-1390	25
0	3	9	737	719	54
1	3	9	526	-534	30
2	3	9	145	-80	-68
3	3	9	470	463	37
4	3	9	240	155	60
5	3	9	955	904	36
6	3	9	76	-5	-76
7	3	9	735	663	47
-13	4	9	135	-32	-135
-12	4	9	467	431	45
-11	4	9	342	-335	52
-10	4	9	377	376	45
-9	4	9	944	-834	32
-8	4	9	97	-134	-97
-7	4	9	928	-904	28
-6	4	9	438	-449	31
-5	4	9	977	-976	26
-4	4	9	670	-650	26
-3	4	9	53	-37	-53
-2	4	9	727	-755	26
-1	4	9	607	598	27
0	4	9	638	-678	22
1	4	9	1240	1273	27
2	4	9	364	-386	36
3	4	9	925	853	32
4	4	9	350	417	48
5	4	9	771	740	38
6	4	9	387	399	55
7	4	9	90	87	-90
-12	5	9	86	-221	-86
-11	5	9	81	72	-81
-10	5	9	806	-722	35
-9	5	9	64	19	-64
-8	5	9	1297	-1248	29
-7	5	9	150	22	-63
-6	5	9	1263	-1242	26
-5	5	9	418	419	30
-4	5	9	618	-660	27
-3	5	9	51	-48	-51
-2	5	9	192	155	38
-1	5	9	443	443	30
0	5	9	1247	1248	18
1	5	9	301	-278	37
2	5	9	1226	1276	29
3	5	9	279	-107	47
4	5	9	1020	1007	33
5	5	9	239	-188	-60
6	5	9	579	424	43
-12	6	9	314	-453	66
-11	6	9	470	-424	44
-10	6	9	356	-400	56
-9	6	9	542	-508	36
-8	6	9	67	-10	-67
-7	6	9	1001	-962	29
-6	6	9	452	478	32
-5	6	9	536	-541	29
-4	6	9	990	972	26
-3	6	9	564	-567	27
-2	6	9	667	639	26
-1	6	9	383	361	32
0	6	9	973	986	35
1	6	9	1140	1068	27
2	6	9	145	-119	-76
3	6	9	940	924	31
4	6	9	333	-315	45
5	6	9	483	506	41
6	6	9	466	-549	45
-12	7	9	78	-48	-78
-11	7	9	764	-738	39
-10	7	9	178	-139	-86
-9	7	9	439	-419	41
-8	7	9	269	-185	41
-7	7	9	61	120	-61
-6	7	9	256	-273	37
-5	7	9	1151	1105	26
-4	7	9	422	-436	28
-3	7	9	1122	1113	25
-2	7	9	374	-392	29
-1	7	9	1225	1190	26
0	7	9	272	-195	25
1	7	9	517	514	30
2	7	9	348	329	38
3	7	9	226	-146	43
4	7	9	152	42	-64
5	7	9	563	-618	37
6	7	9	313	327	52
-12	8	9	743	-675	42
-11	8	9	381	297	45
-10	8	9	227	-325	-75
-9	8	9	711	691	33
-8	8	9	61	-56	-61
-7	8	9	384	348	33
-6	8	9	411	377	34
-5	8	9	340	356	34
-4	8	9	920	892	26
-3	8	9	56	26	-56
-2	8	9	1426	1397	25
-1	8	9	337	-320	32
0	8	9	675	582	21
1	8	9	701	-666	29
2	8	9	292	266	42
3	8	9	645	-592	33
4	8	9	443	-431	38
5	8	9	425	-353	41
6	8	9	737	-727	41
-12	9	9	217	240	-94
-11	9	9	476	-462	47
-10	9	9	688	685	37
-9	9	9	133	-161	-133
-8	9	9	846	803	31
-7	9	9	193	154	-60
-6	9	9	981	1036	27
-5	9	9	233	198	40
-4	9	9	1113	1140	25
-3	9	9	1456	1481	25
-2	9	9	373	391	32
-1	9	9	848	798	26
0	9	9	609	-560	20
1	9	9	483	467	33
2	9	9	1316	-1210	29
3	9	9	234	-106	53
4	9	9	972	-1000	33
5	9	9	71	-193	-71
6	9	9	353	-375	55
-12	10	9	229	77	-65
-11	10	9	739	690	39
-10	10	9	384	315	39
-9	10	9	685	698	34
-8	10	9	66	-16	-66
-7	10	9	1273	1242	28
-6	10	9	315	-339	38
-5	10	9	1032	1083	26
-4	10	9	870	-917	26
-3	10	9	201	161	42
-2	10	9	639	-644	27
-1	10	9	995	-996	26
0	10	9	450	-469	23
1	10	9	1214	-1131	28
2	10	9	207	4	-58
3	10	9	1206	-1124	31
4	10	9	285	327	55
5	10	9	524	-513	42
6	10	9	330	264	52
-12	11	9	191	197	-99
-11	11	9	600	523	37
-10	11	9	506	484	38
-9	11	9	179	169	-57
-8	11	9	596	602	32
-7	11	9	269	-271	45
-6	11	9	708	739	28
-5	11	9	587	-590	28
-4	11	9	437	414	30
-3	11	9	1641	-1636	25
-2	11	9	612	-612	27
-1	11	9	1017	-940	26
0	11	9	536	-515	22
1	11	9	271	-217	47
2	11	9	786	-742	31
3	11	9	358	321	41
4	11	9	418	-362	40
5	11	9	442	445	40
6	11	9	228	-288	-81
-12	12	9	968	885	41
-11	12	9	76	-32	-76
-10	12	9	435	431	43
-9	12	9	67	17	-67
-8	12	9	160	71	-74
-7	12	9	59	-82	-59
-6	12	9	342	-327	34
-5	12	9	124	-125	-87
-4	12	9	1002	-1026	26
-3	12	9	54	69	-54
-2	12	9	2068	-2043	25
-1	12	9	100	-17	-100
0	12	9	884	-797	54
1	12	9	107	153	-107
2	12	9	209	-207	-52
3	12	9	132	-91	-132
4	12	9	599	593	36
5	12	9	77	30	-77
6	12	9	786	836	41
-11	13	9	532	522	43
-10	13	9	397	-416	45
-9	13	9	189	200	-80
-8	13	9	797	-772	31
-7	13	9	121	-86	-121
-6	13	9	1137	-1133	27
-5	13	9	134	-67	-77
-4	13	9	698	-697	27
-3	13	9	961	-966	26
-2	13	9	192	87	42
-1	13	9	639	-620	28
0	13	9	608	574	68
1	13	9	636	-582	31
2	13	9	947	860	30
3	13	9	290	153	41

h	k	l	10Fo	10Fc	10s
4	13	9	644	627	36
5	13	9	389	357	49
-11	14	9	683	-623	37
-10	14	9	142	158	-142
-9	14	9	875	-810	32
-8	14	9	190	14	-49
-7	14	9	987	-985	29
-6	14	9	532	-529	30
-5	14	9	445	-404	31
-4	14	9	703	-670	27
-3	14	9	87	-38	-87
-2	14	9	367	-315	30
-1	14	9	881	867	27
0	14	9	150	-123	-64
1	14	9	1002	938	29
2	14	9	159	25	-94
3	14	9	1277	1201	31
4	14	9	259	142	50
5	14	9	501	568	46
-11	15	9	406	-367	46
-10	15	9	748	-733	36
-9	15	9	209	-106	-53
-8	15	9	1076	-1044	30
-7	15	9	109	-24	-109
-6	15	9	563	-579	29
-5	15	9	89	-67	-89
-4	15	9	397	-358	31
-3	15	9	693	607	27
-2	15	9	461	447	31
-1	15	9	471	447	29
0	15	9	787	766	33
1	15	9	375	366	38
2	15	9	1246	1179	29
3	15	9	189	-19	-64
4	15	9	796	690	35
5	15	9	222	-110	-78
-11	16	9	333	-310	54
-10	16	9	420	-337	45
-9	16	9	629	-653	35
-8	16	9	182	-85	-60
-7	16	9	688	-714	31
-6	16	9	601	631	30
-5	16	9	451	-501	31
-4	16	9	1023	1022	27
-3	16	9	221	-222	51
-2	16	9	1228	1301	27
-1	16	9	287	271	36
0	16	9	671	692	33
1	16	9	556	540	31
2	16	9	170	56	-51
3	16	9	487	514	40
4	16	9	540	-528	40
5	16	9	343	286	48
-11	17	9	673	-695	39
-10	17	9	68	85	-68
-9	17	9	333	-386	47

h	k	l	10Fo	10Fc	10s
-8	17	9	164	174	-68
-7	17	9	282	280	43
-6	17	9	65	-82	-65
-5	17	9	880	896	28
-4	17	9	62	32	-62
-3	17	9	1308	1298	27
-2	17	9	153	76	-61
-1	17	9	1005	967	27
0	17	9	135	85	-62
1	17	9	532	503	32
2	17	9	235	-216	51
3	17	9	409	-395	38
4	17	9	68	-72	-68
5	17	9	410	-378	46
-10	18	9	535	-481	37
-9	18	9	569	524	34
-8	18	9	64	-30	-64
-7	18	9	840	857	30
-6	18	9	390	401	33
-5	18	9	210	198	49
-4	18	9	820	818	28
-3	18	9	301	268	36
-2	18	9	878	859	27
-1	18	9	428	-397	34
0	18	9	626	633	47
1	18	9	686	-644	30
2	18	9	69	-63	-69
3	18	9	794	-780	34
4	18	9	402	-338	42
-10	19	9	656	672	37
-9	19	9	150	21	-92
-8	19	9	1152	1166	31
-7	19	9	97	160	-97
-6	19	9	1057	1073	29
-5	19	9	367	344	32
-4	19	9	365	384	32
-3	19	9	66	104	-66
-2	19	9	285	-241	39
-1	19	9	284	277	37
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1	19	9	325	-127	34
2	19	9	976	-927	31
3	19	9	161	21	-98
4	19	9	642	-629	34
-10	20	9	205	222	-61
-9	20	9	669	697	36
-8	20	9	62	31	-62
-7	20	9	849	880	30
-6	20	9	274	-265	41
-5	20	9	636	641	30
-4	20	9	421	-408	31
-3	20	9	203	164	47
-2	20	9	669	-633	29
-1	20	9	319	-224	34
0	20	9	228	-244	34
1	20	9	945	-901	30

h	k	l	10Fo	10Fc	10s
2	20	9	225	-168	50
3	20	9	732	-719	34
4	20	9	257	154	59
-9	21	9	175	151	-81
-8	21	9	118	155	-118
-7	21	9	390	-380	38
-6	21	9	260	263	41
-5	21	9	554	-566	31
-4	21	9	58	49	-58
-3	21	9	1040	-1080	28
-2	21	9	231	244	50
-1	21	9	861	-842	28
0	21	9	400	-395	43
1	21	9	527	-475	34
2	21	9	143	-217	-100
3	21	9	213	244	-60
-9	22	9	63	-55	-63
-8	22	9	146	35	-72
-7	22	9	319	-257	37
-6	22	9	301	-280	35
-5	22	9	60	-68	-60
-4	22	9	910	-889	29
-3	22	9	64	-45	-64
-2	22	9	887	-909	29
-1	22	9	188	166	-53
0	22	9	631	-615	46
1	22	9	189	99	-56
2	22	9	61	-46	-61
3	22	9	315	279	51
-8	23	9	547	-544	35
-7	23	9	63	13	-63
-6	23	9	548	-585	33
-5	23	9	458	-494	33
-4	23	9	508	-469	31
-3	23	9	564	-527	30
-2	23	9	93	27	-93
-1	23	9	652	-626	30
0	23	9	496	447	48
1	23	9	287	-243	46
2	23	9	727	667	33
-8	24	9	135	57	-135
-7	24	9	750	-734	31
-6	24	9	58	118	-58
-5	24	9	754	-750	30
-4	24	9	95	11	-95
-3	24	9	61	-137	-61
-2	24	9	57	119	-57
-1	24	9	445	430	34
0	24	9	179	-160	-47
1	24	9	791	796	32
2	24	9	146	41	-146
-7	25	9	186	93	-71
-6	25	9	582	-601	34
-5	25	9	496	475	33
-4	25	9	349	-296	34
-3	25	9	583	582	31

h	k	l	10Fo	10Fc	10s
-2	25	9	57	11	-57
-1	25	9	351	351	39
0	25	9	757	681	27
1	25	9	101	6	-101
-6	26	9	294	297	47
-5	26	9	232	-136	43
-4	26	9	761	841	30
-3	26	9	65	-66	-65
-2	26	9	835	824	30
-1	26	9	168	-102	-72
0	26	9	866	836	30
-5	27	9	529	519	33
-4	27	9	178	151	-56
-3	27	9	669	663	32
-2	27	9	231	-198	47
-1	27	9	830	843	31
-12	0	10	746	791	42
-10	0	10	1288	1239	33
-8	0	10	722	704	31
-6	0	10	501	493	31
-4	0	10	903	-885	27
-2	0	10	1260	-1262	27
0	0	10	1552	-1587	28
2	0	10	726	-718	33
4	0	10	162	-131	-114
6	0	10	438	346	46
-12	1	10	91	117	-91
-11	1	10	857	776	37
-10	1	10	80	4	-80
-9	1	10	756	705	33
-8	1	10	579	-482	33
-7	1	10	312	283	37
-6	1	10	884	-861	29
-5	1	10	63	-58	-63
-4	1	10	680	-708	29
-3	1	10	848	-878	28
-2	1	10	178	-213	-57
-1	1	10	1004	-1064	27
0	1	10	159	94	-57
1	1	10	1060	-1055	30
2	1	10	498	470	37
3	1	10	473	-502	36
4	1	10	616	588	39
5	1	10	331	104	50
6	1	10	539	464	44
-12	2	10	261	267	-88
-11	2	10	136	190	-136
-10	2	10	453	443	39
-9	2	10	881	-819	32
-8	2	10	163	196	-78
-7	2	10	925	-897	29
-6	2	10	119	158	-119
-5	2	10	1510	-1495	27
-4	2	10	192	-86	42
-3	2	10	637	-606	28
-2	2	10	58	-121	-58

h	k	l	10Fo	10Fc	10s
-1	2	10	445	-515	34
0	2	10	149	-41	-65
1	2	10	463	440	34
2	2	10	117	-206	-117
3	2	10	692	633	35
4	2	10	147	12	-147
5	2	10	1039	874	37
6	2	10	228	-72	-76
-12	3	10	417	485	53
-11	3	10	353	-451	55
-10	3	10	74	-55	-74
-9	3	10	469	-502	41
-8	3	10	903	-890	31
-7	3	10	61	-30	-61
-6	3	10	1244	-1214	28
-5	3	10	238	269	45
-4	3	10	1218	-1251	27
-3	3	10	412	407	34
-2	3	10	577	-577	30
-1	3	10	472	425	30
0	3	10	354	363	29
1	3	10	210	206	46
2	3	10	722	785	32
3	3	10	317	329	46
4	3	10	863	799	36
5	3	10	141	-109	-141
6	3	10	723	692	44
-12	4	10	608	-585	48
-11	4	10	84	11	-84
-10	4	10	964	-904	35
-9	4	10	69	-188	-69
-8	4	10	443	-441	34
-7	4	10	649	-663	32
-6	4	10	65	-132	-65
-5	4	10	539	-579	30
-4	4	10	1039	1022	27
-3	4	10	676	-715	28
-2	4	10	911	913	27
-1	4	10	91	149	-91
0	4	10	953	906	20
1	4	10	452	488	32
2	4	10	390	387	41
3	4	10	501	441	37
4	4	10	219	273	-75
5	4	10	435	361	46
-12	5	10	80	55	-80
-11	5	10	921	-908	38
-10	5	10	74	117	-74
-9	5	10	911	-896	32
-8	5	10	265	251	49
-7	5	10	515	-526	33
-6	5	10	160	195	-51
-5	5	10	280	254	38
-4	5	10	153	-114	-63
-3	5	10	1054	1099	26
-2	5	10	178	-202	-54

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-1	5	10	1429	1406	27
0	5	10	228	-90	33
1	5	10	998	989	30
2	5	10	131	-151	-106
3	5	10	573	581	35
4	5	10	264	-272	50
5	5	10	264	-209	65
-12	6	10	686	-607	45
-11	6	10	85	-72	-85
-10	6	10	623	-605	36
-9	6	10	633	543	35
-8	6	10	706	-644	32
-7	6	10	770	726	30
-6	6	10	120	-27	-120
-5	6	10	1035	1029	27
-4	6	10	218	114	35
-3	6	10	324	278	35
-2	6	10	1083	1051	27
-1	6	10	241	208	49
0	6	10	981	998	22
1	6	10	589	-583	34
2	6	10	683	701	32
3	6	10	650	-612	36
4	6	10	162	-32	-113
5	6	10	619	-701	41
-12	7	10	230	-235	-90
-11	7	10	75	-70	-75
-10	7	10	82	173	-82
-9	7	10	310	-301	43
-8	7	10	789	775	32
-7	7	10	277	-321	49
-6	7	10	1243	1248	28
-5	7	10	59	-68	-59
-4	7	10	946	937	27
-3	7	10	384	-389	32
-2	7	10	115	192	-115
-1	7	10	105	87	-105
0	7	10	357	-340	31
1	7	10	264	276	45
2	7	10	794	-765	32
3	7	10	76	48	-76
4	7	10	822	-867	36
5	7	10	223	86	-76
-12	8	10	392	355	52
-11	8	10	74	-78	-74
-10	8	10	583	571	40
-9	8	10	279	343	53
-8	8	10	164	149	-66
-7	8	10	1531	1511	29
-6	8	10	569	569	32
-5	8	10	1714	1734	27
-4	8	10	206	-168	45
-3	8	10	1052	1109	27
-2	8	10	501	-508	30
-1	8	10	129	-35	-79
0	8	10	600	-558	39

h	k	l	10Fo	10Fc	10s
1	8	10	566	-558	32
2	8	10	412	-379	37
3	8	10	1019	-995	34
4	8	10	256	-257	-66
5	8	10	793	-856	37
-12	9	10	252	-194	-76
-11	9	10	745	684	39
-10	9	10	73	187	-73
-9	9	10	899	938	34
-8	9	10	454	384	36
-7	9	10	558	526	34
-6	9	10	661	713	31
-5	9	10	378	-352	34
-4	9	10	432	392	31
-3	9	10	950	-975	27
-2	9	10	164	87	-58
-1	9	10	1274	-1279	27
0	9	10	170	-140	-51
1	9	10	956	-827	30
2	9	10	250	-201	50
3	9	10	369	-409	49
4	9	10	238	-186	-60
5	9	10	234	286	-80
-11	10	10	216	181	-86
-10	10	10	789	790	36
-9	10	10	323	-324	45
-8	10	10	1278	1197	31
-7	10	10	571	-523	32
-6	10	10	640	-634	31
-5	10	10	866	-946	27
-4	10	10	917	-875	27
-3	10	10	254	-229	43
-2	10	10	1282	-1280	27
-1	10	10	159	-149	-66
0	10	10	898	-903	21
1	10	10	305	291	43
2	10	10	838	-844	32
3	10	10	294	297	56
4	10	10	66	-23	-66
5	10	10	187	251	-82
-11	11	10	459	395	40
-10	11	10	303	-247	50
-9	11	10	950	873	33
-8	11	10	794	-797	32
-7	11	10	440	501	39
-6	11	10	1198	-1188	28
-5	11	10	538	-551	31
-4	11	10	990	-996	27
-3	11	10	609	-614	30
-2	11	10	209	-165	44
-1	11	10	631	-625	30
0	11	10	222	104	43
1	11	10	713	-633	31
2	11	10	840	778	31
3	11	10	360	-280	46
4	11	10	798	786	36

h	k	l	10Fo	10Fc	10s
5	11	10	86	117	-86
-11	12	10	77	0	-77
-10	12	10	72	-26	-72
-9	12	10	568	-543	34
-8	12	10	67	76	-67
-7	12	10	1243	-1217	29
-6	12	10	64	3	-64
-5	12	10	1280	-1234	27
-4	12	10	58	6	-58
-3	12	10	797	-834	29
-2	12	10	105	-88	-105
-1	12	10	119	28	-119
0	12	10	58	-2	-41
1	12	10	285	281	44
2	12	10	222	-76	51
3	12	10	1127	1097	33
4	12	10	162	-1	-114
5	12	10	759	776	40
-11	13	10	469	-441	40
-10	13	10	84	-90	-84
-9	13	10	949	-973	32
-8	13	10	288	-304	52
-7	13	10	636	-618	30
-6	13	10	927	-902	29
-5	13	10	426	438	33
-4	13	10	853	-872	28
-3	13	10	749	749	29
-2	13	10	316	-338	40
-1	13	10	812	820	29
0	13	10	192	101	37
1	13	10	610	561	31
2	13	10	828	762	32
3	13	10	218	62	-64
4	13	10	822	763	36
-11	14	10	119	-65	-119
-10	14	10	819	-798	36
-9	14	10	123	15	-123
-8	14	10	1212	-1223	31
-7	14	10	126	-101	-89
-6	14	10	61	-52	-61
-5	14	10	92	-127	-92
-4	14	10	466	430	32
-3	14	10	60	-13	-60
-2	14	10	1252	1267	27
-1	14	10	216	35	41
0	14	10	1183	1155	41
1	14	10	215	-63	49
2	14	10	913	847	32
3	14	10	126	155	-126
4	14	10	78	151	-78
-10	15	10	75	-71	-75
-9	15	10	552	-500	35
-8	15	10	132	-25	-132
-7	15	10	61	-55	-61
-6	15	10	61	83	-61
-5	15	10	434	435	30

h	k	l	10Fo	10Fc	10s
-4	15	10	130	112	-79
-3	15	10	869	918	28
-2	15	10	345	347	35
-1	15	10	1029	1033	29
0	15	10	76	-73	-56
1	15	10	911	748	31
2	15	10	262	-204	49
3	15	10	416	301	42
4	15	10	275	-274	58
-10	16	10	518	-534	42
-9	16	10	82	214	-82
-8	16	10	389	-353	36
-7	16	10	997	990	30
-6	16	10	59	-170	-59
-5	16	10	854	783	28
-4	16	10	220	193	46
-3	16	10	1049	1009	28
-2	16	10	544	527	30
-1	16	10	59	-28	-59
0	16	10	390	364	35
1	16	10	437	-457	34
2	16	10	447	413	39
3	16	10	827	-817	35
4	16	10	116	169	-116
-10	17	10	207	312	-73
-9	17	10	66	7	-66
-8	17	10	773	789	33
-7	17	10	66	14	-66
-6	17	10	1068	1109	29
-5	17	10	122	-19	-86
-4	17	10	913	897	28
-3	17	10	57	-31	-57
-2	17	10	461	451	33
-1	17	10	123	-154	-123
0	17	10	231	-250	40
1	17	10	233	-124	53
2	17	10	690	-657	34
3	17	10	306	194	51
-10	18	10	473	479	42
-9	18	10	450	459	39
-8	18	10	505	481	34
-7	18	10	610	611	34
-6	18	10	138	-134	-96
-5	18	10	753	754	29
-4	18	10	276	-274	41
-3	18	10	470	459	32
-2	18	10	801	-852	30
-1	18	10	247	219	44
0	18	10	562	-542	29
1	18	10	299	-365	48
2	18	10	467	-396	39
3	18	10	462	-399	38
-9	19	10	820	813	35
-8	19	10	233	266	-58
-7	19	10	371	419	38
-6	19	10	212	183	46

h	k	l	10Fo	10Fc	10s
-5	19	10	322	-294	37
-4	19	10	262	193	38
-3	19	10	767	-781	30
-2	19	10	61	97	-61
-1	19	10	993	-995	29
0	19	10	62	69	-44
1	19	10	709	-681	33
2	19	10	220	-156	-56
3	19	10	422	-417	41
-9	20	10	327	-340	42
-8	20	10	320	393	47
-7	20	10	463	-544	37
-6	20	10	63	53	-63
-5	20	10	147	-227	-76
-4	20	10	426	-443	32
-3	20	10	357	-349	38
-2	20	10	822	-785	29
-1	20	10	97	79	-97
0	20	10	832	-791	24
1	20	10	133	52	-133
2	20	10	580	-528	38
-8	21	10	590	-606	37
-7	21	10	262	233	47
-6	21	10	833	-818	31
-5	21	10	61	62	-61
-4	21	10	800	-821	30
-3	21	10	229	-229	52
-2	21	10	272	-310	44
-1	21	10	404	-406	36
0	21	10	216	202	41
1	21	10	215	-137	52
2	21	10	746	694	34
-8	22	10	194	-279	-99
-7	22	10	725	-758	32
-6	22	10	173	135	-69
-5	22	10	1037	-1010	30
-4	22	10	158	62	-56
-3	22	10	444	-460	36
-2	22	10	209	238	48
-1	22	10	248	-165	47
0	22	10	61	-13	-43
1	22	10	502	472	36
-7	23	10	332	-263	39
-6	23	10	490	-486	36
-5	23	10	197	143	-50
-4	23	10	361	-386	39
-3	23	10	451	468	38
-2	23	10	252	-266	37
-1	23	10	602	573	33
0	23	10	116	16	-58
1	23	10	588	558	35
-6	24	10	61	-177	-61
-5	24	10	140	50	-80
-4	24	10	565	546	32
-3	24	10	150	42	-66
-2	24	10	659	660	32

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-1	24	10	59	-48	-59
0	24	10	742	748	24
-5	25	10	59	94	-59
-4	25	10	397	361	37
-3	25	10	799	752	32
-2	25	10	59	-24	-59
-1	25	10	702	675	32
-11	0	11	704	698	40
-9	0	11	77	-87	-77
-7	0	11	484	-445	36
-5	0	11	974	-951	29
-3	0	11	1266	-1307	28
-1	0	11	876	-916	30
1	0	11	68	-127	-68
3	0	11	385	387	44
-12	1	11	464	451	47
-11	1	11	352	-339	51
-10	1	11	352	347	49
-9	1	11	728	-713	35
-8	1	11	422	-390	38
-7	1	11	441	-405	38
-6	1	11	556	-547	32
-5	1	11	144	-152	-79
-4	1	11	1058	-1074	28
-3	1	11	255	228	42
-2	1	11	738	-785	31
-1	1	11	482	475	33
0	1	11	370	-399	28
1	1	11	702	668	34
2	1	11	177	74	-56
3	1	11	533	463	43
4	1	11	506	407	42
-12	2	11	311	-440	70
-11	2	11	87	115	-87
-10	2	11	900	-893	35
-9	2	11	108	21	-108
-8	2	11	840	-864	32
-7	2	11	141	-131	-106
-6	2	11	740	-732	30
-5	2	11	232	-186	41
-4	2	11	94	9	-94
-3	2	11	210	-50	40
-2	2	11	269	247	44
-1	2	11	194	-106	-57
0	2	11	1193	1244	44
1	2	11	232	-183	56
2	2	11	821	860	34
3	2	11	175	20	-112
4	2	11	673	642	41
-12	3	11	89	-154	-89
-11	3	11	634	-639	42
-10	3	11	131	-208	-131
-9	3	11	949	-944	34
-8	3	11	239	261	53
-7	3	11	784	-724	31
-6	3	11	256	227	46
-5	3	11	507	-495	32
-4	3	11	740	704	30
-3	3	11	59	-37	-59
-2	3	11	580	672	31
-1	3	11	519	552	34
0	3	11	378	382	26
1	3	11	958	1036	32
2	3	11	72	-30	-72
3	3	11	775	675	36
4	3	11	314	-339	63
-12	4	11	194	-186	-112
-11	4	11	494	-455	46
-10	4	11	388	-426	47
-9	4	11	75	70	-75
-8	4	11	521	-452	34
-7	4	11	635	600	32
-6	4	11	349	-285	38
-5	4	11	1001	951	29
-4	4	11	63	-2	-63
-3	4	11	794	796	30
-2	4	11	417	398	34
-1	4	11	579	564	32
0	4	11	567	578	38
1	4	11	104	-52	-104
2	4	11	571	555	37
3	4	11	369	-325	45
4	4	11	186	109	-113
-11	5	11	82	-58	-82
-10	5	11	366	-328	49
-9	5	11	342	291	43
-8	5	11	459	351	36
-7	5	11	207	-184	-60
-6	5	11	929	899	30
-5	5	11	61	95	-61
-4	5	11	1246	1207	28
-3	5	11	154	35	-68
-2	5	11	967	985	29
-1	5	11	148	-126	-69
0	5	11	494	447	25
1	5	11	224	-245	-61
2	5	11	154	-109	-93
3	5	11	304	-277	50
4	5	11	801	-748	39
-11	6	11	608	-526	38
-10	6	11	673	623	39
-9	6	11	216	-187	-79
-8	6	11	799	768	33
-7	6	11	464	483	37
-6	6	11	364	352	36
-5	6	11	743	748	30
-4	6	11	66	-98	-66
-3	6	11	964	951	29
-2	6	11	463	-430	34
-1	6	11	434	421	35
0	6	11	817	-864	29
1	6	11	65	162	-65
2	6	11	605	-612	35
3	6	11	199	-225	-70
4	6	11	525	-472	41
-11	7	11	658	653	42
-10	7	11	80	91	-80
-9	7	11	1222	1176	33
-8	7	11	158	188	-126
-7	7	11	1143	1133	31
-6	7	11	187	164	-64
-5	7	11	329	299	36
-4	7	11	56	-57	-56
-3	7	11	390	-403	38
-2	7	11	227	187	48
-1	7	11	1039	-1041	30
0	7	11	172	-101	-58
1	7	11	1088	-1098	32
2	7	11	198	4	-54
3	7	11	912	-847	37
4	7	11	263	-87	55
-11	8	11	240	250	-75
-10	8	11	1101	1042	35
-9	8	11	187	178	-84
-8	8	11	1256	1293	32
-7	8	11	192	86	-74
-6	8	11	941	953	30
-5	8	11	587	-576	31
-4	8	11	331	331	40
-3	8	11	451	-437	33
-2	8	11	599	-643	32
-1	8	11	585	-568	32
0	8	11	943	-949	22
1	8	11	199	-37	-66
2	8	11	1050	-1009	33
3	8	11	297	270	48
4	8	11	506	-514	43
-11	9	11	741	667	39
-10	9	11	186	30	-85
-9	9	11	73	19	-73
-8	9	11	636	-688	34
-7	9	11	200	73	-55
-6	9	11	1029	-1074	30
-5	9	11	55	-90	-55
-4	9	11	1254	-1263	28
-3	9	11	65	-112	-65
-2	9	11	907	-920	30
-1	9	11	429	-435	33
0	9	11	382	-377	28
1	9	11	313	-280	45
2	9	11	350	369	40
3	9	11	325	-247	53
4	9	11	734	704	38
-11	10	11	492	497	49
-10	10	11	355	-284	48
-9	10	11	198	-174	-54
-8	10	11	395	-437	36
-7	10	11	904	-860	31
-6	10	11	170	-216	-90
-5	10	11	913	-897	29
-4	10	11	239	225	51
-3	10	11	1151	-1129	29
-2	10	11	192	170	46
-1	10	11	619	-635	32
0	10	11	292	263	33
1	10	11	233	-234	-61
2	10	11	74	136	-74
3	10	11	592	550	40
4	10	11	157	110	-157
-11	11	11	814	-792	39
-10	11	11	208	295	-85
-9	11	11	748	-739	35
-8	11	11	148	9	-91
-7	11	11	840	-823	32
-6	11	11	712	-691	31
-5	11	11	293	-382	43
-4	11	11	662	-688	30
-3	11	11	166	162	-66
-2	11	11	737	-748	30
-1	11	11	698	635	31
0	11	11	273	-283	33
1	11	11	846	775	33
2	11	11	244	169	47
3	11	11	773	732	39
-10	12	11	1032	-1048	35
-9	12	11	282	194	50
-8	12	11	726	-693	33
-7	12	11	130	4	-130
-6	12	11	480	-497	32
-5	12	11	125	-163	-125
-4	12	11	135	-66	-83
-3	12	11	136	-112	-88
-2	12	11	582	633	30
-1	12	11	62	27	-62
0	12	11	850	797	22
1	12	11	160	-15	-84
2	12	11	1031	959	33
3	12	11	78	-9	-78
-10	13	11	132	-111	-132
-9	13	11	700	-673	35
-8	13	11	438	410	34
-7	13	11	814	-801	31
-6	13	11	572	612	34
-5	13	11	443	-399	34
-4	13	11	565	594	31
-3	13	11	216	227	36
-2	13	11	618	628	32
-1	13	11	742	723	32
0	13	11	190	137	46
1	13	11	895	901	33
2	13	11	254	-235	58
3	13	11	712	669	39
-10	14	11	163	118	-93
-9	14	11	200	-328	-84
-8	14	11	183	-138	-67
-7	14	11	447	448	33
-6	14	11	65	-142	-65
-5	14	11	782	808	30
-4	14	11	136	-19	-84
-3	14	11	1270	1251	29
-2	14	11	168	111	-65
-1	14	11	625	664	32
0	14	11	263	242	38
1	14	11	228	229	-69
2	14	11	156	262	-156
3	14	11	349	-383	51
-10	15	11	133	-118	-133
-9	15	11	200	134	-69
-8	15	11	65	125	-65
-7	15	11	144	189	-95
-6	15	11	751	779	31
-5	15	11	62	12	-62
-4	15	11	920	906	30
-3	15	11	232	-204	49
-2	15	11	852	827	30
-1	15	11	369	-380	37
0	15	11	430	405	26
1	15	11	329	-266	42
2	15	11	202	-95	-60
-9	16	11	71	126	-71
-8	16	11	799	723	32
-7	16	11	221	219	-62
-6	16	11	429	467	37
-5	16	11	376	434	40
-4	16	11	159	79	-64
-3	16	11	357	391	40
-2	16	11	526	-522	32
-1	16	11	425	413	37
0	16	11	560	-516	31
1	16	11	261	133	48
2	16	11	613	-592	37
-9	17	11	795	785	35
-8	17	11	185	-63	-58
-7	17	11	827	840	33
-6	17	11	313	-256	44
-5	17	11	205	282	-62
-4	17	11	61	-30	-61
-3	17	11	65	-67	-65
-2	17	11	114	-126	-114
-1	17	11	791	-721	31
0	17	11	280	179	39
1	17	11	879	-838	33
2	17	11	69	-15	-69
-9	18	11	192	23	-70
-8	18	11	569	596	36
-7	18	11	400	-454	41
-6	18	11	401	349	34
-5	18	11	496	-451	31
-4	18	11	60	73	-60
-3	18	11	704	-676	30

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-2	18	11	215	-228	51
-1	18	11	241	-312	59
0	18	11	651	-603	24
1	18	11	316	-142	41
-8	19	11	271	-284	53
-7	19	11	147	97	-78
-6	19	11	641	-631	32
-5	19	11	152	169	-97
-4	19	11	807	-863	32
-3	19	11	62	44	-62
-2	19	11	826	-875	31
-1	19	11	166	-170	-70
0	19	11	634	-557	27
1	19	11	347	-318	46
-8	20	11	197	-302	-75
-7	20	11	459	-460	38
-6	20	11	167	-175	-73
-5	20	11	645	-639	32
-4	20	11	163	-46	-62
-3	20	11	772	-805	31
-2	20	11	279	288	43
-1	20	11	512	-485	34
0	20	11	403	358	40
-7	21	11	661	-688	35
-6	21	11	66	-35	-66
-5	21	11	202	-235	-61
-4	21	11	312	-345	41
-3	21	11	130	172	-130
-2	21	11	320	-335	45
-1	21	11	704	693	33
0	21	11	155	-5	-68
-6	22	11	607	-610	36
-5	22	11	68	152	-68
-4	22	11	82	-37	-82
-3	22	11	144	103	-94
-2	22	11	212	274	-56
-1	22	11	67	26	-67
-5	23	11	264	-153	38
-4	23	11	625	621	34
-3	23	11	204	237	-58
-2	23	11	447	470	35
-10	0	12	511	-497	43
-8	0	12	648	-631	36
-6	0	12	1255	-1260	31
-4	0	12	666	-687	32
-2	0	12	174	-181	-61
0	0	12	721	784	34
2	0	12	648	619	37
-11	1	12	199	-224	-100
-10	1	12	524	-514	43
-9	1	12	509	-515	41
-8	1	12	223	-125	46
-7	1	12	653	-662	34
-6	1	12	281	340	47
-5	1	12	877	-886	31
-4	1	12	716	716	31

h	k	l	10Fo	10Fc	10s
-3	1	12	257	-191	39
-2	1	12	498	516	33
-1	1	12	238	239	51
0	1	12	475	457	28
1	1	12	744	754	34
2	1	12	133	121	-133
3	1	12	481	396	46
-11	2	12	649	-627	42
-10	2	12	165	-188	-124
-9	2	12	533	-528	37
-8	2	12	231	-223	-58
-7	2	12	134	-1	-134
-6	2	12	155	-219	-93
-5	2	12	620	674	35
-4	2	12	207	-215	-58
-3	2	12	1086	1076	30
-2	2	12	116	-49	-116
-1	2	12	1051	1158	31
0	2	12	331	193	59
1	2	12	552	516	36
2	2	12	240	282	-65
3	2	12	121	127	-121
-11	3	12	75	11	-75
-10	3	12	634	-588	39
-9	3	12	416	342	43
-8	3	12	71	-224	-71
-7	3	12	374	368	39
-6	3	12	166	-8	-97
-5	3	12	755	791	33
-4	3	12	674	661	31
-3	3	12	294	240	41
-2	3	12	925	925	31
-1	3	12	157	66	-95
0	3	12	694	740	35
1	3	12	230	-337	-66
2	3	12	377	348	46
3	3	12	281	-347	53
-11	4	12	452	-427	51
-10	4	12	386	298	50
-9	4	12	78	-147	-78
-8	4	12	788	730	33
-7	4	12	66	-45	-66
-6	4	12	1074	1051	31
-5	4	12	299	229	36
-4	4	12	602	651	34
-3	4	12	522	508	35
-2	4	12	67	61	-67
-1	4	12	466	434	36
0	4	12	513	-509	60
1	4	12	239	204	52
2	4	12	660	-658	38
3	4	12	199	137	-79
-11	5	12	264	216	-66
-10	5	12	233	195	-71
-9	5	12	716	713	36
-8	5	12	138	188	-138

h	k	l	10Fo	10Fc	10s
-7	5	12	925	944	32
-6	5	12	186	234	-71
-5	5	12	947	955	31
-4	5	12	64	-100	-64
-3	5	12	383	315	34
-2	5	12	65	-63	-65
-1	5	12	215	-296	-62
0	5	12	223	-261	41
1	5	12	669	-744	35
2	5	12	73	-107	-73
3	5	12	725	-783	41
-11	6	12	628	554	42
-10	6	12	381	401	48
-9	6	12	412	385	43
-8	6	12	624	587	36
-7	6	12	66	-66	-66
-6	6	12	496	508	34
-5	6	12	580	-555	34
-4	6	12	539	554	32
-3	6	12	676	-686	32
-2	6	12	165	42	-69
-1	6	12	827	-870	31
0	6	12	244	-257	39
1	6	12	285	-314	41
2	6	12	667	-691	39
3	6	12	323	-329	46
-10	7	12	1064	1048	37
-9	7	12	281	292	54
-8	7	12	569	576	38
-7	7	12	288	376	55
-6	7	12	228	-240	47
-5	7	12	100	69	-100
-4	7	12	784	-832	32
-3	7	12	100	122	-100
-2	7	12	1120	-1212	31
-1	7	12	293	-349	43
0	7	12	988	-984	25
1	7	12	156	-187	-119
2	7	12	555	-535	40
3	7	12	199	-141	-92
-10	8	12	369	-329	50
-9	8	12	612	601	36
-8	8	12	546	-537	39
-7	8	12	60	-8	-60
-6	8	12	622	-626	32
-5	8	12	593	-567	33
-4	8	12	350	-319	34
-3	8	12	828	-863	32
-2	8	12	70	-34	-70
-1	8	12	650	-667	33
0	8	12	296	261	34
1	8	12	535	-550	38
2	8	12	575	545	41
-10	9	12	78	-98	-78
-9	9	12	902	-918	35
-8	9	12	305	251	51

h	k	l	10Fo	10Fc	10s
-7	9	12	1068	-1054	32
-6	9	12	265	-200	46
-5	9	12	827	-819	32
-4	9	12	182	-180	-60
-3	9	12	225	-227	-56
-2	9	12	473	-495	36
-1	9	12	104	148	-104
0	9	12	312	-317	35
1	9	12	624	600	37
2	9	12	396	-340	47
-10	10	12	432	-394	42
-9	10	12	70	-112	-70
-8	10	12	823	-819	35
-7	10	12	104	-16	-104
-6	10	12	965	-948	31
-5	10	12	267	243	47
-4	10	12	675	-712	31
-3	10	12	225	197	47
-2	10	12	131	-120	-131
-1	10	12	306	369	50
0	10	12	369	348	35
1	10	12	192	-15	-61
2	10	12	1004	905	36
-10	11	12	406	-329	50
-9	11	12	204	-307	-83
-8	11	12	512	-442	35
-7	11	12	787	-783	33
-6	11	12	222	198	51
-5	11	12	535	-575	34
-4	11	12	482	519	33
-3	11	12	430	-382	34
-2	11	12	797	806	32
-1	11	12	147	148	-112
0	11	12	684	655	25
1	11	12	416	402	43
2	11	12	391	223	45
-10	12	12	77	154	-77
-9	12	12	511	-491	38
-8	12	12	74	-76	-74
-7	12	12	61	-81	-61
-6	12	12	69	-70	-69
-5	12	12	616	636	32
-4	12	12	66	-49	-66
-3	12	12	935	937	31
-2	12	12	177	66	-47
-1	12	12	864	890	33
0	12	12	273	-156	45
1	12	12	772	744	35
2	12	12	242	28	50
-9	13	12	385	390	40
-8	13	12	344	-398	51
-7	13	12	599	562	35
-6	13	12	514	506	36
-5	13	12	427	420	36
-4	13	12	509	593	37
-3	13	12	235	243	51

h	k	l	10Fo	10Fc	10s
-2	13	12	800	744	31
-1	13	12	226	-188	54
0	13	12	703	663	43
1	13	12	433	-466	44
-9	14	12	326	-319	44
-8	14	12	902	885	33
-7	14	12	150	-116	-74
-6	14	12	825	854	33
-5	14	12	212	139	41
-4	14	12	483	538	33
-3	14	12	229	232	49
-2	14	12	66	-95	-66
-1	14	12	421	406	40
0	14	12	429	-380	34
1	14	12	366	276	43
-9	15	12	497	442	40
-8	15	12	228	142	53
-7	15	12	779	795	34
-6	15	12	190	-181	-67
-5	15	12	656	664	33
-4	15	12	282	-308	45
-3	15	12	407	444	42
-2	15	12	544	-553	36
-1	15	12	63	-29	-63
0	15	12	436	-401	28
1	15	12	367	-274	41
-8	16	12	448	470	40
-7	16	12	163	-79	-80
-6	16	12	523	528	34
-5	16	12	252	-305	52
-4	16	12	307	310	37
-3	16	12	758	-753	32
-2	16	12	65	-26	-65
-1	16	12	597	-624	35
0	16	12	184	-109	46
-8	17	12	381	378	44
-7	17	12	72	-181	-72
-6	17	12	70	-86	-70
-5	17	12	66	54	-66
-4	17	12	611	-636	33
-3	17	12	189	-115	-74
-2	17	12	995	-1067	33
-1	17	12	268	151	44
0	17	12	455	-479	43
-7	18	12	72	48	-72
-6	18	12	499	-497	37
-5	18	12	274	-289	49
-4	18	12	462	-487	34
-3	18	12	763	-768	34
-2	18	12	121	-45	-121
-1	18	12	579	-618	35
-6	19	12	137	58	-137
-5	19	12	749	-744	33
-4	19	12	180	-182	-72
-3	19	12	436	-437	38
-2	19	12	105	-167	-105

Observed and calculated structure factors for $Re(CO)_3Cl(hhtn)\cdot MeOH$

h	k	l	10Fo	10Fc	10s
-5	20	12	121	144	-121
-4	20	12	325	-395	46
-3	20	12	589	619	34
-9	0	13	794	-768	38
-7	0	13	454	-469	41
-5	0	13	64	-5	-64
-3	0	13	527	569	37
-1	0	13	807	850	34
1	0	13	786	837	36
-10	1	13	702	-700	40
-9	1	13	419	426	48
-8	1	13	574	-511	36
-7	1	13	533	510	37
-6	1	13	336	-274	45
-5	1	13	643	685	35
-4	1	13	410	436	39
-3	1	13	443	397	38
-2	1	13	445	529	39
-1	1	13	316	297	47
0	1	13	820	850	29
1	1	13	295	-238	56
-10	2	13	83	-81	-83
-9	2	13	338	-359	51
-8	2	13	751	807	35
-7	2	13	272	-296	51
-6	2	13	1029	1010	33
-5	2	13	72	143	-72
-4	2	13	998	1009	32
-3	2	13	149	267	-98
-2	2	13	454	498	36
-1	2	13	316	346	46
0	2	13	72	-22	-51
1	2	13	271	244	58
-10	3	13	436	421	47
-9	3	13	209	240	-85
-8	3	13	249	272	-67
-7	3	13	750	725	34
-6	3	13	246	222	52
-5	3	13	1013	1039	33
-4	3	13	297	-294	53
-3	3	13	742	794	34
-2	3	13	239	-218	53
-1	3	13	369	263	35
0	3	13	313	-333	34
1	3	13	203	-261	-68
-10	4	13	78	-4	-78
-9	4	13	895	895	35
-8	4	13	78	140	-78
-7	4	13	631	608	36
-6	4	13	358	375	42
-5	4	13	121	187	-121
-4	4	13	449	404	39
-3	4	13	381	-369	39
-2	4	13	231	225	53
-1	4	13	735	-760	35
0	4	13	196	-69	-54
1	4	13	911	-950	37
-10	5	13	887	812	38
-9	5	13	133	-108	-133
-8	5	13	624	624	37
-7	5	13	225	157	-59
-6	5	13	380	304	42
-5	5	13	68	-86	-68
-4	5	13	432	-393	38
-3	5	13	70	97	-70
-2	5	13	525	-606	38
-1	5	13	179	-285	-86
0	5	13	990	-1029	25
1	5	13	262	-112	52
-9	6	13	370	429	49
-8	6	13	358	-411	51
-7	6	13	456	336	39
-6	6	13	531	-552	37
-5	6	13	69	-59	-69
-4	6	13	793	-792	33
-3	6	13	401	-393	35
-2	6	13	433	-475	39
-1	6	13	627	-641	34
0	6	13	274	-252	42
1	6	13	668	-706	38
-9	7	13	75	-142	-75
-8	7	13	214	197	-66
-7	7	13	666	-641	35
-6	7	13	72	-36	-72
-5	7	13	984	-968	32
-4	7	13	70	82	-70
-3	7	13	851	-853	33
-2	7	13	316	-310	50
-1	7	13	284	-326	54
0	7	13	84	125	-62
1	7	13	254	278	62
-9	8	13	537	-559	43
-8	8	13	474	-492	43
-7	8	13	371	-347	41
-6	8	13	691	-685	35
-5	8	13	72	57	-72
-4	8	13	727	-732	33
-3	8	13	67	245	-67
-2	8	13	367	-433	40
-1	8	13	508	515	38
0	8	13	213	61	39
1	8	13	564	537	42
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-8	9	13	578	-580	39
-7	9	13	288	-253	52
-6	9	13	186	-215	-95
-5	9	13	259	-275	53
-4	9	13	122	96	-122
-3	9	13	447	-495	38
-2	9	13	606	548	34
-1	9	13	127	-77	-127
0	9	13	689	721	33
-9	10	13	858	-814	38
-8	10	13	130	79	-130
-7	10	13	669	-638	36
-6	10	13	69	101	-69
-5	10	13	62	-65	-62
-4	10	13	220	216	54
-3	10	13	481	446	37
-2	10	13	225	201	46
-1	10	13	932	888	34
0	10	13	86	77	-63
-8	11	13	519	-519	39
-7	11	13	539	642	40
-6	11	13	124	-102	-124
-5	11	13	735	750	34
-4	11	13	64	-84	-64
-3	11	13	560	580	36
-2	11	13	518	543	37
-1	11	13	128	166	-128
0	11	13	486	475	28
-8	12	13	436	432	42
-7	12	13	110	82	-110
-6	12	13	921	871	34
-5	12	13	62	-55	-62
-4	12	13	838	832	33
-3	12	13	255	-182	49
-2	12	13	647	628	35
-1	12	13	72	-5	-72
-8	13	13	446	399	43
-7	13	13	711	647	35
-6	13	13	217	197	-64
-5	13	13	465	485	39
-4	13	13	123	-71	-123
-3	13	13	810	778	34
-2	13	13	636	-601	35
-1	13	13	287	244	47
-7	14	13	435	466	44
-6	14	13	188	225	-66
-5	14	13	59	-83	-59
-4	14	13	370	303	39
-3	14	13	581	-636	39
-2	14	13	382	369	46
-1	14	13	909	-922	35
-7	15	13	392	-338	40
-6	15	13	259	239	52
-5	15	13	304	-277	34
-4	15	13	68	-129	-68
-3	15	13	390	-374	43
-2	15	13	602	-602	37
-6	16	13	640	-693	36
-5	16	13	108	-9	-108
-4	16	13	810	-786	34
-3	16	13	74	1	-74
-8	0	14	133	75	-133
-6	0	14	462	479	43
-4	0	14	934	1019	35
-2	0	14	740	788	35
-8	1	14	565	515	41
-7	1	14	159	209	-132
-6	1	14	567	569	38
-5	1	14	586	594	35
-4	1	14	255	214	48
-3	1	14	789	799	35
-2	1	14	196	-115	-72
-1	1	14	513	559	39
-8	2	14	75	16	-75
-7	2	14	725	635	35
-6	2	14	301	259	53
-5	2	14	673	631	37
-4	2	14	221	288	-69
-3	2	14	75	-59	-75
-2	2	14	357	371	43
-1	2	14	267	-346	61
-8	3	14	816	789	35
-7	3	14	172	-157	-62
-6	3	14	865	827	35
-5	3	14	312	-320	49
-4	3	14	312	284	40
-3	3	14	144	-197	-144
-2	3	14	313	-322	52
-1	3	14	212	-160	-60
-8	4	14	73	8	-73
-7	4	14	564	475	38
-6	4	14	308	-349	54
-5	4	14	312	312	48
-4	4	14	795	-814	35
-3	4	14	112	-76	-112
-2	4	14	679	-744	35
-1	4	14	348	-352	49
-8	5	14	250	-143	59
-7	5	14	206	-289	-73
-6	5	14	65	-55	-65
-5	5	14	683	-719	36
-4	5	14	180	92	-75
-3	5	14	933	-885	34
-2	5	14	173	-17	-76
-1	5	14	716	-759	38
-8	6	14	134	-3	-134
-7	6	14	391	-380	45
-6	6	14	532	-525	41
-5	6	14	460	-522	42
-4	6	14	612	-629	40
-3	6	14	74	74	-74
-2	6	14	556	-558	37
-7	7	14	113	5	-113
-6	7	14	669	-589	37
-5	7	14	63	-53	-63
-4	7	14	169	-143	-65
-3	7	14	74	16	-74
-2	7	14	404	463	45
-7	8	14	746	-724	36
-6	8	14	194	187	-83
-5	8	14	373	-368	44
-4	8	14	286	299	49
-3	8	14	69	-103	-69
-2	8	14	353	324	46
-7	9	14	147	234	-147
-6	9	14	234	-183	-59
-5	9	14	566	589	36
-4	9	14	71	-74	-71
-3	9	14	594	618	41
-6	10	14	636	604	37
-5	10	14	78	160	-78
-4	10	14	567	625	39
-3	10	14	73	-20	-73
-5	11	14	402	389	41
-4	11	14	70	176	-70

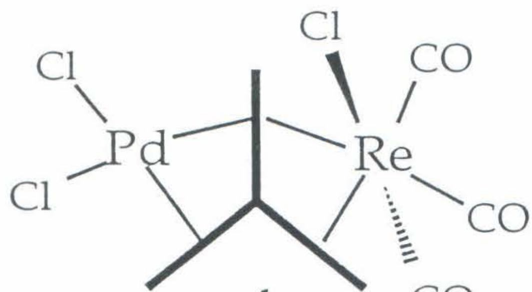

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Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
1	0	0	77	96	77
2	0	0	806	843	17
3	0	0	207	282	59
4	0	0	1655	1595	21
5	0	0	765	792	27
6	0	0	967	1005	29
7	0	0	593	607	35
8	0	0	1226	1217	33
9	0	0	750	670	38
10	0	0	575	616	46
11	0	0	258	269	86
12	0	0	84	54	84
13	0	0	665	703	54
14	0	0	400	456	41
-14	1	0	96	97	96
-13	1	0	0	144	1
-12	1	0	293	184	79
-11	1	0	1729	1634	42
-10	1	0	194	76	107
-9	1	0	257	48	57
-8	1	0	304	371	53
-7	1	0	512	455	37
-6	1	0	130	195	130
-5	1	0	1230	1279	26
-4	1	0	1572	1449	23
-3	1	0	712	790	24
-2	1	0	2012	2190	17
-1	1	0	2090	1916	13
0	1	0	836	628	12
1	1	0	629	727	14
2	1	0	1189	1176	16
3	1	0	1040	1162	20
4	1	0	1826	1899	21
5	1	0	486	428	32
6	1	0	586	596	33
7	1	0	168	43	98
8	1	0	524	602	38
9	1	0	220	196	61
10	1	0	391	341	47
11	1	0	327	271	63
12	1	0	1063	1018	46
13	1	0	151	29	151
14	1	0	247	241	60
15	1	0	219	225	77
-14	2	0	415	392	43
-13	2	0	556	567	33
-12	2	0	438	490	70
-11	2	0	0	179	1
-10	2	0	0	150	1
-9	2	0	764	798	41
-8	2	0	146	74	117
-7	2	0	521	518	40
-6	2	0	717	765	32
-5	2	0	1389	1408	27
-4	2	0	357	319	38
-3	2	0	1558	1563	21
-2	2	0	830	824	22
-1	2	0	455	436	27
0	2	0	1055	964	17
1	2	0	2349	2459	15
2	2	0	283	243	40
3	2	0	463	480	29
4	2	0	700	675	25
5	2	0	609	567	30
6	2	0	949	972	28
7	2	0	1039	1161	30
8	2	0	311	402	57
9	2	0	461	452	44
10	2	0	777	769	40
11	2	0	417	374	55
12	2	0	346	251	56
13	2	0	0	198	1
14	2	0	795	730	56
15	2	0	238	197	59
-13	3	0	78	124	78
-12	3	0	196	185	154
-11	3	0	544	412	46
-10	3	0	633	624	44
-9	3	0	0	39	1
-8	3	0	0	78	1
-7	3	0	1009	1039	34
-6	3	0	585	586	35
-5	3	0	1069	985	29
-4	3	0	1013	988	26
-3	3	0	522	477	29
-2	3	0	999	963	24
-1	3	0	2214	2115	20
0	3	0	509	593	28
1	3	0	207	86	60
2	3	0	646	586	24
3	3	0	1675	1666	20
4	3	0	129	99	128
5	3	0	321	372	44
6	3	0	0	121	1
7	3	0	1137	1124	30
8	3	0	693	704	36
9	3	0	1143	1091	36
10	3	0	254	283	70
11	3	0	185	58	112
12	3	0	303	462	80
13	3	0	613	569	53
14	3	0	317	279	101
15	3	0	115	53	115
-13	4	0	185	272	102
-12	4	0	594	613	33
-11	4	0	237	91	94
-10	4	0	0	60	1
-9	4	0	503	450	47
-8	4	0	969	988	38
-7	4	0	67	23	67
-6	4	0	391	435	44
-5	4	0	292	273	53
-4	4	0	1056	1038	29
-3	4	0	912	888	28
-2	4	0	2045	1956	24
-1	4	0	0	86	1
0	4	0	1106	1098	23
1	4	0	1223	1275	22
2	4	0	1308	1221	22
3	4	0	154	81	105
4	4	0	209	257	68
5	4	0	1350	1288	26
6	4	0	975	976	29
7	4	0	1308	1303	30
8	4	0	677	693	36
9	4	0	330	291	51
10	4	0	158	84	158
11	4	0	1007	981	40
12	4	0	179	216	149
13	4	0	209	158	95
14	4	0	201	130	83
15	4	0	724	703	34
-12	5	0	262	87	44
-11	5	0	262	259	56
-10	5	0	753	682	44
-9	5	0	230	161	68
-8	5	0	73	175	72
-7	5	0	371	386	48
-6	5	0	733	745	38
-5	5	0	615	631	36
-4	5	0	1162	1145	30
-3	5	0	370	302	40
-2	5	0	624	645	32
-1	5	0	262	214	54
0	5	0	2085	2170	24
1	5	0	722	708	27
2	5	0	159	34	102
3	5	0	858	854	27
4	5	0	1578	1689	25
5	5	0	993	1055	28
6	5	0	1016	942	29
7	5	0	651	642	33
8	5	0	433	377	38
9	5	0	485	472	43
10	5	0	634	631	41
11	5	0	150	61	150
12	5	0	197	127	103
13	5	0	771	837	52
14	5	0	359	405	81
15	5	0	413	401	42
-11	6	0	474	490	34
-10	6	0	166	62	166
-9	6	0	0	75	1
-8	6	0	472	524	48
-7	6	0	707	663	39
-6	6	0	115	176	115
-5	6	0	410	394	48
-4	6	0	608	558	36
-3	6	0	610	591	33
-2	6	0	1259	1245	29
-1	6	0	541	593	34
0	6	0	672	655	30
1	6	0	145	127	144
2	6	0	2037	1932	25
3	6	0	886	924	28
4	6	0	1380	1397	27
5	6	0	433	435	38
6	6	0	582	627	34
7	6	0	470	445	43
8	6	0	319	277	41
9	6	0	337	346	54
10	6	0	327	431	64
11	6	0	226	198	102
12	6	0	1266	1217	43
13	6	0	0	61	1
14	6	0	266	135	85
15	6	0	394	382	42
-10	7	0	123	89	122
-9	7	0	751	734	45
-8	7	0	244	270	100
-7	7	0	460	519	48
-6	7	0	274	219	58
-5	7	0	742	768	38
-4	7	0	128	107	127
-3	7	0	594	622	38
-2	7	0	423	339	40
-1	7	0	797	746	31
0	7	0	909	891	31
1	7	0	2047	2043	28
2	7	0	444	424	36
3	7	0	504	554	34
4	7	0	674	702	33
5	7	0	502	456	34
6	7	0	702	699	34
7	7	0	974	982	33
8	7	0	673	610	38
9	7	0	265	363	71
10	7	0	707	726	43
11	7	0	295	279	63
12	7	0	82	72	82
13	7	0	187	105	157
14	7	0	806	866	53
15	7	0	0	41	1
-10	8	0	430	412	37
-9	8	0	0	45	1
-8	8	0	81	27	80
-7	8	0	553	512	47
-6	8	0	313	346	63
-5	8	0	510	415	47
-4	8	0	402	415	48
-3	8	0	661	675	38
-2	8	0	237	220	69
-1	8	0	1334	1362	32
0	8	0	488	516	39
1	8	0	212	318	72
2	8	0	132	231	131
3	8	0	1409	1413	31
4	8	0	369	396	45
5	8	0	428	476	42
6	8	0	921	941	33
7	8	0	861	849	36
8	8	0	69	44	68
9	8	0	712	706	39
10	8	0	163	125	163
11	8	0	242	285	73
12	8	0	661	694	51
13	8	0	589	587	53
14	8	0	92	154	91
15	8	0	109	61	108
-9	9	0	54	43	53
-8	9	0	530	505	30
-7	9	0	225	139	71
-6	9	0	287	261	73
-5	9	0	614	643	47
-4	9	0	679	716	42
-3	9	0	208	233	82
-2	9	0	703	728	39
-1	9	0	0	82	1
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3	9	0	185	219	79
4	9	0	187	79	88
5	9	0	927	1016	35
6	9	0	251	149	60
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10	9	0	166	157	165
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3	10	0	728	615	35
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7	11	0	142	188	142
8	11	0	818	775	39
9	11	0	477	439	49
10	11	0	544	522	47
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3	15	0	328	289	34
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5	15	0	167	168	73
6	15	0	208	121	39
7	15	0	470	464	29
8	15	0	384	407	34
9	15	0	198	272	58
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-3	-15	1	380	394	32
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-10	-10	1	266	316	74
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-8	-10	1	666	597	42
-7	-10	1	421	344	40
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Table 1. Observed and calculated structure factors for 1

Page 2

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7	-10	1	555	583	30
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-12	-9	1	284	155	58
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-9	-9	1	252	292	74
-8	-9	1	650	671	42
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-6	-9	1	628	545	38
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5	-9	1	346	299	52
6	-9	1	628	577	46
7	-9	1	79	86	79
8	-9	1	145	100	118
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h	k	l	10Fo	10Fc	10s
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1	3	1	1007	902	19
2	3	1	263	230	44
3	3	1	1000	975	21
4	3	1	1393	1458	22
5	3	1	680	710	27

h	k	l	10Fo	10Fc	10s
6	3	1	681	685	31
7	3	1	300	304	49
8	3	1	802	855	35
9	3	1	366	219	46
10	3	1	1186	1232	37
11	3	1	223	193	86
12	3	1	0	55	1
13	3	1	306	423	106
14	3	1	702	675	56
15	3	1	234	210	64
-12	4	1	204	204	59
-11	4	1	780	668	51
-10	4	1	178	265	178
-9	4	1	150	101	150
-8	4	1	141	135	141
-7	4	1	938	940	35
-6	4	1	107	91	106
-5	4	1	1164	1122	31
-4	4	1	676	706	32
-3	4	1	887	904	27
-2	4	1	664	611	30
-1	4	1	1659	1628	23
0	4	1	817	832	25
1	4	1	113	81	112
2	4	1	2065	2037	20
3	4	1	2304	2370	21
4	4	1	755	723	26
5	4	1	666	583	28
6	4	1	440	330	34
7	4	1	922	952	31
8	4	1	1318	1354	32
9	4	1	943	961	37
10	4	1	450	429	48
11	4	1	130	64	129
12	4	1	744	720	47
13	4	1	206	177	137
14	4	1	322	345	91
15	4	1	177	119	108
16	4	1	637	622	38
-12	5	1	332	362	50
-11	5	1	177	117	70
-10	5	1	0	138	1
-9	5	1	873	963	42
-8	5	1	604	625	42
-7	5	1	95	126	95
-6	5	1	0	83	1
-5	5	1	138	235	137
-4	5	1	778	757	32
-3	5	1	1577	1648	29
-2	5	1	600	610	32
-1	5	1	920	994	28
0	5	1	225	237	58
1	5	1	1594	1504	23
2	5	1	126	107	125
3	5	1	149	236	149
4	5	1	1152	1100	25
5	5	1	2089	2022	25
6	5	1	0	54	1
7	5	1	852	843	32
8	5	1	0	113	1
9	5	1	160	115	159
10	5	1	850	874	40
11	5	1	964	939	40
12	5	1	0	52	1
13	5	1	364	401	75
14	5	1	308	289	80
15	5	1	458	433	38
16	5	1	363	311	48
-11	6	1	0	52	1
-10	6	1	659	641	48
-9	6	1	0	83	1
-8	6	1	169	14	169
-7	6	1	320	309	59
-6	6	1	872	940	40
-5	6	1	0	85	1
-4	6	1	869	891	34
-3	6	1	262	206	43
-2	6	1	953	1036	31
-1	6	1	1118	1066	28
0	6	1	1719	1687	26
1	6	1	273	209	50
2	6	1	246	266	60
3	6	1	1029	1096	27
4	6	1	1330	1261	26
5	6	1	943	901	28
6	6	1	359	365	49
7	6	1	822	841	33
8	6	1	0	81	1
9	6	1	976	990	37
10	6	1	403	430	50

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
11	6	1	198	132	109
12	6	1	361	351	61
13	6	1	873	809	47
14	6	1	0	62	1
15	6	1	135	80	134
16	6	1	367	351	51
-10	7	1	263	185	40
-9	7	1	0	31	1
-8	7	1	530	573	48
-7	7	1	364	409	63
-6	7	1	341	343	54
-5	7	1	236	214	78
-4	7	1	1023	968	34
-3	7	1	62	33	61
-2	7	1	1427	1438	31
-1	7	1	200	279	85
0	7	1	512	508	35
1	7	1	171	79	79
2	7	1	1380	1387	28
3	7	1	381	326	41
4	7	1	379	286	41
5	7	1	1257	1246	29
6	7	1	1241	1272	30
7	7	1	466	510	40
8	7	1	461	466	43
9	7	1	202	136	63
10	7	1	471	353	46
11	7	1	896	799	43
12	7	1	617	668	51
14	7	1	214	215	141
15	7	1	552	537	37
16	7	1	172	125	87
-10	8	1	173	155	82
-9	8	1	327	363	41
-8	8	1	0	72	1
-7	8	1	289	247	67
-6	8	1	393	416	57
-5	8	1	841	783	40
-4	8	1	436	469	46
-3	8	1	322	311	57
-2	8	1	357	362	46
-1	8	1	522	511	37
0	8	1	1513	1487	30
1	8	1	1061	1043	31
2	8	1	0	65	1
3	8	1	0	83	1
4	8	1	1003	1045	31
5	8	1	474	512	39
6	8	1	354	450	54
7	8	1	684	636	36
8	8	1	736	791	37
9	8	1	169	71	98
10	8	1	839	887	41
11	8	1	0	83	1
12	8	1	296	227	67
13	8	1	390	378	58
14	8	1	538	582	60
15	8	1	195	137	73
-9	9	1	0	189	1
-8	9	1	0	35	1
-7	9	1	572	597	48
-6	9	1	0	73	1
-5	9	1	370	388	59
-4	9	1	0	201	1
-3	9	1	940	924	38
-2	9	1	326	337	56
-1	9	1	1026	1021	35
0	9	1	125	160	124
1	9	1	441	355	39
2	9	1	1012	977	33
3	9	1	1149	1165	32
4	9	1	203	231	79
5	9	1	138	97	138
6	9	1	849	831	35
7	9	1	428	426	45
8	9	1	796	703	38
9	9	1	552	609	46
10	9	1	219	213	86
11	9	1	389	479	54
12	9	1	822	893	45
13	9	1	118	57	118
14	9	1	0	86	1
15	9	1	283	178	46
-8	10	1	355	390	42
-7	10	1	46	89	46
-6	10	1	0	65	1
-5	10	1	529	468	46
-4	10	1	325	344	63
-3	10	1	730	721	41
-2	10	1	342	403	52

h	k	l	10Fo	10Fc	10s
-1	10	1	436	423	46
0	10	1	326	347	58
1	10	1	1074	1098	35
2	10	1	242	168	54
3	10	1	0	84	1
4	10	1	459	436	44
5	10	1	992	1025	35
6	10	1	0	83	1
7	10	1	503	443	42
8	10	1	362	358	52
9	10	1	296	435	62
10	10	1	104	235	104
11	10	1	684	722	46
12	10	1	113	63	112
13	10	1	85	208	84
14	10	1	769	717	28
15	10	1	356	409	39
-6	11	1	615	619	29
-5	11	1	83	63	83
-4	11	1	205	264	105
-3	11	1	465	428	53
-2	11	1	571	611	44
-1	11	1	440	460	48
0	11	1	785	786	39
1	11	1	0	52	1
2	11	1	193	261	139
3	11	1	1204	1198	36
4	11	1	487	479	45
5	11	1	0	78	1
6	11	1	118	98	118
7	11	1	409	377	45
8	11	1	215	231	89
9	11	1	818	863	42
10	11	1	273	322	64
11	11	1	544	541	52
12	11	1	291	169	66
13	11	1	780	762	27
14	11	1	0	34	1
-5	12	1	218	188	49
-4	12	1	369	377	34
-3	12	1	0	58	1
-2	12	1	753	679	44
-1	12	1	211	239	88
0	12	1	658	621	39
1	12	1	248	302	69
2	12	1	966	937	38
3	12	1	0	117	1
4	12	1	186	82	93
5	12	1	526	520	42
6	12	1	384	357	48
7	12	1	163	175	162
8	12	1	467	435	50
9	12	1	185	216	118
10	12	1	563	617	53
11	12	1	680	669	47
12	12	1	272	319	73
13	12	1	86	149	86
14	12	1	129	98	128
-4	13	1	218	215	53
-3	13	1	282	264	41
-2	13	1	167	163	77
-1	13	1	471	475	51
0	13	1	499	576	55
1	13	1	269	216	52
2	13	1	399	341	50
3	13	1	147	114	147
4	13	1	812	855	39
5	13	1	194	176	89
6	13	1	105	290	104
7	13	1	182	131	91
8	13	1	492	521	53
9	13	1	0	126	1
10	13	1	596	585	51
11	13	1	238	218	44
12	13	1	466	464	30
13	13	1	203	193	58
-2	14	1	95	98	95
-1	14	1	535	558	29
0	14	1	137	176	58
1	14	1	520	512	27
2	14	1	505	496	45
3	14	1	240	322	84
4	14	1	0	111	1
5	14	1	0	210	1
6	14	1	565	534	47
7	14	1	549	522	43
8	14	1	448	352	48
9	14	1	174	154	58
10	14	1	332	332	36
11	14	1	83	113	82

h	k	l	10Fo	10Fc	10s
12	14	1	535	540	30
0	15	1	0	13	1
1	15	1	519	504	29
2	15	1	115	96	115
3	15	1	113	236	112
4	15	1	243	273	46
5	15	1	532	582	29
6	15	1	0	28	1
7	15	1	186	182	62
8	15	1	257	199	42
9	15	1	368	434	36
10	15	1	322	310	34
5	16	1	126	126	126
6	16	1	0	78	1
-8	-14	2	337	303	37
-7	-14	2	509	460	29
-6	-14	2	413	377	30
-5	-14	2	153	140	78
-4	-14	2	184	218	57
-3	-14	2	563	606	28
-2	-14	2	160	116	64
-1	-14	2	154	128	68
0	-14	2	229	200	29
-10	-13	2	414	418	30
-9	-13	2	200	102	56
-8	-13	2	441	458	30
-7	-13	2	136	102	79
-6	-13	2	491	511	50
-5	-13	2	381	286	48
-4	-13	2	572	644	47
-3	-13	2	0	96	1
-2	-13	2	0	28	1
-1	-13	2	565	573	26
0	-13	2	372	362	23
1	-13	2	268	325	43
2	-13	2	0	127	1
-11	-12	2	341	394	39
-10	-12	2	196	141	51
-9	-12	2	289	315	41
-8	-12	2	362	307	51
-7	-12	2	262	309	72
-6	-12	2	723	754	43
-5	-12	2	385	379	53
-4	-12	2	319	375	73
-3	-12	2	102	234	102
-2	-12	2	785	831	41
-1	-12	2	72	136	72
0	-12	2	366	408	62
1	-12	2	200	158	105
2	-12	2	496	507	29
3	-12	2	0	84	1
4	-12	2	300	311	38
-12	-11	2	122	34	122
-11	-11	2	259	251	44
-10	-11	2	159	255	158
-9	-11	2	596	650	46
-8	-11	2	0	113	1
-7	-11	2	430	459	53
-6	-11	2	229	311	75
-5	-11	2	74	223	73
-4	-11	2	963	919	38
-3	-11	2	451	417	44
-2	-11	2	0	19	1
-1	-11	2	0	43	1
0	-11	2	655	615	41
1	-11	2	163	242	163
2	-11	2	565	544	45
3	-11	2	171	261	170
4	-11	2	280	392	86
5	-11	2	115	66	114
6	-11	2	408	415	34
-13	-10	2	0	102	1
-12	-10	2	184	67	59
-11	-10	2	550	583	47
-10	-10	2	359	412	52
-9	-10	2	491	552	52
-8	-10	2	221	270	81
-7	-10	2	592	576	46
-6	-10	2	221	101	61
-5	-10	2	668	637	38
-4	-10	2	0	72	1
-3	-10	2	401	342	41
-2	-10	2	626	659	42
-1	-10	2	1097	1081	36
0	-10	2	351	317	51
1	-10	2	0	120	1
2	-10	2	523	499	43
3	-10	2	497	446	48
4	-10	2	351	347	63
5	-10	2	476	433	48

h	k	l	10Fo	10Fc	10s
6	-10	2	0	73	1
7	-10	2	168	152	71
-13	-9	2	451	419	35
-12	-9	2	564	634	53
-11	-9	2	161	12	160
-10	-9	2	134	200	134
-9	-9	2	482	441	48
-8	-9	2	573	600	47
-7	-9	2	644	654	39
-6	-9	2	513	461	42
-5	-9	2	210	233	72
-4	-9	2	0	24	1
-3	-9	2	1126	1111	34
-2	-9	2	598	599	40
-1	-9	2	0	97	1
0	-9	2	263	99	53
1	-9	2	962	986	36
2	-9	2	289	215	53
3	-9	2	529	508	41
4	-9	2	352	384	57
5	-9	2	363	387	57
6	-9	2	108	51	108
7	-9	2	859	773	43
8	-9	2	46	120	45
-14	-8	2	597	596	31
-13	-8	2	346	343	38
-12	-8	2	116	18	115
-11	-8	2	0	75	1
-10	-8	2	682	711	48
-9	-8	2	232	275	77
-8	-8	2	429	426	46
-7	-8	2	682	735	39
-6	-8	2	654	651	39
-5	-8	2	595	536	37
-4	-8	2	948	1005	34
-3	-8	2	0	62	1
-2	-8	2	384	369	44
-1	-8	2	1082	1116	33
0	-8	2	548	589	38
1	-8	2	292	290	54
2	-8	2	311	214	52
3	-8	2	655	593	39
4	-8	2	314	263	55
5	-8	2	623	565	41
6	-8	2	346	444	61
7	-8	2	202	307	142
8	-8	2	0	28	1
9	-8	2	787	739	28
-14	-7	2	207	161	69
-13	-7	2	134	117	134
-12	-7	2	490	541	60
-11	-7	2	426	456	53
-10	-7	2	452	363	49
-9	-7	2	305	221	65
-8	-7	2	847	853	37
-7	-7	2	219	267	85
-6	-7	2	1120	1121	34
-5	-7	2	489	469	37
-4	-7	2	377	402	43
-3	-7	2	61	105	61
-2	-7	2	1302	1297	30
-1	-7	2	102	107	102
0	-7	2	369	278	35
1	-7	2	551	510	36
2	-7	2	1026	1052	34
3	-7	2	89	19	89
4	-7	2	978	967	35
5	-7	2	455	430	45
6	-7	2	529	536	44
7	-7	2	682	747	44
8	-7	2	308	310	72
9	-7	2	114	182	114
10	-7	2	122	67	121
-14	-6	2	180	129	74
-13	-6	2	667	643	49
-12	-6	2	144	157	144
-11	-6	2	261	210	77
-10	-6	2	606	563	48
-9	-6	2	703	714	41
-8	-6	2	427	483	45
-7	-6	2	765	785	36
-6	-6	2	730	750	35
-5	-6	2	929	964	32
-4	-6	2	1235	1188	29
-3	-6	2	156	178	156
-2	-6	2	110	192	110
-1	-6	2	153	186	153
0	-6	2	1803	1806	28
1	-6	2	896	867	31
2	-6	2	172	200	81

h	k	l	10Fo	10Fc	10s
3	-6	2	485	528	39
4	-6	2	791	771	34
5	-6	2	280	324	60
6	-6	2	1419	1493	36
7	-6	2	308	148	48
8	-6	2	279	387	79
9	-6	2	343	243	58
10	-6	2	413	458	63
11	-6	2	224	205	64
-14	-5	2	307	334	44
-13	-5	2	124	44	124
-12	-5	2	218	150	101
-11	-5	2	908	907	46
-10	-5	2	322	350	72
-9	-5	2	0	41	1
-8	-5	2	434	456	44
-7	-5	2	900	946	34
-6	-5	2	0	61	1
-5	-5	2	1931	1927	29
-4	-5	2	247	292	62
-3	-5	2	515	564	34
-2	-5	2	661	675	31
-1	-5	2	1230	1233	27
0	-5	2	178	194	77
1	-5	2	296	298	50
2	-5	2	808	792	29
3	-5	2	526	561	37
4	-5	2	697	697	34
5	-5	2	858	834	32
6	-5	2	412	421	42
7	-5	2	428	403	46
8	-5	2	929	967	39
9	-5	2	215	229	112
10	-5	2	0	35	1
12	-5	2	422	468	40
-14	-4	2	198	234	82
-13	-4	2	519	462	58
-12	-4	2	498	517	54
-11	-4	2	0	111	1
-10	-4	2	104	40	104
-9	-4	2	1009	958	38
-8	-4	2	226	356	92
-7	-4	2	819	874	34
-6	-4	2	731	699	32
-5	-4	2	1025	1100	29
-4	-4	2	791	807	29
-3	-4	2	1748	1763	25
-2	-4	2	467	509	32
-1	-4	2	451	472	34
0	-4	2	947	944	26
1	-4	2	1159	1200	25
2	-4	2	301	282	46
3	-4	2	597	578	31
4	-4	2	180	162	78
5	-4	2	836	879	32
6	-4	2	699	687	35
7	-4	2	925	915	36
8	-4	2	293	274	54
9	-4	2	443	490	51
10	-4	2	536	542	51
11	-4	2	382	490	74
12	-4	2	196	270	73
13	-4	2	146	100	146
-14	-3	2	538	538	36
-13	-3	2	0	63	1
-12	-3	2	250	276	102
-11	-3	2	538	513	51
-10	-3	2	968	905	39
-9	-3	2	284	192	67
-8	-3	2	509	548	45
-7	-3	2	336	348	48
-6	-3	2	1185	1222	30
-5	-3	2	949	988	28
-4	-3	2	1160	1256	26
-3	-3	2	294	315	44
-2	-3	2	1122	1136	23
-1	-3	2	1621	1634	22
0	-3	2	462	519	32
1	-3	2	249	132	50
2	-3	2	590	553	29
3	-3	2	1328	1359	25
4	-3	2	547	543	31
5	-3	2	1047	1054	29
6	-3	2	184	180	67
7	-3	2	660	712	38
8	-3	2	0	74	1
9	-3	2	873	953	40
10	-3	2	438	431	52
11	-3	2	0	183	1
12	-3	2	288	310	89

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
13	-3	2	481	468	38
-14	-2	2	296	256	46
-13	-2	2	367	319	74
-12	-2	2	722	770	52
-11	-2	2	344	229	54
-10	-2	2	0	11	1
-9	-2	2	517	534	45
-8	-2	2	902	903	36
-7	-2	2	660	716	36
-6	-2	2	1178	1206	29
-5	-2	2	286	175	49
-4	-2	2	1226	1206	24
-3	-2	2	701	723	26
-2	-2	2	2000	1937	20
-1	-2	2	289	343	47
0	-2	2	158	86	108
1	-2	2	207	241	64
2	-2	2	1059	1085	22
3	-2	2	765	745	26
4	-2	2	813	790	27
5	-2	2	1041	1023	27
6	-2	2	1777	1747	29
7	-2	2	757	815	34
8	-2	2	975	960	35
9	-2	2	0	129	1
10	-2	2	298	165	71
11	-2	2	1164	1072	43
12	-2	2	0	103	1
13	-2	2	0	216	1
14	-2	2	190	69	80
-14	-1	2	379	362	44
-13	-1	2	576	559	56
-12	-1	2	379	352	61
-11	-1	2	381	394	56
-10	-1	2	514	520	46
-9	-1	2	740	665	38
-8	-1	2	609	567	39
-7	-1	2	779	794	33
-6	-1	2	909	934	29
-5	-1	2	1335	1314	26
-4	-1	2	884	903	25
-3	-1	2	223	130	59
-2	-1	2	390	444	36
-1	-1	2	122	111	122
0	-1	2	2115	2127	17
1	-1	2	549	509	25
2	-1	2	0	173	1
3	-1	2	1120	1102	22
4	-1	2	2072	2118	22
5	-1	2	320	270	40
6	-1	2	1568	1527	27
7	-1	2	1677	1594	30
8	-1	2	227	107	66
9	-1	2	475	572	52
10	-1	2	818	890	42
11	-1	2	874	785	46
12	-1	2	237	199	90
13	-1	2	379	381	79
14	-1	2	351	336	47
-14	0	2	236	245	79
-13	0	2	408	450	38
-12	0	2	297	175	64
-11	0	2	671	700	50
-10	0	2	0	110	1
-9	0	2	271	252	63
-8	0	2	427	550	47
-7	0	2	1708	1689	31
-6	0	2	148	87	108
-5	0	2	788	835	29
-4	0	2	282	251	43
-3	0	2	299	290	39
-2	0	2	1192	1128	21
-1	0	2	1555	1580	18
0	0	2	989	1047	18
1	0	2	584	660	21
2	0	2	2417	2437	16
3	0	2	1043	1029	20
4	0	2	595	658	28
5	0	2	671	812	29
6	0	2	1369	1328	27
7	0	2	98	53	98
8	0	2	1487	1437	32
9	0	2	164	129	163
10	0	2	72	133	71
11	0	2	326	315	69
12	0	2	576	668	55
13	0	2	0	45	1
14	0	2	134	217	134
15	0	2	211	73	61
-13	1	2	617	548	33

h	k	l	10Fo	10Fc	10s
-12	1	2	574	475	55
-11	1	2	303	321	69
-10	1	2	186	27	115
-9	1	2	713	672	42
-8	1	2	495	429	44
-7	1	2	925	915	33
-6	1	2	241	184	65
-5	1	2	1647	1636	27
-4	1	2	630	708	31
-3	1	2	2002	2006	22
-2	1	2	399	314	35
-1	1	2	520	444	26
0	1	2	1092	1100	17
1	1	2	1734	1686	14
2	1	2	483	610	25
3	1	2	631	621	24
4	1	2	868	793	23
5	1	2	1488	1452	23
6	1	2	1030	1007	27
7	1	2	1503	1470	29
8	1	2	867	828	33
9	1	2	1048	1040	35
10	1	2	717	789	42
11	1	2	252	271	85
12	1	2	601	516	50
13	1	2	150	39	149
14	1	2	773	652	59
15	1	2	232	250	69
-13	2	2	227	189	67
-12	2	2	232	84	88
-11	2	2	308	277	77
-10	2	2	463	543	59
-9	2	2	163	158	162
-8	2	2	97	191	97
-7	2	2	797	775	34
-6	2	2	1155	1137	31
-5	2	2	1103	1081	29
-4	2	2	1157	1166	27
-3	2	2	525	535	31
-2	2	2	1236	1112	22
-1	2	2	1153	1079	21
0	2	2	1342	1357	18
1	2	2	177	203	67
2	2	2	914	869	18
3	2	2	2236	2270	18
4	2	2	192	70	68
5	2	2	259	306	51
6	2	2	1081	1058	26
7	2	2	936	951	30
8	2	2	459	435	37
9	2	2	1339	1317	33
10	2	2	250	279	69
11	2	2	484	482	55
12	2	2	751	760	48
13	2	2	759	693	49
14	2	2	0	20	1
15	2	2	280	212	52
-13	3	2	224	176	76
-12	3	2	452	446	38
-11	3	2	291	380	84
-10	3	2	0	130	1
-9	3	2	209	131	99
-8	3	2	1017	1058	38
-7	3	2	225	57	57
-6	3	2	771	757	34
-5	3	2	279	381	57
-4	3	2	1443	1491	28
-3	3	2	0	80	1
-2	3	2	1572	1517	23
-1	3	2	465	508	33
0	3	2	654	656	25
1	3	2	1564	1577	18
2	3	2	1760	1765	18
3	3	2	117	128	116
4	3	2	976	1003	22
5	3	2	762	724	27
6	3	2	1169	1168	26
7	3	2	994	990	29
8	3	2	650	699	34
9	3	2	633	605	36
10	3	2	511	477	43
11	3	2	1193	1187	41
12	3	2	210	174	114
13	3	2	168	31	167
14	3	2	348	304	75
15	3	2	630	601	35
16	3	2	0	75	1
-12	4	2	153	183	123
-11	4	2	86	116	85
-10	4	2	639	654	48

h	k	l	10Fo	10Fc	10s
-9	4	2	527	576	54
-8	4	2	0	106	1
-7	4	2	0	94	1
-6	4	2	962	1020	34
-5	4	2	689	723	34
-4	4	2	966	954	29
-3	4	2	412	350	34
-2	4	2	401	404	37
-1	4	2	49	178	49
0	4	2	2235	2210	21
1	4	2	383	391	36
2	4	2	1168	1142	22
3	4	2	1678	1659	21
4	4	2	1177	1142	23
5	4	2	0	113	1
6	4	2	1254	1273	27
7	4	2	576	572	33
8	4	2	1452	1404	31
9	4	2	993	990	35
10	4	2	720	725	41
11	4	2	127	125	127
12	4	2	0	64	1
13	4	2	733	755	52
14	4	2	320	382	89
15	4	2	415	323	41
16	4	2	0	43	1
-12	5	2	57	22	57
-11	5	2	664	661	30
-10	5	2	184	49	86
-9	5	2	112	152	111
-8	5	2	417	368	50
-7	5	2	888	854	39
-6	5	2	0	68	1
-5	5	2	567	727	36
-4	5	2	156	116	107
-3	5	2	1504	1481	29
-2	5	2	1113	1112	28
-1	5	2	901	857	27
0	5	2	176	72	82
1	5	2	418	358	36
2	5	2	1340	1336	23
3	5	2	1404	1416	23
4	5	2	919	903	25
5	5	2	707	686	30
6	5	2	1103	1140	28
7	5	2	692	669	32
8	5	2	1367	1345	32
9	5	2	0	158	1
10	5	2	496	485	44
11	5	2	255	285	76
12	5	2	797	813	46
13	5	2	166	102	105
14	5	2	176	110	175
15	5	2	257	170	60
16	5	2	605	548	38
-11	6	2	129	191	128
-10	6	2	112	133	111
-9	6	2	694	732	51
-8	6	2	315	318	66
-7	6	2	0	162	1
-6	6	2	317	316	63
-5	6	2	798	852	37
-4	6	2	513	506	40
-3	6	2	1167	1110	31
-2	6	2	56	98	56
-1	6	2	1178	1080	28
0	6	2	970	945	28
1	6	2	1194	1248	27
2	6	2	445	423	34
3	6	2	211	123	61
4	6	2	1465	1455	26
5	6	2	1506	1483	27
6	6	2	243	289	64
7	6	2	326	433	51
8	6	2	341	323	47
9	6	2	610	642	38
10	6	2	1097	1102	37
11	6	2	515	553	47
12	6	2	0	109	1
13	6	2	246	96	81
14	6	2	664	629	55
15	6	2	133	103	132
16	6	2	162	161	118
-10	7	2	271	314	53
-9	7	2	0	35	1
-8	7	2	138	72	137
-7	7	2	745	682	43
-6	7	2	838	889	40
-5	7	2	292	349	64
-4	7	2	244	199	62

h	k	l	10Fo	10Fc	10s
-3	7	2	0	105	1
-2	7	2	427	412	42
-1	7	2	1626	1640	30
0	7	2	809	789	31
1	7	2	619	600	33
2	7	2	231	242	60
3	7	2	1283	1267	28
4	7	2	420	401	34
5	7	2	511	574	34
6	7	2	538	534	36
7	7	2	1379	1371	31
8	7	2	0	106	1
9	7	2	934	920	36
10	7	2	426	276	43
11	7	2	332	373	73
12	7	2	530	486	49
13	7	2	501	688	64
14	7	2	261	192	86
15	7	2	108	92	108
16	7	2	437	364	36
-9	8	2	224	178	50
-8	8	2	441	400	51
-7	8	2	137	40	136
-6	8	2	150	143	149
-5	8	2	190	134	83
-4	8	2	1185	1208	36
-3	8	2	350	362	52
-2	8	2	1007	959	34
-1	8	2	381	348	43
0	8	2	595	495	35
1	8	2	938	970	32
2	8	2	782	819	32
3	8	2	0	35	1
4	8	2	213	211	62
5	8	2	1324	1345	30
6	8	2	868	886	33
7	8	2	836	898	35
8	8	2	275	265	52
9	8	2	655	689	40
10	8	2	301	199	56
11	8	2	909	903	40
12	8	2	134	202	134
13	8	2	0	56	1
14	8	2	122	51	121
15	8	2	664	693	33
16	8	2	176	151	77
-9	9	2	207	212	58
-8	9	2	112	96	111
-7	9	2	115	51	114
-6	9	2	599	672	51
-5	9	2	534	576	49
-4	9	2	630	629	42
-3	9	2	196	86	87
-2	9	2	680	664	40
-1	9	2	0	62	1
0	9	2	1259	1215	33
1	9	2	611	548	36
2	9	2	243	207	60
3	9	2	255	301	55
4	9	2	1198	1223	31
5	9	2	275	319	51
6	9	2	679	564	36
7	9	2	765	797	36
8	9	2	923	941	38
9	9	2	121	158	120
10	9	2	361	329	59
11	9	2	199	163	87
12	9	2	236	153	89
13	9	2	1050	951	44
14	9	2	559	495	54
15	9	2	0	6	1
16	9	2	78	43	77
-8	10	2	184	195	73
-7	10	2	516	568	33
-6	10	2	280	193	75
-5	10	2	281	336	68
-4	10	2	290	348	79
-3	10	2	843	838	41
-2	10	2	499	449	45
-1	10	2	305	231	62
0	10	2	312	276	54
1	10	2	159	114	158
2	10	2	1336	1251	33
3	10	2	912	904	35
4	10	2	190	170	80
5	10	2	214	175	78
6	10	2	850	869	36
7	10	2	150	212	149
8	10	2	706	670	41
9	10	2	465	411	46

h	k	l	10Fo	10Fc	10s
10	10	2	465	476	53
11	10	2	253	180	76
12	10	2	749	792	46
13	10	2	0	161	1
14	10	2	229	310	138
15	10	2	412	458	43
-6	11	2	170	179	78
-5	11	2	765	724	47
-4	11	2	175	49	109
-3	11	2	478	524	51
-2	11	2	463	437	53
-1	11	2	725	655	41
0	11	2	447	408	50
1	11	2	1129	1069	36
2	11	2	0	55	1
3	11	2	328	343	50
4	11	2	834	834	36
5	11	2	658	646	38
6	11	2	245	210	59
7	11	2	455	376	44
8	11	2	460	454	48
9	11	2	678	557	40
10	11	2	720	681	45
11	11	2	220	187	77
12	11	2	196	186	121
13	11	2	0	34	1
14	11	2	787	804	29
15	11	2	193	152	65
-5	12	2	176	252	81
-4	12	2	281	183	36
-3	12	2	431	492	57
-2	12	2	333	283	62
-1	12	2	624	684	42
0	12	2	0	156	1
1	12	2	214	232	86
2	12	2	0	127	1
3	12	2	1025	964	38
4	12	2	0	297	1
5	12	2	0	33	1
6	12	2	235	289	75
7	12	2	531	584	45
8	12	2	207	174	82
9	12	2	691	689	44
10	12	2	203	78	93
11	12	2	585	597	50
12	12	2	391	442	65
13	12	2	290	318	45
14	12	2	264	139	36
-4	13	2	406	363	32
-3	13	2	208	173	56
-2	13	2	228	292	49
-1	13	2	173	212	173
0	13	2	709	692	42
1	13	2	633	527	42
2	13	2	479	412	45
3	13	2	126	120	126
4	13	2	0	33	1
5	13	2	745	768	42
6	13	2	563	495	44
7	13	2	432	340	44
8	13	2	301	273	54
9	13	2	350	424	55
10	13	2	134	124	134
11	13	2	723	748	45
12	13	2	66	64	66
13	13	2	285	336	42
14	13	2	209	115	53
-2	14	2	527	498	3[illegible]
-1	14	2	0	52	1
0	14	2	703	695	2[illegible]
1	14	2	219	152	6[illegible]
2	14	2	392	399	5[illegible]
3	14	2	422	448	5[illegible]
4	14	2	490	496	5[illegible]
5	14	2	0	54	[illegible]
6	14	2	152	192	15[illegible]
7	14	2	366	313	6[illegible]
8	14	2	599	602	4[illegible]
9	14	2	414	408	5[illegible]
10	14	2	330	270	3[illegible]
11	14	2	260	252	3[illegible]
12	14	2	179	235	7[illegible]
13	14	2	438	497	3[illegible]
0	15	2	243	250	3[illegible]
1	15	2	200	246	5[illegible]
2	15	2	551	573	2[illegible]
3	15	2	102	182	10[illegible]
4	15	2	63	128	6[illegible]
5	15	2	44	209	4[illegible]
6	15	2	527	570	2[illegible]

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
7	15	2	167	191	63
8	15	2	355	405	34
9	15	2	0	56	1
10	15	2	535	565	30
11	15	2	0	173	1
3	16	2	150	185	100
4	16	2	431	433	30
5	16	2	456	429	27
6	16	2	50	71	50
7	16	2	50	101	50
8	16	2	395	356	33
9	16	2	385	300	32
-5	-14	3	401	451	33
-4	-14	3	0	32	1
-3	-14	3	131	163	89
-2	-14	3	422	477	32
-9	-13	3	341	342	38
-8	-13	3	94	100	93
-7	-13	3	577	557	27
-6	-13	3	223	241	48
-5	-13	3	454	428	31
-4	-13	3	0	38	1
-3	-13	3	661	617	25
-2	-13	3	0	80	1
-1	-13	3	43	84	42
0	-13	3	414	409	22
1	-13	3	472	462	29
-10	-12	3	386	410	35
-9	-12	3	244	137	41
-8	-12	3	420	386	29
-7	-12	3	308	260	60
-6	-12	3	450	531	60
-5	-12	3	687	707	48
-4	-12	3	279	264	69
-3	-12	3	196	162	91
-2	-12	3	76	193	75
-1	-12	3	644	676	45
0	-12	3	0	182	1
1	-12	3	381	354	32
2	-12	3	178	141	59
3	-12	3	473	373	27
4	-12	3	106	15	106
-11	-11	3	325	248	35
-10	-11	3	108	197	107
-9	-11	3	314	320	63
-8	-11	3	612	593	47
-7	-11	3	0	97	1
-6	-11	3	619	567	44
-4	-11	3	457	485	51
-3	-11	3	482	519	47
-2	-11	3	495	589	47
-1	-11	3	239	86	56
0	-11	3	193	242	90
1	-11	3	533	506	46
2	-11	3	646	562	44
3	-11	3	467	385	45
4	-11	3	211	111	42
5	-11	3	206	187	49
-12	-10	3	0	19	1
-11	-10	3	275	258	43
-10	-10	3	559	472	51
-9	-10	3	614	662	49
-8	-10	3	283	341	75
-7	-10	3	221	94	69
-6	-10	3	472	456	45
-5	-10	3	0	73	1
-4	-10	3	1039	1042	37
-3	-10	3	303	409	64
-2	-10	3	120	173	119
-1	-10	3	138	104	137
0	-10	3	658	685	41
1	-10	3	0	37	1
2	-10	3	650	563	39
3	-10	3	197	259	128
4	-10	3	671	643	45
5	-10	3	0	221	1
6	-10	3	488	488	32
7	-10	3	136	37	91
-13	-9	3	188	164	74
-12	-9	3	181	216	71
-11	-9	3	337	468	72
-10	-9	3	176	122	103
-9	-9	3	437	465	53
-8	-9	3	347	403	64
-7	-9	3	904	849	40
-6	-9	3	712	693	41
-5	-9	3	274	300	59
-4	-9	3	336	356	56
-3	-9	3	96	110	95
-2	-9	3	981	963	36

h	k	l	10Fo	10Fc	10s
-1	-9	3	616	617	40
0	-9	3	0	124	1
1	-9	3	166	148	166
2	-9	3	839	808	37
3	-9	3	0	157	1
4	-9	3	552	503	45
5	-9	3	326	234	51
6	-9	3	318	232	63
7	-9	3	125	48	124
8	-9	3	570	578	31
-13	-8	3	459	486	35
-12	-8	3	360	382	39
-11	-8	3	230	124	73
-10	-8	3	191	138	190
-9	-8	3	707	735	44
-8	-8	3	228	237	94
-7	-8	3	772	701	39
-6	-8	3	191	216	79
-5	-8	3	593	533	40
-4	-8	3	170	289	104
-3	-8	3	1254	1289	33
-2	-8	3	191	184	62
-1	-8	3	0	249	1
0	-8	3	693	693	37
1	-8	3	881	838	35
2	-8	3	433	355	45
3	-8	3	377	382	50
4	-8	3	340	285	55
5	-8	3	591	600	43
6	-8	3	407	407	49
7	-8	3	510	465	46
8	-8	3	124	38	123
9	-8	3	0	78	1
-13	-7	3	325	216	37
-12	-7	3	253	119	79
-11	-7	3	387	380	58
-10	-7	3	806	723	43
-9	-7	3	362	330	56
-8	-7	3	326	286	56
-7	-7	3	749	716	38
-6	-7	3	436	455	44
-5	-7	3	906	924	36
-4	-7	3	392	395	38
-3	-7	3	259	280	67
-2	-7	3	0	64	1
-1	-7	3	1420	1433	31
0	-7	3	456	399	37
1	-7	3	152	29	105
2	-7	3	208	173	70
3	-7	3	798	803	36
4	-7	3	174	62	90
5	-7	3	765	728	40
6	-7	3	363	383	49
7	-7	3	678	651	44
8	-7	3	525	435	47
9	-7	3	630	708	49
10	-7	3	275	241	41
-14	-6	3	290	272	59
-13	-6	3	128	40	128
-12	-6	3	716	773	55
-11	-6	3	402	381	65
-10	-6	3	187	148	107
-9	-6	3	252	208	62
-8	-6	3	983	936	37
-7	-6	3	248	253	62
-6	-6	3	777	840	37
-5	-6	3	793	769	34
-4	-6	3	798	752	33
-3	-6	3	600	673	35
-2	-6	3	1071	1086	30
-1	-6	3	179	228	88
0	-6	3	142	78	87
1	-6	3	1051	1022	32
2	-6	3	817	807	33
3	-6	3	349	294	48
4	-6	3	631	640	38
5	-6	3	492	462	40
6	-6	3	297	332	58
7	-6	3	960	1046	38
8	-6	3	198	202	71
9	-6	3	262	176	67
10	-6	3	186	281	185
11	-6	3	508	523	34
-14	-5	3	366	292	42
-13	-5	3	399	350	36
-12	-5	3	147	43	147
-11	-5	3	140	101	140
-10	-5	3	1030	1016	42
-9	-5	3	484	535	48
-8	-5	3	503	399	42

h	k	l	10Fo	10Fc	10s
-7	-5	3	205	270	100
-6	-5	3	946	930	34
-5	-5	3	296	283	51
-4	-5	3	1462	1526	29
-3	-5	3	448	428	36
-2	-5	3	634	700	32
-1	-5	3	956	919	30
0	-5	3	1367	1344	28
1	-5	3	309	296	46
2	-5	3	147	252	146
3	-5	3	579	538	33
4	-5	3	640	696	36
5	-5	3	367	347	45
6	-5	3	612	613	38
7	-5	3	0	76	1
8	-5	3	484	563	46
9	-5	3	1071	945	41
10	-5	3	434	357	54
11	-5	3	0	12	1
12	-5	3	0	118	1
-14	-4	3	0	83	1
-13	-4	3	176	109	83
-12	-4	3	305	348	85
-11	-4	3	856	846	45
-10	-4	3	76	54	75
-9	-4	3	0	65	1
-8	-4	3	557	560	43
-7	-4	3	968	854	35
-6	-4	3	573	580	35
-5	-4	3	906	910	31
-4	-4	3	396	345	39
-3	-4	3	901	958	28
-2	-4	3	1930	1937	26
-1	-4	3	672	684	29
0	-4	3	284	269	49
1	-4	3	259	203	48
2	-4	3	986	984	28
3	-4	3	576	579	32
4	-4	3	862	801	30
5	-4	3	0	99	1
6	-4	3	839	843	36
7	-4	3	270	382	75
8	-4	3	981	1020	38
9	-4	3	182	190	182
10	-4	3	458	453	53
11	-4	3	373	295	64
12	-4	3	442	458	37
13	-4	3	166	107	107
-14	-3	3	263	264	65
-13	-3	3	553	478	34
-12	-3	3	255	292	97
-11	-3	3	254	110	82
-10	-3	3	369	249	50
-9	-3	3	1107	1036	38
-8	-3	3	434	451	45
-7	-3	3	551	559	40
-6	-3	3	283	243	51
-5	-3	3	959	952	30
-4	-3	3	770	854	31
-3	-3	3	1876	1859	26
-2	-3	3	388	488	38
-1	-3	3	900	829	26
0	-3	3	442	404	33
1	-3	3	869	767	26
2	-3	3	184	120	74
3	-3	3	1047	1076	26
4	-3	3	832	792	28
5	-3	3	1081	1110	30
6	-3	3	1212	1171	31
7	-3	3	373	312	45
8	-3	3	369	428	56
9	-3	3	407	329	51
10	-3	3	766	742	46
11	-3	3	497	428	53
12	-3	3	124	16	123
13	-3	3	173	194	106
-14	-2	3	534	464	38
-13	-2	3	262	189	54
-12	-2	3	436	324	54
-11	-2	3	608	723	48
-10	-2	3	619	596	45
-9	-2	3	174	19	133
-8	-2	3	313	282	53
-7	-2	3	768	771	36
-6	-2	3	733	773	33
-5	-2	3	1556	1570	29
-4	-2	3	238	287	58
-3	-2	3	1553	1605	24
-2	-2	3	214	95	58
-1	-2	3	1044	1139	24

h	k	l	10Fo	10Fc	10s
0	-2	3	147	273	147
1	-2	3	699	659	26
2	-2	3	699	721	27
3	-2	3	1719	1785	24
4	-2	3	129	173	128
5	-2	3	461	463	34
6	-2	3	384	343	41
7	-2	3	1001	995	32
8	-2	3	816	784	36
9	-2	3	1045	1081	38
10	-2	3	643	561	44
11	-2	3	0	42	1
12	-2	3	655	666	55
13	-2	3	273	269	44
14	-2	3	518	471	35
-14	-1	3	450	428	45
-13	-1	3	216	51	59
-12	-1	3	502	519	57
-11	-1	3	292	252	70
-10	-1	3	202	74	86
-9	-1	3	669	713	46
-8	-1	3	1448	1386	35
-7	-1	3	0	16	1
-6	-1	3	662	587	34
-5	-1	3	0	106	1
-4	-1	3	1228	1177	26
-3	-1	3	1557	1537	24
-2	-1	3	926	957	25
-1	-1	3	1314	1317	22
0	-1	3	124	47	124
1	-1	3	1230	1155	21
2	-1	3	771	862	24
3	-1	3	868	937	24
4	-1	3	649	606	29
5	-1	3	1758	1755	26
6	-1	3	585	573	35
7	-1	3	1445	1478	31
8	-1	3	201	240	102
9	-1	3	436	427	51
10	-1	3	649	688	46
11	-1	3	1015	1025	43
12	-1	3	119	142	119
13	-1	3	154	33	154
14	-1	3	159	172	159
-13	0	3	133	158	132
-12	0	3	348	347	77
-11	0	3	0	128	1
-10	0	3	811	869	42
-9	0	3	708	729	42
-8	0	3	441	501	42
-7	0	3	349	348	48
-6	0	3	942	961	30
-5	0	3	56	51	56
-4	0	3	1871	1885	25
-3	0	3	316	378	45
-2	0	3	1647	1667	22
-1	0	3	620	654	27
0	0	3	1707	1635	19
1	0	3	169	122	80
2	0	3	437	456	30
3	0	3	599	632	26
4	0	3	1367	1383	23
5	0	3	831	819	27
6	0	3	865	816	29
7	0	3	255	246	59
8	0	3	883	864	34
9	0	3	1004	1022	36
10	0	3	594	562	43
11	0	3	0	54	1
12	0	3	233	192	102
13	0	3	706	708	51
14	0	3	0	62	1
15	0	3	234	308	87
-13	1	3	349	327	50
-12	1	3	448	403	58
-11	1	3	430	351	61
-10	1	3	134	117	134
-9	1	3	75	31	75
-8	1	3	397	427	52
-7	1	3	1165	1218	35
-6	1	3	763	789	32
-5	1	3	447	453	42
-4	1	3	935	976	28
-3	1	3	256	168	53
-2	1	3	943	943	25
-1	1	3	1381	1299	21
0	1	3	722	737	23
1	1	3	387	407	30
2	1	3	1926	1891	18
3	1	3	216	160	61

h	k	l	10Fo	10Fc	10s
4	1	3	484	477	31
5	1	3	643	575	28
6	1	3	1519	1515	26
7	1	3	323	345	54
8	1	3	519	525	39
9	1	3	433	345	48
10	1	3	416	385	45
11	1	3	930	878	43
12	1	3	1095	1060	45
13	1	3	0	46	1
14	1	3	158	72	158
15	1	3	287	238	50
-13	2	3	243	271	71
-12	2	3	189	187	75
-11	2	3	428	451	60
-10	2	3	0	67	1
-9	2	3	1018	1029	41
-8	2	3	69	94	68
-7	2	3	653	618	39
-6	2	3	173	149	93
-5	2	3	1549	1543	29
-4	2	3	385	371	39
-3	2	3	1036	1007	27
-2	2	3	428	414	39
-1	2	3	691	746	26
0	2	3	1975	1983	19
1	2	3	2056	2110	18
2	2	3	0	141	1
3	2	3	267	353	47
4	2	3	909	932	24
5	2	3	524	464	31
6	2	3	1237	1225	26
7	2	3	1044	1088	30
8	2	3	859	897	32
9	2	3	643	634	38
10	2	3	1375	1357	37
11	2	3	0	106	1
12	2	3	298	258	87
13	2	3	370	290	67
14	2	3	661	654	56
15	2	3	284	211	55
16	2	3	384	340	53
-12	3	3	0	101	1
-11	3	3	650	664	51
-10	3	3	686	614	45
-9	3	3	75	102	74
-8	3	3	285	285	67
-7	3	3	729	831	38
-6	3	3	427	364	45
-5	3	3	1154	1215	32
-4	3	3	837	819	31
-3	3	3	1426	1442	27
-2	3	3	389	346	38
-1	3	3	1104	1067	24
0	3	3	255	192	51
1	3	3	287	220	44
2	3	3	796	770	23
3	3	3	1711	1703	20
4	3	3	103	156	102
5	3	3	268	250	56
6	3	3	1189	1126	26
7	3	3	948	992	30
8	3	3	1266	1253	31
9	3	3	851	856	35
10	3	3	257	321	80
11	3	3	763	752	43
12	3	3	899	916	45
13	3	3	367	365	68
14	3	3	296	124	85
15	3	3	366	354	47
16	3	3	378	370	47
-12	4	3	368	396	40
-11	4	3	124	161	124
-10	4	3	0	100	1
-9	4	3	245	242	83
-8	4	3	1057	1114	39
-7	4	3	300	318	64
-6	4	3	186	234	106
-5	4	3	852	799	35
-4	4	3	1005	1025	31
-3	4	3	927	908	29
-2	4	3	1016	980	28
-1	4	3	316	359	44
0	4	3	1307	1286	23
1	4	3	1561	1540	22
2	4	3	530	515	28
3	4	3	965	944	23
4	4	3	1027	1038	24
5	4	3	902	872	26
6	4	3	1043	1000	27

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
7	4	3	1288	1329	29
8	4	3	144	187	143
9	4	3	1396	1380	34
10	4	3	529	474	44
11	4	3	1052	1086	41
12	4	3	222	174	125
13	4	3	81	192	81
14	4	3	500	385	57
15	4	3	571	547	64
16	4	3	0	32	1
-11	5	3	0	4	1
-10	5	3	688	665	47
-9	5	3	288	311	73
-8	5	3	0	74	1
-7	5	3	0	122	1
-6	5	3	989	967	37
-5	5	3	182	102	88
-4	5	3	893	894	33
-3	5	3	489	498	39
-2	5	3	1523	1470	28
-1	5	3	232	194	61
0	5	3	557	570	31
1	5	3	130	109	129
2	5	3	261	303	54
3	5	3	2092	2004	23
4	5	3	1966	1984	23
5	5	3	238	121	61
6	5	3	265	145	54
7	5	3	437	484	41
8	5	3	207	348	86
9	5	3	1515	1533	33
10	5	3	529	527	45
11	5	3	693	656	43
12	5	3	233	185	97
13	5	3	674	613	49
14	5	3	151	105	150
15	5	3	308	307	95
16	5	3	181	136	93
-11	6	3	439	396	35
-10	6	3	134	66	134
-9	6	3	0	40	1
-8	6	3	701	759	46
-7	6	3	689	739	41
-6	6	3	100	77	100
-5	6	3	0	65	1
-4	6	3	651	716	37
-3	6	3	387	389	46
-2	6	3	1700	1659	29
-1	6	3	392	403	37
0	6	3	778	780	29
1	6	3	254	236	54
2	6	3	1067	1079	26
3	6	3	590	544	29
4	6	3	431	431	34
5	6	3	835	839	30
6	6	3	1786	1774	28
7	6	3	357	349	48
8	6	3	1003	1038	33
9	6	3	224	213	74
10	6	3	966	934	38
11	6	3	874	831	41
12	6	3	452	474	59
13	6	3	142	177	142
14	6	3	172	26	172
15	6	3	485	387	56
16	6	3	420	407	43
-10	7	3	203	153	63
-9	7	3	646	709	29
-8	7	3	0	43	1
-7	7	3	243	223	79
-6	7	3	179	138	151
-5	7	3	931	864	38
-4	7	3	382	414	50
-3	7	3	617	655	40
-2	7	3	250	255	56
-1	7	3	1067	1070	31
0	7	3	1085	1156	29
1	7	3	310	330	48
2	7	3	0	166	1
3	7	3	534	538	33
4	7	3	1189	1133	28
5	7	3	1104	1163	30
6	7	3	906	980	32
7	7	3	187	165	79
8	7	3	1221	1211	33
9	7	3	217	182	67
10	7	3	1034	1066	38
11	7	3	180	295	180
12	7	3	380	400	61
13	7	3	306	263	77

h	k	l	10Fo	10Fc	10s
14	7	3	603	669	56
15	7	3	240	120	92
16	7	3	125	228	125
-9	8	3	0	47	1
-8	8	3	0	40	1
-7	8	3	554	574	48
-6	8	3	437	410	51
-5	8	3	371	423	57
-4	8	3	68	170	67
-3	8	3	942	959	38
-2	8	3	213	202	79
-1	8	3	831	826	34
0	8	3	377	404	41
1	8	3	679	654	34
2	8	3	966	948	31
3	8	3	1289	1293	30
4	8	3	56	41	56
5	8	3	590	563	34
6	8	3	575	601	37
7	8	3	1333	1330	32
8	8	3	892	875	36
9	8	3	321	288	54
10	8	3	392	447	56
11	8	3	210	320	137
12	8	3	744	782	44
13	8	3	490	450	54
14	8	3	227	99	111
15	8	3	0	40	1
16	8	3	478	479	38
-8	9	3	412	412	35
-7	9	3	217	26	88
-6	9	3	136	65	136
-5	9	3	428	408	52
-4	9	3	1046	1013	40
-3	9	3	594	644	44
-2	9	3	301	304	56
-1	9	3	638	572	37
0	9	3	141	46	140
1	9	3	975	947	33
2	9	3	598	604	35
3	9	3	147	143	99
4	9	3	268	263	53
5	9	3	1272	1264	32
6	9	3	291	329	63
7	9	3	571	580	40
8	9	3	386	374	52
9	9	3	982	891	37
10	9	3	436	333	46
11	9	3	749	712	42
12	9	3	0	62	1
13	9	3	163	269	162
14	9	3	297	312	95
15	9	3	521	502	35
16	9	3	111	109	110
-7	10	3	0	43	1
-6	10	3	644	664	48
-5	10	3	135	87	135
-4	10	3	465	422	50
-3	10	3	105	160	105
-2	10	3	988	1030	38
-1	10	3	681	701	40
0	10	3	542	575	40
1	10	3	368	398	46
2	10	3	0	184	1
3	10	3	704	676	35
4	10	3	1087	1076	34
5	10	3	416	411	45
6	10	3	145	85	145
7	10	3	1265	1267	35
8	10	3	448	524	50
9	10	3	576	584	45
10	10	3	253	100	51
11	10	3	331	347	67
12	10	3	209	150	101
13	10	3	1025	986	45
14	10	3	192	114	151
15	10	3	206	89	66
16	10	3	283	226	49
-6	11	3	426	383	34
-5	11	3	126	71	125
-4	11	3	793	740	42
-3	11	3	445	444	52
-2	11	3	376	310	49
-1	11	3	373	318	55
0	11	3	390	422	50
1	11	3	410	423	49
2	11	3	1342	1360	35
3	11	3	164	241	136
4	11	3	0	129	1
5	11	3	420	395	51

h	k	l	10Fo	10Fc	10s
6	11	3	792	729	37
7	11	3	154	63	154
8	11	3	360	345	52
9	11	3	382	307	51
10	11	3	615	649	45
11	11	3	664	669	47
12	11	3	429	459	52
13	11	3	145	36	145
14	11	3	0	160	1
15	11	3	496	522	33
-5	12	3	523	481	31
-4	12	3	423	419	32
-3	12	3	0	100	1
-2	12	3	287	209	60
-1	12	3	519	470	47
0	12	3	469	473	46
1	12	3	418	398	48
2	12	3	225	245	95
3	12	3	198	127	74
4	12	3	1017	963	37
5	12	3	444	394	47
6	12	3	198	242	92
7	12	3	189	73	67
8	12	3	596	678	45
9	12	3	129	67	129
10	12	3	758	727	41
11	12	3	192	179	100
12	12	3	362	500	71
13	12	3	188	240	188
14	12	3	538	522	31
15	12	3	161	33	91
-4	13	3	0	124	1
-3	13	3	400	440	36
-2	13	3	46	43	45
-1	13	3	0	98	1
0	13	3	132	286	131
1	13	3	673	579	43
2	13	3	355	341	45
3	13	3	885	929	41
4	13	3	162	151	116
5	13	3	193	65	100
6	13	3	473	558	50
7	13	3	495	494	47
8	13	3	390	418	46
9	13	3	341	418	57
10	13	3	390	442	63
11	13	3	339	388	61
12	13	3	643	660	48
13	13	3	0	57	1
14	13	3	148	169	147
-2	14	3	217	125	46
-1	14	3	627	610	28
0	14	3	322	370	45
1	14	3	741	703	43
2	14	3	188	161	114
3	14	3	153	133	152
4	14	3	392	357	53
5	14	3	785	789	43
6	14	3	0	159	1
7	14	3	263	254	63
8	14	3	75	78	75
9	14	3	630	655	49
10	14	3	139	269	139
11	14	3	457	462	31
12	14	3	86	137	85
13	14	3	347	353	38
0	15	3	400	375	22
1	15	3	106	153	105
2	15	3	204	254	54
3	15	3	508	514	30
4	15	3	192	337	155
5	15	3	0	25	1
6	15	3	0	139	1
7	15	3	566	566	46
8	15	3	449	487	51
9	15	3	453	435	31
10	15	3	95	60	95
11	15	3	400	418	33
12	15	3	0	139	1
2	16	3	501	475	30
3	16	3	224	161	50
4	16	3	0	110	1
5	16	3	258	290	42
6	16	3	484	465	29
7	16	3	0	85	1
8	16	3	158	146	55
9	16	3	137	162	110
10	16	3	534	519	30
-7	-13	4	305	261	34
-6	-13	4	509	469	28

h	k	l	10Fo	10Fc	10s
-5	-13	4	333	296	32
-4	-13	4	172	185	59
-3	-13	4	189	71	41
-2	-13	4	588	622	28
-1	-13	4	139	101	83
0	-13	4	67	72	66
-9	-12	4	440	482	34
-8	-12	4	67	67	66
-7	-12	4	431	425	32
-6	-12	4	193	183	46
-5	-12	4	504	489	26
-4	-12	4	490	486	28
-3	-12	4	415	459	55
-2	-12	4	109	57	108
-1	-12	4	134	129	84
0	-12	4	437	415	38
1	-12	4	373	334	32
2	-12	4	343	326	37
3	-12	4	0	108	1
-10	-11	4	252	306	48
-9	-11	4	259	277	46
-8	-11	4	249	204	41
-7	-11	4	533	435	47
-6	-11	4	200	181	104
-5	-11	4	813	733	42
-4	-11	4	0	179	1
-3	-11	4	504	434	41
-2	-11	4	233	269	89
-1	-11	4	565	544	46
0	-11	4	0	58	1
1	-11	4	271	392	68
2	-11	4	202	216	114
3	-11	4	636	626	26
4	-11	4	228	215	48
5	-11	4	302	346	36
-11	-10	4	0	23	1
-10	-10	4	199	196	52
-9	-10	4	447	488	54
-8	-10	4	713	691	46
-7	-10	4	446	389	52
-6	-10	4	275	312	68
-5	-10	4	371	338	59
-4	-10	4	202	253	75
-3	-10	4	781	787	40
-2	-10	4	275	321	61
-1	-10	4	0	26	1
0	-10	4	304	262	60
1	-10	4	786	783	42
2	-10	4	232	288	84
3	-10	4	462	425	52
4	-10	4	216	105	99
5	-10	4	437	458	29
6	-10	4	263	215	37
-12	-9	4	0	43	1
-11	-9	4	170	220	76
-10	-9	4	625	623	50
-9	-9	4	269	245	77
-8	-9	4	436	402	44
-7	-9	4	75	75	74
-6	-9	4	777	710	41
-5	-9	4	436	507	47
-4	-9	4	719	718	41
-3	-9	4	400	386	41
-2	-9	4	153	147	152
-1	-9	4	497	485	45
0	-9	4	913	927	38
1	-9	4	311	409	71
2	-9	4	254	226	63
3	-9	4	368	388	56
4	-9	4	615	551	45
5	-9	4	362	428	61
6	-9	4	233	259	83
7	-9	4	216	219	52
8	-9	4	130	56	129
-12	-8	4	322	304	41
-11	-8	4	434	423	35
-10	-8	4	112	182	112
-9	-8	4	171	172	171
-8	-8	4	645	631	43
-7	-8	4	548	545	48
-6	-8	4	692	737	40
-5	-8	4	237	198	66
-4	-8	4	547	576	41
-3	-8	4	302	322	59
-2	-8	4	933	944	36
-1	-8	4	340	415	57
0	-8	4	0	9	1
1	-8	4	134	156	134
2	-8	4	935	978	37
3	-8	4	98	141	97

h	k	l	10Fo	10Fc	10s
4	-8	4	769	675	38
5	-8	4	262	227	66
6	-8	4	493	467	49
7	-8	4	320	257	66
8	-8	4	336	292	37
9	-8	4	140	100	86
-13	-7	4	396	371	40
-12	-7	4	333	296	35
-11	-7	4	117	89	117
-10	-7	4	237	68	86
-9	-7	4	878	885	42
-8	-7	4	243	232	83
-7	-7	4	609	582	40
-6	-7	4	697	711	41
-5	-7	4	708	783	39
-4	-7	4	799	746	35
-3	-7	4	515	466	39
-2	-7	4	218	247	71
-1	-7	4	126	32	125
0	-7	4	871	883	34
1	-7	4	773	739	36
2	-7	4	481	432	43
3	-7	4	115	173	115
4	-7	4	852	800	37
5	-7	4	434	388	45
6	-7	4	605	603	43
7	-7	4	289	309	68
8	-7	4	220	207	75
9	-7	4	349	335	31
10	-7	4	647	626	28
-13	-6	4	120	114	120
-12	-6	4	102	81	101
-11	-6	4	514	461	51
-10	-6	4	423	468	58
-9	-6	4	368	395	56
-8	-6	4	420	383	44
-7	-6	4	1451	1433	35
-6	-6	4	248	150	58
-5	-6	4	729	726	37
-4	-6	4	270	269	51
-3	-6	4	265	236	59
-2	-6	4	595	614	36
-1	-6	4	1463	1521	31
0	-6	4	354	288	39
1	-6	4	263	269	52
2	-6	4	753	772	35
3	-6	4	761	695	35
4	-6	4	642	624	38
5	-6	4	584	599	37
6	-6	4	208	249	104
7	-6	4	653	549	41
8	-6	4	646	666	48
9	-6	4	239	220	74
10	-6	4	0	49	1
11	-6	4	269	179	50
-13	-5	4	474	439	35
-12	-5	4	552	601	55
-11	-5	4	218	43	111
-10	-5	4	109	101	109
-9	-5	4	332	353	58
-8	-5	4	776	719	38
-7	-5	4	668	713	39
-6	-5	4	443	497	44
-5	-5	4	1082	1079	33
-4	-5	4	490	523	39
-3	-5	4	1170	1136	30
-2	-5	4	389	357	42
-1	-5	4	188	52	62
0	-5	4	228	233	65
1	-5	4	1731	1678	29
2	-5	4	493	543	36
3	-5	4	435	435	38
4	-5	4	149	110	149
5	-5	4	527	515	35
6	-5	4	404	385	46
7	-5	4	797	809	38
8	-5	4	0	71	1
9	-5	4	740	704	45
10	-5	4	293	440	95
11	-5	4	303	389	44
12	-5	4	94	40	94
-13	-4	4	77	87	76
-12	-4	4	193	27	152
-11	-4	4	0	70	1
-10	-4	4	902	900	43
-9	-4	4	222	223	86
-8	-4	4	69	185	68
-7	-4	4	392	394	48
-6	-4	4	895	933	35
-5	-4	4	235	184	62

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
-4	-4	4	1108	1130	30
-3	-4	4	576	465	32
-2	-4	4	549	633	33
-1	-4	4	1105	1166	28
0	-4	4	983	922	29
1	-4	4	240	121	47
2	-4	4	460	463	37
3	-4	4	601	651	31
4	-4	4	936	898	30
5	-4	4	740	758	33
6	-4	4	397	397	45
7	-4	4	538	573	40
8	-4	4	235	136	81
9	-4	4	864	840	42
10	-4	4	79	107	79
11	-4	4	0	117	1
12	-4	4	216	200	63
13	-4	4	541	503	33
-13	-3	4	385	350	40
-12	-3	4	425	444	65
-11	-3	4	657	679	47
-10	-3	4	110	21	110
-9	-3	4	179	59	179
-8	-3	4	1190	1126	36
-7	-3	4	415	415	43
-6	-3	4	673	689	36
-5	-3	4	167	263	105
-4	-3	4	1200	1222	29
-3	-3	4	234	59	50
-2	-3	4	1698	1664	27
-1	-3	4	126	102	125
0	-3	4	303	270	47
1	-3	4	1085	987	27
2	-3	4	1362	1440	27
3	-3	4	189	77	70
4	-3	4	481	424	34
5	-3	4	128	144	127
6	-3	4	873	882	33
7	-3	4	1082	1062	34
8	-3	4	539	522	43
9	-3	4	529	513	46
10	-3	4	337	380	72
11	-3	4	551	625	55
12	-3	4	390	401	76
13	-3	4	180	113	81
-13	-2	4	483	530	37
-12	-2	4	0	181	1
-11	-2	4	0	167	1
-10	-2	4	635	561	46
-9	-2	4	965	1009	40
-8	-2	4	0	59	1
-7	-2	4	260	308	67
-6	-2	4	464	505	40
-5	-2	4	894	1009	32
-4	-2	4	1092	1129	29
-3	-2	4	1051	1019	28
-2	-2	4	743	729	29
-1	-2	4	399	419	36
0	-2	4	1224	1284	25
1	-2	4	573	591	29
2	-2	4	117	124	117
3	-2	4	402	414	36
4	-2	4	1227	1190	27
5	-2	4	425	432	36
6	-2	4	1028	1049	31
7	-2	4	240	248	63
8	-2	4	887	927	37
9	-2	4	490	528	46
10	-2	4	907	899	44
11	-2	4	241	260	80
12	-2	4	256	85	88
13	-2	4	485	423	34
14	-2	4	486	500	42
-13	-1	4	212	199	74
-12	-1	4	151	206	151
-11	-1	4	708	618	50
-10	-1	4	280	224	78
-9	-1	4	0	35	1
-8	-1	4	294	370	64
-7	-1	4	1527	1497	34
-6	-1	4	173	259	133
-5	-1	4	1120	1097	30
-4	-1	4	179	284	93
-3	-1	4	1031	977	27
-2	-1	4	1320	1245	26
-1	-1	4	1610	1592	24
0	-1	4	205	180	77
1	-1	4	383	358	36
2	-1	4	273	291	44
3	-1	4	1788	1759	24

h	k	l	10Fo	10Fc	10s
4	-1	4	1166	1101	26
5	-1	4	665	664	31
6	-1	4	1150	1127	30
7	-1	4	829	833	35
8	-1	4	1059	1077	35
9	-1	4	301	281	68
10	-1	4	0	100	1
11	-1	4	0	190	1
12	-1	4	650	715	57
13	-1	4	125	165	124
14	-1	4	403	342	40
-13	0	4	308	379	55
-12	0	4	452	426	34
-11	0	4	187	129	122
-10	0	4	0	82	1
-9	0	4	480	471	45
-8	0	4	763	722	38
-7	0	4	580	550	41
-6	0	4	326	325	47
-5	0	4	1210	1285	31
-4	0	4	580	621	34
-3	0	4	1285	1263	27
-2	0	4	208	204	60
-1	0	4	249	317	60
0	0	4	1618	1625	22
1	0	4	784	754	25
2	0	4	1189	1196	22
3	0	4	213	226	65
4	0	4	196	159	64
5	0	4	2068	2119	25
6	0	4	559	578	35
7	0	4	488	464	35
8	0	4	354	345	46
9	0	4	260	265	58
10	0	4	664	671	43
11	0	4	608	569	49
12	0	4	218	292	108
13	0	4	86	209	86
14	0	4	471	492	42
15	0	4	291	339	57
-13	1	4	216	106	66
-12	1	4	236	208	54
-11	1	4	168	143	168
-10	1	4	483	470	57
-9	1	4	0	129	1
-8	1	4	200	97	76
-7	1	4	0	180	1
-6	1	4	1706	1729	32
-5	1	4	337	357	45
-4	1	4	0	239	1
-3	1	4	424	451	40
-2	1	4	427	393	36
-1	1	4	2248	2222	22
0	1	4	2109	2098	21
1	1	4	556	521	29
2	1	4	675	772	26
3	1	4	908	935	24
4	1	4	673	668	27
5	1	4	1265	1253	26
6	1	4	404	347	38
7	1	4	1405	1399	29
8	1	4	306	241	54
9	1	4	1064	1091	36
10	1	4	308	271	54
11	1	4	330	395	73
12	1	4	243	225	97
13	1	4	981	904	48
14	1	4	0	21	1
15	1	4	129	164	129
-12	2	4	499	553	37
-11	2	4	257	294	89
-10	2	4	291	243	68
-9	2	4	323	337	57
-8	2	4	702	763	43
-7	2	4	678	695	41
-6	2	4	837	853	35
-5	2	4	466	391	37
-4	2	4	1522	1486	29
-3	2	4	599	550	31
-2	2	4	959	969	26
-1	2	4	896	927	26
0	2	4	918	879	24
1	2	4	507	506	29
2	2	4	1894	1810	20
3	2	4	492	467	31
4	2	4	393	488	36
5	2	4	761	768	27
6	2	4	1252	1218	27
7	2	4	1137	1137	29
8	2	4	441	469	41

h	k	l	10Fo	10Fc	10s
9	2	4	526	515	39
10	2	4	355	416	54
11	2	4	1119	1110	41
12	2	4	444	432	60
13	2	4	148	43	147
14	2	4	0	102	1
15	2	4	534	507	39
16	2	4	207	177	89
-12	3	4	288	236	42
-11	3	4	340	338	39
-10	3	4	184	181	184
-9	3	4	879	919	44
-8	3	4	105	228	105
-7	3	4	249	280	72
-6	3	4	719	802	40
-5	3	4	1166	1198	33
-4	3	4	1036	1044	32
-3	3	4	330	344	45
-2	3	4	1036	1012	28
-1	3	4	162	161	132
0	3	4	1250	1268	23
1	3	4	1429	1425	22
2	3	4	295	350	47
3	3	4	314	307	42
4	3	4	1370	1373	23
5	3	4	462	434	36
6	3	4	1127	1136	27
7	3	4	484	510	40
8	3	4	1272	1326	31
9	3	4	89	78	89
10	3	4	1098	1130	37
11	3	4	148	122	148
12	3	4	210	147	134
13	3	4	610	704	62
14	3	4	586	618	56
15	3	4	0	78	1
16	3	4	195	186	76
-11	4	4	576	561	33
-10	4	4	278	307	89
-9	4	4	195	100	126
-8	4	4	0	71	1
-7	4	4	1152	1095	38
-6	4	4	0	126	1
-5	4	4	436	443	43
-4	4	4	716	725	34
-3	4	4	1277	1267	30
-2	4	4	429	418	36
-1	4	4	1446	1431	26
0	4	4	156	218	115
1	4	4	153	197	124
2	4	4	1173	1187	24
3	4	4	747	799	27
4	4	4	220	94	57
5	4	4	50	95	49
6	4	4	1147	1166	27
7	4	4	683	726	32
8	4	4	1479	1521	31
9	4	4	356	305	45
10	4	4	791	718	40
11	4	4	0	45	1
12	4	4	844	870	47
13	4	4	322	334	75
14	4	4	0	63	1
15	4	4	210	303	209
16	4	4	388	366	45
-11	5	4	184	167	81
-10	5	4	0	134	1
-9	5	4	605	651	51
-8	5	4	583	637	49
-7	5	4	302	301	64
-6	5	4	221	139	80
-5	5	4	1113	1144	35
-4	5	4	206	122	79
-3	5	4	917	901	32
-2	5	4	437	405	36
-1	5	4	1134	1093	28
0	5	4	158	92	101
1	5	4	1580	1565	24
2	5	4	531	496	29
3	5	4	249	194	53
4	5	4	1124	1095	25
5	5	4	1157	1187	26
6	5	4	878	830	29
7	5	4	803	775	31
8	5	4	616	612	39
9	5	4	1586	1482	33
10	5	4	863	890	38
11	5	4	521	524	43
12	5	4	0	78	1
13	5	4	0	29	1

h	k	l	10Fo	10Fc	10s
14	5	4	708	605	51
15	5	4	369	402	79
16	5	4	0	97	1
-10	6	4	637	686	31
-9	6	4	188	99	187
-8	6	4	0	55	1
-7	6	4	427	498	56
-6	6	4	955	987	39
-5	6	4	393	449	53
-4	6	4	536	591	44
-3	6	4	475	444	37
-2	6	4	846	912	32
-1	6	4	922	937	30
0	6	4	579	576	34
1	6	4	49	99	48
2	6	4	124	120	123
3	6	4	1600	1584	25
4	6	4	738	771	29
5	6	4	710	640	30
6	6	4	464	408	32
7	6	4	1246	1220	30
8	6	4	258	131	60
9	6	4	1303	1284	33
10	6	4	119	194	119
11	6	4	729	781	44
12	6	4	518	435	49
13	6	4	712	688	53
14	6	4	229	152	92
15	6	4	274	228	107
16	6	4	253	178	62
-10	7	4	0	130	1
-9	7	4	111	33	111
-8	7	4	952	937	44
-7	7	4	366	270	57
-6	7	4	150	211	149
-5	7	4	189	108	81
-4	7	4	685	695	42
-3	7	4	252	310	79
-2	7	4	555	607	38
-1	7	4	221	326	64
0	7	4	1015	980	30
1	7	4	403	386	39
2	7	4	837	867	30
3	7	4	192	173	75
4	7	4	0	166	1
5	7	4	924	969	29
6	7	4	1454	1484	30
7	7	4	994	986	32
8	7	4	124	91	124
9	7	4	758	803	38
10	7	4	230	219	81
11	7	4	1204	1165	39
12	7	4	506	538	54
13	7	4	325	276	74
14	7	4	172	88	171
15	7	4	488	450	64
16	7	4	0	102	1
-9	8	4	467	490	36
-8	8	4	133	152	132
-7	8	4	197	37	83
-6	8	4	537	561	45
-5	8	4	697	647	42
-4	8	4	283	236	60
-3	8	4	225	74	70
-2	8	4	745	713	36
-1	8	4	226	278	81
0	8	4	1203	1255	32
1	8	4	880	831	31
2	8	4	797	799	32
3	8	4	80	89	79
4	8	4	898	936	31
5	8	4	183	176	88
6	8	4	1177	1154	31
7	8	4	629	609	35
8	8	4	1505	1497	33
9	8	4	597	556	41
10	8	4	329	302	52
11	8	4	417	344	62
12	8	4	245	263	82
13	8	4	438	380	59
14	8	4	574	608	57
15	8	4	237	154	86
16	8	4	0	90	1
-8	9	4	87	79	86
-7	9	4	636	605	29
-6	9	4	113	31	113
-5	9	4	153	112	152
-4	9	4	275	306	80
-3	9	4	1064	1055	38
-2	9	4	631	666	37

h	k	l	10Fo	10Fc	10s
-1	9	4	649	601	39
0	9	4	691	677	35
1	9	4	416	376	44
2	9	4	772	755	35
3	9	4	498	475	38
4	9	4	438	437	38
5	9	4	0	114	1
6	9	4	1629	1591	32
7	9	4	994	945	35
8	9	4	876	851	35
9	9	4	226	214	87
10	9	4	829	840	40
11	9	4	106	143	105
12	9	4	870	804	42
13	9	4	356	316	66
14	9	4	0	18	1
16	9	4	521	471	35
-7	10	4	152	209	90
-6	10	4	181	52	61
-5	10	4	665	685	50
-4	10	4	419	472	52
-3	10	4	384	409	58
-2	10	4	102	130	102
-1	10	4	878	903	38
0	10	4	356	371	53
1	10	4	908	846	35
2	10	4	946	859	35
3	10	4	221	248	76
4	10	4	512	513	39
5	10	4	1222	1175	33
6	10	4	531	617	42
7	10	4	133	70	132
8	10	4	768	744	40
9	10	4	930	946	37
10	10	4	544	530	45
11	10	4	530	548	52
12	10	4	207	51	68
13	10	4	117	12	116
14	10	4	612	583	58
15	10	4	388	382	38
16	10	4	136	71	135
-6	11	4	565	615	32
-5	11	4	459	400	32
-4	11	4	224	71	94
-3	11	4	422	450	59
-2	11	4	488	470	52
-1	11	4	502	533	51
0	11	4	484	472	44
1	11	4	308	341	59
2	11	4	0	16	1
3	11	4	932	922	37
4	11	4	468	398	43
5	11	4	0	127	1
6	11	4	0	169	1
7	11	4	1185	1201	37
8	11	4	428	444	53
9	11	4	698	663	42
10	11	4	75	113	75
11	11	4	516	582	48
12	11	4	194	41	83
13	11	4	614	591	52
14	11	4	273	234	78
15	11	4	0	7	1
16	11	4	441	477	39
-5	12	4	283	215	46
-4	12	4	681	675	28
-3	12	4	416	442	48
-2	12	4	279	308	70
-1	12	4	76	81	76
0	12	4	424	376	51
1	12	4	216	64	75
2	12	4	334	275	52
3	12	4	392	358	46
4	12	4	408	333	48
5	12	4	791	759	37
6	12	4	955	1000	39
7	12	4	538	453	41
8	12	4	230	157	66
9	12	4	750	715	42
10	12	4	274	157	68
11	12	4	621	654	47
12	12	4	80	171	79
13	12	4	168	189	167
14	12	4	114	36	114
15	12	4	580	589	33
-4	13	4	495	504	32
-3	13	4	0	43	1
-2	13	4	410	381	33
-1	13	4	135	20	135
0	13	4	133	121	133

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
1	13	4	169	204	131
2	13	4	649	593	42
3	13	4	71	148	71
4	13	4	1325	1240	37
5	13	4	193	136	107
6	13	4	0	95	1
7	13	4	522	595	46
8	13	4	718	722	43
9	13	4	387	382	55
10	13	4	556	492	46
11	13	4	138	157	138
12	13	4	500	478	47
13	13	4	490	504	32
14	13	4	256	257	52
15	13	4	57	29	57
-2	14	4	230	186	44
-1	14	4	69	91	69
0	14	4	288	412	89
1	14	4	428	408	52
2	14	4	643	592	45
3	14	4	600	539	43
4	14	4	200	101	97
5	14	4	75	108	75
6	14	4	786	766	42
7	14	4	304	276	63
8	14	4	408	372	52
9	14	4	135	147	135
10	14	4	569	594	48
11	14	4	0	51	1
12	14	4	556	514	29
13	14	4	0	64	1
14	14	4	192	286	80
0	15	4	69	115	68
1	15	4	467	438	30
2	15	4	82	80	82
3	15	4	316	283	59
4	15	4	351	418	66
5	15	4	508	553	48
7	15	4	156	148	155
8	15	4	428	441	54
9	15	4	501	502	48
10	15	4	436	443	32
11	15	4	0	130	1
12	15	4	286	348	44
13	15	4	188	138	65
2	16	4	68	150	67
3	16	4	593	584	27
4	16	4	96	119	96
5	16	4	96	90	96
6	16	4	254	238	42
7	16	4	662	635	26
8	16	4	0	39	1
9	16	4	199	136	51
10	16	4	53	89	52
11	16	4	516	508	33
-7	-12	5	50	10	49
-6	-12	5	563	507	28
-5	-12	5	329	304	34
-4	-12	5	370	386	33
-3	-12	5	241	164	38
-2	-12	5	474	487	29
-1	-12	5	65	64	65
0	-12	5	0	103	1
1	-12	5	303	308	40
2	-12	5	538	487	28
-9	-11	5	398	378	34
-8	-11	5	284	269	42
-7	-11	5	303	269	36
-6	-11	5	391	364	31
-5	-11	5	398	295	62
-4	-11	5	550	568	48
-3	-11	5	281	228	61
-2	-11	5	238	184	60
-1	-11	5	327	210	54
0	-11	5	620	673	46
1	-11	5	290	261	36
2	-11	5	327	282	34
3	-11	5	0	82	1
4	-11	5	515	517	29
-10	-10	5	214	144	41
-9	-10	5	213	137	43
-8	-10	5	82	161	81
-7	-10	5	573	509	49
-6	-10	5	312	356	62
-5	-10	5	549	551	44
-4	-10	5	232	273	82
-3	-10	5	399	409	46
-2	-10	5	483	575	49
-1	-10	5	459	550	44
0	-10	5	0	102	1

h	k	l	10Fo	10Fc	10s
1	-10	5	314	285	58
2	-10	5	365	366	63
3	-10	5	505	518	52
4	-10	5	464	467	29
5	-10	5	67	119	66
6	-10	5	348	396	37
-11	-9	5	0	14	1
-10	-9	5	175	114	69
-9	-9	5	580	563	28
-8	-9	5	280	374	83
-7	-9	5	479	493	45
-6	-9	5	234	128	64
-5	-9	5	530	580	45
-4	-9	5	0	126	1
-3	-9	5	783	811	40
-2	-9	5	315	289	54
-1	-9	5	121	82	121
0	-9	5	186	227	108
1	-9	5	743	750	40
2	-9	5	73	49	72
3	-9	5	408	424	54
4	-9	5	415	398	52
5	-9	5	466	511	53
6	-9	5	426	391	30
7	-9	5	197	151	54
-11	-8	5	291	274	38
-10	-8	5	476	533	33
-9	-8	5	224	16	61
-8	-8	5	306	246	67
-7	-8	5	469	490	50
-6	-8	5	587	585	45
-5	-8	5	725	731	41
-4	-8	5	137	247	137
-3	-8	5	453	479	44
-2	-8	5	166	222	166
-1	-8	5	808	833	38
0	-8	5	765	796	38
1	-8	5	503	442	38
2	-8	5	317	213	49
3	-8	5	712	687	39
4	-8	5	190	20	86
5	-8	5	0	219	1
6	-8	5	295	197	52
7	-8	5	561	567	44
8	-8	5	325	316	35
9	-8	5	468	534	34
-12	-7	5	427	406	32
-11	-7	5	0	201	1
-10	-7	5	354	238	55
-9	-7	5	156	74	155
-8	-7	5	908	888	41
-7	-7	5	192	128	74
-6	-7	5	513	404	42
-5	-7	5	580	567	39
-4	-7	5	798	799	38
-3	-7	5	653	707	41
-2	-7	5	1084	1095	34
-1	-7	5	146	180	145
0	-7	5	217	64	62
1	-7	5	315	226	49
2	-7	5	997	989	37
3	-7	5	377	406	52
4	-7	5	330	219	49
5	-7	5	767	756	41
6	-7	5	221	241	92
7	-7	5	498	524	51
8	-7	5	79	237	79
9	-7	5	0	148	1
10	-7	5	0	31	1
-12	-6	5	136	59	136
-11	-6	5	0	103	1
-10	-6	5	449	400	55
-9	-6	5	395	395	56
-8	-6	5	571	510	44
-7	-6	5	214	73	62
-6	-6	5	1100	1026	36
-5	-6	5	328	376	57
-4	-6	5	892	916	35
-3	-6	5	753	723	36
-2	-6	5	495	507	39
-1	-6	5	187	236	89
0	-6	5	1336	1336	33
1	-6	5	107	72	107
2	-6	5	429	452	46
3	-6	5	223	203	62
4	-6	5	887	973	36
5	-6	5	192	162	100
6	-6	5	515	519	44
7	-6	5	311	304	54
8	-6	5	317	357	68

h	k	l	10Fo	10Fc	10s
9	-6	5	557	567	50
10	-6	5	248	258	55
11	-6	5	117	143	116
-12	-5	5	293	318	47
-11	-5	5	429	487	66
-10	-5	5	254	230	86
-9	-5	5	204	266	111
-8	-5	5	103	106	103
-7	-5	5	1019	1016	37
-6	-5	5	234	221	79
-5	-5	5	326	348	51
-4	-5	5	799	814	35
-3	-5	5	325	309	49
-2	-5	5	590	521	36
-1	-5	5	1012	1044	32
0	-5	5	0	109	1
1	-5	5	0	91	1
2	-5	5	1201	1230	32
3	-5	5	626	596	36
4	-5	5	533	577	40
5	-5	5	363	275	41
6	-5	5	456	452	41
7	-5	5	0	133	1
8	-5	5	504	535	45
9	-5	5	77	159	77
10	-5	5	183	267	183
11	-5	5	209	316	72
12	-5	5	521	543	35
-13	-4	5	328	317	42
-12	-4	5	324	254	37
-11	-4	5	120	159	119
-10	-4	5	265	253	89
-9	-4	5	945	888	41
-8	-4	5	398	435	53
-7	-4	5	68	112	67
-6	-4	5	397	297	42
-5	-4	5	1364	1325	34
-4	-4	5	183	188	79
-3	-4	5	1000	1051	32
-2	-4	5	225	268	75
-1	-4	5	392	434	41
0	-4	5	651	661	35
1	-4	5	1607	1564	30
2	-4	5	0	39	1
3	-4	5	0	53	1
4	-4	5	599	602	35
5	-4	5	744	749	37
6	-4	5	947	916	36
7	-4	5	264	391	77
8	-4	5	419	464	48
9	-4	5	402	364	51
10	-4	5	767	721	46
11	-4	5	147	190	147
12	-4	5	50	28	49
-13	-3	5	0	62	1
-12	-3	5	203	189	71
-11	-3	5	207	244	157
-10	-3	5	1128	1079	42
-9	-3	5	214	121	82
-8	-3	5	74	68	73
-7	-3	5	846	805	38
-6	-3	5	602	576	41
-5	-3	5	835	867	35
-4	-3	5	908	908	33
-3	-3	5	919	930	31
-2	-3	5	564	578	34
-1	-3	5	1181	1105	29
0	-3	5	577	604	33
1	-3	5	227	259	64
2	-3	5	370	377	40
3	-3	5	1277	1300	29
4	-3	5	327	281	42
5	-3	5	767	733	33
6	-3	5	234	250	65
7	-3	5	844	849	37
8	-3	5	531	563	43
9	-3	5	527	543	50
10	-3	5	191	184	110
11	-3	5	219	295	90
12	-3	5	411	356	76
13	-3	5	580	598	34
-13	-2	5	174	197	116
-12	-2	5	498	559	39
-11	-2	5	239	249	90
-10	-2	5	139	33	139
-9	-2	5	293	263	82
-8	-2	5	1193	1153	38
-7	-2	5	192	92	73
-6	-2	5	414	416	42
-5	-2	5	618	667	36

h	k	l	10Fo	10Fc	10s
-4	-2	5	1254	1264	31
-3	-2	5	614	647	33
-2	-2	5	1108	1132	29
-1	-2	5	217	167	64
0	-2	5	352	370	40
1	-2	5	1106	1096	27
2	-2	5	1447	1402	27
3	-2	5	182	287	91
4	-2	5	571	554	32
5	-2	5	783	786	32
6	-2	5	715	724	35
7	-2	5	1166	1166	33
8	-2	5	98	88	97
9	-2	5	822	791	40
10	-2	5	0	35	1
11	-2	5	803	785	46
12	-2	5	298	273	81
13	-2	5	340	391	46
14	-2	5	312	187	51
-12	-1	5	0	54	1
-11	-1	5	224	71	105
-10	-1	5	860	758	47
-9	-1	5	526	596	57
-8	-1	5	74	27	74
-7	-1	5	225	142	78
-6	-1	5	884	858	36
-5	-1	5	301	316	50
-4	-1	5	1344	1286	30
-3	-1	5	484	519	39
-2	-1	5	1296	1320	28
-1	-1	5	467	509	35
0	-1	5	1253	1225	26
1	-1	5	161	200	112
2	-1	5	1046	936	26
3	-1	5	973	1034	28
4	-1	5	1449	1466	27
5	-1	5	359	357	45
6	-1	5	128	123	128
7	-1	5	488	383	39
8	-1	5	595	557	39
9	-1	5	1312	1296	37
10	-1	5	610	632	49
11	-1	5	347	261	57
12	-1	5	267	116	69
13	-1	5	310	247	77
14	-1	5	313	244	47
-12	0	5	176	131	80
-11	0	5	593	635	52
-10	0	5	0	116	1
-9	0	5	170	115	100
-8	0	5	694	624	40
-7	0	5	847	902	38
-6	0	5	0	140	1
-5	0	5	301	206	54
-4	0	5	253	268	66
-3	0	5	891	880	31
-2	0	5	1444	1406	27
-1	0	5	1431	1419	26
0	0	5	632	607	31
1	0	5	166	72	92
2	0	5	1431	1431	24
3	0	5	533	515	33
4	0	5	1106	1097	26
5	0	5	279	238	53
6	0	5	1586	1642	29
7	0	5	146	14	145
8	0	5	487	466	43
9	0	5	368	391	56
10	0	5	505	560	48
11	0	5	155	297	154
12	0	5	938	909	49
13	0	5	0	51	1
14	0	5	54	68	53
15	0	5	185	191	102
-12	1	5	472	406	34
-11	1	5	230	149	94
-10	1	5	142	23	142
-9	1	5	851	776	44
-8	1	5	194	72	95
-7	1	5	301	201	53
-6	1	5	217	163	72
-5	1	5	1401	1395	32
-4	1	5	285	257	55
-3	1	5	817	803	31
-2	1	5	968	971	28
-1	1	5	1109	1059	26
0	1	5	1126	1085	25
1	1	5	1822	1791	23
2	1	5	227	168	62
3	1	5	535	499	30

h	k	l	10Fo	10Fc	10s
4	1	5	930	952	27
5	1	5	1741	1771	26
6	1	5	809	871	30
7	1	5	100	147	99
8	1	5	703	728	37
9	1	5	118	87	117
10	1	5	998	974	38
11	1	5	552	588	50
12	1	5	0	112	1
13	1	5	213	35	111
14	1	5	732	766	60
15	1	5	0	120	1
-12	2	5	345	253	44
-11	2	5	368	421	40
-10	2	5	454	410	57
-9	2	5	136	90	135
-8	2	5	106	30	105
-7	2	5	676	688	42
-6	2	5	1164	1126	35
-5	2	5	714	654	38
-4	2	5	214	240	85
-3	2	5	1244	1205	29
-2	2	5	282	222	47
-1	2	5	1423	1457	25
0	2	5	1415	1339	25
1	2	5	413	413	35
2	2	5	40	89	40
3	2	5	1774	1744	23
4	2	5	203	66	69
5	2	5	149	204	148
6	2	5	313	328	44
7	2	5	1321	1293	30
8	2	5	767	787	35
9	2	5	726	715	38
10	2	5	243	247	81
11	2	5	0	98	1
12	2	5	520	518	53
13	2	5	739	739	52
14	2	5	0	13	1
15	2	5	160	66	128
16	2	5	368	410	48
-11	3	5	246	212	56
-10	3	5	222	215	115
-9	3	5	0	83	1
-8	3	5	908	978	44
-7	3	5	160	144	159
-6	3	5	289	312	63
-5	3	5	825	823	35
-4	3	5	1245	1216	32
-3	3	5	710	681	34
-2	3	5	678	663	32
-1	3	5	934	876	27
0	3	5	0	39	1
1	3	5	1322	1283	24
2	3	5	2267	2252	22
3	3	5	471	451	34
4	3	5	954	949	26
5	3	5	1278	1249	26
6	3	5	0	61	1
7	3	5	1036	1071	30
8	3	5	643	612	35
9	3	5	929	901	36
10	3	5	0	148	1
11	3	5	886	827	40
12	3	5	137	174	137
13	3	5	188	67	134
14	3	5	497	399	59
15	3	5	765	647	58
16	3	5	0	53	1
-11	4	5	107	106	106
-10	4	5	600	630	56
-9	4	5	658	664	48
-8	4	5	0	41	1
-7	4	5	381	358	51
-6	4	5	991	1009	39
-5	4	5	0	145	1
-4	4	5	1010	1007	33
-3	4	5	842	863	33
-2	4	5	1374	1357	29
-1	4	5	262	163	51
0	4	5	477	551	34
1	4	5	273	300	50
2	4	5	473	552	33
3	4	5	1267	1277	24
4	4	5	2099	2083	24
5	4	5	1119	1069	27
6	4	5	197	78	67
7	4	5	658	652	33
8	4	5	1019	946	32
9	4	5	870	827	34

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
10	4	5	624	663	42
11	4	5	472	447	47
12	4	5	111	110	110
13	4	5	871	811	47
14	4	5	249	268	109
15	4	5	133	86	132
16	4	5	238	49	59
-11	5	5	302	370	52
-10	5	5	179	168	76
-9	5	5	187	204	117
-8	5	5	262	286	95
-7	5	5	1008	1077	43
-6	5	5	622	566	43
-5	5	5	254	244	62
-4	5	5	1094	1030	35
-3	5	5	845	793	35
-2	5	5	337	316	44
-1	5	5	764	780	31
0	5	5	0	137	1
1	5	5	0	54	1
2	5	5	1962	1912	25
3	5	5	782	805	28
4	5	5	122	183	121
5	5	5	387	352	43
6	5	5	1660	1685	28
7	5	5	128	78	127
8	5	5	1443	1354	31
9	5	5	330	438	59
10	5	5	633	600	42
11	5	5	395	409	59
12	5	5	617	649	49
13	5	5	141	189	141
14	5	5	0	65	1
15	5	5	497	453	67
16	5	5	587	614	38
-10	6	5	159	17	79
-9	6	5	824	788	28
-8	6	5	423	350	56
-7	6	5	173	267	172
-6	6	5	223	172	100
-5	6	5	1219	1166	37
-4	6	5	423	426	44
-3	6	5	988	904	35
-2	6	5	762	793	34
-1	6	5	316	328	53
0	6	5	686	709	33
1	6	5	198	227	74
2	6	5	0	109	1
3	6	5	585	567	31
4	6	5	1340	1282	27
5	6	5	1294	1259	28
6	6	5	541	572	36
7	6	5	0	83	1
8	6	5	711	693	35
9	6	5	260	274	57
10	6	5	1469	1404	35
11	6	5	496	431	47
12	6	5	692	678	47
13	6	5	201	142	99
14	6	5	481	523	59
15	6	5	93	158	92
16	6	5	204	269	87
17	6	5	156	102	124
-9	7	5	0	59	1
-8	7	5	435	361	62
-7	7	5	714	719	49
-6	7	5	607	594	48
-5	7	5	364	328	51
-4	7	5	404	328	52
-3	7	5	806	820	36
-2	7	5	180	35	110
-1	7	5	840	849	35
0	7	5	144	169	143
1	7	5	673	658	34
2	7	5	463	387	35
3	7	5	1418	1475	28
4	7	5	616	530	32
5	7	5	0	143	1
6	7	5	724	695	33
7	7	5	1225	1174	32
8	7	5	764	739	34
9	7	5	753	816	38
10	7	5	666	579	40
11	7	5	677	652	46
12	7	5	518	586	55
13	7	5	391	394	64
14	7	5	173	65	172
15	7	5	0	164	1
16	7	5	502	441	40
17	7	5	350	372	52

h	k	l	10Fo	10Fc	10s
-9	8	5	130	44	130
-8	8	5	788	776	29
-7	8	5	217	82	95
-6	8	5	237	146	77
-5	8	5	549	528	44
-4	8	5	703	611	41
-3	8	5	310	414	65
-2	8	5	496	481	39
-1	8	5	737	717	34
0	8	5	991	969	33
1	8	5	1122	1112	32
2	8	5	653	606	34
3	8	5	0	98	1
4	8	5	208	263	73
5	8	5	1503	1524	30
6	8	5	614	655	36
7	8	5	762	751	36
8	8	5	183	203	111
9	8	5	1324	1279	36
10	8	5	298	406	78
11	8	5	935	918	42
12	8	5	0	353	1
13	8	5	215	225	119
14	8	5	0	74	1
15	8	5	691	565	54
16	8	5	167	120	92
17	8	5	0	64	1
-8	9	5	0	56	1
-7	9	5	0	93	1
-6	9	5	697	668	51
-5	9	5	206	162	86
-4	9	5	249	194	89
-3	9	5	362	173	42
-2	9	5	834	912	40
-1	9	5	222	230	75
0	9	5	1001	983	35
1	9	5	373	344	44
2	9	5	417	399	41
3	9	5	538	556	38
4	9	5	1120	1110	32
5	9	5	247	177	59
6	9	5	188	188	84
7	9	5	834	822	36
8	9	5	837	855	38
9	9	5	945	915	37
10	9	5	304	299	59
11	9	5	689	647	46
12	9	5	0	150	1
13	9	5	462	506	59
14	9	5	436	545	71
15	9	5	237	162	116
16	9	5	135	78	135
17	9	5	593	557	36
-7	10	5	401	422	38
-6	10	5	99	87	98
-5	10	5	255	93	57
-4	10	5	454	528	55
-3	10	5	463	473	48
-2	10	5	440	477	57
-1	10	5	289	236	63
0	10	5	823	769	38
1	10	5	0	24	1
2	10	5	877	856	36
3	10	5	648	646	37
4	10	5	0	49	1
5	10	5	113	95	113
6	10	5	1671	1612	33
7	10	5	695	648	39
8	10	5	572	569	40
9	10	5	243	298	67
10	10	5	631	643	44
11	10	5	130	212	130
12	10	5	527	488	49
13	10	5	246	290	105
14	10	5	0	58	1
15	10	5	476	476	62
16	10	5	345	361	48
-6	11	5	136	151	135
-5	11	5	827	858	27
-4	11	5	379	302	53
-3	11	5	260	332	79
-2	11	5	452	447	58
-1	11	5	447	418	48
0	11	5	378	344	52
1	11	5	413	373	42
2	11	5	283	299	60
3	11	5	262	214	67
4	11	5	857	879	37
5	11	5	483	456	41
6	11	5	518	540	43

h	k	l	10Fo	10Fc	10s
7	11	5	397	407	48
8	11	5	1021	1054	38
9	11	5	545	570	45
10	11	5	562	561	44
11	11	5	362	396	54
13	11	5	274	350	81
14	11	5	512	519	53
15	11	5	200	119	61
16	11	5	324	363	47
-5	12	5	183	191	68
-4	12	5	0	66	1
-3	12	5	991	903	44
-2	12	5	158	216	157
-1	12	5	588	526	50
0	12	5	130	215	130
1	12	5	72	121	72
2	12	5	472	481	43
3	12	5	432	420	50
4	12	5	158	171	158
5	12	5	1079	1090	37
6	12	5	174	184	134
7	12	5	1610	1562	37
8	12	5	550	569	43
9	12	5	651	759	45
10	12	5	923	922	43
11	12	5	0	118	1
12	12	5	323	354	61
13	12	5	336	298	63
15	12	5	121	135	120
16	12	5	571	573	35
-4	13	5	656	631	31
-3	13	5	311	355	43
-2	13	5	311	328	36
-1	13	5	632	624	47
0	13	5	174	51	120
1	13	5	304	304	64
2	13	5	0	241	1
3	13	5	0	79	1
4	13	5	447	442	50
5	13	5	1155	1099	39
6	13	5	311	334	61
7	13	5	129	186	129
8	13	5	451	376	47
9	13	5	841	872	45
10	13	5	0	148	1
11	13	5	670	752	47
12	13	5	308	226	70
13	13	5	226	210	92
14	13	5	272	292	49
15	13	5	333	329	40
-2	14	5	473	446	30
-1	14	5	269	200	40
0	14	5	91	112	90
1	14	5	158	268	157
2	14	5	448	372	49
3	14	5	368	377	56
4	14	5	790	761	42
5	14	5	229	228	93
6	14	5	108	143	108
7	14	5	667	689	45
8	14	5	257	240	98
9	14	5	476	432	50
10	14	5	288	321	80
11	14	5	650	596	46
12	14	5	303	257	56
13	14	5	484	457	33
14	14	5	0	55	1
0	15	5	388	436	24
1	15	5	285	250	40
2	15	5	454	491	32
3	15	5	196	53	74
4	15	5	223	48	80
5	15	5	209	200	120
6	15	5	864	866	43
7	15	5	0	35	1
8	15	5	0	74	1
9	15	5	241	260	77
10	15	5	526	515	53
11	15	5	472	440	31
12	15	5	333	313	40
13	15	5	148	109	147
2	16	5	273	161	35
3	16	5	277	321	42
4	16	5	523	516	29
5	16	5	334	328	37
6	16	5	0	62	1
7	16	5	0	117	1
8	16	5	586	562	29
9	16	5	46	94	46
10	16	5	329	316	35

h	k	l	10Fo	10Fc	10s
11	16	5	115	55	114
12	16	5	468	451	34
6	17	5	373	367	36
7	17	5	560	494	28
8	17	5	140	152	113
-4	-12	6	302	289	36
-3	-12	6	146	170	69
-2	-12	6	138	36	73
-1	-12	6	689	647	26
-7	-11	6	93	185	93
-6	-11	6	371	357	31
-5	-11	6	287	285	33
-4	-11	6	358	333	31
-3	-11	6	472	468	29
-2	-11	6	436	399	27
-1	-11	6	0	37	1
0	-11	6	59	29	58
1	-11	6	579	510	27
2	-11	6	336	350	36
3	-11	6	277	294	40
-9	-10	6	238	200	45
-8	-10	6	191	180	51
-7	-10	6	146	212	95
-6	-10	6	410	466	32
-5	-10	6	0	26	1
-4	-10	6	574	581	43
-3	-10	6	167	187	80
-2	-10	6	299	206	60
-1	-10	6	211	296	113
0	-10	6	631	665	46
1	-10	6	0	88	1
2	-10	6	214	248	44
3	-10	6	311	330	37
4	-10	6	482	495	30
5	-10	6	340	327	36
-10	-9	6	0	77	1
-9	-9	6	45	34	45
-8	-9	6	523	530	30
-7	-9	6	446	423	49
-6	-9	6	437	450	50
-5	-9	6	248	249	73
-4	-9	6	388	338	49
-3	-9	6	218	96	65
-2	-9	6	692	725	42
-1	-9	6	432	446	38
0	-9	6	144	18	144
1	-9	6	273	183	61
2	-9	6	697	685	42
3	-9	6	225	133	81
4	-9	6	402	273	52
5	-9	6	158	138	66
6	-9	6	572	565	29
7	-9	6	437	466	33
-10	-8	6	247	241	43
-9	-8	6	617	581	28
-8	-8	6	0	47	1
-7	-8	6	202	296	122
-6	-8	6	183	146	104
-5	-8	6	697	703	41
-4	-8	6	521	522	46
-3	-8	6	865	857	40
-2	-8	6	421	440	51
-1	-8	6	0	101	1
0	-8	6	350	313	42
1	-8	6	704	636	40
2	-8	6	235	232	75
3	-8	6	0	206	1
4	-8	6	855	832	40
5	-8	6	327	301	60
6	-8	6	514	524	46
7	-8	6	0	59	1
8	-8	6	200	174	49
-11	-7	6	449	400	32
-10	-7	6	314	228	35
-9	-7	6	227	205	85
-8	-7	6	0	168	1
-7	-7	6	830	887	42
-6	-7	6	164	100	163
-5	-7	6	877	815	38
-4	-7	6	140	149	140
-3	-7	6	465	500	44
-2	-7	6	167	92	92
-1	-7	6	1004	1052	36
0	-7	6	734	740	38
1	-7	6	117	201	117
2	-7	6	629	625	41
3	-7	6	771	748	40
4	-7	6	761	731	39
5	-7	6	162	68	162
6	-7	6	360	346	55

h	k	l	10Fo	10Fc	10s
7	-7	6	557	624	48
8	-7	6	286	327	42
9	-7	6	547	515	30
-11	-6	6	203	255	55
-10	-6	6	248	218	46
-9	-6	6	516	549	53
-8	-6	6	375	432	67
-7	-6	6	728	729	41
-6	-6	6	248	195	69
-5	-6	6	334	346	59
-4	-6	6	667	669	38
-3	-6	6	297	375	62
-2	-6	6	820	800	35
-1	-6	6	194	266	94
0	-6	6	173	212	80
1	-6	6	1025	981	35
2	-6	6	597	622	38
3	-6	6	553	469	42
4	-6	6	296	260	65
5	-6	6	799	782	39
6	-6	6	280	254	59
7	-6	6	402	334	51
8	-6	6	0	112	1
10	-6	6	235	126	52
-12	-5	6	331	313	41
-11	-5	6	278	230	44
-10	-5	6	811	700	48
-9	-5	6	0	84	1
-8	-5	6	547	556	47
-7	-5	6	163	140	163
-6	-5	6	852	882	39
-5	-5	6	118	57	118
-4	-5	6	0	93	1
-3	-5	6	563	524	39
-2	-5	6	708	670	37
-1	-5	6	397	481	47
0	-5	6	1726	1667	32
1	-5	6	0	43	1
2	-5	6	319	287	48
3	-5	6	678	733	38
4	-5	6	508	402	42
5	-5	6	733	742	37
6	-5	6	349	344	51
7	-5	6	675	675	43
8	-5	6	251	328	97
9	-5	6	509	525	49
10	-5	6	0	103	1
11	-5	6	0	14	1
-12	-4	6	379	392	38
-11	-4	6	497	553	33
-10	-4	6	115	144	114
-9	-4	6	377	360	53
-8	-4	6	542	512	48
-7	-4	6	543	544	45
-6	-4	6	379	354	43
-5	-4	6	784	797	38
-4	-4	6	1150	1183	33
-3	-4	6	372	454	50
-2	-4	6	928	906	33
-1	-4	6	524	478	39
0	-4	6	0	31	1
1	-4	6	0	96	1
2	-4	6	1629	1631	31
3	-4	6	85	155	85
4	-4	6	299	352	54
5	-4	6	574	512	37
6	-4	6	602	654	42
7	-4	6	408	402	46
8	-4	6	535	553	45
9	-4	6	231	192	72
10	-4	6	334	315	64
11	-4	6	535	491	59
12	-4	6	408	384	39
-12	-3	6	214	123	56
-11	-3	6	159	60	74
-10	-3	6	0	51	1
-9	-3	6	1010	1009	44
-8	-3	6	167	64	166
-7	-3	6	214	118	78
-6	-3	6	877	886	38
-5	-3	6	897	925	37
-4	-3	6	369	465	50
-3	-3	6	977	917	33
-2	-3	6	447	441	41
-1	-3	6	304	273	48
0	-3	6	1017	1058	31
1	-3	6	1011	1037	30
2	-3	6	256	234	59
3	-3	6	0	127	1
4	-3	6	1160	1175	32

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
5	-3	6	336	319	50
6	-3	6	688	651	38
7	-3	6	364	415	55
8	-3	6	600	590	42
9	-3	6	132	31	131
10	-3	6	700	750	48
11	-3	6	146	68	146
12	-3	6	136	8	136
13	-3	6	206	114	71
-12	-2	6	194	184	72
-11	-2	6	529	546	32
-10	-2	6	500	507	59
-9	-2	6	247	126	55
-8	-2	6	0	47	1
-7	-2	6	1041	1040	38
-6	-2	6	244	54	66
-5	-2	6	428	460	47
-4	-2	6	681	685	37
-3	-2	6	895	902	32
-2	-2	6	143	40	143
-1	-2	6	1630	1638	29
0	-2	6	0	101	1
1	-2	6	55	195	55
2	-2	6	860	851	30
3	-2	6	1182	1181	29
4	-2	6	275	345	58
5	-2	6	170	230	108
6	-2	6	868	839	35
7	-2	6	645	642	41
8	-2	6	863	919	39
9	-2	6	408	339	50
10	-2	6	338	370	60
11	-2	6	0	167	1
12	-2	6	417	449	69
13	-2	6	360	365	44
14	-2	6	280	287	62
-12	-1	6	534	535	35
-11	-1	6	0	69	1
-10	-1	6	144	148	144
-9	-1	6	572	623	49
-8	-1	6	602	685	49
-7	-1	6	266	298	69
-6	-1	6	0	85	1
-5	-1	6	934	922	35
-4	-1	6	649	568	34
-3	-1	6	904	907	32
-2	-1	6	732	771	32
-1	-1	6	257	200	53
0	-1	6	277	237	51
1	-1	6	820	849	30
2	-1	6	608	591	31
3	-1	6	251	360	54
4	-1	6	625	591	34
5	-1	6	1766	1813	29
6	-1	6	507	477	41
7	-1	6	612	643	37
8	-1	6	166	135	166
9	-1	6	830	822	39
10	-1	6	184	217	184
11	-1	6	591	590	50
12	-1	6	296	230	72
13	-1	6	0	152	1
14	-1	6	347	280	47
-12	0	6	217	224	62
-11	0	6	90	231	90
-10	0	6	775	744	50
-9	0	6	0	78	1
-8	0	6	169	137	120
-7	0	6	578	611	46
-6	0	6	1100	1144	38
-5	0	6	325	312	56
-4	0	6	230	284	62
-3	0	6	337	270	47
-2	0	6	1441	1386	29
-1	0	6	0	85	1
0	0	6	1589	1495	26
1	0	6	629	586	30
2	0	6	262	302	49
3	0	6	1657	1623	26
4	0	6	1180	1225	28
5	0	6	732	680	33
6	0	6	234	107	54
7	0	6	964	948	33
8	0	6	482	416	40
9	0	6	904	924	39
10	0	6	296	238	71
11	0	6	0	219	1
12	0	6	0	78	1
13	0	6	737	724	55
14	0	6	324	297	45
15	0	6	132	216	132
-12	1	6	0	141	1
-11	1	6	449	435	35
-10	1	6	0	48	1
-8	1	6	1214	1109	41
-7	1	6	400	437	50
-6	1	6	0	130	1
-5	1	6	0	121	1
-4	1	6	616	610	36
-3	1	6	512	485	37
-2	1	6	1059	1125	30
-1	1	6	944	921	29
0	1	6	1160	1156	27
1	1	6	629	637	31
2	1	6	1728	1759	25
3	1	6	650	616	30
4	1	6	451	414	37
5	1	6	821	835	30
6	1	6	1481	1430	30
7	1	6	1027	1006	32
8	1	6	92	106	92
9	1	6	506	432	41
10	1	6	206	175	98
11	1	6	595	523	44
12	1	6	754	786	51
13	1	6	230	35	115
14	1	6	0	96	1
15	1	6	506	501	38
-11	2	6	432	460	36
-10	2	6	307	237	66
-9	2	6	499	555	57
-8	2	6	0	117	1
-7	2	6	341	170	51
-6	2	6	476	531	50
-5	2	6	1396	1359	35
-4	2	6	642	669	36
-3	2	6	308	314	50
-2	2	6	899	912	31
-1	2	6	192	151	72
0	2	6	1481	1470	26
1	2	6	1533	1592	25
2	2	6	0	58	1
3	2	6	504	553	34
4	2	6	1458	1524	26
5	2	6	569	515	32
6	2	6	843	843	31
7	2	6	219	264	74
8	2	6	1230	1182	34
9	2	6	0	188	1
10	2	6	703	684	40
11	2	6	274	227	66
12	2	6	81	19	80
13	2	6	0	171	1
14	2	6	670	735	61
15	2	6	160	165	160
16	2	6	0	46	1
-11	3	6	503	486	33
-10	3	6	239	190	53
-9	3	6	0	110	1
-8	3	6	0	41	1
-7	3	6	1073	1037	40
-6	3	6	212	223	88
-5	3	6	344	341	53
-4	3	6	364	372	43
-3	3	6	983	970	32
-2	3	6	480	489	37
-1	3	6	1345	1346	28
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1	3	6	894	932	29
2	3	6	1075	1064	26
3	3	6	1218	1202	26
4	3	6	1263	1240	26
5	3	6	239	211	57
6	3	6	1650	1590	29
7	3	6	1128	1103	31
8	3	6	460	482	43
9	3	6	186	240	119
10	3	6	273	286	68
11	3	6	0	52	1
12	3	6	952	953	46
13	3	6	479	464	62
14	3	6	88	118	88
15	3	6	0	98	1
16	3	6	614	642	36
-11	4	6	121	94	120
-10	4	6	427	391	36
-9	4	6	336	244	72
-8	4	6	667	579	46
-7	4	6	284	300	82
-6	4	6	280	295	70
-5	4	6	1063	1100	38
-4	4	6	797	865	38
-3	4	6	327	356	44
-2	4	6	378	253	41
-1	4	6	427	429	35
0	4	6	0	62	1
1	4	6	1652	1680	26
2	4	6	1176	1177	26
3	4	6	306	242	44
4	4	6	494	461	34
5	4	6	1896	1841	27
6	4	6	555	504	36
7	4	6	731	689	33
8	4	6	709	713	35
9	4	6	637	665	37
10	4	6	171	208	170
11	4	6	893	816	42
12	4	6	224	65	89
13	4	6	265	174	100
14	4	6	686	678	53
15	4	6	513	569	74
16	4	6	55	151	54
-10	5	6	657	593	31
-8	5	6	162	132	161
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-3	5	6	1250	1213	33
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-1	5	6	889	838	31
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1	5	6	265	247	48
2	5	6	820	870	30
3	5	6	1559	1586	27
4	5	6	478	492	35
5	5	6	718	618	32
6	5	6	58	81	58
7	5	6	1252	1187	31
8	5	6	350	289	51
9	5	6	491	567	46
10	5	6	703	670	41
11	5	6	490	484	50
12	5	6	234	275	103
13	5	6	898	936	49
14	5	6	303	154	72
15	5	6	0	89	1
16	5	6	0	146	1
17	5	6	532	553	40
-10	6	6	0	47	1
-9	6	6	116	203	116
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-7	6	6	364	343	57
-6	6	6	151	196	151
-5	6	6	0	76	1
-4	6	6	1170	1184	38
-3	6	6	63	211	62
-2	6	6	524	583	38
-1	6	6	837	893	34
0	6	6	416	445	43
1	6	6	676	615	33
2	6	6	1613	1655	28
3	6	6	1198	1125	28
4	6	6	448	477	40
5	6	6	112	128	112
6	6	6	1495	1437	29
7	6	6	118	178	117
8	6	6	0	208	1
9	6	6	1057	1079	36
10	6	6	381	458	53
11	6	6	985	901	40
12	6	6	523	505	54
13	6	6	0	45	1
14	6	6	124	22	123
15	6	6	754	658	48
16	6	6	357	328	45
17	6	6	0	181	1
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-8	7	6	213	199	52
-7	7	6	231	287	105
-6	7	6	415	415	46
-5	7	6	773	737	44
-4	7	6	122	33	122
-3	7	6	69	268	68
-2	7	6	943	953	36
-1	7	6	301	272	60
0	7	6	1047	1020	32
1	7	6	588	596	35
2	7	6	114	63	113
3	7	6	710	638	32
4	7	6	1853	1970	29
5	7	6	653	587	34
6	7	6	167	88	96
7	7	6	266	255	56
8	7	6	1038	1069	34
9	7	6	258	225	60
10	7	6	1042	1028	38
11	7	6	363	401	57
12	7	6	695	645	47
13	7	6	456	481	54
14	7	6	524	593	67
15	7	6	0	117	1
16	7	6	0	77	1
17	7	6	82	207	82
-8	8	6	236	42	47
-7	8	6	954	916	44
-6	8	6	139	188	139
-5	8	6	205	236	142
-4	8	6	346	375	60
-3	8	6	466	498	49
-2	8	6	390	338	53
-1	8	6	1050	1073	36
0	8	6	466	478	44
1	8	6	1011	1080	32
2	8	6	672	650	33
3	8	6	1025	1002	31
4	8	6	197	209	78
5	8	6	225	205	67
6	8	6	1214	1194	32
7	8	6	945	886	34
8	8	6	721	737	38
9	8	6	151	132	151
10	8	6	699	743	43
11	8	6	104	55	103
12	8	6	786	836	44
13	8	6	433	507	61
14	8	6	122	101	121
15	8	6	203	37	159
16	8	6	512	523	39
17	8	6	0	58	1
-7	9	6	114	47	114
-6	9	6	83	52	83
-5	9	6	748	805	48
-4	9	6	375	238	52
-3	9	6	234	243	72
-2	9	6	317	272	66
-1	9	6	644	631	39
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1	9	6	1082	1030	34
2	9	6	472	469	41
3	9	6	563	469	36
4	9	6	271	270	55
5	9	6	1234	1196	33
6	9	6	156	191	155
7	9	6	411	373	46
8	9	6	573	577	45
9	9	6	1083	1042	38
10	9	6	645	645	42
11	9	6	418	424	47
12	9	6	350	300	58
13	9	6	183	106	130
14	9	6	470	396	58
15	9	6	525	483	59
16	9	6	0	147	1
17	9	6	0	43	1
-7	10	6	256	268	48
-6	10	6	571	578	30
-5	10	6	165	30	165
-4	10	6	0	62	1
-3	10	6	515	488	48
-2	10	6	822	723	41
-1	10	6	773	777	40
0	10	6	457	519	50
1	10	6	460	483	41
2	10	6	491	547	46
3	10	6	816	808	35
4	10	6	392	463	51
5	10	6	335	295	54
6	10	6	0	194	1
7	10	6	1676	1580	35
8	10	6	153	173	153
9	10	6	413	467	47
10	10	6	194	210	111
11	10	6	216	223	98
12	10	6	78	246	78
13	10	6	691	673	50
14	10	6	345	363	70
15	10	6	299	229	86
16	10	6	201	164	68
-6	11	6	0	39	1
-5	11	6	47	158	47
-4	11	6	662	671	48
-3	11	6	210	289	87
-2	11	6	335	249	60
-1	11	6	326	287	63
0	11	6	504	521	51
1	11	6	572	587	45
2	11	6	1064	1076	37
3	11	6	119	72	118
4	11	6	387	394	51
5	11	6	206	194	76
6	11	6	742	757	38
7	11	6	279	293	66
8	11	6	201	201	93
9	11	6	697	594	41
10	11	6	556	565	49
11	11	6	396	365	52
12	11	6	494	614	55
13	11	6	540	487	61
14	11	6	0	62	1
15	11	6	719	724	32
16	11	6	0	56	1
-5	12	6	369	381	40
-4	12	6	86	6	85
-3	12	6	202	123	107
-2	12	6	505	568	60
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0	12	6	593	608	42
1	12	6	492	469	44
2	12	6	650	628	44
3	12	6	0	16	1
4	12	6	1018	939	38
5	12	6	294	278	65
6	12	6	417	328	45
7	12	6	495	437	46
8	12	6	1157	1180	39
9	12	6	422	451	48
10	12	6	243	134	68
11	12	6	1040	1037	42
12	12	6	315	246	64
13	12	6	701	761	49
14	12	6	796	838	51
15	12	6	334	326	49
16	12	6	283	227	52
-3	13	6	527	572	31
-2	13	6	0	32	1
-1	13	6	0	73	1
0	13	6	697	694	48
1	13	6	309	298	70
2	13	6	698	757	44
3	13	6	613	592	46
4	13	6	365	307	58
5	13	6	561	556	47
6	13	6	684	667	42
7	13	6	466	408	48
8	13	6	284	273	56
9	13	6	368	398	58
10	13	6	719	707	49
11	13	6	0	39	1
12	13	6	397	491	64
13	13	6	173	291	172
14	13	6	273	269	57
15	13	6	213	169	68
-2	14	6	0	150	1
-1	14	6	638	586	28
0	14	6	51	44	51
1	14	6	424	397	54
2	14	6	138	111	137
3	14	6	426	326	50
4	14	6	77	39	76
5	14	6	1064	1012	42
6	14	6	421	330	48
7	14	6	134	88	134
8	14	6	413	440	56
9	14	6	344	435	59
10	14	6	0	223	1
11	14	6	403	382	54
12	14	6	208	278	118
13	14	6	339	330	38
14	14	6	530	533	33
15	14	6	323	269	47
0	15	6	154	194	51
1	15	6	155	265	84
2	15	6	369	375	35
3	15	6	613	566	49
4	15	6	160	229	160
5	15	6	114	29	113
6	15	6	111	126	110
7	15	6	729	729	46
8	15	6	180	33	113

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
9	15	6	215	165	92
10	15	6	489	410	50
11	15	6	550	521	30
12	15	6	0	64	1
13	15	6	394	416	37
14	15	6	112	79	112
2	16	6	390	386	34
3	16	6	0	57	1
4	16	6	226	242	53
5	16	6	564	505	29
6	16	6	537	513	29
7	16	6	143	85	83
8	16	6	0	101	1
9	16	6	515	524	30
10	16	6	212	238	58
11	16	6	298	353	46
12	16	6	157	153	101
5	17	6	0	51	1
6	17	6	0	158	1
7	17	6	305	282	40
8	17	6	504	554	31
9	17	6	0	41	1
-4	-11	7	227	126	43
-3	-11	7	273	252	39
-2	-11	7	166	244	71
-1	-11	7	515	554	29
0	-11	7	0	69	1
1	-11	7	0	38	1
-7	-10	7	125	53	100
-6	-10	7	168	184	67
-5	-10	7	382	391	32
-4	-10	7	223	157	44
-3	-10	7	717	642	25
-2	-10	7	295	235	33
-1	-10	7	134	70	84
0	-10	7	236	191	44
1	-10	7	698	650	26
2	-10	7	65	49	65
3	-10	7	207	78	44
4	-10	7	156	211	90
-8	-9	7	96	42	95
-7	-9	7	363	354	33
-6	-9	7	425	368	30
-5	-9	7	353	343	59
-4	-9	7	580	615	45
-3	-9	7	168	212	117
-2	-9	7	415	360	49
-1	-9	7	524	548	45
0	-9	7	440	439	46
1	-9	7	198	143	85
2	-9	7	272	179	58
3	-9	7	589	619	26
4	-9	7	359	295	32
5	-9	7	290	270	35
6	-9	7	159	108	61
-9	-8	7	138	134	137
-8	-8	7	691	650	26
-7	-8	7	240	199	39
-6	-8	7	384	404	56
-5	-8	7	250	189	65
-4	-8	7	322	366	62
-3	-8	7	193	226	89
-2	-8	7	804	833	40
-1	-8	7	388	309	49
0	-8	7	239	119	70
1	-8	7	517	444	44
2	-8	7	706	739	44
3	-8	7	257	205	64
4	-8	7	130	51	129
5	-8	7	564	484	43
6	-8	7	453	468	29
7	-8	7	545	536	28
-10	-7	7	554	507	30
-9	-7	7	502	484	30
-8	-7	7	227	193	118
-7	-7	7	232	235	95
-6	-7	7	283	334	76
-5	-7	7	444	343	48
-4	-7	7	633	706	45
-3	-7	7	595	607	41
-2	-7	7	307	256	52
-1	-7	7	251	131	65
0	-7	7	614	601	39
1	-7	7	377	326	47
2	-7	7	0	24	1
3	-7	7	295	209	53
4	-7	7	1187	1134	39
5	-7	7	223	143	77
6	-7	7	440	514	58
7	-7	7	113	153	113

h	k	l	10Fo	10Fc	10s
8	-7	7	69	48	69
9	-7	7	0	154	1
-10	-6	7	142	116	142
-9	-6	7	117	130	116
-8	-6	7	507	390	51
-7	-6	7	1062	982	42
-6	-6	7	393	414	46
-5	-6	7	876	845	41
-4	-6	7	307	198	55
-3	-6	7	0	71	1
-2	-6	7	168	133	130
-1	-6	7	325	390	57
0	-6	7	759	766	37
1	-6	7	601	648	41
2	-6	7	960	976	39
3	-6	7	757	732	39
4	-6	7	860	903	38
5	-6	7	143	180	143
6	-6	7	680	682	42
7	-6	7	153	128	153
8	-6	7	251	368	99
9	-6	7	146	207	146
10	-6	7	0	52	1
-11	-5	7	289	318	43
-10	-5	7	181	180	68
-9	-5	7	647	654	49
-8	-5	7	368	351	52
-7	-5	7	755	733	44
-6	-5	7	104	135	104
-5	-5	7	729	730	39
-4	-5	7	228	233	78
-3	-5	7	270	277	61
-2	-5	7	639	634	39
-1	-5	7	430	369	44
0	-5	7	0	111	1
1	-5	7	1331	1330	34
2	-5	7	174	117	173
3	-5	7	220	81	63
4	-5	7	712	726	39
5	-5	7	940	983	37
6	-5	7	436	399	49
7	-5	7	497	406	41
8	-5	7	289	161	68
9	-5	7	81	109	81
10	-5	7	455	404	34
11	-5	7	463	429	34
-11	-4	7	127	215	126
-10	-4	7	707	671	30
-9	-4	7	140	64	139
-8	-4	7	157	59	156
-7	-4	7	501	462	49
-6	-4	7	840	848	40
-5	-4	7	298	154	48
-4	-4	7	541	502	41
-3	-4	7	741	675	37
-2	-4	7	0	192	1
-1	-4	7	1221	1175	34
0	-4	7	1088	1092	34
1	-4	7	188	185	65
2	-4	7	111	135	110
3	-4	7	1079	1040	35
4	-4	7	113	71	113
5	-4	7	449	451	44
6	-4	7	450	455	48
7	-4	7	704	710	42
8	-4	7	0	34	1
9	-4	7	585	603	48
10	-4	7	142	126	142
11	-4	7	126	59	126
12	-4	7	263	230	59
-11	-3	7	389	336	34
-10	-3	7	0	117	1
-9	-3	7	0	163	1
-8	-3	7	748	687	44
-7	-3	7	106	49	106
-6	-3	7	405	385	46
-5	-3	7	653	652	39
-4	-3	7	934	973	35
-3	-3	7	348	354	50
-2	-3	7	950	998	34
-1	-3	7	223	206	67
0	-3	7	361	428	51
1	-3	7	679	641	35
2	-3	7	1485	1397	31
3	-3	7	319	373	47
4	-3	7	165	130	83
5	-3	7	928	897	34
6	-3	7	361	252	51
7	-3	7	680	630	40
8	-3	7	496	486	50

h	k	l	10Fo	10Fc	10s
9	-3	7	537	484	48
10	-3	7	342	365	64
11	-3	7	685	683	52
12	-3	7	148	90	118
13	-3	7	186	144	107
-11	-2	7	314	223	44
-10	-2	7	434	423	36
-9	-2	7	706	719	47
-8	-2	7	0	123	1
-7	-2	7	0	59	1
-6	-2	7	789	755	39
-5	-2	7	96	149	96
-4	-2	7	557	558	40
-3	-2	7	869	872	34
-2	-2	7	696	750	35
-1	-2	7	524	471	38
0	-2	7	1248	1239	31
1	-2	7	155	87	116
2	-2	7	0	95	1
3	-2	7	636	672	35
4	-2	7	1161	1176	32
5	-2	7	207	59	70
6	-2	7	481	390	41
7	-2	7	417	416	52
8	-2	7	760	722	39
9	-2	7	382	400	60
10	-2	7	718	653	45
11	-2	7	82	46	82
12	-2	7	153	134	152
13	-2	7	387	393	41
-11	-1	7	631	645	33
-10	-1	7	101	147	101
-9	-1	7	0	174	1
-8	-1	7	300	279	75
-7	-1	7	909	895	40
-6	-1	7	309	305	56
-5	-1	7	473	441	42
-4	-1	7	722	734	37
-3	-1	7	916	856	34
-2	-1	7	343	324	46
-1	-1	7	921	894	32
0	-1	7	429	470	39
1	-1	7	682	678	34
2	-1	7	1343	1396	29
3	-1	7	734	757	32
4	-1	7	55	110	55
5	-1	7	121	73	121
6	-1	7	1205	1120	34
7	-1	7	246	248	71
8	-1	7	1059	1055	38
9	-1	7	451	424	48
10	-1	7	243	308	103
11	-1	7	0	146	1
12	-1	7	635	516	50
13	-1	7	0	51	1
14	-1	7	53	26	52
-11	0	7	168	54	78
-10	0	7	159	106	96
-9	0	7	942	927	46
-8	0	7	374	319	59
-7	0	7	0	129	1
-6	0	7	224	187	73
-5	0	7	692	709	40
-4	0	7	0	113	1
-3	0	7	1028	1061	33
-2	0	7	902	900	33
-1	0	7	532	628	37
0	0	7	194	122	75
1	0	7	630	688	32
2	0	7	251	189	53
3	0	7	756	773	30
4	0	7	1617	1572	29
5	0	7	1969	1857	30
6	0	7	436	425	41
7	0	7	546	572	40
8	0	7	388	434	48
9	0	7	295	177	64
10	0	7	792	700	44
11	0	7	375	407	64
12	0	7	317	244	87
13	0	7	269	132	64
14	0	7	387	425	46
15	0	7	146	195	145
-11	1	7	0	101	1
-10	1	7	452	445	33
-9	1	7	0	94	1
-8	1	7	343	382	66
-7	1	7	863	933	42
-6	1	7	664	694	40
-5	1	7	465	459	46

h	k	l	10Fo	10Fc	10s
-4	1	7	595	613	40
-3	1	7	398	323	44
-2	1	7	983	951	32
-1	1	7	1185	1168	30
0	1	7	751	770	32
1	1	7	769	748	31
2	1	7	244	328	58
3	1	7	1844	1817	28
4	1	7	347	329	41
5	1	7	568	591	33
6	1	7	206	193	84
7	1	7	1633	1602	33
8	1	7	116	196	116
9	1	7	664	718	43
10	1	7	149	236	148
11	1	7	0	37	1
12	1	7	0	226	1
13	1	7	705	647	55
14	1	7	132	180	131
15	1	7	83	102	82
-11	2	7	203	99	66
-10	2	7	341	310	38
-9	2	7	203	28	94
-8	2	7	863	833	44
-7	2	7	169	73	169
-6	2	7	102	176	101
-5	2	7	259	374	84
-4	2	7	1091	1032	34
-3	2	7	258	212	63
-2	2	7	838	821	33
-1	2	7	596	654	35
0	2	7	483	405	35
1	2	7	955	993	29
2	2	7	1398	1448	28
3	2	7	294	239	53
4	2	7	577	575	33
5	2	7	1722	1678	28
6	2	7	765	749	32
7	2	7	792	717	34
8	2	7	0	203	1
9	2	7	832	710	40
10	2	7	192	24	83
11	2	7	794	798	43
12	2	7	260	398	109
13	2	7	0	34	1
14	2	7	184	88	184
15	2	7	689	660	35
16	2	7	148	164	147
-10	3	7	484	475	34
-9	3	7	424	354	59
-8	3	7	227	46	86
-7	3	7	243	85	80
-6	3	7	787	789	41
-5	3	7	552	540	44
-4	3	7	469	508	43
-3	3	7	621	554	37
-2	3	7	848	843	33
-1	3	7	215	227	65
0	3	7	1170	1273	30
1	3	7	622	524	32
2	3	7	313	408	47
3	3	7	308	243	42
4	3	7	1623	1625	27
5	3	7	165	142	136
6	3	7	544	555	37
7	3	7	524	562	39
8	3	7	981	959	35
9	3	7	530	510	45
10	3	7	615	628	47
11	3	7	276	246	87
12	3	7	313	165	67
13	3	7	476	512	60
14	3	7	535	611	57
15	3	7	186	195	81
16	3	7	204	161	86
-10	4	7	0	90	1
-9	4	7	548	381	30
-8	4	7	246	265	93
-7	4	7	575	588	52
-6	4	7	75	111	74
-5	4	7	349	333	58
-4	4	7	791	807	38
-3	4	7	1111	1078	34
-2	4	7	566	590	40
-1	4	7	317	375	53
0	4	7	878	838	32
1	4	7	304	359	48
2	4	7	1397	1378	28
3	4	7	866	930	30
4	4	7	228	200	60

h	k	l	10Fo	10Fc	10s
5	4	7	373	385	42
6	4	7	1646	1646	29
7	4	7	390	382	42
8	4	7	604	586	38
9	4	7	806	801	39
10	4	7	596	541	43
11	4	7	0	78	1
12	4	7	644	688	51
13	4	7	254	110	78
14	4	7	0	197	1
15	4	7	400	441	91
16	4	7	706	672	37
-9	5	7	561	588	32
-8	5	7	237	268	99
-7	5	7	138	31	137
-6	5	7	171	173	171
-5	5	7	1017	981	40
-4	5	7	138	61	138
-3	5	7	403	505	50
-2	5	7	668	668	38
-1	5	7	1326	1318	32
0	5	7	0	51	1
1	5	7	1441	1385	29
2	5	7	264	297	58
3	5	7	0	33	1
4	5	7	1463	1429	28
5	5	7	1287	1299	30
6	5	7	606	671	36
7	5	7	331	289	51
8	5	7	611	647	38
9	5	7	605	565	40
10	5	7	420	402	47
11	5	7	450	451	56
12	5	7	209	265	116
13	5	7	0	117	1
14	5	7	1132	1115	50
15	5	7	294	164	74
16	5	7	140	82	140
17	5	7	0	40	1
-9	6	7	0	45	1
-8	6	7	0	85	1
-7	6	7	337	332	70
-6	6	7	508	479	51
-5	6	7	259	227	74
-4	6	7	189	107	87
-3	6	7	1057	1023	36
-2	6	7	549	581	41
-1	6	7	477	463	38
0	6	7	373	378	45
1	6	7	203	111	72
2	6	7	0	46	1
3	6	7	2401	2425	28
4	6	7	412	397	41
5	6	7	0	121	1
6	6	7	188	105	99
7	6	7	417	436	39
8	6	7	0	62	1
9	6	7	398	416	48
10	6	7	836	778	39
11	6	7	1087	1098	40
12	6	7	236	341	95
13	6	7	930	893	45
14	6	7	419	237	52
15	6	7	159	37	158
16	6	7	628	604	36
17	6	7	168	256	168
-8	7	7	730	704	29
-7	7	7	0	201	1
-6	7	7	267	234	87
-5	7	7	421	397	50
-4	7	7	554	577	43
-3	7	7	273	224	57
-2	7	7	387	320	45
-1	7	7	707	680	38
0	7	7	1048	1007	34
1	7	7	692	701	35
2	7	7	1182	1231	31
3	7	7	257	236	64
4	7	7	381	473	44
5	7	7	1737	1761	30
6	7	7	404	418	40
7	7	7	66	150	65
8	7	7	566	583	38
9	7	7	829	810	38
10	7	7	404	383	46
11	7	7	939	913	40
12	7	7	193	202	96
13	7	7	453	387	50
14	7	7	313	216	82
15	7	7	815	806	52

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
16	7	7	0	32	1
17	7	7	156	110	124
-8	8	7	0	47	1
-7	8	7	174	102	69
-6	8	7	740	697	46
-5	8	7	112	111	111
-4	8	7	0	89	1
-3	8	7	537	516	47
-2	8	7	913	908	39
-1	8	7	271	239	76
0	8	7	900	937	36
1	8	7	0	127	1
2	8	7	508	454	36
3	8	7	619	595	38
4	8	7	1564	1497	32
5	8	7	139	271	139
6	8	7	274	140	51
7	8	7	756	756	36
8	8	7	520	519	41
9	8	7	673	632	41
10	8	7	548	603	44
11	8	7	538	511	50
12	8	7	485	511	57
13	8	7	547	611	56
14	8	7	386	296	63
15	8	7	92	144	92
16	8	7	111	77	111
17	8	7	642	599	39
-7	9	7	428	472	34
-6	9	7	0	94	1
-5	9	7	182	245	182
-4	9	7	651	579	46
-3	9	7	485	489	54
-2	9	7	301	337	73
-1	9	7	474	523	48
0	9	7	484	474	42
1	9	7	871	781	37
2	9	7	1373	1398	34
3	9	7	223	179	61
4	9	7	143	143	143
5	9	7	0	49	1
6	9	7	1517	1483	34
7	9	7	175	219	103
8	9	7	193	218	115
9	9	7	244	274	76
10	9	7	745	771	43
11	9	7	314	386	76
12	9	7	829	833	46
13	9	7	80	59	80
14	9	7	86	216	85
15	9	7	181	203	180
16	9	7	424	440	44
17	9	7	62	168	61
-6	10	7	224	189	49
-5	10	7	705	653	28
-4	10	7	141	105	141
-3	10	7	192	162	136
-2	10	7	213	337	134
-1	10	7	569	588	44
0	10	7	226	172	85
1	10	7	1004	1002	39
2	10	7	217	178	72
3	10	7	513	503	43
4	10	7	882	852	35
5	10	7	863	873	38
6	10	7	0	167	1
7	10	7	217	88	69
8	10	7	644	733	43
9	10	7	360	370	58
10	10	7	639	571	48
11	10	7	203	176	105
12	10	7	365	350	62
13	10	7	220	176	141
14	10	7	379	463	75
15	10	7	203	201	142
16	10	7	0	42	1
17	10	7	0	78	1
-5	11	7	126	20	125
-4	11	7	120	33	119
-3	11	7	592	645	51
-2	11	7	458	344	53
-1	11	7	572	532	47
0	11	7	258	242	77
1	11	7	558	575	47
2	11	7	161	35	112
3	11	7	1027	1006	38
4	11	7	0	120	1
5	11	7	350	225	53
6	11	7	525	441	42
7	11	7	988	983	38

h	k	l	10Fo	10Fc	10s
8	11	7	0	217	1
9	11	7	208	61	87
10	11	7	0	155	1
11	11	7	743	704	44
12	11	7	0	166	1
13	11	7	420	544	68
14	11	7	503	405	58
15	11	7	74	156	73
16	11	7	764	776	33
-4	12	7	469	455	36
-3	12	7	0	35	1
-1	12	7	337	296	61
0	12	7	786	747	44
1	12	7	845	803	42
2	12	7	573	548	45
3	12	7	264	318	84
4	12	7	0	130	1
5	12	7	855	836	41
6	12	7	412	438	55
7	12	7	220	261	113
8	12	7	0	70	1
9	12	7	919	798	41
10	12	7	173	102	173
11	12	7	195	185	117
12	12	7	348	403	67
13	12	7	545	508	52
14	12	7	234	180	130
15	12	7	1078	1074	30
16	12	7	0	62	1
-3	13	7	244	252	56
-2	13	7	554	576	30
-1	13	7	0	73	1
0	13	7	290	267	75
1	13	7	78	66	77
2	13	7	601	624	43
3	13	7	314	248	66
4	13	7	1162	1215	41
5	13	7	108	48	108
6	13	7	151	181	150
7	13	7	401	397	56
8	13	7	243	218	73
9	13	7	543	498	49
10	13	7	210	237	115
11	13	7	546	524	49
12	13	7	466	369	57
13	13	7	378	418	59
14	13	7	213	278	68
15	13	7	52	25	51
-2	14	7	261	196	50
-1	14	7	101	43	101
0	14	7	559	577	21
1	14	7	305	315	71
2	14	7	596	608	50
3	14	7	335	277	72
4	14	7	0	94	1
5	14	7	110	225	110
6	14	7	785	781	46
7	14	7	0	57	1
8	14	7	79	30	78
9	14	7	504	486	53
10	14	7	527	521	46
11	14	7	0	113	1
12	14	7	297	327	74
13	14	7	181	105	65
14	14	7	365	346	42
15	14	7	390	338	42
0	15	7	95	154	94
1	15	7	178	210	70
2	15	7	0	68	1
3	15	7	432	382	57
4	15	7	627	572	49
5	15	7	484	503	53
6	15	7	0	46	1
7	15	7	0	170	1
8	15	7	665	622	50
9	15	7	0	175	1
10	15	7	118	187	118
11	15	7	314	272	40
12	15	7	429	430	36
13	15	7	161	163	84
14	15	7	609	570	34
2	16	7	143	101	89
3	16	7	611	610	30
4	16	7	0	45	1
5	16	7	280	268	41
6	16	7	300	292	37
7	16	7	588	582	31
8	16	7	0	135	1
9	16	7	0	26	1
10	16	7	391	386	33

h	k	l	10Fo	10Fc	10s
11	16	7	305	338	42
12	16	7	160	239	110
5	17	7	595	595	29
6	17	7	99	46	98
7	17	7	122	155	121
8	17	7	175	96	65
9	17	7	462	468	34
10	17	7	147	98	99
-4	-10	8	276	311	41
-3	-10	8	321	360	37
-2	-10	8	427	465	31
-1	-10	8	370	345	33
0	-10	8	127	130	62
1	-10	8	92	124	91
2	-10	8	581	596	27
-6	-9	8	275	276	39
-5	-9	8	344	374	36
-4	-9	8	0	33	1
-3	-9	8	643	634	26
-2	-9	8	0	65	1
-1	-9	8	173	189	55
0	-9	8	558	574	19
1	-9	8	581	567	26
2	-9	8	0	21	1
3	-9	8	177	81	58
4	-9	8	380	371	35
5	-9	8	328	299	34
-8	-8	8	109	35	108
-7	-8	8	400	432	31
-6	-8	8	81	157	80
-5	-8	8	460	439	29
-4	-8	8	323	368	65
-3	-8	8	345	336	56
-2	-8	8	150	130	150
-1	-8	8	779	781	42
0	-8	8	0	152	1
1	-8	8	0	23	1
2	-8	8	461	444	45
3	-8	8	644	623	45
4	-8	8	0	20	1
5	-8	8	173	139	62
6	-8	8	189	176	55
-9	-7	8	277	286	46
-8	-7	8	605	585	28
-7	-7	8	45	153	44
-6	-7	8	174	322	173
-5	-7	8	341	289	52
-4	-7	8	168	382	167
-3	-7	8	662	704	47
-2	-7	8	584	597	46
-1	-7	8	103	112	102
0	-7	8	0	108	1
1	-7	8	569	554	47
2	-7	8	363	212	47
3	-7	8	233	176	75
4	-7	8	0	90	1
5	-7	8	742	774	45
6	-7	8	364	361	33
7	-7	8	501	482	29
8	-7	8	280	304	45
-9	-6	8	109	237	109
-8	-6	8	173	171	61
-7	-6	8	209	302	97
-6	-6	8	670	593	45
-5	-6	8	249	228	65
-4	-6	8	553	637	50
-3	-6	8	144	230	143
-2	-6	8	318	322	71
-1	-6	8	404	421	50
0	-6	8	492	489	44
1	-6	8	69	94	68
2	-6	8	403	401	45
3	-6	8	275	269	55
4	-6	8	1155	1147	38
5	-6	8	0	20	1
6	-6	8	313	313	66
7	-6	8	580	511	48
8	-6	8	0	75	1
9	-6	8	526	536	31
-10	-5	8	145	90	78
-9	-5	8	147	129	75
-8	-5	8	280	360	76
-7	-5	8	820	846	44
-6	-5	8	0	9	1
-5	-5	8	474	472	47
-4	-5	8	407	379	51
-3	-5	8	0	48	1
-2	-5	8	659	675	42
-1	-5	8	552	542	40
0	-5	8	606	577	42

h	k	l	10Fo	10Fc	10s
1	-5	8	326	262	50
2	-5	8	1285	1245	36
3	-5	8	0	255	1
4	-5	8	221	222	79
5	-5	8	372	401	54
6	-5	8	639	662	46
7	-5	8	0	31	1
8	-5	8	575	532	47
9	-5	8	295	332	39
10	-5	8	47	103	47
-10	-4	8	136	46	135
-9	-4	8	647	645	29
-8	-4	8	0	76	1
-7	-4	8	246	214	90
-6	-4	8	238	340	92
-5	-4	8	843	789	41
-4	-4	8	172	113	106
-3	-4	8	522	645	45
-2	-4	8	413	508	53
-1	-4	8	503	463	41
0	-4	8	903	970	36
1	-4	8	1013	976	36
2	-4	8	271	288	63
3	-4	8	164	177	163
4	-4	8	872	901	38
5	-4	8	368	382	53
6	-4	8	569	494	40
7	-4	8	322	275	62
8	-4	8	522	514	48
9	-4	8	140	223	139
10	-4	8	595	625	30
11	-4	8	137	165	137
-10	-3	8	457	430	34
-9	-3	8	0	27	1
-8	-3	8	139	39	139
-7	-3	8	612	619	45
-6	-3	8	454	451	51
-5	-3	8	434	381	50
-4	-3	8	335	377	58
-3	-3	8	648	643	40
-2	-3	8	149	117	148
-1	-3	8	830	843	36
0	-3	8	321	387	52
1	-3	8	0	192	1
2	-3	8	246	256	62
3	-3	8	1332	1377	34
4	-3	8	172	205	96
5	-3	8	66	97	66
6	-3	8	645	701	42
7	-3	8	297	299	61
8	-3	8	336	253	51
9	-3	8	588	536	53
10	-3	8	0	67	1
11	-3	8	388	377	35
12	-3	8	542	543	34
-10	-2	8	0	158	1
-9	-2	8	0	233	1
-8	-2	8	810	778	44
-7	-2	8	135	57	134
-6	-2	8	209	41	66
-5	-2	8	677	627	42
-4	-2	8	685	590	38
-3	-2	8	579	570	41
-2	-2	8	864	790	35
-1	-2	8	180	203	102
0	-2	8	508	519	42
1	-2	8	1261	1234	32
2	-2	8	635	594	37
3	-2	8	125	69	124
4	-2	8	0	124	1
5	-2	8	919	939	35
6	-2	8	0	35	1
7	-2	8	542	600	45
8	-2	8	452	406	50
9	-2	8	580	601	50
10	-2	8	0	83	1
11	-2	8	714	728	51
12	-2	8	0	74	1
13	-2	8	0	61	1
-10	-1	8	630	562	32
-9	-1	8	335	369	90
-8	-1	8	78	43	78
-7	-1	8	173	181	172
-6	-1	8	714	767	41
-5	-1	8	0	103	1
-4	-1	8	398	403	51
-3	-1	8	754	737	38
-2	-1	8	769	723	36
-1	-1	8	87	205	87
0	-1	8	1108	1152	33

h	k	l	10Fo	10Fc	10s
1	-1	8	218	90	65
2	-1	8	487	566	36
3	-1	8	970	958	33
4	-1	8	643	640	37
5	-1	8	92	87	91
6	-1	8	115	221	114
7	-1	8	747	812	39
8	-1	8	784	731	38
9	-1	8	705	671	43
10	-1	8	535	516	47
11	-1	8	312	268	78
12	-1	8	0	23	1
13	-1	8	600	618	37
14	-1	8	0	66	1
-10	0	8	0	73	1
-9	0	8	326	295	75
-8	0	8	731	660	45
-7	0	8	408	505	49
-6	0	8	223	113	80
-5	0	8	334	314	58
-4	0	8	582	668	43
-3	0	8	365	437	51
-2	0	8	1000	1028	35
-1	0	8	399	396	44
0	0	8	662	602	35
1	0	8	249	215	65
2	0	8	1643	1649	30
3	0	8	166	146	98
4	0	8	178	192	94
5	0	8	718	715	34
6	0	8	1285	1345	34
7	0	8	0	108	1
8	0	8	839	827	40
9	0	8	284	288	73
10	0	8	507	561	51
11	0	8	566	549	52
12	0	8	545	531	55
13	0	8	182	143	182
14	0	8	0	19	1
-10	1	8	0	43	1
-9	1	8	722	710	29
-8	1	8	0	51	1
-7	1	8	108	43	108
-6	1	8	395	341	48
-5	1	8	761	709	40
-4	1	8	0	102	1
-3	1	8	669	686	37
-2	1	8	431	466	43
-1	1	8	746	736	34
0	1	8	1413	1387	31
1	1	8	714	732	33
2	1	8	0	67	1
3	1	8	0	223	1
4	1	8	1323	1354	30
5	1	8	999	976	33
6	1	8	433	351	43
7	1	8	215	222	89
8	1	8	722	705	40
9	1	8	190	30	88
10	1	8	942	947	43
11	1	8	300	362	69
12	1	8	339	353	79
13	1	8	0	37	1
14	1	8	587	552	33
15	1	8	297	228	51
-10	2	8	205	175	61
-9	2	8	143	126	103
-8	2	8	0	43	1
-7	2	8	848	830	43
-6	2	8	573	504	48
-5	2	8	161	63	161
-4	2	8	298	262	60
-3	2	8	355	381	50
-2	2	8	166	15	117
-1	2	8	1408	1416	31
0	2	8	760	749	34
1	2	8	1311	1336	30
2	2	8	503	498	35
3	2	8	972	993	30
4	2	8	442	474	38
5	2	8	314	266	49
6	2	8	940	948	33
7	2	8	1025	1093	34
8	2	8	134	134	134
9	2	8	558	539	47
10	2	8	0	203	1
11	2	8	274	294	75
12	2	8	825	746	49
13	2	8	481	507	66
14	2	8	0	30	1

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
15	2	8	182	41	99
-10	3	8	435	506	39
-9	3	8	380	351	36
-8	3	8	520	462	55
-7	3	8	0	89	1
-6	3	8	132	140	131
-5	3	8	734	692	42
-4	3	8	599	631	40
-3	3	8	240	382	86
-2	3	8	562	578	37
-1	3	8	677	661	35
0	3	8	742	795	32
1	3	8	1592	1624	30
2	3	8	422	376	38
3	3	8	517	539	39
4	3	8	162	111	104
5	3	8	1318	1287	31
6	3	8	105	170	104
7	3	8	405	466	45
8	3	8	416	401	44
9	3	8	945	941	38
10	3	8	423	418	51
11	3	8	818	751	44
12	3	8	184	165	184
13	3	8	172	154	172
14	3	8	182	199	181
15	3	8	536	510	40
16	3	8	178	232	133
-9	4	8	164	56	70
-7	4	8	214	268	151
-6	4	8	834	831	43
-5	4	8	296	271	69
-4	4	8	352	409	66
-3	4	8	303	309	56
-2	4	8	893	984	38
-1	4	8	795	740	35
0	4	8	1093	1052	32
1	4	8	716	727	33
2	4	8	1029	989	31
3	4	8	663	712	34
4	4	8	890	917	31
5	4	8	763	797	34
6	4	8	137	129	136
7	4	8	1632	1651	33
8	4	8	674	703	42
9	4	8	417	415	48
10	4	8	264	199	74
11	4	8	153	66	152
12	4	8	0	30	1
13	4	8	1040	1046	46
14	4	8	179	159	179
15	4	8	268	279	90
16	4	8	0	51	1
-9	5	8	295	266	41
-8	5	8	485	453	32
-7	5	8	308	267	59
-6	5	8	250	138	78
-5	5	8	214	292	98
-4	5	8	800	817	42
-3	5	8	659	620	40
-2	5	8	671	666	40
-1	5	8	298	257	55
0	5	8	516	530	40
1	5	8	299	37	46
2	5	8	1561	1586	30
3	5	8	523	547	38
4	5	8	155	263	155
5	5	8	408	357	42
6	5	8	1174	1099	32
7	5	8	609	570	39
8	5	8	647	637	39
9	5	8	619	623	41
10	5	8	539	553	50
11	5	8	110	48	110
12	5	8	470	516	54
13	5	8	0	42	1
14	5	8	495	512	62
15	5	8	731	777	57
16	5	8	400	406	44
-8	6	8	49	105	48
-7	6	8	238	234	79
-6	6	8	267	218	77
-5	6	8	740	696	42
-4	6	8	346	308	57
-3	6	8	235	128	76
-2	6	8	809	765	38
-1	6	8	784	768	37
0	6	8	528	463	38
1	6	8	558	535	38
2	6	8	378	339	45
3	6	8	553	578	39
4	6	8	1638	1679	31
5	6	8	242	319	69
6	6	8	283	254	63
7	6	8	506	463	36
8	6	8	1320	1256	35
9	6	8	301	237	56
10	6	8	377	439	52
11	6	8	186	188	124
12	6	8	487	463	55
13	6	8	265	98	71
14	6	8	1029	979	49
15	6	8	0	41	1
16	6	8	212	226	75
17	6	8	518	451	40
-8	7	8	184	74	75
-7	7	8	578	584	30
-6	7	8	370	314	59
-5	7	8	209	99	97
-4	7	8	239	309	85
-3	7	8	1029	1034	38
-2	7	8	242	74	61
-1	7	8	819	791	38
0	7	8	263	173	48
1	7	8	675	706	38
2	7	8	293	373	60
3	7	8	1313	1343	32
4	7	8	174	116	108
5	7	8	352	348	45
6	7	8	1331	1275	33
7	7	8	711	728	38
8	7	8	223	286	86
9	7	8	662	662	40
10	7	8	460	468	48
11	7	8	451	416	51
12	7	8	871	866	47
13	7	8	205	190	142
14	7	8	277	168	76
15	7	8	0	79	1
16	7	8	701	706	35
17	7	8	117	117	116
-7	8	8	0	46	1
-6	8	8	158	117	95
-5	8	8	598	611	48
-4	8	8	455	367	50
-3	8	8	495	458	49
-2	8	8	289	257	62
-1	8	8	655	678	41
0	8	8	554	534	41
1	8	8	995	1005	36
2	8	8	291	243	54
3	8	8	314	386	53
4	8	8	0	44	1
5	8	8	1639	1723	33
6	8	8	0	61	1
7	8	8	0	47	1
8	8	8	369	366	54
9	8	8	674	729	43
10	8	8	220	234	88
11	8	8	864	810	43
12	8	8	81	133	80
13	8	8	737	684	51
14	8	8	586	533	52
15	8	8	330	371	92
16	8	8	210	220	71
17	8	8	168	23	105
-6	9	8	574	550	32
-5	9	8	187	84	118
-4	9	8	256	183	79
-3	9	8	331	269	56
-2	9	8	504	521	51
-1	9	8	342	299	55
0	9	8	887	913	41
1	9	8	441	410	50
2	9	8	1022	978	36
3	9	8	757	763	39
4	9	8	558	531	42
5	9	8	0	32	1
6	9	8	488	458	45
7	9	8	1102	1088	37
8	9	8	690	621	42
9	9	8	287	299	68
10	9	8	0	246	1
11	9	8	444	490	60
12	9	8	212	178	121
13	9	8	924	854	47
14	9	8	0	66	1
15	9	8	130	129	130
16	9	8	303	197	44
17	9	8	424	363	45
-6	10	8	242	133	49
-5	10	8	190	25	60
-4	10	8	660	654	52
-3	10	8	214	189	92
-2	10	8	411	381	59
-1	10	8	321	285	65
0	10	8	796	782	43
1	10	8	215	109	71
2	10	8	989	967	39
3	10	8	208	270	77
4	10	8	572	532	44
5	10	8	886	946	39
6	10	8	953	952	38
7	10	8	173	183	131
8	10	8	0	155	1
9	10	8	440	391	48
10	10	8	642	633	43
11	10	8	655	599	46
12	10	8	229	272	91
13	10	8	0	159	1
14	10	8	382	398	67
15	10	8	420	461	70
16	10	8	314	228	49
17	10	8	0	52	1
-5	11	8	381	426	40
-4	11	8	124	123	123
-3	11	8	0	47	1
-2	11	8	242	279	87
-1	11	8	638	615	46
0	11	8	680	664	43
1	11	8	388	437	54
2	11	8	459	425	48
3	11	8	409	441	52
4	11	8	1100	1092	38
5	11	8	190	136	120
6	11	8	0	135	1
7	11	8	423	377	53
8	11	8	930	951	42
9	11	8	359	265	58
10	11	8	429	369	63
11	11	8	210	103	98
12	11	8	511	521	52
13	11	8	240	301	109
14	11	8	632	646	54
15	11	8	294	261	48
16	11	8	312	343	56
-4	12	8	117	148	116
-3	12	8	629	581	31
-2	12	8	0	216	1
-1	12	8	461	514	58
0	12	8	136	187	136
1	12	8	693	735	46
2	12	8	567	553	46
3	12	8	684	608	41
4	12	8	196	205	111
5	12	8	297	255	62
6	12	8	634	667	44
7	12	8	701	692	44
8	12	8	214	333	137
9	12	8	0	74	1
10	12	8	438	560	60
11	12	8	141	188	140
12	12	8	633	588	51
13	12	8	259	260	75
14	12	8	201	185	158
15	12	8	265	159	47
16	12	8	628	651	38
-3	13	8	0	178	1
-2	13	8	0	47	1
-1	13	8	489	452	32
0	13	8	233	296	97
1	13	8	719	721	48
2	13	8	307	198	69
3	13	8	499	471	46
4	13	8	154	32	153
5	13	8	597	584	45
6	13	8	0	93	1
7	13	8	256	92	69
8	13	8	578	523	47
9	13	8	923	841	45
10	13	8	180	245	180
11	13	8	142	259	142
12	13	8	0	61	1
13	13	8	215	194	96
14	13	8	438	399	38
15	13	8	381	377	39
16	13	8	0	81	1
-1	14	8	239	224	52
0	14	8	149	126	59
1	14	8	148	127	86
2	14	8	418	426	56
3	14	8	598	578	47
4	14	8	391	395	65
5	14	8	139	250	139
6	14	8	0	178	1
7	14	8	844	760	44
8	14	8	0	155	1
9	14	8	303	176	67
10	14	8	261	224	70
11	14	8	491	555	56
12	14	8	123	39	123
13	14	8	615	469	31
14	14	8	146	54	104
15	14	8	356	338	44
0	15	8	601	573	21
1	15	8	0	7	1
2	15	8	503	491	31
3	15	8	225	139	41
4	15	8	444	355	55
5	15	8	247	305	96
6	15	8	528	605	52
7	15	8	231	160	77
8	15	8	142	87	141
9	15	8	538	489	55
10	15	8	338	388	76
11	15	8	264	229	47
12	15	8	272	283	46
13	15	8	217	271	76
14	15	8	289	310	51
2	16	8	298	309	44
3	16	8	123	188	123
4	16	8	544	563	30
5	16	8	0	131	1
6	16	8	72	108	71
7	16	8	131	137	130
8	16	8	659	649	29
9	16	8	0	42	1
10	16	8	0	115	1
11	16	8	291	248	49
12	16	8	378	344	37
13	16	8	0	88	1
6	17	8	575	563	33
7	17	8	305	253	36
8	17	8	153	128	92
9	17	8	154	71	82
10	17	8	311	299	40
-4	-9	9	394	359	33
-3	-9	9	162	104	69
-2	-9	9	593	575	28
-1	-9	9	65	82	65
0	-9	9	6	148	6
1	-9	9	362	345	34
2	-9	9	524	501	29
3	-9	9	125	39	124
-6	-8	9	305	339	41
-5	-8	9	363	379	34
-4	-8	9	310	237	31
-3	-8	9	405	380	29
-2	-8	9	79	153	79
-1	-8	9	233	247	46
0	-8	9	751	765	17
1	-8	9	224	235	44
2	-8	9	0	89	1
3	-8	9	258	267	37
4	-8	9	443	458	30
5	-8	9	164	116	57
-7	-7	9	555	537	27
-6	-7	9	215	129	45
-5	-7	9	405	393	32
-4	-7	9	0	207	1
-3	-7	9	584	492	45
-2	-7	9	320	297	60
-1	-7	9	625	658	47
0	-7	9	0	53	1
1	-7	9	0	50	1
2	-7	9	559	529	47
3	-7	9	294	338	73
4	-7	9	0	140	1
5	-7	9	146	92	69
6	-7	9	281	273	40
7	-7	9	479	498	31
-8	-6	9	394	388	34
-7	-6	9	0	55	1
-6	-6	9	276	237	45
-5	-6	9	467	437	50
-4	-6	9	379	249	52
-3	-6	9	735	677	41
-2	-6	9	276	292	58
-1	-6	9	350	394	60
0	-6	9	0	43	1
1	-6	9	628	642	45
2	-6	9	103	168	102
3	-6	9	164	27	119
4	-6	9	268	222	65
5	-6	9	829	717	43
6	-6	9	0	128	1
7	-6	9	330	315	33
8	-6	9	312	356	41
9	-6	9	338	327	41
-8	-5	9	177	93	65
-7	-5	9	443	380	29
-6	-5	9	538	567	47
-5	-5	9	79	59	78
-4	-5	9	259	283	65
-3	-5	9	319	351	66
-2	-5	9	711	735	42
-1	-5	9	821	797	39
0	-5	9	585	581	43
1	-5	9	122	153	122
2	-5	9	69	33	68
3	-5	9	892	893	39
4	-5	9	439	426	48
5	-5	9	391	433	57
6	-5	9	108	209	108
7	-5	9	620	610	49
8	-5	9	157	193	82
9	-5	9	473	489	33
10	-5	9	0	135	1
-9	-4	9	0	107	1
-8	-4	9	509	465	31
-7	-4	9	475	467	53
-6	-4	9	206	149	96
-5	-4	9	215	290	104
-4	-4	9	702	706	44
-3	-4	9	190	37	90
-2	-4	9	725	672	40
-1	-4	9	140	172	140
0	-4	9	331	357	57
1	-4	9	591	644	44
2	-4	9	923	961	38
3	-4	9	207	37	73
4	-4	9	99	118	98
5	-4	9	433	405	48
6	-4	9	497	542	52
7	-4	9	253	313	71
8	-4	9	418	362	49
9	-4	9	260	210	89
10	-4	9	168	141	60
11	-4	9	390	460	41
-9	-3	9	549	509	32
-8	-3	9	85	148	85
-7	-3	9	239	120	84
-6	-3	9	459	435	55
-5	-3	9	634	703	47
-4	-3	9	300	396	61
-3	-3	9	174	232	93
-2	-3	9	501	460	43
-1	-3	9	97	94	96
0	-3	9	994	990	36
1	-3	9	587	585	42
2	-3	9	267	269	72
3	-3	9	0	170	1
4	-3	9	1018	965	37
5	-3	9	172	208	111
6	-3	9	432	484	53
7	-3	9	451	468	52
8	-3	9	637	567	47
9	-3	9	301	179	64
10	-3	9	628	587	49
11	-3	9	127	113	126
12	-3	9	211	179	59
-9	-2	9	168	255	86
-8	-2	9	0	46	1
-7	-2	9	596	587	48
-6	-2	9	133	43	133
-5	-2	9	473	411	47
-4	-2	9	667	670	41
-3	-2	9	923	907	37
-2	-2	9	227	202	80
-1	-2	9	547	569	41
0	-2	9	0	76	1
1	-2	9	352	300	45
2	-2	9	1056	1067	35
3	-2	9	779	813	38
4	-2	9	0	43	1
5	-2	9	0	53	1
6	-2	9	726	716	39
7	-2	9	299	224	59
8	-2	9	378	407	61
9	-2	9	344	333	57

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
10	-2	9	359	365	60
11	-2	9	287	331	84
12	-2	9	771	712	30
13	-2	9	224	79	65
-9	-1	9	534	549	32
-8	-1	9	627	541	46
-7	-1	9	211	61	65
-6	-1	9	188	57	74
-5	-1	9	748	716	42
-4	-1	9	335	265	56
-3	-1	9	523	554	44
-2	-1	9	491	459	43
-1	-1	9	557	537	42
0	-1	9	0	34	1
1	-1	9	1369	1397	34
2	-1	9	61	104	60
3	-1	9	389	391	49
4	-1	9	439	545	42
5	-1	9	1041	980	36
6	-1	9	0	83	1
7	-1	9	475	402	41
8	-1	9	533	485	47
9	-1	9	776	776	46
10	-1	9	396	422	61
11	-1	9	576	580	55
13	-1	9	0	134	1
-9	0	9	279	230	43
-8	0	9	187	199	187
-7	0	9	300	290	65
-6	0	9	626	534	43
-5	0	9	307	174	58
-4	0	9	383	409	55
-3	0	9	560	523	40
-2	0	9	841	824	37
-1	0	9	709	726	40
0	0	9	510	441	39
1	0	9	0	87	1
2	0	9	176	141	89
3	0	9	1545	1551	33
4	0	9	807	790	36
5	0	9	0	84	1
6	0	9	397	345	48
7	0	9	743	668	40
8	0	9	0	91	1
9	0	9	1005	996	41
10	0	9	275	260	82
11	0	9	613	602	50
12	0	9	0	120	1
13	0	9	556	528	33
14	0	9	0	109	1
-9	1	9	0	46	1
-8	1	9	789	703	46
-7	1	9	418	375	57
-6	1	9	328	236	48
-5	1	9	269	271	74
-4	1	9	478	577	54
-3	1	9	96	164	95
-2	1	9	733	748	38
-1	1	9	478	460	42
0	1	9	864	871	35
1	1	9	490	484	42
2	1	9	953	989	34
3	1	9	0	81	1
4	1	9	151	148	150
5	1	9	1177	1164	33
6	1	9	766	743	36
7	1	9	70	196	70
8	1	9	439	470	49
9	1	9	372	353	50
10	1	9	562	471	49
11	1	9	748	690	46
12	1	9	258	251	133
13	1	9	0	192	1
14	1	9	111	94	110
15	1	9	599	555	35
-9	2	9	631	609	31
-8	2	9	0	37	1
-7	2	9	181	58	180
-6	2	9	736	699	44
-5	2	9	398	426	52
-4	2	9	277	256	66
-3	2	9	249	236	64
-2	2	9	778	729	36
-1	2	9	566	591	38
0	2	9	1441	1427	33
1	2	9	0	263	1
2	2	9	551	551	40
3	2	9	407	373	45
4	2	9	1333	1348	33
5	2	9	422	475	44

h	k	l	10Fo	10Fc	10s
6	2	9	266	107	55
7	2	9	65	175	64
8	2	9	834	869	38
9	2	9	293	335	79
10	2	9	768	757	44
11	2	9	214	212	104
12	2	9	488	479	62
13	2	9	557	498	53
14	2	9	341	328	45
15	2	9	200	33	78
-9	3	9	294	229	47
-8	3	9	230	200	49
-7	3	9	598	530	48
-6	3	9	209	199	87
-5	3	9	340	208	52
-4	3	9	383	341	58
-3	3	9	862	753	38
-2	3	9	560	537	45
-1	3	9	800	761	36
0	3	9	405	418	42
1	3	9	978	973	34
2	3	9	1359	1398	32
3	3	9	562	602	40
4	3	9	400	487	49
5	3	9	0	79	1
6	3	9	976	963	34
7	3	9	804	743	37
8	3	9	921	945	39
9	3	9	127	101	126
10	3	9	643	639	48
11	3	9	0	53	1
12	3	9	721	725	52
13	3	9	362	242	71
15	3	9	256	248	58
16	3	9	481	486	43
-9	4	9	424	395	38
-8	4	9	286	183	39
-7	4	9	168	208	167
-6	4	9	140	126	139
-5	4	9	637	600	46
-4	4	9	367	405	57
-3	4	9	714	682	42
-2	4	9	296	220	53
-1	4	9	852	923	38
0	4	9	157	142	128
1	4	9	1270	1252	32
2	4	9	524	539	38
3	4	9	395	415	45
4	4	9	515	499	39
5	4	9	1003	940	33
6	4	9	0	125	1
7	4	9	350	375	47
8	4	9	715	676	42
9	4	9	831	900	42
10	4	9	572	548	48
11	4	9	612	692	48
12	4	9	0	73	1
13	4	9	0	187	1
14	4	9	474	469	65
15	4	9	99	120	99
16	4	9	144	74	143
-8	5	9	295	317	50
-7	5	9	356	336	38
-6	5	9	271	262	85
-5	5	9	292	178	61
-4	5	9	334	325	57
-3	5	9	585	564	43
-2	5	9	993	971	38
-1	5	9	715	701	38
0	5	9	0	103	1
1	5	9	838	841	34
2	5	9	0	93	1
3	5	9	1267	1327	33
4	5	9	350	253	44
5	5	9	127	11	126
6	5	9	169	265	168
7	5	9	1225	1245	35
8	5	9	152	43	152
9	5	9	511	451	45
10	5	9	247	244	94
11	5	9	710	636	45
12	5	9	260	249	91
13	5	9	719	706	53
15	5	9	299	393	91
16	5	9	486	437	40
-8	6	9	444	464	36
-7	6	9	0	130	1
-6	6	9	0	64	1
-5	6	9	0	82	1
-4	6	9	875	862	42

h	k	l	10Fo	10Fc	10s
-3	6	9	194	267	131
-2	6	9	245	187	56
-1	6	9	183	260	93
0	6	9	948	901	37
1	6	9	693	643	39
2	6	9	1181	1238	34
3	6	9	289	303	58
4	6	9	658	625	38
5	6	9	901	856	35
6	6	9	677	687	40
7	6	9	220	302	84
8	6	9	463	444	48
9	6	9	861	916	40
10	6	9	558	551	46
11	6	9	672	760	50
12	6	9	408	297	56
13	6	9	256	185	85
14	6	9	88	51	88
15	6	9	864	811	53
16	6	9	0	34	1
-7	7	9	188	191	86
-6	7	9	573	493	30
-5	7	9	316	382	74
-4	7	9	464	456	53
-3	7	9	415	325	56
-2	7	9	1004	953	39
-1	7	9	479	481	47
0	7	9	894	795	37
1	7	9	201	141	83
2	7	9	577	608	42
3	7	9	454	487	49
4	7	9	1456	1436	34
5	7	9	93	194	92
6	7	9	0	217	1
7	7	9	309	307	51
8	7	9	1010	974	38
9	7	9	443	345	51
10	7	9	876	844	42
11	7	9	428	407	53
12	7	9	671	621	46
13	7	9	557	616	52
14	7	9	320	261	71
15	7	9	0	185	1
16	7	9	179	195	102
17	7	9	535	523	40
-7	8	9	391	467	43
-6	8	9	0	65	1
-5	8	9	0	113	1
-4	8	9	179	228	130
-3	8	9	584	608	53
-2	8	9	425	367	49
-1	8	9	75	247	74
0	8	9	437	405	49
1	8	9	508	501	40
2	8	9	819	824	37
3	8	9	751	744	38
4	8	9	394	336	47
5	8	9	335	279	48
6	8	9	1133	1125	36
7	8	9	154	154	154
8	8	9	301	286	59
9	8	9	816	702	42
10	8	9	754	706	44
11	8	9	514	407	46
12	8	9	723	699	50
13	8	9	209	178	147
14	8	9	306	384	66
15	8	9	472	427	68
16	8	9	523	531	38
17	8	9	0	21	1
-6	9	9	216	230	60
-5	9	9	432	381	34
-4	9	9	0	49	1
-3	9	9	0	181	1
-2	9	9	372	386	56
-1	9	9	927	957	41
0	9	9	220	84	69
1	9	9	474	601	50
2	9	9	186	173	121
3	9	9	632	651	43
4	9	9	884	891	38
5	9	9	1124	1135	37
6	9	9	260	229	80
7	9	9	0	57	1
8	9	9	707	736	42
9	9	9	437	450	47
10	9	9	723	615	43
11	9	9	306	431	77
12	9	9	440	429	61
13	9	9	564	511	54

h	k	l	10Fo	10Fc	10s
14	9	9	632	681	58
15	9	9	0	115	1
16	9	9	0	102	1
17	9	9	0	117	1
-5	10	9	104	46	104
-4	10	9	242	216	48
-3	10	9	564	531	48
-2	10	9	488	486	52
-1	10	9	530	506	50
0	10	9	202	302	122
1	10	9	519	485	45
2	10	9	264	389	85
3	10	9	1088	1065	39
4	10	9	215	104	69
5	10	9	385	386	51
6	10	9	259	291	66
7	10	9	892	950	40
8	10	9	0	204	1
9	10	9	542	500	49
10	10	9	79	172	79
11	10	9	941	849	44
12	10	9	307	363	74
13	10	9	392	457	71
14	10	9	0	48	1
15	10	9	445	357	66
16	10	9	410	409	42
17	10	9	280	281	52
-4	11	9	481	392	32
-3	11	9	0	34	1
-2	11	9	84	93	83
-1	11	9	214	268	98
0	11	9	827	914	43
1	11	9	353	376	65
2	11	9	657	622	47
3	11	9	471	356	46
4	11	9	286	353	70
5	11	9	923	925	40
6	11	9	424	405	52
7	11	9	196	12	86
8	11	9	400	326	49
9	11	9	669	568	44
10	11	9	594	573	47
11	11	9	584	622	52
12	11	9	221	85	89
13	11	9	540	567	65
14	11	9	0	105	1
15	11	9	623	581	33
16	11	9	152	92	152
-3	12	9	186	137	65
-2	12	9	483	511	33
-1	12	9	345	336	63
0	12	9	483	528	59
1	12	9	113	65	112
2	12	9	805	801	43
3	12	9	336	363	68
4	12	9	825	822	44
5	12	9	286	206	65
6	12	9	0	77	1
7	12	9	531	510	47
8	12	9	644	715	50
9	12	9	236	159	70
10	12	9	138	107	138
11	12	9	218	169	133
12	12	9	478	497	62
13	12	9	539	634	58
14	12	9	375	321	76
15	12	9	147	148	116
16	12	9	0	102	1
-2	13	9	173	185	69
-1	13	9	114	55	114
0	13	9	207	162	95
1	13	9	340	384	69
2	13	9	728	701	48
3	13	9	252	226	76
4	13	9	633	588	49
5	13	9	209	109	75
6	13	9	666	633	45
7	13	9	272	195	79
8	13	9	0	172	1
9	13	9	139	153	138
10	13	9	807	825	50
11	13	9	0	10	1
12	13	9	376	437	69
13	13	9	0	77	1
14	13	9	420	378	37
15	13	9	171	308	171
16	13	9	427	377	45
-1	14	9	577	590	33
0	14	9	102	61	102
1	14	9	364	353	35

h	k	l	10Fo	10Fc	10s
2	14	9	291	167	72
3	14	9	488	528	57
4	14	9	462	549	59
5	14	9	487	379	50
6	14	9	197	121	103
7	14	9	142	111	141
8	14	9	295	415	73
9	14	9	582	585	52
10	14	9	444	443	52
11	14	9	320	160	71
12	14	9	583	522	53
13	14	9	284	259	45
14	14	9	503	514	35
15	14	9	0	85	1
1	15	9	577	533	30
2	15	9	0	114	1
3	15	9	444	465	34
4	15	9	130	153	129
5	15	9	166	271	166
6	15	9	263	179	71
7	15	9	594	598	51
8	15	9	169	33	168
9	15	9	280	111	59
10	15	9	393	406	65
11	15	9	608	568	31
12	15	9	219	235	64
13	15	9	190	171	71
14	15	9	206	56	70
3	16	9	262	210	44
4	16	9	190	218	68
5	16	9	596	564	30
6	16	9	432	369	34
7	16	9	0	44	1
8	16	9	0	57	1
9	16	9	566	510	29
10	16	9	0	62	1
11	16	9	225	209	58
12	16	9	109	131	108
13	16	9	346	414	52
6	17	9	217	266	60
7	17	9	153	289	126
8	17	9	394	384	37
9	17	9	129	41	129
10	17	9	119	32	118
-3	-8	10	156	185	74
-2	-8	10	421	439	33
-1	-8	10	131	141	130
0	-8	10	300	252	37
1	-8	10	620	546	28
2	-8	10	376	355	32
3	-8	10	0	51	1
-5	-7	10	185	164	54
-4	-7	10	511	468	28
-3	-7	10	326	340	35
-2	-7	10	483	490	31
-1	-7	10	0	17	1
0	-7	10	608	567	19
1	-7	10	185	65	46
2	-7	10	127	17	71
3	-7	10	359	383	35
4	-7	10	467	425	29
5	-7	10	115	104	115
6	-7	10	0	122	1
-6	-6	10	0	18	1
-5	-6	10	294	269	35
-4	-6	10	358	326	34
-3	-6	10	482	486	49
-2	-6	10	615	572	44
-1	-6	10	338	318	58
0	-6	10	226	243	75
1	-6	10	0	154	1
2	-6	10	676	671	44
3	-6	10	273	240	71
4	-6	10	108	103	107
5	-6	10	159	189	78
6	-6	10	660	634	26
7	-6	10	285	244	37
-7	-5	10	119	17	119
-6	-5	10	350	329	35
-5	-5	10	703	677	26
-4	-5	10	0	117	1
-3	-5	10	558	543	46
-2	-5	10	0	109	1
-1	-5	10	677	540	43
0	-5	10	477	423	46
1	-5	10	595	627	43
2	-5	10	220	263	83
3	-5	10	148	147	147
4	-5	10	633	581	44
5	-5	10	500	555	51

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
6	-5	10	293	404	81
7	-5	10	236	204	41
8	-5	10	213	193	58
9	-5	10	201	127	55
-8	-4	10	0	117	1
-7	-4	10	499	543	32
-6	-4	10	573	518	29
-5	-4	10	305	274	70
-4	-4	10	0	144	1
-3	-4	10	570	516	43
-2	-4	10	194	214	120
-1	-4	10	664	722	42
0	-4	10	394	329	43
1	-4	10	436	475	53
2	-4	10	277	153	59
3	-4	10	699	684	42
4	-4	10	163	45	126
5	-4	10	388	473	58
6	-4	10	0	251	1
7	-4	10	670	643	49
8	-4	10	215	67	58
9	-4	10	316	284	41
10	-4	10	155	152	87
-8	-3	10	410	409	35
-7	-3	10	138	140	100
-6	-3	10	0	248	1
-5	-3	10	350	364	60
-4	-3	10	950	924	42
-3	-3	10	339	291	56
-2	-3	10	124	261	124
-1	-3	10	326	426	66
0	-3	10	393	312	43
1	-3	10	763	785	41
2	-3	10	541	537	44
3	-3	10	0	133	1
4	-3	10	0	58	1
5	-3	10	730	799	43
6	-3	10	429	481	51
7	-3	10	413	330	50
8	-3	10	238	257	115
9	-3	10	287	322	71
10	-3	10	0	70	1
11	-3	10	522	514	35
-8	-2	10	166	28	65
-7	-2	10	129	127	128
-6	-2	10	664	728	50
-5	-2	10	597	490	44
-4	-2	10	467	319	46
-3	-2	10	147	152	146
-2	-2	10	631	585	42
-1	-2	10	350	381	51
0	-2	10	813	792	39
1	-2	10	336	364	51
2	-2	10	398	489	51
3	-2	10	496	461	43
4	-2	10	878	897	40
5	-2	10	384	319	53
6	-2	10	400	380	49
7	-2	10	451	356	46
8	-2	10	589	596	46
9	-2	10	257	177	79
10	-2	10	377	337	60
11	-2	10	259	286	50
12	-2	10	145	234	144
-8	-1	10	272	254	47
-7	-1	10	572	601	30
-6	-1	10	0	106	1
-5	-1	10	77	172	76
-4	-1	10	627	595	44
-3	-1	10	636	624	42
-2	-1	10	648	583	43
-1	-1	10	218	301	79
0	-1	10	273	301	70
1	-1	10	179	169	102
2	-1	10	1065	1017	35
3	-1	10	399	350	44
4	-1	10	0	35	1
5	-1	10	363	285	54
6	-1	10	884	907	41
7	-1	10	275	198	69
8	-1	10	572	639	48
9	-1	10	80	286	80
10	-1	10	609	601	48
11	-1	10	274	128	70
12	-1	10	560	569	33
13	-1	10	111	34	111
-8	0	10	350	316	38
-7	0	10	145	7	144
-6	0	10	139	229	139
-5	0	10	804	792	45
-4	0	10	0	21	1
-3	0	10	228	176	86
-2	0	10	465	450	43
-1	0	10	695	710	41
0	0	10	605	622	41
1	0	10	546	578	41
2	0	10	95	123	94
3	0	10	188	101	74
4	0	10	916	931	38
5	0	10	569	632	43
6	0	10	0	100	1
7	0	10	375	331	48
8	0	10	708	682	42
9	0	10	391	411	59
10	0	10	642	694	50
11	0	10	147	146	147
12	0	10	0	255	1
13	0	10	221	138	59
14	0	10	482	473	41
-8	1	10	87	78	87
-7	1	10	594	610	54
-6	1	10	585	608	47
-5	1	10	269	206	80
-4	1	10	182	67	109
-3	1	10	831	833	41
-2	1	10	407	397	50
-1	1	10	880	887	37
0	1	10	162	107	123
1	1	10	504	452	41
2	1	10	284	274	53
3	1	10	1343	1380	35
4	1	10	0	261	1
5	1	10	212	230	86
6	1	10	552	530	44
7	1	10	781	747	41
8	1	10	0	108	1
9	1	10	680	684	46
10	1	10	0	78	1
11	1	10	713	684	51
12	1	10	597	586	57
13	1	10	180	188	83
14	1	10	140	146	140
-8	2	10	676	693	31
-7	2	10	236	240	50
-6	2	10	0	153	1
-5	2	10	427	498	51
-4	2	10	373	415	55
-3	2	10	382	353	53
-2	2	10	567	634	43
-1	2	10	354	383	53
0	2	10	788	773	37
1	2	10	1040	1100	36
2	2	10	463	352	43
3	2	10	266	338	65
4	2	10	0	95	1
5	2	10	1178	1225	36
6	2	10	797	778	40
7	2	10	321	294	55
8	2	10	146	191	146
9	2	10	598	589	50
10	2	10	0	67	1
11	2	10	709	767	48
12	2	10	301	132	88
13	2	10	588	579	59
14	2	10	381	312	42
15	2	10	325	387	54
-8	3	10	157	45	83
-7	3	10	149	162	121
-6	3	10	775	711	46
-5	3	10	249	260	95
-4	3	10	213	22	77
-3	3	10	0	74	1
-2	3	10	671	614	44
-1	3	10	375	362	51
0	3	10	1113	1103	36
1	3	10	472	494	50
2	3	10	798	849	36
3	3	10	569	627	41
4	3	10	704	739	39
5	3	10	115	36	114
6	3	10	505	479	44
7	3	10	610	545	42
8	3	10	1154	1091	39
9	3	10	383	372	56
10	3	10	259	315	99
11	3	10	603	475	51
12	3	10	0	36	1
13	3	10	705	694	53
14	3	10	0	124	1
15	3	10	0	95	1
-8	4	10	284	324	49
-7	4	10	423	342	34
-6	4	10	0	70	1
-5	4	10	79	32	78
-4	4	10	488	513	50
-3	4	10	656	602	42
-2	4	10	633	616	43
-1	4	10	250	228	66
0	4	10	1031	953	36
1	4	10	0	98	1
2	4	10	1095	1090	34
3	4	10	205	132	74
4	4	10	378	293	51
5	4	10	413	352	48
6	4	10	1382	1354	35
7	4	10	302	347	62
8	4	10	454	499	49
9	4	10	167	152	167
10	4	10	616	569	48
11	4	10	591	637	52
12	4	10	425	366	66
13	4	10	234	345	164
14	4	10	579	461	56
15	4	10	535	517	35
16	4	10	297	271	58
-7	5	10	0	123	1
-6	5	10	477	480	57
-5	5	10	719	801	49
-4	5	10	134	153	133
-3	5	10	167	138	167
-2	5	10	206	226	97
-1	5	10	609	712	43
0	5	10	733	738	40
1	5	10	592	580	40
2	5	10	980	995	37
3	5	10	741	667	38
4	5	10	635	671	39
5	5	10	665	715	39
6	5	10	618	592	42
7	5	10	230	183	67
8	5	10	950	897	39
9	5	10	643	629	44
10	5	10	577	601	50
11	5	10	279	152	64
12	5	10	497	477	59
13	5	10	233	162	100
14	5	10	698	657	58
15	5	10	252	114	54
16	5	10	275	277	62
-7	6	10	351	375	41
-6	6	10	520	477	30
-5	6	10	0	111	1
-4	6	10	225	213	94
-3	6	10	874	897	43
-2	6	10	182	198	125
-1	6	10	655	632	43
0	6	10	0	91	1
1	6	10	1023	1048	37
2	6	10	223	164	83
3	6	10	954	988	37
4	6	10	580	554	39
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6	6	10	743	799	39
7	6	10	1164	1118	38
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3	7	10	554	587	42
4	7	10	0	54	1
5	7	10	1012	1051	38
6	7	10	587	557	40
7	7	10	244	295	86
8	7	10	124	158	123
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11	7	10	508	561	58
12	7	10	354	240	68
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3	8	10	421	481	50
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6	8	10	290	241	60
7	8	10	937	895	39
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9	8	10	301	351	70
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11	8	10	624	613	55
12	8	10	322	357	84
13	8	10	769	825	52
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3	9	10	192	192	91
4	9	10	517	447	47
5	9	10	322	313	47
6	9	10	985	1047	40
7	9	10	0	115	1
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13	9	10	123	168	123
14	9	10	570	549	54
15	9	10	440	628	86
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7	10	10	259	338	98
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2	11	10	0	97	1
3	11	10	607	633	48
4	11	10	0	100	1
5	11	10	230	349	95
6	11	10	985	936	43
7	11	10	1052	1021	41
8	11	10	220	57	77
9	11	10	137	126	136
10	11	10	228	148	81
11	11	10	274	396	96
12	11	10	784	791	51
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14	11	10	555	544	60
15	11	10	250	205	56
16	11	10	456	471	42
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2	12	10	0	179	1
3	12	10	534	553	51
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5	12	10	528	551	54
6	12	10	260	282	73
7	12	10	0	61	1
8	12	10	373	390	63
9	12	10	866	872	45
10	12	10	0	135	1
11	12	10	468	440	52
12	12	10	150	101	150
13	12	10	655	608	54
14	12	10	320	392	76
15	12	10	234	209	58
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3	13	10	411	358	59
4	13	10	216	161	94
5	13	10	0	237	1
6	13	10	0	129	1
7	13	10	681	654	47
8	13	10	743	692	45
9	13	10	358	241	62
10	13	10	166	50	166
11	13	10	460	520	58
12	13	10	90	137	89
13	13	10	708	666	50
14	13	10	0	106	1
15	13	10	418	414	42
0	14	10	368	394	29
1	14	10	200	93	51
2	14	10	423	384	34
3	14	10	169	197	168
4	14	10	632	647	47
5	14	10	289	267	80
6	14	10	397	457	63
7	14	10	0	94	1
8	14	10	81	168	81
9	14	10	314	279	68
10	14	10	760	789	49
11	14	10	327	359	74
12	14	10	154	44	154
13	14	10	294	324	47
14	14	10	227	229	56
15	14	10	536	491	40
2	15	10	447	423	34
3	15	10	48	168	48
4	15	10	493	499	33
5	15	10	309	310	40
6	15	10	268	261	77
7	15	10	0	45	1
8	15	10	646	620	51
9	15	10	0	83	1
10	15	10	357	362	40
11	15	10	0	58	1
12	15	10	712	686	32
13	15	10	0	126	1
14	15	10	320	320	53
4	16	10	0	149	1
5	16	10	170	132	70
6	16	10	271	285	48
7	16	10	285	380	50
8	16	10	0	43	1
9	16	10	116	122	116
10	16	10	541	587	34
11	16	10	346	440	49
12	16	10	449	406	37
8	17	10	107	124	106
9	17	10	502	522	36
-2	-7	11	382	308	30
-1	-7	11	309	275	35
0	-7	11	157	76	82
1	-7	11	601	646	28
2	-7	11	191	185	60
3	-7	11	0	4	1
-4	-6	11	208	298	58
-3	-6	11	371	322	32
-2	-6	11	604	617	28
-1	-6	11	339	343	36

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
0	-6	11	502	487	20
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4	-6	11	402	376	31
5	-6	11	0	26	1
6	-6	11	235	138	47
-5	-5	11	240	196	46
-4	-5	11	491	472	29
-3	-5	11	245	232	48
-2	-5	11	624	635	27
-1	-5	11	265	298	70
0	-5	11	544	617	47
1	-5	11	304	177	61
2	-5	11	573	465	42
3	-5	11	254	76	62
4	-5	11	256	268	64
5	-5	11	307	325	41
6	-5	11	585	603	29
7	-5	11	168	150	64
8	-5	11	244	242	44
-6	-4	11	450	436	32
-5	-4	11	613	672	29
-4	-4	11	155	193	91
-3	-4	11	233	264	77
-2	-4	11	286	315	71
-1	-4	11	398	407	56
0	-4	11	594	623	44
1	-4	11	196	334	151
2	-4	11	268	253	71
3	-4	11	0	55	1
4	-4	11	636	645	46
5	-4	11	355	358	57
6	-4	11	378	367	57
7	-4	11	0	57	1
8	-4	11	497	489	31
9	-4	11	0	108	1
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-6	-3	11	336	310	39
-5	-3	11	254	219	46
-4	-3	11	303	184	56
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-2	-3	11	282	267	64
-1	-3	11	554	528	46
0	-3	11	382	343	53
1	-3	11	432	446	55
2	-3	11	263	324	68
3	-3	11	730	664	40
4	-3	11	0	31	1
5	-3	11	321	255	58
6	-3	11	470	468	54
7	-3	11	532	462	49
8	-3	11	357	362	64
9	-3	11	223	176	53
10	-3	11	323	366	44
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-3	-2	11	456	406	46
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-1	-2	11	716	700	41
1	-2	11	818	817	39
2	-2	11	319	352	60
4	-2	11	205	71	82
5	-2	11	664	696	43
6	-2	11	0	31	1
7	-2	11	404	423	56
8	-2	11	402	416	62
9	-2	11	708	643	52
10	-2	11	314	238	40
11	-2	11	300	252	42
-7	-1	11	46	127	46
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-5	-1	11	0	24	1
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3	-1	11	822	786	39
4	-1	11	753	764	42
5	-1	11	72	125	72
6	-1	11	106	159	106
7	-1	11	635	620	47
8	-1	11	112	100	112
9	-1	11	410	407	66
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2	0	11	892	911	40
3	0	11	0	87	1
4	0	11	211	191	104
5	0	11	394	370	56
6	0	11	980	928	39
7	0	11	300	312	78
8	0	11	311	372	73
9	0	11	428	414	61
10	0	11	556	512	51
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13	0	11	99	116	99
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5	1	11	576	468	42
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7	1	11	306	216	62
8	1	11	721	731	43
9	1	11	0	72	1
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11	1	11	84	168	84
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13	1	11	483	422	40
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6	2	11	675	680	42
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9	5	11	893	895	45
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15	5	11	515	535	39
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16	8	11	143	65	143
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3	9	11	641	658	46
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7	9	11	795	834	42
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9	9	11	473	401	48
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13	9	11	294	274	81
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3	10	11	175	160	174
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5	10	11	752	699	43
6	10	11	1122	1103	44
7	10	11	280	96	82
8	10	11	138	122	137
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14	10	11	319	206	87
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13	11	11	596	614	59
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14	13	11	603	638	35
15	13	11	249	112	66
1	14	11	330	328	43
2	14	11	232	216	52
3	14	11	568	536	32
4	14	11	85	158	85
5	14	11	542	545	59
6	14	11	86	41	86
7	14	11	517	521	56
8	14	11	87	174	86
9	14	11	173	261	172
10	14	11	0	97	1
11	14	11	926	854	48
12	14	11	304	305	42
13	14	11	279	191	43
14	14	11	164	175	110
2	15	11	192	169	60
3	15	11	297	322	45
4	15	11	367	352	37
5	15	11	367	336	35
6	15	11	285	316	49
7	15	11	0	82	1
8	15	11	0	48	1
9	15	11	610	616	32
10	15	11	493	500	34
11	15	11	364	362	44
12	15	11	240	104	54
13	15	11	504	463	39
5	16	11	240	218	50
6	16	11	251	249	47
7	16	11	196	98	58
8	16	11	529	553	34
9	16	11	130	199	130
10	16	11	76	21	76
11	16	11	306	271	43
12	16	11	609	586	35
-1	-6	12	493	457	28
0	-6	12	165	53	36
1	-6	12	524	498	28
2	-6	12	133	160	133
3	-6	12	0	34	1
-3	-5	12	363	348	34
-2	-5	12	286	317	39
-1	-5	12	416	455	31
0	-5	12	341	333	24
1	-5	12	260	301	43
2	-5	12	0	58	1
3	-5	12	621	607	27
4	-5	12	215	259	48
5	-5	12	150	116	88
6	-5	12	109	50	108
-4	-4	12	433	426	32
-3	-4	12	231	157	45
-2	-4	12	388	428	34
-1	-4	12	375	361	31
0	-4	12	520	534	24
1	-4	12	289	346	68
2	-4	12	462	432	49
3	-4	12	0	120	1
4	-4	12	138	120	80
5	-4	12	363	373	34
6	-4	12	379	446	39

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
7	-4	12	218	263	56
8	-4	12	0	76	1
-5	-3	12	409	397	33
-4	-3	12	224	254	52
-3	-3	12	82	130	81
-2	-3	12	575	565	48
0	-3	12	557	566	45
1	-3	12	380	338	53
2	-3	12	331	295	50
3	-3	12	275	179	73
4	-3	12	678	626	44
5	-3	12	176	45	176
6	-3	12	226	270	107
7	-3	12	259	248	46
8	-3	12	584	606	30
9	-3	12	396	355	37
-5	-2	12	0	26	1
-4	-2	12	456	442	30
-3	-2	12	683	676	43
-2	-2	12	445	458	51
-1	-2	12	241	278	81
0	-2	12	501	447	51
1	-2	12	225	223	89
2	-2	12	395	449	56
3	-2	12	504	477	44
4	-2	12	0	27	1
5	-2	12	173	169	172
6	-2	12	682	714	46
7	-2	12	0	48	1
8	-2	12	203	296	136
9	-2	12	73	57	73
10	-2	12	440	510	39
-6	-1	12	70	123	69
-5	-1	12	708	708	27
-4	-1	12	95	191	95
-3	-1	12	342	257	60
-2	-1	12	0	125	1
-1	-1	12	728	726	44
0	-1	12	343	322	51
1	-1	12	780	785	41
2	-1	12	442	485	53
3	-1	12	222	144	80
4	-1	12	0	89	1
5	-1	12	500	546	51
6	-1	12	543	451	42
7	-1	12	0	106	1
8	-1	12	675	718	49
9	-1	12	536	541	56
10	-1	12	386	389	37
11	-1	12	160	136	131
-6	0	12	309	313	43
-5	0	12	146	180	108
-4	0	12	0	45	1
-3	0	12	1010	966	42
-2	0	12	490	555	49
-1	0	12	516	458	44
0	0	12	323	353	58
1	0	12	366	328	50
2	0	12	164	148	163
3	0	12	782	707	40
4	0	12	389	392	52
5	0	12	73	39	72
6	0	12	78	192	78
7	0	12	802	807	43
8	0	12	113	112	113
9	0	12	264	295	104
10	0	12	260	322	94
11	0	12	461	474	35
12	0	12	325	291	52
-6	1	12	54	96	53
-5	1	12	0	162	1
-4	1	12	913	897	46
-3	1	12	0	120	1
-2	1	12	358	329	52
-1	1	12	551	633	49
0	1	12	411	381	53
1	1	12	587	628	43
2	1	12	492	497	47
3	1	12	73	73	72
4	1	12	103	203	103
5	1	12	855	844	42
6	1	12	414	473	60
7	1	12	191	159	105
8	1	12	309	227	75
9	1	12	650	675	53
10	1	12	121	133	120
11	1	12	307	442	90
12	1	12	171	134	98
13	1	12	324	354	53
-6	2	12	605	656	32

h	k	l	10Fo	10Fc	10s
-5	2	12	315	315	41
-4	2	12	115	247	114
-3	2	12	315	190	59
-2	2	12	770	674	42
-1	2	12	0	81	1
0	2	12	377	421	62
1	2	12	290	224	59
2	2	12	347	307	53
3	2	12	100	70	100
4	2	12	1133	1093	39
5	2	12	106	71	105
6	2	12	0	65	1
7	2	12	391	385	60
8	2	12	657	602	47
9	2	12	536	493	53
10	2	12	267	257	84
11	2	12	589	523	50
12	2	12	508	432	55
13	2	12	526	524	35
14	2	12	216	126	51
-6	3	12	161	43	84
-5	3	12	276	212	44
-4	3	12	326	405	80
-3	3	12	318	363	70
-2	3	12	408	370	54
-1	3	12	338	301	48
0	3	12	760	830	43
1	3	12	473	576	53
2	3	12	556	498	46
3	3	12	367	263	53
4	3	12	0	51	1
5	3	12	0	156	1
6	3	12	957	1029	42
7	3	12	388	435	59
8	3	12	260	214	69
9	3	12	79	114	78
10	3	12	503	626	60
11	3	12	359	403	81
12	3	12	570	435	60
13	3	12	156	110	156
14	3	12	441	407	41
-6	4	12	180	122	73
-5	4	12	773	762	28
-4	4	12	0	117	1
-3	4	12	0	22	1
-2	4	12	175	241	126
-1	4	12	712	770	45
0	4	12	0	224	1
1	4	12	805	822	44
2	4	12	301	377	65
3	4	12	423	418	54
4	4	12	218	264	80
5	4	12	541	576	49
6	4	12	130	77	130
7	4	12	0	141	1
8	4	12	835	896	47
9	4	12	581	550	50
10	4	12	650	563	47
11	4	12	0	126	1
12	4	12	579	520	53
13	4	12	0	92	1
14	4	12	544	515	36
15	4	12	281	313	59
-6	5	12	253	271	53
-5	5	12	177	107	62
-4	5	12	186	142	58
-3	5	12	941	924	44
-2	5	12	354	281	58
-1	5	12	458	468	54
0	5	12	303	154	50
1	5	12	842	790	41
2	5	12	222	235	101
3	5	12	774	841	42
4	5	12	575	522	44
5	5	12	149	76	148
6	5	12	747	691	45
7	5	12	872	854	44
8	5	12	207	172	112
9	5	12	160	201	159
10	5	12	262	233	95
11	5	12	947	1011	48
12	5	12	828	830	51
13	5	12	629	600	56
14	5	12	245	255	60
15	5	12	0	12	1
-5	6	12	360	296	38
-4	6	12	595	585	30
-3	6	12	145	83	144
-2	6	12	198	163	149
-1	6	12	511	531	48

h	k	l	10Fo	10Fc	10s
0	6	12	1087	1068	44
1	6	12	1032	967	41
2	6	12	1056	1042	39
3	6	12	129	144	129
4	6	12	384	482	55
5	6	12	289	286	71
6	6	12	226	122	99
7	6	12	275	251	84
8	6	12	248	109	70
9	6	12	1418	1295	42
10	6	12	165	284	164
11	6	12	382	478	75
12	6	12	198	136	136
13	6	12	315	424	93
14	6	12	229	286	67
15	6	12	489	525	43
-5	7	12	0	81	1
-4	7	12	137	93	136
-3	7	12	0	46	1
-2	7	12	1068	1018	44
-1	7	12	242	163	103
0	7	12	505	548	55
1	7	12	154	220	154
2	7	12	324	264	62
3	7	12	550	515	47
4	7	12	481	420	51
5	7	12	170	175	118
6	7	12	0	52	1
7	7	12	256	175	64
8	7	12	1040	1002	44
9	7	12	180	224	180
10	7	12	360	313	67
11	7	12	734	751	52
12	7	12	341	277	65
13	7	12	738	653	55
14	7	12	515	445	57
15	7	12	129	157	128
16	7	12	0	111	1
-4	8	12	485	438	32
-3	8	12	688	655	30
-2	8	12	223	255	128
-1	8	12	0	49	1
0	8	12	517	501	55
1	8	12	0	58	1
2	8	12	221	350	129
3	8	12	378	347	59
4	8	12	496	538	49
5	8	12	244	153	76
6	8	12	884	902	43
7	8	12	383	294	56
8	8	12	80	168	80
9	8	12	334	304	61
10	8	12	891	954	48
11	8	12	172	245	171
12	8	12	248	191	123
13	8	12	314	317	89
14	8	12	264	322	99
15	8	12	375	383	44
16	8	12	469	418	41
-3	9	12	49	86	48
-2	9	12	244	205	51
-1	9	12	748	713	51
0	9	12	310	311	70
1	9	12	0	102	1
2	9	12	494	484	53
3	9	12	433	384	49
4	9	12	531	572	51
5	9	12	755	777	45
6	9	12	112	115	111
7	9	12	397	328	64
8	9	12	950	896	46
9	9	12	523	470	53
10	9	12	383	332	56
11	9	12	171	169	171
12	9	12	720	717	55
13	9	12	181	24	180
14	9	12	487	523	70
15	9	12	214	57	61
16	9	12	157	206	156
-3	10	12	535	537	34
-2	10	12	75	168	75
-1	10	12	183	229	84
0	10	12	122	223	122
1	10	12	571	632	58
2	10	12	0	81	1
3	10	12	397	506	69
4	10	12	0	209	1
5	10	12	212	255	89
6	10	12	213	186	128
7	10	12	1128	1079	44

h	k	l	10Fo	10Fc	10s
8	10	12	216	151	70
9	10	12	0	30	1
10	10	12	597	670	55
11	10	12	653	579	54
12	10	12	451	385	58
13	10	12	0	190	1
14	10	12	124	185	124
15	10	12	286	222	54
16	10	12	409	461	51
-2	11	12	121	108	120
-1	11	12	601	584	31
0	11	12	466	430	23
1	11	12	226	253	106
2	11	12	188	158	188
3	11	12	187	179	115
4	11	12	297	111	74
5	11	12	722	778	52
6	11	12	586	551	51
7	11	12	0	19	1
8	11	12	0	48	1
9	11	12	805	814	50
10	11	12	0	229	1
11	11	12	276	198	73
12	11	12	87	70	86
13	11	12	688	660	57
14	11	12	230	136	60
15	11	12	518	484	35
16	11	12	0	71	1
-1	12	12	57	180	57
0	12	12	0	89	1
1	12	12	327	341	40
2	12	12	521	565	60
3	12	12	284	143	73
4	12	12	501	624	56
5	12	12	0	54	1
6	12	12	0	43	1
7	12	12	557	539	48
8	12	12	369	329	72
9	12	12	0	9	1
10	12	12	450	417	58
11	12	12	483	514	60
12	12	12	442	433	61
13	12	12	682	633	33
14	12	12	310	272	50
15	12	12	347	379	53
0	13	12	582	596	46
1	13	12	207	163	63
2	13	12	450	446	36
3	13	12	286	279	47
4	13	12	245	256	108
5	13	12	0	23	1
6	13	12	507	602	63
7	13	12	210	50	112
8	13	12	229	242	118
9	13	12	274	192	81
10	13	12	839	735	49
11	13	12	219	223	123
12	13	12	225	87	85
13	13	12	267	276	52
14	13	12	604	530	37
15	13	12	355	427	51
2	14	12	278	299	53
3	14	12	412	391	36
4	14	12	410	364	37
5	14	12	288	239	45
6	14	12	150	113	150
7	14	12	0	84	1
8	14	12	691	654	53
9	14	12	352	445	89
10	14	12	268	243	95
11	14	12	200	150	73
12	14	12	593	612	33
13	14	12	247	143	53
14	14	12	482	385	39
3	15	12	285	333	47
4	15	12	219	186	66
5	15	12	269	332	45
6	15	12	245	243	58
7	15	12	441	429	34
8	15	12	129	86	128
9	15	12	0	96	1
10	15	12	364	355	41
11	15	12	496	518	36
12	15	12	327	375	45
13	15	12	201	37	86
6	16	12	244	138	46
7	16	12	0	67	1
8	16	12	150	98	100
9	16	12	640	621	32
10	16	12	190	29	70

h	k	l	10Fo	10Fc	10s
11	16	12	0	112	1
-2	-4	13	50	56	50
-1	-4	13	394	407	36
0	-4	13	287	258	28
1	-4	13	369	360	32
2	-4	13	156	181	88
3	-4	13	506	536	30
4	-4	13	0	63	1
5	-4	13	85	25	84
6	-4	13	269	267	48
-3	-3	13	84	203	84
-2	-3	13	213	178	49
-1	-3	13	384	384	35
0	-3	13	269	238	28
1	-3	13	492	526	30
2	-3	13	346	396	35
3	-3	13	81	225	81
4	-3	13	116	61	115
5	-3	13	552	576	29
6	-3	13	129	97	128
7	-3	13	238	195	47
8	-3	13	0	96	1
-4	-2	13	100	141	99
-3	-2	13	209	213	56
-2	-2	13	455	492	30
-1	-2	13	250	205	42
0	-2	13	503	490	48
1	-2	13	375	418	64
2	-2	13	339	350	57
3	-2	13	414	320	55
4	-2	13	465	517	60
5	-2	13	0	149	1
6	-2	13	46	57	46
7	-2	13	534	523	32
8	-2	13	330	349	39
9	-2	13	367	373	39
-4	-1	13	516	527	29
-3	-1	13	295	366	42
-2	-1	13	375	384	36
-1	-1	13	207	239	102
0	-1	13	505	519	50
1	-1	13	108	23	108
2	-1	13	505	507	53
3	-1	13	438	438	55
4	-1	13	173	80	173
5	-1	13	307	295	66
6	-1	13	730	788	48
7	-1	13	368	287	54
8	-1	13	0	42	1
9	-1	13	267	237	43
10	-1	13	450	406	35
-5	0	13	477	501	33
-4	0	13	139	134	139
-3	0	13	70	53	69
-2	0	13	465	385	52
-1	0	13	451	532	52
0	0	13	310	292	63
1	0	13	646	621	45
2	0	13	477	484	50
3	0	13	0	6	1
4	0	13	792	818	43
5	0	13	294	283	72
6	0	13	276	323	78
7	0	13	142	118	142
8	0	13	671	754	50
9	0	13	0	41	1
10	0	13	149	171	149
11	0	13	283	265	50
-5	1	13	88	122	88
-4	1	13	203	52	54
-3	1	13	799	820	27
-2	1	13	0	61	1
-1	1	13	314	346	67
0	1	13	483	491	52
1	1	13	241	288	111
2	1	13	274	343	74
3	1	13	686	760	47
4	1	13	0	58	1
5	1	13	0	127	1
6	1	13	0	278	1
7	1	13	615	580	50
8	1	13	470	410	65
9	1	13	226	128	87
10	1	13	475	535	58
11	1	13	387	333	37
12	1	13	417	373	41
-5	2	13	397	355	36
-4	2	13	407	373	36
-3	2	13	301	293	41
-2	2	13	289	179	65

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
-1	2	13	634	738	51
0	2	13	269	178	67
1	2	13	404	424	55
2	2	13	305	237	71
3	2	13	78	226	78
4	2	13	0	129	1
5	2	13	960	891	43
6	2	13	110	137	110
7	2	13	310	94	56
8	2	13	339	334	65
9	2	13	562	627	54
10	2	13	0	169	1
11	2	13	320	272	40
12	2	13	0	170	1
13	2	13	262	282	61
-5	3	13	0	36	1
-4	3	13	72	10	71
-3	3	13	429	400	34
-2	3	13	614	610	48
-1	3	13	177	74	138
0	3	13	397	346	57
1	3	13	297	322	69
2	3	13	389	382	60
3	3	13	542	528	49
4	3	13	876	874	43
5	3	13	134	202	133
6	3	13	407	318	54
7	3	13	639	661	45
8	3	13	0	174	1
9	3	13	461	357	60
10	3	13	261	258	120
11	3	13	690	642	54
12	3	13	172	91	91
13	3	13	379	412	44
14	3	13	0	48	1
-5	4	13	238	200	52
-4	4	13	524	551	34
-3	4	13	184	51	67
-2	4	13	258	227	65
-1	4	13	524	445	51
0	4	13	802	855	44
1	4	13	108	82	108
2	4	13	660	606	45
3	4	13	264	119	58
4	4	13	397	334	51
5	4	13	387	330	59
6	4	13	921	947	43
7	4	13	239	68	83
8	4	13	84	145	83
9	4	13	616	579	52
10	4	13	572	488	53
11	4	13	690	649	52
12	4	13	390	275	74
13	4	13	292	277	51
14	4	13	347	345	46
-4	5	13	163	161	95
-3	5	13	166	136	74
-2	5	13	370	408	63
-1	5	13	493	496	55
0	5	13	0	163	1
1	5	13	542	678	53
2	5	13	576	573	48
3	5	13	475	460	47
4	5	13	865	844	43
5	5	13	291	258	79
6	5	13	110	82	110
7	5	13	358	426	66
8	5	13	1030	994	46
9	5	13	236	178	100
10	5	13	463	465	62
11	5	13	0	106	1
12	5	13	465	547	62
13	5	13	0	39	1
14	5	13	389	390	43
-4	6	13	215	214	57
-3	6	13	804	782	28
-2	6	13	205	71	93
-1	6	13	0	233	1
0	6	13	181	220	181
1	6	13	679	650	45
2	6	13	222	37	78
3	6	13	737	694	45
4	6	13	426	426	60
5	6	13	176	205	176
6	6	13	1022	1043	43
7	6	13	376	289	55
8	6	13	777	752	49
9	6	13	508	517	54
10	6	13	243	208	99
11	6	13	385	404	67
12	6	13	314	283	76
13	6	13	337	388	88
14	6	13	537	506	38
15	6	13	0	23	1
-4	7	13	250	247	60
-3	7	13	180	131	78
-2	7	13	201	186	57
-1	7	13	461	400	54
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1	7	13	472	457	53
2	7	13	631	578	48
3	7	13	435	561	64
4	7	13	0	186	1
5	7	13	485	437	54
6	7	13	277	254	72
7	7	13	243	140	111
8	7	13	0	155	1
9	7	13	917	1051	48
10	7	13	211	165	113
11	7	13	124	53	123
12	7	13	240	352	142
13	7	13	336	353	78
14	7	13	331	248	45
15	7	13	481	475	38
-3	8	13	359	352	44
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0	8	13	118	85	118
1	8	13	166	294	165
2	8	13	283	305	71
3	8	13	590	496	51
4	8	13	607	573	50
5	8	13	524	384	47
6	8	13	334	346	72
7	8	13	869	864	45
8	8	13	0	271	1
9	8	13	386	414	76
11	8	13	999	988	51
12	8	13	0	9	1
13	8	13	0	256	1
14	8	13	0	217	1
15	8	13	54	169	53
-2	9	13	159	165	94
-1	9	13	201	161	66
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2	9	13	251	322	96
3	9	13	397	327	61
4	9	13	339	316	61
5	9	13	260	307	105
6	9	13	934	874	44
7	9	13	262	263	96
8	9	13	0	172	1
9	9	13	646	605	53
10	9	13	659	669	58
11	9	13	235	291	115
12	9	13	181	161	180
13	9	13	551	500	59
14	9	13	171	96	116
15	9	13	403	473	43
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3	10	13	0	57	1
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5	10	13	428	395	66
6	10	13	221	101	79
7	10	13	0	91	1
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9	10	13	209	175	148
10	10	13	214	89	139
11	10	13	464	473	64
12	10	13	616	612	58
13	10	13	310	219	69
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15	10	13	143	52	143
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3	11	13	357	292	68
4	11	13	285	178	80
5	11	13	343	376	83
6	11	13	504	584	63
7	11	13	553	552	54
8	11	13	228	244	154
9	11	13	194	151	194
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11	11	13	179	38	178
12	11	13	160	239	159
13	11	13	0	101	1
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15	11	13	237	207	73
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2	12	13	247	283	58
3	12	13	217	337	217
4	12	13	232	21	96
5	12	13	689	631	51
6	12	13	173	54	173
7	12	13	389	336	64
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9	12	13	709	690	52
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11	12	13	129	136	129
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13	12	13	458	459	40
14	12	13	271	190	53
15	12	13	287	252	55
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2	13	13	235	289	63
3	13	13	233	216	63
4	13	13	428	412	37
6	13	13	293	174	86
7	13	13	861	865	52
8	13	13	267	62	79
9	13	13	0	71	1
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11	13	13	532	569	33
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13	13	13	394	401	43
14	13	13	249	171	57
3	14	13	163	214	122
4	14	13	416	410	37
5	14	13	276	223	46
6	14	13	358	368	45
7	14	13	0	33	1
8	14	13	205	229	64
9	14	13	671	654	33
10	14	13	275	344	59
11	14	13	212	299	65
12	14	13	0	40	1
13	14	13	432	392	42
5	15	13	230	53	54
6	15	13	283	264	52
7	15	13	0	23	1
8	15	13	576	595	34
9	15	13	162	121	90
10	15	13	0	9	1
11	15	13	175	189	91
12	15	13	530	527	39
1	-3	14	362	361	34
2	-3	14	329	346	35
3	-3	14	367	364	37
4	-3	14	85	27	85
5	-3	14	177	38	64
-1	-2	14	384	353	34
0	-2	14	0	23	1
1	-2	14	515	530	31
2	-2	14	115	211	115
3	-2	14	302	287	35
4	-2	14	267	256	42
5	-2	14	596	572	28
6	-2	14	0	23	1
7	-2	14	0	29	1
-2	-1	14	280	275	42
-1	-1	14	308	308	38
0	-1	14	230	198	43
1	-1	14	406	428	33
2	-1	14	0	185	1
3	-1	14	566	563	29
4	-1	14	316	365	41
5	-1	14	136	44	98
6	-1	14	155	116	78
7	-1	14	779	755	28
8	-1	14	87	73	87
9	-1	14	219	215	66
-3	0	14	122	128	122
-2	0	14	0	226	1
-1	0	14	185	207	59
0	0	14	388	406	24
1	0	14	277	236	70
2	0	14	505	538	47
3	0	14	376	390	62
4	0	14	227	300	109
5	0	14	620	580	49
6	0	14	440	500	63
7	0	14	466	505	35
8	0	14	49	166	48
9	0	14	426	434	37
10	0	14	0	214	1
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-2	1	14	586	597	28
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0	1	14	215	252	130
1	1	14	300	231	67
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3	1	14	0	145	1
4	1	14	859	874	45
5	1	14	0	110	1
6	1	14	185	189	145
7	1	14	189	227	189
8	1	14	525	534	58
9	1	14	308	278	41
10	1	14	162	53	79
11	1	14	328	307	54
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-1	2	14	180	196	69
0	2	14	335	422	77
1	2	14	240	216	81
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3	2	14	422	567	59
4	2	14	212	168	93
5	2	14	345	365	74
6	2	14	653	733	53
7	2	14	204	264	101
8	2	14	257	73	71
9	2	14	0	149	1
10	2	14	591	580	33
11	2	14	0	18	1
12	2	14	321	320	56
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3	3	14	536	437	51
4	3	14	278	343	92
5	3	14	825	828	45
7	3	14	205	268	134
8	3	14	561	582	57
9	3	14	401	365	66
10	3	14	200	220	200
11	3	14	272	218	51
12	3	14	393	406	40
13	3	14	252	269	72
-3	4	14	455	455	33
-2	4	14	207	228	54
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2	4	14	370	344	60
3	4	14	732	620	47
4	4	14	266	263	85
5	4	14	182	189	132
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7	4	14	944	970	48
8	4	14	226	53	103
9	4	14	174	75	174
10	4	14	410	420	63
11	4	14	460	438	38
12	4	14	394	287	41
13	4	14	498	480	40
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1	5	14	85	126	84
2	5	14	510	518	58
3	5	14	0	196	1
4	5	14	544	514	50
5	5	14	764	738	50
6	5	14	529	538	57
7	5	14	250	89	74
8	5	14	0	197	1
9	5	14	714	655	50
10	5	14	0	84	1
11	5	14	622	653	54
12	5	14	97	58	97
13	5	14	180	195	87
14	5	14	145	119	144
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2	6	14	717	730	49
3	6	14	0	17	1
4	6	14	700	669	48
5	6	14	0	124	1
6	6	14	262	300	99
7	6	14	551	486	54
8	6	14	657	649	54
9	6	14	443	364	53
11	6	14	0	164	1
12	6	14	233	256	55
13	6	14	112	146	111
14	6	14	155	107	154
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1	7	14	307	378	95
2	7	14	265	298	94
3	7	14	0	156	1
4	7	14	447	377	53
5	7	14	264	243	93
6	7	14	891	905	45
7	7	14	339	252	77
8	7	14	0	44	1
9	7	14	0	51	1
10	7	14	882	754	50
11	7	14	183	21	182
12	7	14	310	346	88
13	7	14	170	211	138
14	7	14	318	360	49
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3	8	14	735	614	49
4	8	14	478	377	59
5	8	14	523	497	60
7	8	14	171	245	171
8	8	14	775	748	50
9	8	14	650	640	57
10	8	14	346	301	73
11	8	14	128	101	127
12	8	14	416	464	67
13	8	14	0	96	1
14	8	14	392	438	45
15	8	14	307	311	49
-1	9	14	186	71	78
0	9	14	183	156	48
1	9	14	426	389	34
2	9	14	152	102	152
3	9	14	441	499	62
4	9	14	210	292	137
5	9	14	298	482	88
6	9	14	211	85	94
7	9	14	778	746	47
8	9	14	276	228	85
9	9	14	293	58	75
10	9	14	500	422	54
11	9	14	667	576	56
12	9	14	348	171	57
13	9	14	149	172	148
14	9	14	184	241	90
15	9	14	290	215	47
0	10	14	591	556	23
1	10	14	152	154	151
2	10	14	216	132	52
3	10	14	451	332	53
4	10	14	363	371	76
5	10	14	668	606	55
6	10	14	419	372	63
7	10	14	0	65	1
8	10	14	266	262	93
9	10	14	790	813	53
10	10	14	0	54	1
11	10	14	131	193	130
12	10	14	287	251	47
13	10	14	423	435	45
14	10	14	0	26	1
15	10	14	381	401	46
0	11	14	188	113	48
1	11	14	225	223	56
2	11	14	568	550	34
3	11	14	94	8	93
4	11	14	507	481	64
5	11	14	282	109	83
6	11	14	294	330	73
7	11	14	319	380	89
8	11	14	709	658	53
9	11	14	91	252	91
10	11	14	203	177	149

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
11	11	14	570	570	59
12	11	14	282	280	58
13	11	14	0	160	1
14	11	14	0	138	1
1	12	14	261	270	54
2	12	14	110	159	109
3	12	14	78	128	77
4	12	14	194	184	83
5	12	14	183	130	80
6	12	14	895	910	51
7	12	14	0	206	1
8	12	14	239	219	118
9	12	14	181	48	181
10	12	14	420	489	75
11	12	14	220	174	64
12	12	14	0	204	1
13	12	14	323	345	51
14	12	14	399	454	48
3	13	14	390	368	39
4	13	14	155	147	89
5	13	14	161	224	110
6	13	14	0	96	1
7	13	14	411	395	39
8	13	14	799	780	31
9	13	14	285	293	51
10	13	14	0	28	1
11	13	14	0	87	1
12	13	14	396	414	43
13	13	14	174	106	76
4	14	14	156	46	98
5	14	14	388	387	38
6	14	14	50	118	50
7	14	14	500	603	40
8	14	14	171	95	78
9	14	14	255	278	53
10	14	14	317	306	43
11	14	14	404	396	44
12	14	14	222	240	67
7	15	14	95	99	95
8	15	14	183	132	70
9	15	14	607	612	36
10	15	14	0	59	-1
1	-1	15	345	346	42
2	-1	15	269	189	42
3	-1	15	231	297	55
4	-1	15	391	394	37
5	-1	15	285	332	48
6	-1	15	0	27	1
0	0	15	163	133	50
1	0	15	455	435	33
2	0	15	213	123	50
3	0	15	536	548	31
4	0	15	111	160	110
5	0	15	213	110	46
6	0	15	337	390	43
7	0	15	566	591	32
8	0	15	74	120	73
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0	1	15	154	151	52
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2	1	15	306	303	41
3	1	15	318	335	40
4	1	15	72	190	72
5	1	15	537	542	33
6	1	15	237	129	46
7	1	15	0	89	1
8	1	15	210	174	54
9	1	15	558	583	34
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1	2	15	97	106	97
2	2	15	278	303	45
3	2	15	419	383	32
4	2	15	599	536	50
5	2	15	209	184	135
6	2	15	400	354	37
7	2	15	669	631	29
8	2	15	389	406	41
9	2	15	151	182	122
10	2	15	59	160	58
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2	3	15	501	472	31
3	3	15	393	279	52
4	3	15	367	313	59
5	3	15	0	72	1
6	3	15	907	879	48
7	3	15	0	39	1
8	3	15	137	100	137
9	3	15	343	356	46
10	3	15	364	389	45
11	3	15	127	80	127
-2	4	15	365	338	37
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2	4	15	294	276	86
3	4	15	377	303	64
4	4	15	638	671	52
5	4	15	561	433	51
6	4	15	0	251	1
7	4	15	350	206	57
8	4	15	667	631	56
9	4	15	108	55	107
10	4	15	197	233	76
11	4	15	441	426	40
12	4	15	386	382	45
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3	5	15	519	574	58
4	5	15	0	56	1
5	5	15	456	460	67
6	5	15	506	566	65
7	5	15	607	612	51
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11	5	15	278	184	51
12	5	15	431	483	46
13	5	15	194	160	83
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2	6	15	230	299	148
3	6	15	323	393	83
4	6	15	228	264	162
5	6	15	716	760	55
6	6	15	123	76	122
7	6	15	153	154	152
8	6	15	201	269	200
9	6	15	574	562	55
11	6	15	0	117	1
12	6	15	0	67	1
13	6	15	454	388	39
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3	7	15	547	501	57
4	7	15	592	511	52
5	7	15	89	82	89
6	7	15	305	362	98
7	7	15	595	580	56
8	7	15	402	335	54
9	7	15	92	61	91
10	7	15	160	99	159
11	7	15	553	573	40
12	7	15	271	235	57
13	7	15	546	547	36
0	8	15	407	428	28
1	8	15	77	43	76
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3	8	15	0	222	1
4	8	15	632	575	55
5	8	15	0	146	1
6	8	15	495	435	60
7	8	15	0	79	1
8	8	15	0	151	1
9	8	15	577	511	57
10	8	15	792	698	48
11	8	15	135	163	134
12	8	15	246	262	59
13	8	15	164	169	120
14	8	15	158	123	157
0	9	15	161	119	69
1	9	15	0	137	1
2	9	15	336	260	41
3	9	15	365	437	43
4	9	15	703	653	52
5	9	15	156	158	156
6	9	15	422	372	67
7	9	15	129	64	129
8	9	15	711	694	59
9	9	15	0	72	1
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11	9	15	54	56	53
12	9	15	530	530	37
13	9	15	116	6	115
14	9	15	329	371	52
1	10	15	393	441	45
2	10	15	269	171	50
3	10	15	403	368	39
4	10	15	279	282	49
5	10	15	541	546	64
6	10	15	490	360	60
7	10	15	387	419	68
8	10	15	205	80	130
9	10	15	0	119	1
10	10	15	609	610	33
11	10	15	442	391	38
12	10	15	247	224	59
13	10	15	0	123	1
14	10	15	0	142	1
2	11	15	231	105	51
3	11	15	459	482	37
4	11	15	0	57	1
5	11	15	590	603	35
6	11	15	217	148	75
7	11	15	334	303	43
8	11	15	96	141	96
9	11	15	594	607	33
10	11	15	229	118	64
11	11	15	110	62	110
12	11	15	372	335	40
13	11	15	333	384	52
3	12	15	308	329	46
4	12	15	0	199	1
5	12	15	191	206	87
6	12	15	363	360	40
7	12	15	571	613	33
8	12	15	279	140	53
9	12	15	165	55	91
10	12	15	125	99	124
11	12	15	624	580	33
12	12	15	0	100	1
13	12	15	234	138	62
5	13	15	167	101	100
6	13	15	564	582	36
7	13	15	0	56	1
8	13	15	462	410	37
9	13	15	328	379	46
10	13	15	177	262	117
11	13	15	80	110	79
12	13	15	101	118	100
7	14	15	0	116	1
8	14	15	469	574	41
9	14	15	0	39	1
10	14	15	0	127	1
3	1	16	281	311	49
4	1	16	0	128	1
5	1	16	73	63	72
6	1	16	505	481	32
2	2	16	0	84	1
3	2	16	408	364	36
4	2	16	258	234	54
5	2	16	423	508	39
6	2	16	203	172	65
7	2	16	178	126	63
8	2	16	350	303	42
1	3	16	392	384	37
2	3	16	55	159	55
3	3	16	484	442	34
4	3	16	269	288	44
5	3	16	296	236	42
6	3	16	0	102	1
7	3	16	660	625	32
8	3	16	77	102	77
9	3	16	0	74	1
1	4	16	196	142	63
2	4	16	330	305	43
3	4	16	89	138	89
4	4	16	452	387	36
5	4	16	551	486	33
6	4	16	516	487	34
7	4	16	161	75	102
8	4	16	196	120	57
9	4	16	494	498	37
10	4	16	359	284	47
1	5	16	199	127	76
2	5	16	450	361	35
3	5	16	118	53	118
4	5	16	614	597	32
5	5	16	160	134	101
6	5	16	369	364	39
7	5	16	186	197	91
8	5	16	606	588	34
9	5	16	165	40	104
10	5	16	219	215	70
11	5	16	258	263	54
1	6	16	476	400	34
2	6	16	50	151	49
3	6	16	213	169	65
4	6	16	106	160	105
5	6	16	282	331	51
6	6	16	760	759	32
7	6	16	282	335	56
8	6	16	274	179	41
9	6	16	175	100	73
10	6	16	335	358	46
11	6	16	0	76	1
12	6	16	393	361	44
1	7	16	257	279	56
2	7	16	109	156	108
3	7	16	615	618	33
4	7	16	154	123	124
5	7	16	512	447	36
6	7	16	0	62	1
7	7	16	171	174	80
8	7	16	639	601	34
9	7	16	435	410	43
10	7	16	127	16	126
11	7	16	127	100	126
12	7	16	241	229	71
2	8	16	468	391	36
3	8	16	531	542	34
4	8	16	143	97	143
5	8	16	267	300	52
6	8	16	189	67	75
7	8	16	696	681	33
8	8	16	227	131	59
9	8	16	184	138	82
10	8	16	127	99	126
11	8	16	406	428	43
12	8	16	62	59	61
2	9	16	401	315	40
3	9	16	137	201	136
4	9	16	545	549	35
5	9	16	612	565	35
6	9	16	246	195	45
7	9	16	167	135	105
8	9	16	0	111	1
9	9	16	407	410	41
10	9	16	566	511	36
11	9	16	200	174	97
12	9	16	115	93	115
3	10	16	0	35	1
4	10	16	416	408	39
5	10	16	0	154	1
6	10	16	519	541	39
7	10	16	209	246	72
8	10	16	464	510	40
9	10	16	97	57	96
10	10	16	81	99	81
11	10	16	257	278	57
12	10	16	423	516	44
4	11	16	369	329	45
5	11	16	0	134	1
6	11	16	625	660	35
7	11	16	210	195	74
8	11	16	169	161	88
9	11	16	139	75	139
10	11	16	505	540	36
11	11	16	0	119	1
12	11	16	291	250	48
5	12	16	323	305	47
6	12	16	226	170	59
7	12	16	339	316	43
8	12	16	440	334	37
9	12	16	241	317	70
10	12	16	80	129	79
11	12	16	0	40	1
9	13	16	278	214	46
5	4	17	264	281	50
6	4	17	208	227	68
7	4	17	472	445	37
4	5	17	0	89	1
5	5	17	328	371	49
6	5	17	222	205	72
7	5	17	224	199	69
8	5	17	0	35	1
4	6	17	186	206	97
5	6	17	59	52	59
6	6	17	307	285	55
7	6	17	446	410	40
8	6	17	416	440	44
9	6	17	142	146	142
4	7	17	239	327	66
5	7	17	0	27	1
6	7	17	542	521	38
7	7	17	171	112	91
8	7	17	172	180	119
9	7	17	165	215	164
10	7	17	453	469	44
4	8	17	580	373	36
5	8	17	151	161	150
6	8	17	160	178	160
7	8	17	0	55	1
8	8	17	427	515	47
9	8	17	327	298	51
10	8	17	119	40	118
5	9	17	522	501	40
6	9	17	258	276	70
7	9	17	325	279	46
8	9	17	183	149	86
9	9	17	0	56	1
10	9	17	387	341	44
6	10	17	216	77	61
7	10	17	0	157	1
8	10	17	164	96	111
9	10	17	439	465	43