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Task No. NR 053-559

Technical Report No. 22

Synthesis, Characterization, and Structure of
Tri- μ -halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids,
by

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Prepared for Publication
in the

Journal of American Chemical Society

11 15 March 1978

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Technical Report No. 22	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Synthesis, Characterization, and Structure of Tri- μ -halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids		5. TYPE OF REPORT & PERIOD COVERED Interim
7. AUTHOR(s) C.P. Hrung, M. Tsutsui, D.L. Cullen, and E.F. Meyer, Jr. and C.N. Morimoto, Syntex Analytical Instruments, Inc.		6. PERFORMING ORG. REPORT NUMBER
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Chemistry Texas A&M University College Station, Texas 77843		8. CONTRACT OR GRANT NUMBER(s) N00014-75-C-0417
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Department of the Navy Arlington, Virginia 22217		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		12. REPORT DATE March 15, 1978
		13. NUMBER OF PAGES 73
		15. SECURITY CLASS. (of this report)
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report)		
DISTRIBUTION STATEMENT A Approved for public release; Distribution Unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES Prepared for publication in the Journal of American Chemical Society		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Monocationic Porphyrin Acids Tri- μ -halogeno-hexacarbonyldirhenate(I) Octaethylporphyrin		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Two new compounds, μ -[2,3,7,8,12,13,17,18-octaethylporphyrin]-bis-[tricarbonylrhenium(I)], $(C_{36}H_{44}N_4)[Re(CO)_3]_2$ and a salt of a monocationic porphyrin acid, octaethylporphyrinium tri- μ -chlorohexacarbonyldirhenate(I), $(C_{36}H_{47}N_4)[Re_2(CO)_6Cl_3]^+$, have been synthesized by the reaction of a 2:1 mole ratio of rhenium pentacarbonyl and octaethylporphyrin in refluxing decalin under argon. The structure of the latter was determined from three-dimensional diffractometer data.		

Synthesis, Characterization, and Structure of
Tri- μ -halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids

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ABSTRACT

Two new compounds, μ -[2,3,7,8,12,13,17,18-octaethylporphyrin]-bis-[tricarbonylrhenium(I)], $(C_{36}H_{44}N_4)[Re(CO)_3]_2$ and a salt of a monocationic porphyrin acid, octaethylporphinium tri- μ -chlorohexacarbonyl-dirhenate(I), $(C_{36}H_{47}N_4)^+[Re_2(CO)_6Cl_3]^-$, have been synthesized by the reaction of a 2:1 mole ratio of rhenium pentacarbonyl and octaethylporphyrin in refluxing decalin under argon. The structure of the latter was determined from three-dimensional diffractometer data. A total of 10,792 independent reflections was measured. The compound crystallizes in the monoclinic space group $P2_1/a$ with a unit cell of $a = 18.140(3)$, $b = 19.847(3)$, $c = 13.625(2) \text{ \AA}$, $\beta = 111.64(2)^\circ$. There are four molecules in the unit cell. The structure was solved by heavy-atom methods and refined by least-squares techniques to a conventional R index of 0.045 for the 5995 reflections having $I \geq 3\sigma_I$. The porphyrin monoacid cation has three coplanar pyrrole rings with the plane of the fourth ring tilted by 8.6° from the mean plane of the other three. Evidence indicates that the nitrogen atom in the tilted ring has sp^3 hybridization. The anion, which was hitherto unknown, consists of two rhenium atoms bridged by three chlorine atoms. Three carbonyl groups complete the octahedral coordination on each metal atom. There is a water molecule of crystallization which is involved in hydrogen bonding with the pyrrole nitrogen atoms of the cation. The salt could also be prepared using a 1.5/1 $Re(CO)_5Cl/H_2OEP$ mixture with $(H-OEP)Re(CO)_3$ as the other product. Analogous compounds could be made using mesoporphyrin IX dimethyl ester and $Re(CO)_5Br$, but the monocationic porphyrin species could not be ob-

tained when meso-tetraphenylporphyrin was used.

INTRODUCTION

The metal-carbonyl insertion method² has been found useful for the preparation of bimetallic porphyrin complexes of rhodium, rhenium, and technetium.^{3,4} Metal carbonyl halides are more reactive reagents than metal carbonyls for the synthesis of bimetallic complexes of porphyrins as well as bimetallic salts of porphyrin acids.⁵⁻⁸ For example, dimeric rhodium dicarbonyl chloride reacts with porphyrin in benzene at ambient temperature or in boiling chloroform to form a dirhodium porphyrin complex or a dirhodium salt of a porphyrin diacid.^{9,10} In the present work it was discovered that dimeric rhenium tetracarbonyl halides are also capable of reacting with porphyrin in refluxing decalin to form a monorhenium or a dirhenium porphyrin complex as well as a salt complex of a porphyrin monoacid.¹¹ This salt contains a hitherto unreported anionic dimeric halocarbonyl rhenium complex, tri- μ -halogeno-hexacarbonyldirhenate(I). The structure of the salt containing chlorine as the halogen and octaethylporphinium monoacid as the cation has been elucidated by several means, primary among them being an x-ray structural analysis. A preliminary communication on this work has been published.¹¹

Only a few porphyrin acid structures have been reported. Most of these have been porphyrin diacids. The earlier studies revealed macrocycles with large deviations from planarity, presumably because of the non-bonded interactions between the four imino hydrogen atoms.⁷ However a more recent report on the structure of an H_4OEP^{2+} salt (OEP = octaethylporphyrin anion) showed that the macrocycle in that case was nearly planar.¹⁰ Monoacid porphyrin cations are uncommon. Samuels, Shuttleworth, and Stevens¹² reported the preparation of a tri-iodo de-

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rivative of octaethylporphyrin. A later x-ray structure determination, reported by Hirayama et. al. in a short communication, revealed that this compound should be formulated as $(H_3OEP)^+I_3^-$.⁵ While the macrocycle in this case shows some deviations from planarity, the H-H contacts inside the porphyrin "hole" are still too short if the pyrrole nitrogen atoms are assumed to be trigonally hybridized. Thus partial sp^3 hybridization of the nitrogen atoms has been proposed for both the monocationic and dicationic octaethylporphyrin salts.^{5,10} Such a hybridization would be necessary to explain the proposed hydrogen bonding in the H_4OEP^{2+} structure.¹⁰

In all of the porphyrin acid structures so far reported, the data have not been of sufficient quality to examine these suggestions adequately. However in the present case, crystals of excellent quality were available. Thus in addition to elucidating the nature of the material obtained in the synthetic procedure, a full x-ray analysis promised to shed some light on the nature and conformations of the porphyrin acids.

RESULTS AND DISCUSSION

Monocation Porphyrinium Tri- μ -halogeno-hexacarbonyldirhenate(I).

When a mixture of $Re(CO)_5Cl$ and H_2OEP in a 2:1 mole ratio was refluxed in decalin under argon and then allowed to stand at room temperature, a large quantity of burgundy colored crystals formed, leaving a solution of dirhenium octaethylporphyrin complex, $OEP[Re(CO)_3]_2$. The burgundy colored substance was recrystallized from dichloromethane/cyclohexane as dark red crystals, (I), mp 215-220°. The

structure of the new compound was formulated as $(H_3OEP)^+ [Re_2(CO)_6Cl_3]^-$, monocation octaethylporphinium tri- μ -chlorohexacarbonyldirhenate(I), based on elemental analysis, spectroscopic data, and a single-crystal x-ray diffraction analysis.

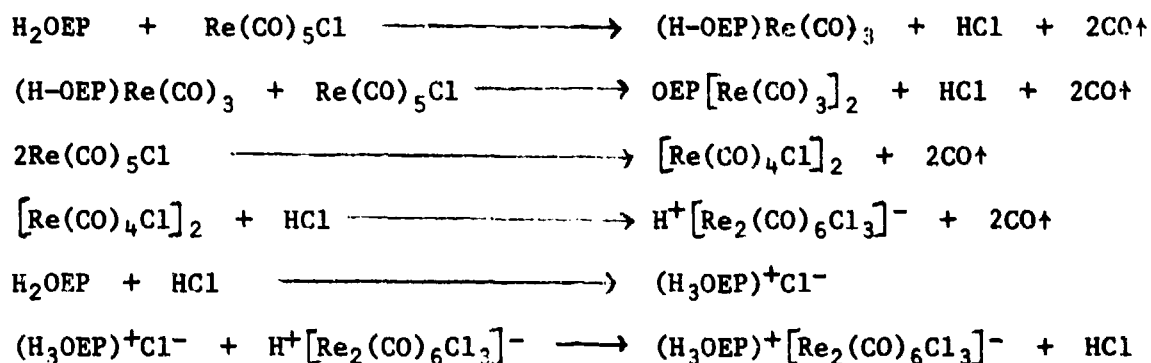
Compound I has visible absorptions in dichloromethane at 390 (Soret band), 530, 555, 570, and 602 nm. The visible spectrum is extremely similar to that of monocation octaethylporphinium triiodide, $(H_3OEP)^+ \cdot I_3^-$ (the only previously known porphyrin monocation salt)⁵, and is distinctly different from that of the dication salt, $(H_4OEP)^{++} \cdot 2Cl^-$ (Figure 1).⁶ When ethanol is added to the dichloromethane solution of I, the visible spectrum reverts to that of metal free octaethylporphyrin H_2OEP . The infrared spectrum of I in the solid state (KBr pellet) has two broad peaks at 3350 and 3375 cm^{-1} attributed to stretching vibrations of the two chemically independent N-H bonds, and three strong metal-carbonyl stretching bands at 1950, 2020, and 2050 cm^{-1} . The far-infrared spectrum of I (in Nujol) has two broad metal-halide stretching peaks at 200 and 250 cm^{-1} . The pmr solution of I in deuteriochloroform shows two sharp peaks at 1.90 (t) and 4.20 (q) δ for the ethyl substituents and two broad peaks at 10.70 and -3.50 δ for the bridged methine protons and the pyrrolic N-H protons, respectively.

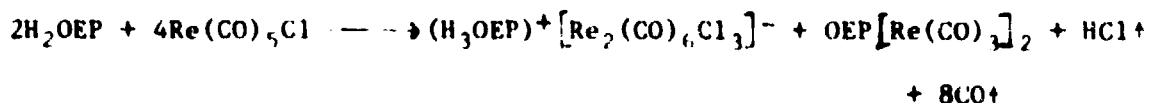
The new compound I is moisture sensitive and thermally unstable. It is fairly stable in dry methylene chloride, tetrahydrofuran, and ethylacetate but decomposes immediately in alcohols, acetone, and water to free octaethylporphyrin, H_2OEP . It can be kept under argon for several days without decomposition in a vacuum desiccator stored in a refrigerator. However, it decomposes gradually to dirhenium octaethyl-

porphyrin as indicated by its visible absorption spectrum. This behavior was confirmed by heating a purified sample of I in decalin under argon (Figure 2). Dirhenium octaethylporphyrin formed in the supernatant while the undecomposed burgundy colored solid of I remained at the bottom of the reaction flask. The amount of the dirhenium octaethylporphyrin varied with the heating time and temperature. Prolonged heating of I in refluxing decalin caused further decomposition to monorhenium octaethylporphyrin, $(H-OEP)Re(CO)_3$, as indicated by its visible absorption spectrum.¹¹

By reaction of $H_2MPIXDME$ with stoichiometric quantities of $Re(CO)_5Br$ or $[Re(CO)_4Br]_2$ in refluxing decalin under argon, an analogous salt-like complex of I was prepared: $(H_3MPIXDME)^+[Re_2(CO)_6Br_3]^-$, (II), monocation mesoporphyrinium IX dimethyl ester tri- μ -bromo-hexacarbonyl dirhenate(I). This complex has chemical and spectroscopic properties similar to that of I (Figure 3). Therefore, a structure identical to that of I is proposed for II.

On the basis of the stepwise changes of visible absorption spectra of the reaction mixture and the x-ray crystal structure of I, the following reaction scheme was proposed.





Because of the instability of meso-tetraphenylporphine monocation,^{6,7} none of the corresponding monocation tetraphenylporphinium analogues could be prepared; possible reasons for this instability are outlined by Fleischer.⁶

X-Ray Structural Data

A preliminary study on the single crystal x-ray diffraction analysis of (I) has already been reported.¹¹ It is an ionic compound with the porphyrin moiety present as a monocationic species, H_3OEP^+ . In the anionic species $[\text{Re}_2(\text{CO})_6\text{Cl}_3]^-$, the two rhenium ions have octahedral coordination. They are joined by three bridging chlorine atoms. Three carbonyl groups on each metal ion complete the coordination. ORTEP¹³ drawings of the compound are shown in Figure 4. Figure 4a also shows the nomenclature for the different types of carbon atoms and the designations for the four rings. A stereoview of the entire formula unit, including a water molecule of crystallization, is shown in Figure 5.

A. Cation

The imino hydrogen atoms appear to be localized on Rings A, B, and C. Such a localization was postulated for the H_3OEP^+ cation as found in the tri-iodide salt.⁵ The hydrogen atoms in that study were not located directly, but the $\text{C}_a\text{-N-C}_a$ angle for one ring was reported as 102° as compared to the values of 109° and 110° for the other two crystallographically independent rings, which presumably bear imino hydrogen atoms. A similar difference is noted in the present case. Bond lengths and angles are tabulated in Table I. Some non-bonded con-

tacts of interest are also shown. Ring D, the pyrrollenine ring, has a C_a-N-C_a bond angle of $105.3(6)^\circ$, while the analogous angles on the other three rings are $110.6(6)^\circ$, $108.3(6)^\circ$, and $110.8(6)^\circ$. These values correspond to those tabulated by Hoard¹⁴ for pyrrole rings respectively lacking and carrying an N-H bond in free base porphyrins.

Unlike the earlier studies, electron density peaks corresponding to the imino hydrogen atoms were found in the present case, thus confirming the localization of the hydrogen atoms. No evidence of any electron density corresponding to a hydrogen atom bonded to N(4) (Ring D) was found.

Of particular interest is the planarity of the cation. The free base of octaethylporphyrin is essentially planar. The structure of meso-tetraphenylporphyrin, H_2TPP , has been reported as planar in a triclinic crystalline modification¹⁵ and as non-planar in a tetragonal crystalline modification.¹⁶ Three structures of divalent cationic porphyrin species have been reported. In the two earlier studies, both of which involved meso-substituted porphyrins, the cations are decidedly non-planar.⁷ In these non-planar species, the symmetry of the cations may be described as S_4 . The non-planarity of these cations has been postulated as a mechanism for relieving the crowding of the imino hydrogen atoms. In a much more recent study, the H_4OEP^{2+} cation, as observed in a crystalline salt formulated as $(H_4OEP^{2+})[Rh(Cl_2)(CO)_2^-]_2$, is nearly planar.¹⁰

As in the earlier study,⁵ the monovalent H_3OEP^+ cation in the present work has three of the four pyrrole rings (A,C,D) approximately coplanar. Information on least squares planes is given in Table II.

As is normally found the individual pyrrole rings are planar. For rings A, C, and D the interplanar angles between adjacent pyrrole rings are 3.2° and 2.7° . The maximum deviation of an atom from the mean plane of these three rings is $0.07\text{\AA}$ (for C(2)). The fourth ring (B) is tilted by 8.6° from the plane of the other three rings. By way of comparison, this angle is 14° in the triiodide salt. In the current study, interplanar angles between Ring B and the adjacent rings are 7.9° and 9.8° .

It is believed that this deviation from planarity is due in part to the tight H-H contacts of the imino hydrogens. Ring B, the one which is not coplanar, bears the imino hydrogen atom which comes in closest contact with the other two imino hydrogen atoms. However this deviation from planarity is still not sufficient to relieve the tight contacts completely. In the present case, the H-H contacts are still $\sim 1.5\text{--}1.6\text{\AA}$ if we assume trigonal hybridization and a N-H bond length of $1.0\text{\AA}$. The minimum H-H non-bonded contact is usually taken to be $1.9\text{--}2.0\text{\AA}$.¹⁷

In both the $\text{H}_4\text{OEP}^{2+}$ salt¹⁰ and in the triiodide salt of H_3OEP^+ ,⁵ sp^3 hybridization of the nitrogen atoms has been postulated. Such a hybridization would be advantageous for a number of reasons. Most importantly, such a hybridization would relieve the tight H-H contacts. A second reason would be to explain the hydrogen bonding arrangement found in some of these compounds.

In the case of the $\text{H}_4\text{OEP}^{2+}$ salt,¹⁰ hydrogen bonds are postulated between the pyrrole nitrogen atoms and one of the chlorine atoms of the anion. For this to occur, the N-H bonds need to point more or less directly towards the chlorine atoms, as would be the case if there were sp^3 hybridization of the nitrogen atoms.

In the triiodide salt of H_3OEP^+ ,⁵, no hydrogen-bonding is reported. In the present case there is hydrogen bonding between the pyrrole nitrogen atoms and the water molecule of solvation. Intermolecular contacts between pyrrole nitrogen atoms and the oxygen atom of the water molecule are shown schematically in Figure 6. N...O distances are 2.97, 2.99 and $3.05\text{\AA}$ for N(1), N(2) and N(4) respectively. These are short enough to be considered hydrogen bonding distances. The fourth N..O distance (N(3)...O(7)) is $3.22\text{\AA}$, probably too long to be considered a hydrogen bond. There are also fairly short intermolecular distances between the water molecule and two of the chlorine atoms of the anion (O(7)-Cl(1) $3.43\text{\AA}$; O(7)-Cl(2), $3.46\text{\AA}$) but these are probably too long to be considered O...Cl hydrogen bonds.

At least one of the hydrogen bonds should involve an imino hydrogen atom, especially since N(4) has no hydrogen atom of its own, and yet is implicated in the hydrogen bonding scheme. The observed hydrogen atom positions would indicate that N(2) has at least some degree of sp^3 hybridization, whereas N(1) and N(3) are trigonally hybridized. H(1) and H(3) are $0.13\text{\AA}$ and $0.04\text{\AA}$ respectively out of the planes defined by the pyrrole rings to which they are bonded. The bond angles also indicate trigonal hybridization. On the other hand H(2) is $0.67\text{\AA}$ out of the plane of Ring B in the direction of the water molecule. The N(2)-H(2)...O(7) angle is 148° . The problem of tight H-H contacts is also eliminated. The three H-H contacts are now $2.62\text{\AA}$ (H(1)-H(2)); $3.00\text{\AA}$ (H(1)-H(3)); and $2.34\text{\AA}$ (H(2)-H(3)). If the hydrogen atom positions are given idealized values (assuming sp^3 hybridization for N(2), trigonal hybridization for N(1) and N(3), and a N-H bond length of $1.0\text{\AA}$) the corresponding H-H contacts are 2.22, 2.23 and $2.19\text{\AA}$.

A caveat should be observed here. The positions of hydrogen atoms are difficult to locate when heavy, highly scattering atoms such as rhenium and chlorine are present and the accuracy of these positions is quite low. The N-H observed bond lengths in this case are certainly underestimated and the angles involving H(2) differ considerably from ideal values. Thus the observed hydrogen atom positions should be viewed as merely an indication of the nature of the nitrogen atom hybridization. However, other supportive geometric evidence for the suggested hybridization is available.

The C_a-N-C_a angle in Ring B ($108.3(6)^\circ$) is considerably less than that found in Rings A and C ($110.6(6)^\circ$ and $110.8(5)^\circ$). In an N-substituted porphyrin, ethoxycarbonylmethyloctaethylporphyrin,¹⁸ the C_a-N-C_a angle is 107° on the pyrrole ring which has the substituent on the nitrogen atom. There is little doubt the nitrogen atom in this ring has sp^3 hybridization. On the other hand the angle is 110° in the ring in which the nitrogen atom is trigonally hybridized and bears a hydrogen atom.

The C_a-N bond lengths provide inconclusive evidence for this hybridization scheme. One would expect a bond length of $\sim 1.41\text{\AA}$ if sp^3 hybridization were present, as opposed to $\sim 1.38\text{\AA}$ if there were trigonal hybridization.^{4,18} The C_a-N distances are slightly longer in Ring B than in the other rings, but this difference is not statistically significant. Given the e.s.d. of $\sim 0.01\text{\AA}$ in a bond length, it is not unexpected that a difference, if there is one, cannot be observed.

The average C_a-C_b distance of $1.42(1)\text{\AA}$ is somewhat shorter than the usual $1.44\text{\AA}$, but once again it is difficult to judge the statistical significance of the difference. The C_b-C_b distances fall within

the range tabulated by Hoard.¹⁴ With the exception of the $C_a-C_m-C_a$ angles, other bond parameters in the macrocyclic skeleton agree well with those tabulated. These angles are larger than expected, especially those involving atoms in Ring B. Opening of the $C_a-C_m-C_a$ angle would further increase the distance between the hydrogen atoms. In an oxo-dipyrromethene where both pyrrole rings bear imino hydrogen atoms, the angle is 133° , presumably to relieve the close H-H contacts.¹⁹ Since Ring D does not bear an imino hydrogen atom, the need for an extension of the $C_a-C_m-C_a$ angle is eliminated and the angles involving this ring are smaller.

The values for terminal C-C bonds are unusually short. This is a common observation for octaethylporphyrin complexes and is probably due to thermal shortening. Previous experience has shown that when these bond distances are corrected for thermal motion assuming a "riding" model, more reasonable values are obtained.²⁰ However, thermal shortening does not completely explain the short C(35)-C(36) distance. This is undoubtedly short because of the unusually long C(18)-C(35) distance. No explanation for this long bond length is readily available. The large thermal ellipsoids and standard deviations for C(35) and C(36) may indicate some disorder, but attempts to resolve this possible disorder failed. This bond length was long in separate refinements using both the copper and molybdenum radiation data (see experimental section).

B. Complex Anion

The preparative, ²¹⁻²⁶ mechanistic^{27,28} and spectroscopic²⁹⁻³¹ properties of halocarbonyls of rhenium(I) have been extensively studied in the past. Four series of halocarbonyl anions of rhenium(I) have been reported: $[Re(CO)_3X_3]^{2-}$, $[Re(CO)_4X_2]^-$, $[Re_2(CO)_7X_3]^-$, and $[Re_2(CO)_6X_4]^{2-}$.^{32,33}

The structure of these anions were deduced from infrared spectroscopic data. To our knowledge anions of the type found in the present study, $[\text{Re}_2(\text{CO})_6\text{X}_3]^-$, have not been previously reported. No structural data have been reported for these anionic rhenium(I) halocarbonyls. However the structure of a closely related neutral complex has been reported. In this compound one of the bridging chlorine atoms has been replaced by a bis(di phenylarsino)methane group (abbreviated as dam). In the anion in the present work the average Re-Cl distance is $2.51(1)\text{\AA}$, the average Re-C distance is $1.88(2)\text{\AA}$, while the average C-O distance is $1.15(2)\text{\AA}$. These numbers agree well with those found in $\text{Re}_2(\text{CO})_6(\text{dam})\text{Cl}_2$ as do many of the other bond parameters.³⁵ The Re-C and C-O distances also agree with those found in $\text{TPP}[\text{Re}(\text{CO})_3]_2$.⁴ The Re(1)-Re(2) distance of $3.375(1)\text{\AA}$ is too long to postulate any sort of metal-metal interactions. None would be expected.

C. Molecular Packing

A stereoview of the packing in the unit cell is shown in Figure 7. The reason for all eight terminal carbon atoms being pointed in one direction with respect to the porphyrin ring is apparent from this figure. With this arrangement steric interactions with the porphyrin cation related by a center of symmetry are avoided. This was also observed in N-ethoxycarbonylmethyl-octaethylporphyrin.¹⁸ The interplanar separation between the cation and its centrosymmetrically related nearest neighbor is $3.4\text{\AA}$, which is the approximate layer separation in graphite. However there are no unusually close contacts between atoms in the two macrocycles. A listing of the intermolecular contacts $\leq 3.5\text{\AA}$ are given in Table III.

With the obvious exception of the hydrogen bonding distances between the cation and the water molecule, and with the possible exception of the Cl(2)-O(7) and Cl(3)-O(7) distances which, though unlikely, may correspond to weak O...Cl hydrogen-bonding distances, none of these contacts is expected to have any significant effect on the observed structure.

EXPERIMENTAL SECTION

Materials

Octaethylporphyrin, H_2OEP , was purchased from Strem Chemical Co.; Dirhenium decacarbonyl, $Re_2(CO)_{10}$, and rhenium pentacarbonyl chloride, $Re(CO)_5Cl$, were purchased from Pressure Chemical Co.; Decahydronaphthalene (decalin) was purchased from J. T. Baker Chemical Co., treated with concentrated sulfuric acid, neutralized with sodium bicarbonate solution, washed with distilled water, dried over anhydrous calcium chloride overnight, filtered, and further dried over sodium wire; finally it was distilled under vacuum and stored in a Schlenk tube under argon before use. Other organic solvents were reagent grade chemicals, dried over type 4A molecular sieve and distilled under argon before use.

Rhenium pentacarbonyl bromide, $Re(CO)_5Br$, and dimeric rhenium tetracarbonyl bromide, $[Re(CO)_4Br]_2$, were prepared by literature procedures.³⁶⁻³⁸

Physical Measurements

Elemental analyses were performed by Schwarzkopf Microanalytical Laboratory, Woodside, New York, 11377. Visible spectra were measured with a Cary 14 spectrophotometer. Infrared spectra were measured with a Beckman IR-8 spectrophotometer. Mass spectra were obtained on a CEC-21-104 mass spectrometer. Proton Magnetic resonance spectra were ob-

tained using Varian T-60 spectrometers.

Monocation Octaethylporphirium Tri- μ -chlorohexacarbonyldirhenate(I),
 $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$, (I)

A mixture of 95 mg (0.26 mmol) $Re(CO)_5Cl$ and 65.5 mg (0.13 mmol) H_2OEP was refluxed in decalin under argon. The progress of the reaction was followed by visible spectroscopy. The reaction was complete after 20 hr of refluxing. The decalin solution was then allowed to stand at room temperature. A large quantity of burgundy colored crystals were collected by centrifugation and washed with decalin and n-pentane. Finally, the crude product was recrystallized from dichloromethane/cyclohexane to give 84 mg (0.07 mmol) dark red crystals, (I), mp. 215-220°. Anal. Calcd for $Re_2C_{42}H_{47}N_4O_6Cl_3$: Re, 31.50; N, 4.74; Cl, 8.98. Found: Re, 26.25; N, 4.81; Cl, 8.91. The supernatant contained only dirhenium octaethylporphyrin complex, $OEP[Re(CO)_3]_2$, as indicated by its visible spectrum. About 55 mg (0.05 mmol) of the dirhenium octaethylporphyrin complex was isolated from the supernatant solution.

The new complex I was also prepared by heating H_2OEP and $Re(CO)_5Cl$ in a 1:1.5 mole ratio in decalin under argon for approximately 5 hr. The supernatant contained only the monorhenium octaethylporphyrin complex, $(H-OEP)Re(CO)_3$, as indicated by its visible absorption spectrum. When equimolar quantities of H_2OEP and $Re(CO)_5Cl$ were refluxed in decalin under argon for approximately 3 hr, only the monorhenium octaethylporphyrin complex was formed.

Monocation Mesoporphyrinium IX Dimethyl Ester Tri- μ -bromohexacarbonyldirhenate(I), $(H_3MPIXDME)^+[Re_2(CO)_6Br_3]^-$, (II).

The reaction was carried out in essentially the same manner as that described above, with rhenium pentacarbonyl bromide, $Re(CO)_5Br$, substi-

tuted for $\text{Re}(\text{CO})_5\text{Cl}$ as the metal source. A 120 mg sample of $\text{H}_2\text{MPIXDME}$ (0.21 mmol) and 180 mg (0.44 mmol) of $\text{Re}(\text{CO})_5\text{Br}$ in about 20 ml of decalin were heated under argon in an oil bath. The reaction was observed to proceed at a temperature of ca. 120° and the progress of the reaction was followed by visible absorption spectroscopy. A stepwise change in the absorption spectra (Figure 3) and a continuous change of color in the reaction mixture was observed. After 5 hr of heating, the decalin solution was cooled to room temperature. A large quantity of burgundy colored substance crystallized out and was collected by centrifugation, washed with decalin and n-pentane, and finally recrystallized from ethyl acetate/cyclohexane/dichloromethane to give 186 mg (0.14 mmol) dark red crystals, (II), mp $180\text{--}185^\circ$. Anal. Calcd for $\text{Re}_2\text{C}_{42}\text{H}_{43}\text{N}_4\text{O}_{10}\text{Br}_3$: C, 36.63; H, 3.13; Re, 27.10; N, 4.07; Br, 17.82. Found: C, 35.74; H, 3.26; Re, 29.74; N, 4.31; Br, 19.58. The supernatant contained only the dirhenium mesoporphyrin complex, $\text{MP}[\text{Re}(\text{CO})_3]_2$, as indicated by its visible absorption spectrum. About 75 mg (0.067 mmol) of the dirhenium mesoporphyrin complex was isolated from the supernatant solution.

Compound II can also be prepared in essentially the same manner as that described above, with dimeric rhenium tetracarbonyl bromide, $[\text{Re}(\text{CO})_4\text{Br}]_2$, substituted for $\text{Re}(\text{CO})_5\text{Br}$ as the metal source. $\text{H}_2\text{MPIXDME}$ (198 mg, 0.33 mmol) and $[\text{Re}(\text{CO})_4\text{Br}]_2$ (304 mg, 0.40 mmol) were mixed in about 20 ml of decalin and heated under argon in an oil bath. The reaction was observed to proceed at a temperature of ca. 105° and the progress of the reaction was followed by visible absorption spectroscopy.

Attempted Preparation of meso-Tetraphenylporphyrin Monocation Salt

The reaction of stoichiometric quantities of $\text{Re}(\text{CO})_5\text{Cl}$ with H_2TTP in

refluxing decalin under argon, in a manner similar to that used in preparing the salt-like complex I, resulted in a mixture of the meso-tetraphenylporphyrin dication salt, $(H_4TPP)^{++} \cdot 2Cl^-$, and the monorhenium tetraphenylporphyrin complex, $(H-TPP)Re(CO)_3$.

X-Ray Study

The crystals of I grew as parallelepipeds elongated along c and bounded by {110}. The crystal chosen for intensity measurements measured 0.23x0.34x0.44 mm. The crystal was mounted in a capillary at an arbitrary orientation,³⁹ but with the c axis approximately parallel to the spindle axis. In the capillary the crystal has remained stable for over two years.

Crystal data are listed in Table IV. Cell dimensions were determined by least squares, minimizing the differences between observed and calculated 2θ values. 24 Cu K_α ($\lambda = 1.54178\text{\AA}$) reflections, all having 2θ in the range $50-52.5^\circ$, were measured at both $+$ and $- 2\theta$. A Syntex-Datex automated diffractometer equipped with a graphite monochromator was used. The systematic absences uniquely determined the space group as $P2_1/a$.

A set of intensity data were collected on the Datex-Syntex diffractometer using Cu K_α radiation, using the $\theta-2\theta$ method. A total of 4946 independent reflections were measured out to $ca. 100^\circ$ in 2θ , the machine limit. Of these 3463 were considered observed and were used in the analysis. They were corrected for absorption effects using a Gaussian integration method.

From these data the structure was elucidated, which provided the basis for the preliminary communication.¹¹ However for a number of reasons it was decided to recollect the data using Mo K_α radiation

($\lambda = 0.71069\text{\AA}$). At the machine limit of 100° in 2θ , a large percentage of the reflections still had intensities which were considered to be observed. Collection of the data to a higher $\sin \theta/\lambda$ limit would increase the accuracy of the structural parameters. Also, the high linear absorption coefficient for Cu K_α radiation (119.5 cm^{-1}) introduces a large systematic error which an absorption correction could only approximately correct. Low order reflections are the most affected by absorption effects. It is these same reflections which contain a significant contribution from the scattering power of the hydrogen atoms. One of the hopes of this study was to locate the imino hydrogen atoms. In the presence of rhenium and chlorine atoms, which have a high scattering power, locating the hydrogen atoms would require a good set of data as free from systematic error as possible.

Therefore the data were recollected on a Syntex P2₁ diffractometer using Mo K_α radiation. The same crystal was used. Intensity data for 10,792 unique reflections, ($2\theta_{\text{max}} = 55^\circ$, $(\sin \theta/\lambda)_{\text{max}} = 0.65$) were obtained; the ω scan method was employed with a scan range of 0.6° . The scan rate varied from $2^\circ/\text{minute}$ to $12^\circ/\text{minute}$, depending on the number of counts accumulated in a rapid preliminary scan. The intensities were normalized to counts/min. Background measurements were taken at both ends of the scan with ω displaced by 0.7° from the K_α peak; each measurement was made for one-half of the scan time. The intensities of the four standard reflections were monitored after every 89 reflections. Only statistical variations were observed and no corrections were applied.

Only the 5995 reflections with $I \geq 3\sigma_I$ were used in the analysis. The standard deviation σ_I was determined in terms of the statistical

variances of the counts as $\sigma_I^2 = \sigma_I^2(\text{count}) + (0.03 F_o)^2$ where F_o is the observed structure factor and $\sigma_I^2(\text{count})$ is the standard deviation based solely on counting statistics.

Absorption corrections were made to the data using a ψ scan technique, observing the change of intensity of the $52\bar{1}$ reflection. The minimum intensity observed for this reflection was 62% of the maximum. A scan of several other reflections gave similar results. Structure factors were calculated in the usual way assuming a 50% ideally perfect-50% ideally imperfect monochromator mounted in a parallel orientation.

Determination and Refinement of the Structure

Because there are four molecules in the unit cell of space group $P2_1/a$, no crystallographic symmetry is imposed on the molecule. The positions of the rhenium atoms were found from a Patterson synthesis, using the data collected with $\text{Cu K}\alpha$ radiation. The positions of the remaining 56 non-hydrogen atoms were found from a series of difference Fourier maps. Included among these atoms was a peak attributable to a water molecule of crystallization.

Least-squares refinements using block diagonal and finally full-matrix methods were carried out. The function minimized was $\sum w(F_o - F_c)^2$ where $w = 1/\sigma_F^2$. Refinement using the $\text{Cu K}\alpha$ data was not carried beyond the stage where isotropic temperature factors were used. At this stage $R = \sum |F_o| - |F_c| / \sum F_o$ was 0.106.

Further refinement utilized the $\text{Mo K}\alpha$ data. The thermal parameters of the non-hydrogen atoms were refined anisotropically. The large number of parameters required refining the formula unit in blocks, alternately refining the anion and then the cation and water molecule.

After several cycles of refinement, ΔF syntheses were calculated in an effort to locate hydrogen atoms. The three imino hydrogen atoms were thus found. However many of the hydrogens on the peripheral atoms were not located or were in chemically unreasonable positions. The positional parameters of the imino hydrogen atoms were refined. The thermal parameters for these three atoms were not refined, but were set as $B = 4.0\text{\AA}^2$, as was the case for all hydrogen atoms. Idealized positions for the other hydrogen atoms were calculated except for those on the water molecule. A C-H bond length of $1.0\text{\AA}$ and a staggered configuration for the methyl hydrogens was assumed. The contributions from these were added to the calculated structure factors but the positions were not refined. However, before the final cycles of refinement, new positions were calculated and used. The refinement converged with $R = 0.046$ and $R_w = \sum w ||F_o| - |F_c|| / \sum w F_o^2 = 0.047$. The final value of the standard deviation of an observation of unit weight, defined as $[\sum w ||F_o| - |F_c||^2 / (N_o - N_v)]^{1/2}$ was 1.72 for $N_o = 5995$ reflections and $N_v = 532$ variables. In the last cycle of refinement all shifts were considerably less than one standard deviation. There were five peaks on the final difference Fourier which were above $1\text{ e/\AA}^3$. These were all close to the rhenium atoms. Neither they nor any other peak in the final difference Fourier were believed to have any physical significance.

Correction for anomalous dispersion were made for all non-hydrogen atoms.⁴⁰ Scattering factors were from Ref. 41. The rhenium and chlorine atoms were assumed to be in the zero ionization state. No evidence of secondary extinction was found.

The structure was solved and the initial refinement performed on

the IBM 360/65 and its successor at Texas A&M, the Amdahl 470 v/6. Most of the programs used have been listed elsewhere.^{42,43} In addition the data collection and data reduction programs used for the molybdenum data are those supplied by Syntex Analytical Instruments. Most of the final refinements and calculations were performed on a PDP 11/40 computer using the Enraf-Nonius Structure Determination Package (SDP).

The final positional and thermal parameters for the non-hydrogen atoms and the three imino hydrogen atoms are given in Table V. The final calculated positions of the other hydrogen atoms are given in Table VI. Tables VII and VIII contain the root-mean-square-components of thermal displacement along the principal axes of the thermal ellipsoids and the observed and calculated structure factors respectively. Tables VI-VIII are available as supplementary material.

Acknowledgement. The authors wish to thank Professor Shinzi Kato for many helpful and stimulating discussions. We wish to acknowledge support of this research project by the Office of Naval Research, the Robert A. Welch Foundation, (A-328), and the Texas Agricultural Experiment Station (H-1668). In the later phases support was also given by the National Institutes of Health (AM20051) and the National Science Foundation (CHE76-15557).

Supplementary Material Available: Table VI-VIII containing the calculated hydrogen atom positions, the root-mean-square components along the principal axes of the thermal ellipsoids, and observed and calculated structure factors. Ordering information is given on any current masthead page.

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TABLE I

Bond Lengths (Å) and Angles (deg)^a

A. Cation

N(1) -C(1)	1.377(9)	C(1) -N(1) -C(4)	110.6(6)
N(1) -C(4)	1.351(9)	C(6) -N(2) -C(9)	108.3(6)
N(2) -C(6)	1.382(8)	C(11) -N(3) -C(14)	110.8(5)
N(2) -C(9)	1.391(8)	C(16) -N(4) -C(19)	105.3(6)
N(3) -C(11)	1.378(8)	N(1) -C(1) -C(2)	106.4(6)
N(3) -C(14)	1.363(8)	N(1) -C(1) -C(20)	125.3(6)
N(4) -C(16)	1.367(8)	C(2) -C(1) -C(20)	128.2(6)
N(4) -C(19)	1.364(8)	C(1) -C(2) -C(3)	107.9(6)
C(1) -C(2)	1.406(9)	C(1) -C(2) -C(21)	124.6(7)
C(1) -C(20)	1.366(10)	C(3) -C(2) -C(21)	127.5(7)
C(2) -C(3)	1.381(9)	C(2) -C(3) -C(4)	107.7(6)
C(2) -C(21)	1.496(9)	C(2) -C(3) -C(23)	126.3(6)
C(3) -C(4)	1.407(9)	C(4) -C(3) -C(23)	126.0(6)
C(3) -C(23)	1.504(10)	N(1) -C(4) -C(3)	107.2(6)
C(4) -C(5)	1.391(9)	N(1) -C(4) -C(5)	124.6(6)
C(5) -C(6)	1.381(9)	C(3) -C(4) -C(5)	128.1(7)
C(6) -C(7)	1.417(9)	C(4) -C(5) -C(6)	131.3(6)
C(7) -C(8)	1.348(9)	N(2) -C(6) -C(5)	123.3(6)
C(7) -C(25)	1.523(10)	N(2) -C(6) -C(7)	107.4(6)
C(8) -C(9)	1.410(9)	C(5) -C(6) -C(7)	128.8(6)
C(8) -C(27)	1.516(9)	C(6) -C(7) -C(8)	108.2(6)
C(9) -C(10)	1.381(9)	C(6) -C(7) -C(25)	123.8(6)
C(10) -C(11)	1.352(9)	C(8) -C(7) -C(25)	128.0(6)
C(11) -C(12)	1.435(9)	C(7) -C(8) -C(9)	108.8(6)
C(12) -C(13)	1.358(9)	C(7) -C(8) -C(27)	127.6(6)
C(12) -C(29)	1.520(9)	C(9) -C(8) -C(27)	123.6(6)
C(13) -C(14)	1.421(8)	N(2) -C(9) -C(8)	107.1(6)
C(13) -C(31)	1.520(9)	N(2) -C(9) -C(10)	123.5(6)
C(14) -C(15)	1.392(9)	C(8) -C(9) -C(10)	129.2(6)
C(15) -C(16)	1.392(9)	C(9) -C(10) -C(11)	130.0(6)
C(16) -C(17)	1.425(9)	N(3) -C(11) -C(10)	125.6(6)
C(17) -C(18)	1.341(10)	N(3) -C(11) -C(12)	105.5(6)
C(17) -C(33)	1.495(10)	C(10) -C(11) -C(12)	129.0(6)
C(18) -C(19)	1.419(10)	C(11) -C(12) -C(13)	108.7(6)
C(18) -C(35)	1.698(20)	C(11) -C(12) -C(29)	123.3(6)
C(19) -C(20)	1.407(10)	C(13) -C(12) -C(29)	127.9(6)
C(21) -C(22)	1.458(13)	C(12) -C(13) -C(14)	107.9(6)
		C(12) -C(13) -C(31)	128.3(6)
C(23) -C(24)	1.467(12)	C(14) -C(13) -C(31)	123.6(6)
		N(3) -C(14) -C(13)	107.1(6)
C(25) -C(26)	1.449(12)	N(3) -C(14) -C(15)	125.2(6)
		C(13) -C(14) -C(15)	127.7(6)
C(27) -C(28)	1.480(13)	C(14) -C(15) -C(16)	129.0(6)
		N(4) -C(16) -C(15)	124.1(6)
C(29) -C(30)	1.486(11)	N(4) -C(16) -C(17)	110.8(6)

C(31)-C(32)	1.472(10)	C(15)-C(16)-C(17)	125.1(6)
C(33)-C(34)	1.472(12)	C(16)-C(17)-C(18)	105.9(6)
C(35)-C(36)	1.262(18)	C(16)-C(17)-C(33)	125.3(6)
N(1) -H(1)	0.62(7)	C(18)-C(17)-C(33)	128.7(7)
N(2) -H(2)	0.84(7)	C(17)-C(18)-C(19)	108.1(6)
N(3) -H(3)	0.62(8)	C(17)-C(18)-C(35)	127.4(7)
N(1) -N(2)	3.002(9)	C(19)-C(18)-C(35)	122.7(18)
N(1) -N(4)	2.908(9)	N(4) -C(19)-C(18)	109.9(6)
N(2) -N(3)	2.940(9)	N(4) -C(19)-C(20)	125.2(7)
N(3) -N(4)	2.945(9)	C(18)-C(19)-C(20)	124.7(7)
N(1) -N(3)	4.226(8)	C(1) -C(20)-C(19)	127.2(7)
N(2) -N(4)	4.113(9)	C(2) -C(21)-C(22)	112.5(8)
C(5)-C(15)	6.782(10)	C(3) -C(23)-C(24)	114.3(7)
C(10)-C(20)	6.883(10)	C(7) -C(25)-C(26)	113.4(8)
		C(8) -C(27)-C(28)	112.0(7)
		C(12)-C(29)-C(30)	113.3(6)
		C(13)-C(31)-C(32)	113.8(6)
		C(17)-C(33)-C(34)	110.8(7)
		C(18)-C(35)-C(36)	93.4(15)
		C(1) -N(1) -H(1)	124 (8)
		C(4) -N(1) -H(1)	124 (8)
		C(6) -N(2) -H(2)	118 (5)
		C(9) -N(2) -H(2)	98 (5)
		C(11)-N(3)-H(3)	124 (9)
		C(14)-N(3) H(3)	125 (9)

B. Anion

Re(1)-Cl(1)	2.517(2)	Cl(1)-Re(1)-Cl(2)	79.06(5)
Re(1)-Cl(2)	2.501(2)	Cl(1)-Re(1)-Cl(3)	79.87(6)
Re(1)-Cl(3)	2.493(2)	Cl(1)-Re(1)-C(37)	171.0(2)
Re(1)-C(37)	1.889(8)	Cl(1)-Re(1)-C(38)	95.6(3)
Re(1)-C(38)	1.852(10)	Cl(1)-Re(1)-C(39)	97.1(2)
Re(1)-C(39)	1.877(8)	Cl(2)-Re(1)-C(37)	94.6(2)
Re(2)-Cl(1)	2.530(2)	Cl(2)-Re(1)-C(38)	93.8(2)
Re(2)-Cl(2)	2.509(2)	Cl(2)-Re(1)-C(39)	175.1(2)
Re(2)-Cl(3)	2.501(2)	Cl(3)-Re(1)-C(37)	92.9(2)
Re(2)-C(40)	1.091(9)	Cl(3)-Re(1)-C(38)	173.4(3)
Re(2)-C(41)	1.897(9)	Cl(3)-Re(1)-C(39)	95.7(2)
Re(2)-C(42)	1.867(9)	C(37)-Re(1)-C(38)	91.2(3)
C(37)-O(1)	1.142(8)	C(37)-Re(1)-C(39)	88.9(3)
C(38)-O(2)	1.191(9)	C(38)-Re(1)-C(39)	89.5(3)
C(39)-O(3)	1.138(8)	Cl(1)-Re(2)-Cl(2)	76.68(5)
C(40)-O(4)	1.158(9)	Cl(1)-Re(2)-Cl(3)	79.47(6)
C(41)-O(5)	1.125(8)	Cl(1)-Re(2)-C(40)	96.57(2)
C(41)-O(6)	1.159(9)	Cl(1)-Re(2)-C(41)	170.9(2)
Re(1)-Re(2)	3.375(1)	Cl(1)-Re(2)-C(42)	97.5(3)
		Cl(2)-Re(2)-Cl(3)	80.37(6)
		Cl(2)-Re(2)-C(40)	174.8(2)
		Cl(2)-Re(2)-C(41)	95.6(2)
		Cl(2)-Re(2)-C(42)	93.9(3)

C1(3)-Re(2)-C(40)	96.8(3)
C1(3)-Re(2)-C(41)	92.7(2)
C1(3)-Re(2)-C(42)	173.9(3)
C(40)-Re(2)-C(41)	88.9(3)
C(40)-Re(2)-C(42)	88.7(4)
C(41)-Re(2)-C(42)	89.9(3)
Re(1)-C1(1)-Re(2)	83.93(6)
Re(1)-C1(2)-Re(2)	84.70(6)
Re(1)-C1(3)-Re(2)	85.02(6)
Re(1)-C(37)-O(1)	177.7(7)
Re(1)-C(38)-O(2)	177.8(8)
Re(1)-C(39)-O(3)	179.2(7)
Re(2)-C(40)-O(4)	179.1(8)
Re(2)-C(41)-O(5)	177.5(8)
Re(2)-C(42)-O(6)	178.7(8)

^a Some nonbonded distances of interest are also given. Asterisks indicate corrections for thermal motion.

TABLE II

Least Squares Planes

A. Deviations (A) From Planes

	Plane 1	Plane 2	Plane 3	Plane 4	Plane 5	Plane 6	Plane 7
N(1)	0.007	-0.027	-0.008	-0.003	-0.298	0.106	0.102
N(2)	0.127	0.027	0.092	0.208	-0.009	0.095	0.183
N(3)	-0.013	-0.027	-0.024	0.109	-0.504	-0.002	0.016
N(4)	-0.024	0.027	-0.015	0.009	-0.677	0.117	0.013
C(1)	0.040	0.044	0.036	-0.008	-0.373	0.203	0.148
C(2)	0.102	0.082	0.091	0.016	-0.196	0.273	0.243
C(3)	0.050	-0.020	0.026	-0.018	-0.072	0.165	0.199
C(4)	0.035	-0.043	0.008	0.014	-0.094	0.105	0.154
C(5)	-0.107	-0.226	-0.147	-0.100	-0.111	-0.096	0.006
C(6)	0.002	-0.133	-0.042	0.057	0.018	-0.040	0.088
C(7)	-0.189	-0.371	-0.247	-0.105	-0.022	-0.295	-0.107
C(8)	-0.091	-0.266	-0.147	0.036	0.017	-0.225	-0.039
C(9)	0.078	-0.047	0.035	0.204	-0.005	-0.011	0.112
C(10)	0.094	-0.007	0.058	0.255	-0.108	-0.001	0.095
C(11)	0.052	0.001	0.030	0.213	-0.331	0.000	0.036
C(12)	0.060	0.034	0.045	0.258	-0.444	0.001	0.011
C(13)	0.009	0.024	0.000	0.183	-0.674	-0.002	-0.055
C(14)	-0.041	-0.009	-0.038	0.094	-0.708	0.002	-0.067
C(15)	-0.049	0.027	-0.035	0.054	-0.860	0.057	-0.071
C(16)	-0.023	0.064	-0.004	0.034	-0.830	0.130	-0.016
C(17)	0.004	0.139	0.036	0.033	-0.958	0.221	0.013
C(18)	-0.046	0.082	-0.016	-0.059	-0.946	0.198	-0.005
C(19)	-0.062	0.014	-0.046	-0.073	-0.771	0.135	-0.004
C(20)	-0.007	0.047	0.003	-0.055	-0.603	0.200	0.084
O(7)	2.254	2.228	2.241	2.304	1.844	2.311	2.304

B. Angles (deg) between Least-Squares Planes

	Plane 2	Plane 3	Plane 4	Plane 5	Plane 6	Plane 7
Plane 1	2.1	0.6	1.9	7.7	2.7	1.4
Plane 2		1.5	3.2	9.8	1.5	2.9
Plane 3			2.2	8.3	2.2	1.7
Plane 4				7.9	4.3	3.2
Plane 5					9.8	7.1
Plane 6						2.7

C. Equations of Planes^a

Plane 1 Macrocycle: N(1)-N(4), C(1)-C(20)

$$11.711x + 12.286y - 8.909z = -2.725$$

Plane 2 N(1)-N(4)

$$11.992x + 11.703y - 9.197z = -2.854$$

Plane 3 N(1), N(3), N(4), C(1)-C(5), C(10)-C(20)

$$11.796x + 12.121y - 8.990z = -2.755$$

Plane 4 Ring A: N(1), C(1)-C(4)

$$11.274x + 12.454y - 9.063z = -2.909$$

Plane 5 Ring B: N(2), C(6)-C(9)

$$10.883x + 14.155y - 7.604z = -1.625$$

Plane 6 Ring C: N(3), C(11)-C(14)

$$12.296x + 11.627y - 9.032z = -2.812$$

Plane 7 Ring D: N(4), C(16)-C(19)

$$11.899x + 12.36y - 8.693z = -2.628$$

^a All planes are unweighted. x, y, z are in monoclinic fractional coordinates.

TABLE III

Intermolecular Contacts ($\text{\AA}$) $\leq 3.5\text{\AA}$

C1(2)-O(7)	3.43	O(1) -C(33) ^a	3.47
C1(3)-O(7)	3.47	O(1) -C(34) ^a	3.20
C(38)-O(7)	3.46	C(5) -C(31) ^b	3.45
N(1) -O(7)	2.97*	C(27)-C(33) ^b	3.47
N(2) -O(7)	2.99*	O(1) -C(24) ^c	3.30
N(3) -O(7)	3.22	O(2) -O(4) ^d	3.09
N(4) -O(7)	3.05*	O(3) -C(21) ^e	3.38
O(2) -C(10)	3.19		
O(2) -C(11)	3.24		
O(6) -C(36)	3.42		

Superscripts denote the following equivalent positions relative to positions given in Table V. No superscript indicates only the identity transformation has been made. Asterisks indicate hydrogen-bonding distances.

- a $-x, -y, -z$
- b $-x, -y, 1-z$
- c $-\frac{1}{2}+x, \frac{1}{2}-y, -1+z$
- d $-\frac{1}{2}+x, \frac{1}{2}-y, z$
- e $\frac{1}{2}-x, \frac{1}{2}+y, -1+z$

TABLE IV

Crystal Data for $(C_{36}H_{47}N_4)^+[Re_2(CO)_6Cl_3]^- \cdot H_2O^a$

$a = 18.140(3)\text{\AA}$	F.W. = 1200.6
$b = 19.847(3)\text{\AA}$	$Z = 4$
$c = 13.625(2)\text{\AA}$	$d_{\text{calcd}} = 1.75 \text{ g/cm}^3$
$\beta = 111.64(2)$	$\mu = 58.4 \text{ cm}^{-1}(\text{Mo K}_{\alpha} \text{ radiation})$
$V = 4559\text{\AA}^3$	

SYSTEMATIC ABSENCES: $h0\ell(h \text{ odd}); 0k0(k \text{ odd})$

SPACE GROUP: $P2_1/a$

^a Estimated standard deviation of least significant figures shown in parentheses

Table V
Fractional Coordinates and Thermal Motion Parameters Derived from the
Least-Squares Refinement^a

^aIn this and subsequent tables estimated standard deviations for the least significant figure are in parentheses. The Debye-Waller factor is defined as $T = \exp[-2\pi^2(U_{11}a^2h^2 + U_{22}b^2k^2 + U_{33}c^2l^2 + U_{12}a^*b^*hk + U_{13}a^*c^*hl + U_{23}b^*c^*kl)]$.

The values for U have been multiplied by 10^3 , except for those of Re which have been multiplied by 10^4 . For those atoms refined isotropically, the values for B (multiplied by a factor of 10) are given in the column labeled U_{11} . Isotropic temperature factors are defined by $T = \exp[-B(\sin^2\theta)/\lambda^2]$.

ATOM	X	Y	Z	U(11)	U(22)	U(33)	U(12)	U(13)	U(23)
26(1)	0.12959(1)	0.19511(1)	0.16057(2)	475(1)	517(1)	626(1)	-46(3)	299(2)	-21(3)
26(2)	0.29152(2)	0.21982(1)	0.21982(2)	486(1)	524(1)	542(1)	-21(3)	155(2)	-99(3)
26(3)	0.2647(1)	0.2022(1)	0.3048(1)	51(1)	52(1)	57(1)	-17(1)	22(1)	-21(1)
26(4)	0.1520(1)	0.0741(1)	0.2135(1)	56(1)	40(1)	61(1)	-19(1)	31(1)	-6(1)
26(5)	0.2147(1)	0.1435(1)	0.0594(1)	56(1)	64(1)	52(1)	2(2)	35(1)	-2(2)
26(6)	0.2250(3)	0.0576(3)	0.6760(5)	37(3)	69(4)	60(4)	17(6)	-13(4)	-13(7)
26(7)	0.0901(3)	0.1398(3)	0.5997(4)	42(3)	95(4)	39(3)	15(6)	25(4)	-13(6)
26(8)	0.0159(3)	0.0529(3)	0.4024(4)	38(3)	64(4)	40(3)	-8(6)	5(5)	-7(6)
26(9)	0.1677(3)	-0.0275(3)	0.4853(5)	48(3)	43(3)	63(4)	9(6)	0(7)	-4(8)
26(10)	0.2488(4)	0.0107(4)	0.6951(6)	38(4)	63(3)	60(5)	18(8)	-8(7)	-7(8)
26(11)	0.3459(4)	0.0700(4)	0.7918(5)	32(3)	61(5)	65(5)	3(7)	4(7)	-17(8)
26(12)	0.3154(4)	0.0821(4)	0.8307(6)	37(3)	56(4)	46(4)	-20(7)	-2(6)	-17(8)
26(13)	0.2412(4)	0.0997(4)	0.7552(6)	52(4)	59(5)	49(4)	6(8)	24(6)	-4(8)
26(14)	0.1809(4)	0.1490(4)	0.7598(6)	47(4)	75(5)	43(4)	12(8)	10(6)	-17(8)
26(15)	0.1155(4)	0.1676(4)	0.6889(6)	45(4)	76(5)	49(4)	28(8)	24(6)	-6(8)
26(16)	0.0509(4)	0.2144(4)	0.7029(6)	52(4)	78(5)	56(4)	33(8)	24(6)	-2(8)
26(17)	-0.0020(4)	0.2174(4)	0.4121(6)	-7(4)	68(5)	57(4)	33(8)	30(6)	-2(8)
26(18)	-0.0065(4)	0.1702(4)	0.5404(6)	35(3)	40(5)	44(4)	27(8)	26(6)	13(8)
26(19)	-0.0047(4)	0.1512(4)	0.4424(6)	34(3)	71(5)	44(4)	25(7)	10(6)	0(8)
26(20)	-0.0027(4)	0.0403(4)	0.3756(6)	35(3)	60(4)	52(4)	13(7)	20(6)	4(8)
26(21)	-0.0020(4)	0.0097(4)	0.2782(5)	34(3)	67(5)	44(4)	11(7)	15(6)	0(7)
26(22)	-0.0020(4)	0.0244(4)	0.2442(5)	34(3)	55(4)	46(4)	-10(7)	16(6)	4(7)
26(23)	0.0015(4)	0.0077(3)	0.3225(5)	34(3)	49(4)	45(4)	0(7)	14(6)	0(7)
26(24)	0.0521(4)	-0.0445(4)	0.3189(6)	49(4)	44(4)	51(4)	-13(7)	11(7)	1(7)
26(25)	0.1271(4)	-0.0607(3)	0.3919(6)	43(4)	42(4)	62(4)	0(7)	17(7)	-3(7)
26(26)	0.1174(5)	-0.1134(4)	0.3400(7)	52(4)	57(4)	77(5)	39(8)	-10(8)	-29(9)
26(27)	0.2404(5)	-0.1141(4)	0.4455(8)	45(5)	64(5)	111(7)	71(9)	-52(11)	-57(10)
26(28)	0.2328(5)	-0.0411(4)	0.5247(7)	60(5)	67(5)	78(6)	37(9)	-4(9)	-29(9)
26(29)	0.2916(5)	-0.0421(4)	0.6216(7)	49(4)	74(6)	81(6)	54(8)	-19(9)	-25(10)
26(30)	0.4371(5)	-0.0017(5)	0.8404(7)	52(5)	74(6)	90(6)	13(10)	-21(9)	-22(11)
26(31)	0.4867(6)	0.0320(7)	0.8082(13)	50(5)	110(9)	254(15)	28(13)	58(15)	-1(22)
26(32)	0.4867(6)	0.0320(7)	0.5736(7)	62(5)	97(7)	65(5)	41(10)	28(8)	7(10)
26(33)	0.3916(7)	0.1144(6)	0.9233(10)	89(6)	102(8)	115(9)	-36(14)	-17(15)	-24(15)
26(34)	0.0749(7)	0.2522(5)	0.8054(7)	55(5)	36(6)	75(5)	15(10)	22(8)	4(11)
26(35)	0.1275(6)	0.3095(6)	0.8207(9)	92(7)	92(7)	118(8)	11(13)	37(13)	-1(13)
26(36)	-0.0751(5)	0.2625(1)	0.6872(7)	61(5)	90(6)	68(5)	27(9)	24(8)	-24(9)
26(37)	-0.0674(7)	0.3295(6)	0.5441(9)	32(7)	102(9)	102(9)	60(13)	-12(14)	9(14)
26(38)	-0.1749(4)	0.1205(5)	0.2196(6)	67(5)	30(6)	30(6)	74(10)	38(9)	57(11)
26(39)	-0.1544(5)	0.1702(5)	0.1441(6)	41(4)	67(5)	63(4)	-15(8)	8(7)	1(9)
26(40)	-0.1004(3)	-0.0116(4)	0.1401(6)	43(5)	62(5)	61(5)	-38(10)	37(8)	-23(10)
26(41)	-0.0744(5)	0.0064(5)	0.0620(6)	61(5)	63(5)	63(4)	20(9)	4(11)	-6(12)
26(42)	0.1506(5)	-0.1551(4)	0.2825(8)	51(6)	99(6)	103(7)	23(11)	4(11)	-39(12)
26(43)	0.1911(6)	-0.1190(5)	0.3052(8)	163(10)	217(13)	91(7)	-190(19)	58(14)	-39(12)
26(44)	0.3077(8)	-0.1774(8)	0.5156(9)	246(15)	115(11)	134(9)	4(22)	170(17)	17(17)
26(45)	0.7570(10)	-0.1500(7)	0.4439(11)	54(4)	67(5)	70(5)	-3(8)	31(7)	14(9)
26(46)	0.0747(4)	0.1781(4)	0.0446(6)	95(4)	53(5)	69(5)	-59(9)	29(9)	-1(9)
26(47)	0.0724(5)	0.2119(4)	0.2474(7)	45(3)	64(5)	103(5)	25(8)	62(7)	-7(9)
26(48)	0.1205(4)	0.2466(4)	0.1224(7)	55(4)	60(5)	38(6)	9(9)	22(5)	-34(10)
26(49)	0.2062(5)	0.1217(4)	0.2252(7)	49(4)	59(5)	43(5)	-11(8)	7(8)	-28(9)
26(50)	0.2064(4)	0.0201(4)	0.1386(7)	75(6)	56(5)	49(5)	-14(10)	5(7)	-9(10)
26(51)	0.3401(4)	0.0369(4)	0.3434(9)	61(4)	107(5)	107(5)	-34(8)	-16(9)	18(9)
26(52)	-0.0212(1)	0.1670(3)	-0.0272(6)	10(3)	104(5)	118(4)	3(7)	142(8)	-5(8)
26(53)	0.0754(3)	0.2237(3)	0.3005(5)	103(4)	53(5)	154(5)	32(7)	47(8)	25(8)
26(54)	0.1544(3)	0.3419(3)	0.0947(5)	50(3)	113(5)	163(6)	-44(7)	49(7)	-54(10)
26(55)	0.4561(3)	0.1777(4)	0.2273(6)	45(4)	73(4)	121(4)	1(7)	52(6)	-82(7)
26(56)	0.2007(3)	-0.0237(3)	0.0477(5)	140(7)	99(5)	104(5)	24(11)	-36(10)	61(9)
26(57)	0.3707(5)	0.0150(6)	0.4191(6)	79(7)	79(4)	31(7)	-2(6)	73(5)	0(6)
26(58)	0.1847(3)	0.1214(3)	0.4704(4)	40					
26(59)	0.197(3)	0.042(3)	0.642(4)	40					
26(60)	0.100(3)	0.140(3)	0.544(4)	40					
26(61)	0.046(3)	0.052(3)	0.445(4)	40					

CAPTIONS FOR FIGURES

Figure 1. Visible Spectra of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$ and $(H_4OEP)^{++}2Cl^-$.

Figure 2. Thermal Decomposition of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$ to Form $OEP[Re(CO)_3]_2$ in Refluxing Decalin.

Figure 3. Repeated Scan Spectrophotometry Showing Progress of the Formation of $(H-MP)Re(CO)_3$, $MP[Re(CO)_3]_2$ and $(H_3MPIXDME)^+[Re_2(CO)_6Br_3]^-$.

Figure 4. a. ORTEP¹³ drawing of the porphyrin cation, H_3OEP^+ . Numbering scheme is shown. Shown in parentheses are the designations for the various types of carbon atoms. The thermal ellipsoids are drawn for 50% probability, except those of the hydrogen atoms which are not drawn to scale. H(21) and H(40) are hidden behind C(26) and C(34) respectively.

b. ORTEP Drawing of the complex anion.

Figure 5. A stereoview of the formula unit of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^- \cdot H_2O$. The water of crystallization is illustrated by a large circle. Imino hydrogen atoms are indicated by small circles. Other hydrogen atoms have been omitted. The notation of the pyrrole rings is shown. Note the tilt of Ring B with respect to the macrocycle.

Figure 6. Schematic drawing showing the significant contacts between the porphyrins cation and the oxygen atom of the water of crystallization. The lines between nitrogen atoms signify the planes of the macrocycle. Of the hydrogen atoms shown, it is believed that only H(2) is involved in hydrogen-bonding. This is indicated by a solid line between H(2) and O(7). The N(2)-H(2)-O(7) bond angle is also shown.

Figure 7. Steroview of the packing in the unit cell. Circles of increasing size represent rhenium, chlorine and oxygen atoms respectively.

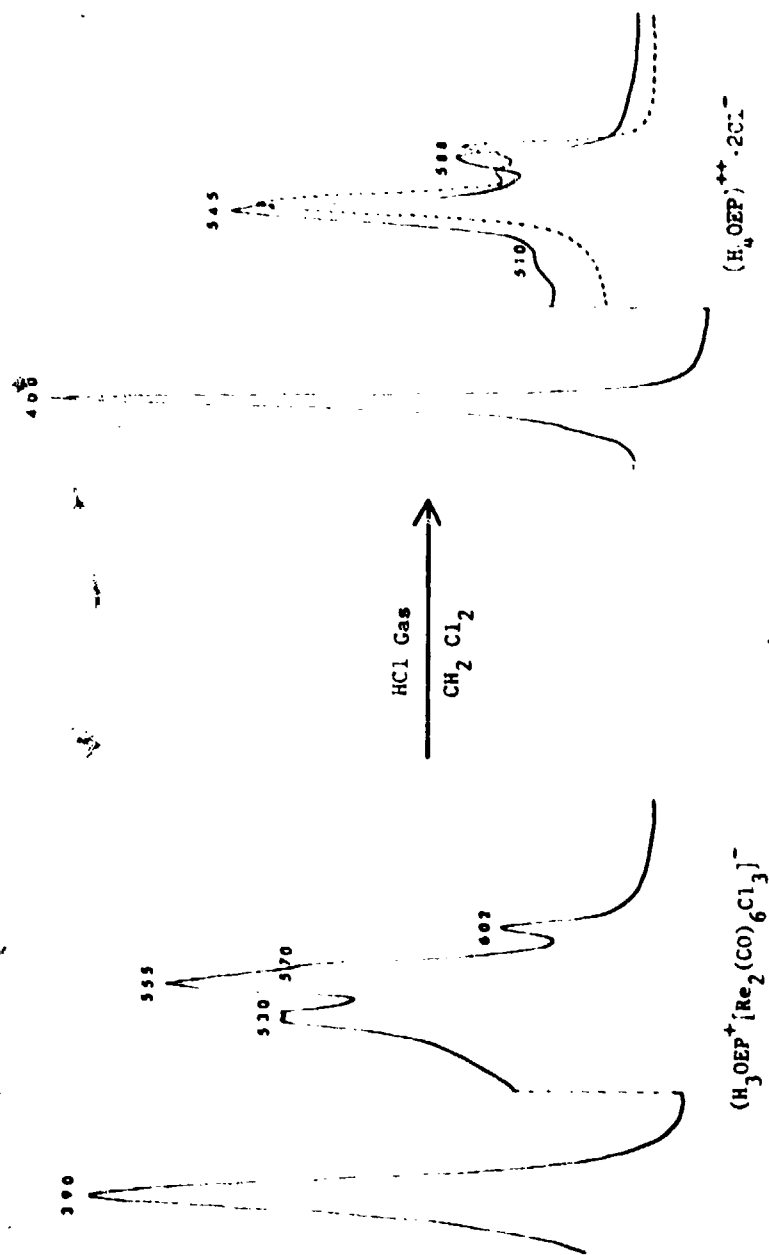


Figure 1. Visible Spectra of $(\text{H}_3\text{OEP})^+[\text{Re}_2(\text{CO})_6\text{Cl}_3]^-$ and $(\text{H}_4\text{OEP})^{++}2\text{Cl}^-$.

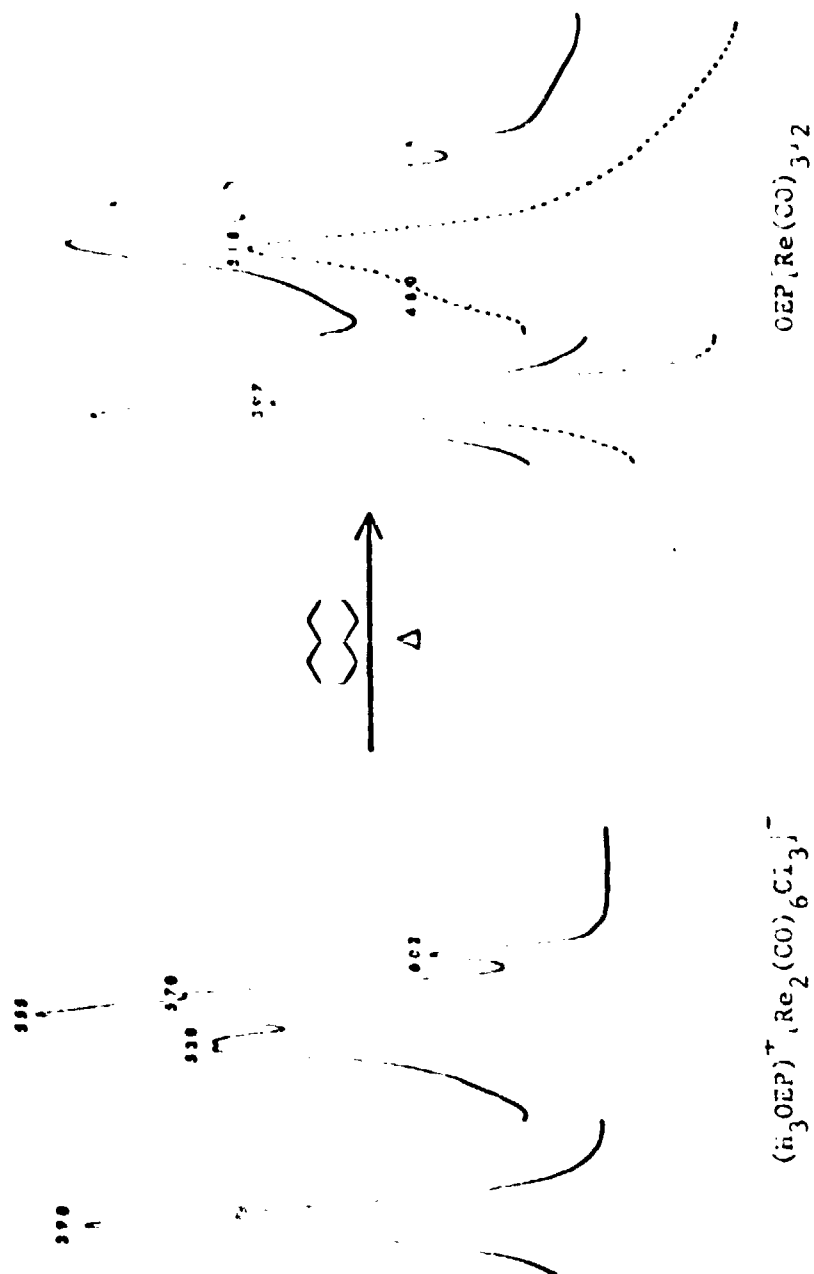


Figure 2. Thermal Decomposition of $(n_3OEP)^+ [Re_2(CO)_6Cl_3]^-$ to Form $OEP[Re(CO)_3]_2$ in Refluxing Decalin.

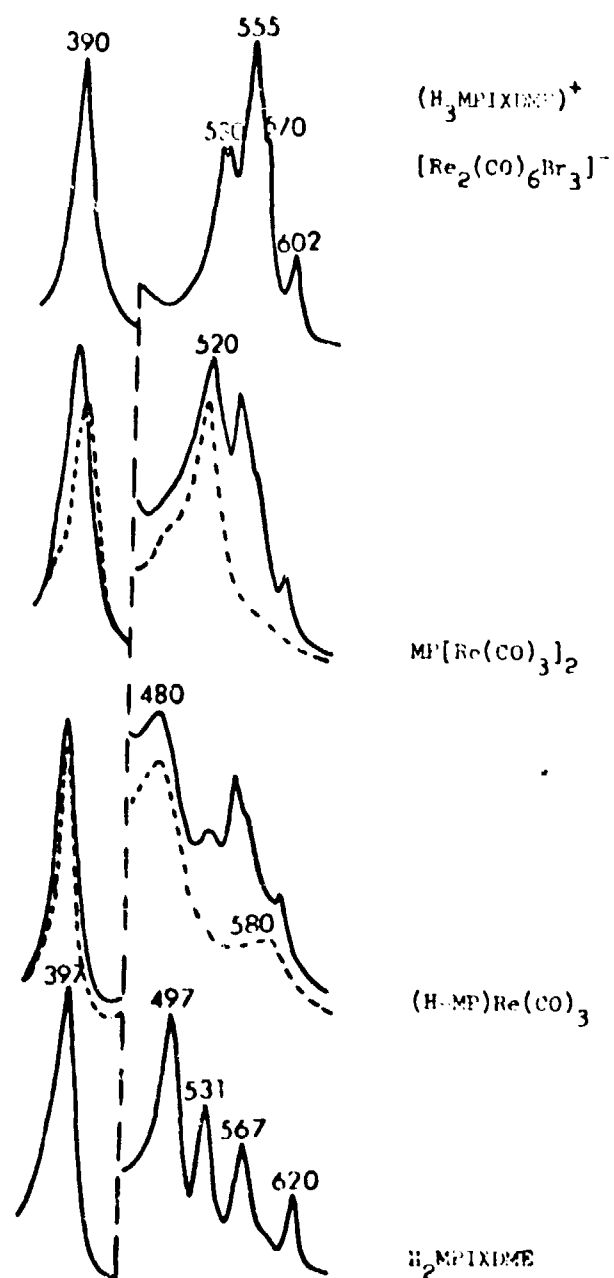


Figure 3. Repeated Scan Spectrophotometry Showing Progress of the Formation of $(H-MP)Re(CO)_3$, $MP[Re(CO)_3]_2$, and $(H_3MP)IXDME^+[Re(CO)_6Br_3]^-$.

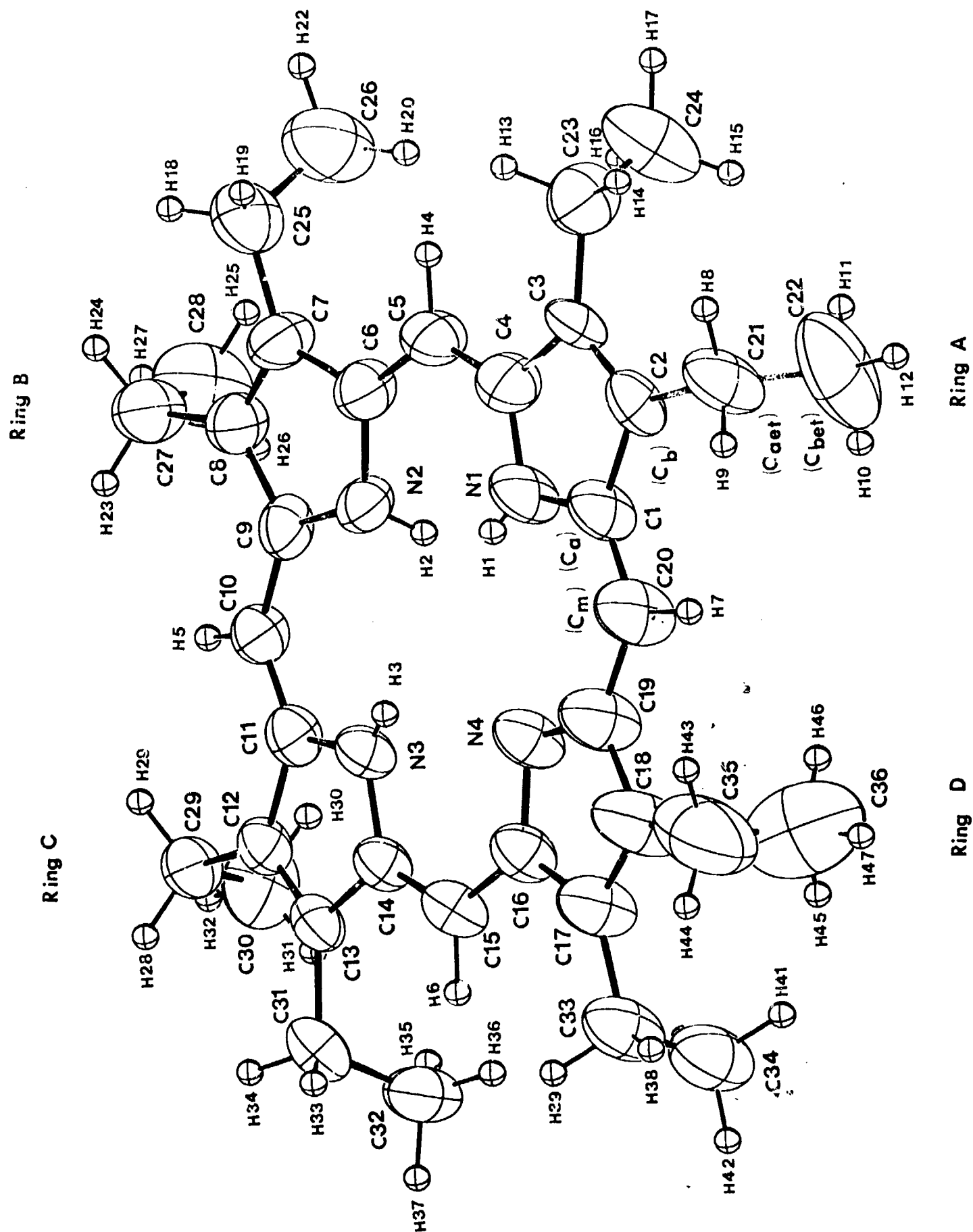


Figure 4A

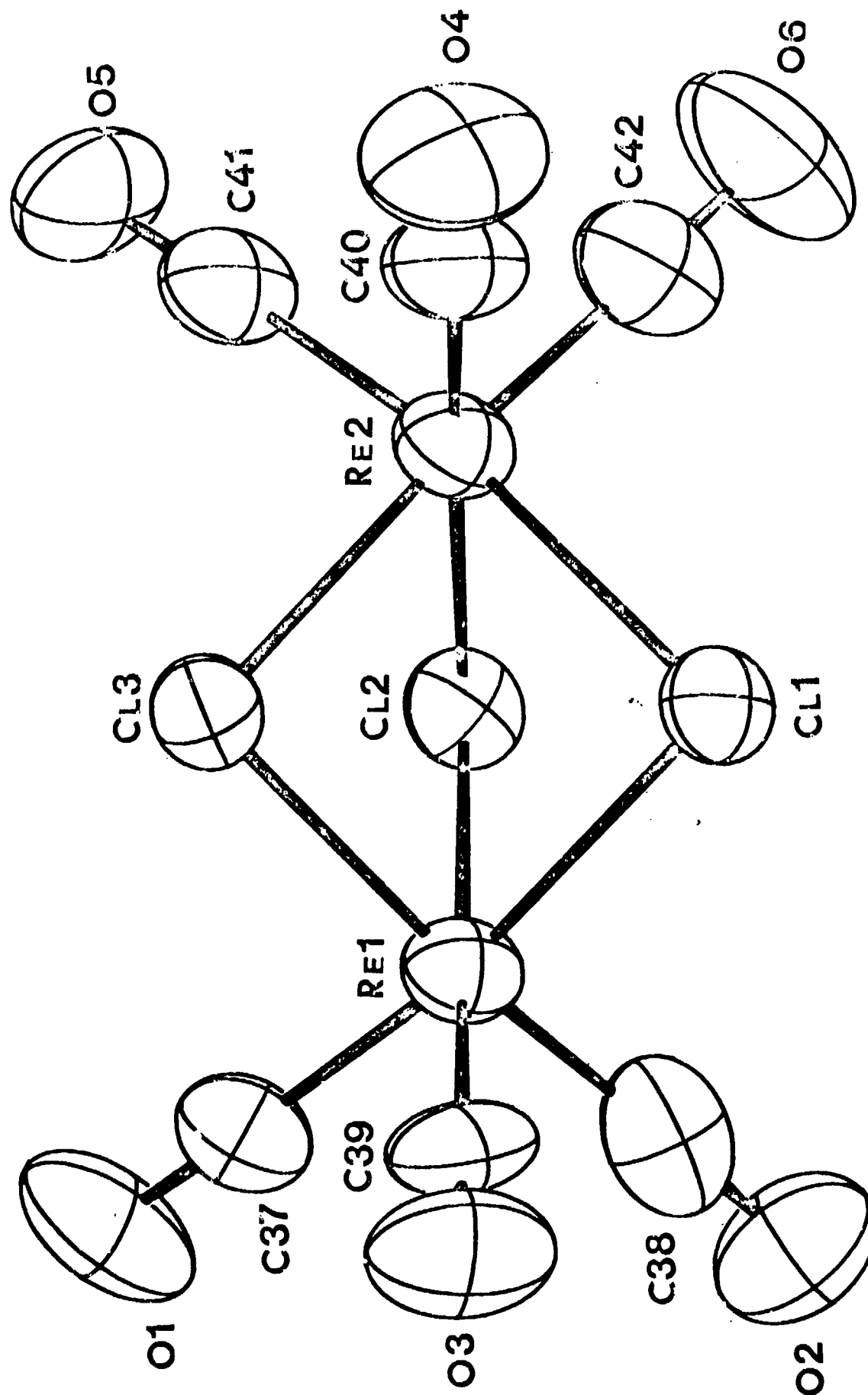


Figure 4B

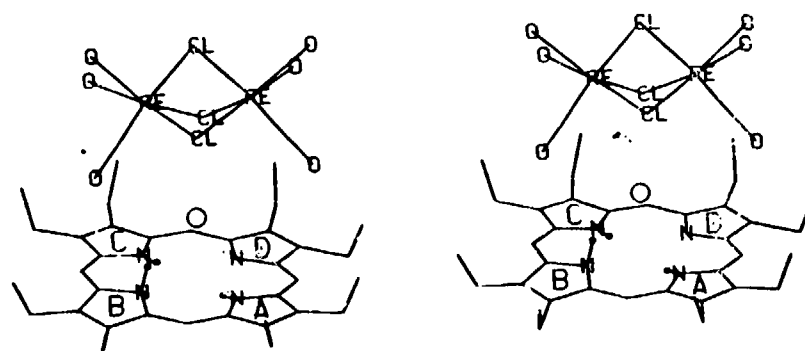


Figure 5

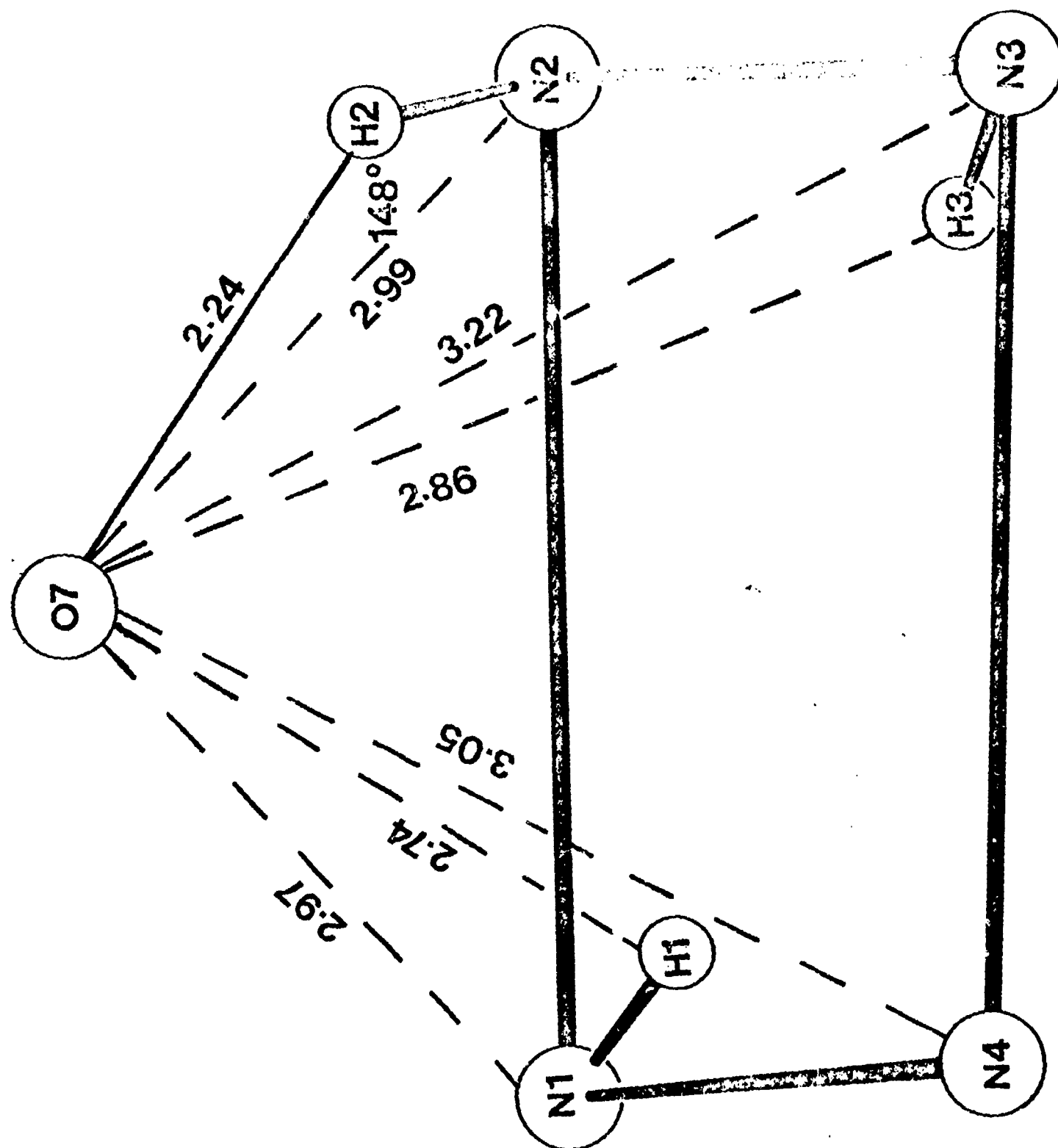


Figure 6

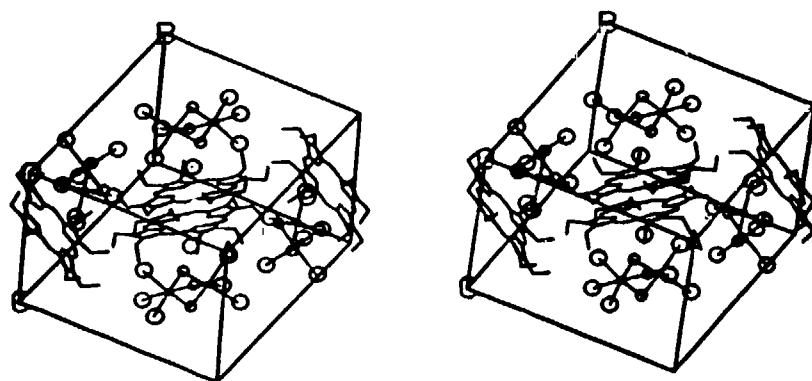


Figure 7

S U P P L E M E N T A R Y M A T E R I A L

Synthesis, Characterization, and Structure of
Tri- μ -halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids

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SUPPLEMENTARY MATERIAL

TABLE VI
Calculated Hydrogen Atom Positions

ATOM	$\bar{X}$	$\bar{Y}$	$\bar{Z}$	ATOM	$\bar{X}$	$\bar{Y}$	$\bar{Z}$
H(4)	0.2085	0.1764	0.8261	H(25)	-0.0170	0.3521	0.5971
H(5)	-0.0949	0.1803	0.4134	H(26)	-0.0534	0.3213	0.4776
H(6)	0.0323	-0.0741	0.2552	H(27)	-0.1121	0.3566	0.5290
H(7)	0.3407	-0.0706	0.6568	H(28)	-0.2180	0.0886	0.1792
H(8)	0.4251	0.0020	0.9189	H(29)	-0.1909	0.1456	0.2722
H(9)	0.4241	-0.0496	0.8190	H(30)	-0.1220	0.2032	0.1826
H(10)	0.4704	0.0287	0.7294	H(31)	-0.1490	0.1462	0.0897
H(11)	0.4914	0.0803	0.3294	H(32)	-0.2154	0.1951	0.1076
H(12)	0.5393	0.0092	0.8425	H(33)	-0.1024	-0.0613	0.1535
H(13)	0.579	0.1272	0.9678	H(34)	-0.1675	-0.0009	0.1096
H(14)	0.611	0.0898	0.9801	H(35)	-0.0818	0.0561	0.0470
H(15)	0.4322	0.1777	0.8903	H(36)	-0.0167	-0.0043	0.0909
H(16)	0.3491	0.2150	0.8780	H(37)	-0.1014	-0.0191	-0.0046
H(17)	0.4179	0.2051	0.9949	H(38)	0.1902	-0.1984	0.3017
H(18)	0.0226	0.2690	0.8048	H(39)	0.1018	-0.1653	0.2501
H(19)	0.0986	0.2207	0.8652	H(40)	0.1538	-0.0757	0.1852
H(20)	0.1802	0.2939	0.8223	H(41)	0.2422	-0.1088	0.2368
H(21)	0.1041	0.3421	0.7610	H(42)	0.1729	-0.1473	0.1496
H(22)	0.1340	0.3323	0.8888	H(43)	0.3257	-0.1812	0.5936
H(23)	-0.1217	0.2397	0.5341	H(44)	0.2862	-0.2207	0.4811
H(24)	-0.0853	0.2705	0.6536	H(45)	0.3349	-0.1451	0.4054
				H(46)	0.3744	-0.1057	0.5179
				H(47)	0.4052	-0.1810	0.5036

^aAll hydrogen atoms were assumed to have an isotropic thermal parameter, $B = 4.0 \text{ \AA}^2$

TABLE VII

ROOT-MEAN-SQUARE AMPLITUDES OF THERMAL VIBRATION IN ANGSTROMS.

ATOM	MIN.	INT'ED.	MAX.	ATOM	MIN.	INT'ED.	MAX.
N1	0.167	0.250	0.313	RE1	0.207	0.229	0.258
N2	0.194	0.204	0.259	RE2	0.212	0.227	0.283
N3	0.174	0.241	0.256	CL1	0.195	0.246	0.264
N4	0.195	0.209	0.301	CL2	0.205	0.245	0.265
C1	0.173	0.247	0.304	CL3	0.228	0.241	0.255
C2	0.174	0.248	0.286	C37	0.232	0.250	0.288
C3	0.157	0.247	0.264	C38	0.196	0.263	0.356
C4	0.215	0.243	0.268	C39	0.185	0.272	0.325
C5	0.193	0.237	0.290	C40	0.228	0.234	0.348
C6	0.199	0.224	0.293	C41	0.201	0.249	0.328
C7	0.205	0.212	0.309	C42	0.227	0.261	0.354
C8	0.204	0.234	0.281	O1	0.204	0.319	0.419
C9	0.177	0.224	0.290	O2	0.249	0.330	0.367
C10	0.170	0.229	0.280	O3	0.220	0.327	0.399
C11	0.183	0.242	0.250	O4	0.219	0.334	0.424
C12	0.182	0.229	0.260	O5	0.221	0.292	0.395
C13	0.181	0.222	0.246	O6	0.233	0.342	0.476
C14	0.187	0.219	0.236				
C15	0.197	0.220	0.268				
C16	0.206	0.213	0.275				
C17	0.186	0.227	0.356				
C18	0.172	0.237	0.456				
C19	0.210	0.234	0.358				
C20	0.172	0.257	0.374				
C21	0.195	0.265	0.360				
C22	0.217	0.337	0.529				
C23	0.225	0.272	0.330				
C24	0.242	0.333	0.422				
C25	0.227	0.293	0.303				
C26	0.275	0.298	0.396				
C27	0.232	0.246	0.324				
C28	0.227	0.327	0.417				
C29	0.172	0.245	0.332				
C30	0.192	0.314	0.350				
C31	0.191	0.252	0.287				
C32	0.214	0.293	0.320				
C33	0.218	0.242	0.358				
C34	0.239	0.254	0.401				
C35	0.272	0.326	0.543				
C36	0.330	0.356	0.496				
O7	0.263	0.282	0.293				

TABLE VIII

Values of $10 |F_o|$ and $10 |F_c|$

For $(H_3OEP)^+[Re_2(CO)_6Cl_3]^{--}$

A. Data having $2\theta \leq 45^\circ$

B. Data having $45^\circ < 2\theta \leq 55^\circ$

MODEP+ REZ(CO)ECL3- MD DATA 0-40 DEG IN 2THETA 10 FO AND 10FC										PAGE 1									
H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
0-10	0	0	753	730	11-13	0	0	611	597	2	-8	0	261	238	10	-5	0	419	342
1-18	0	0	769	798	1-12	0	0	2159	2114	3	-8	0	749	711	11	-5	0	1355	1281
3-18	0	0	769	759	2-12	0	0	422	428	4	-8	0	1749	1701	13	-5	0	378	839
4-18	0	0	878	894	3-12	0	0	186	155	6	-8	0	382	331	14	-5	0	351	307
5-18	0	0	295	329	4-12	0	0	969	914	7	-9	0	229	170	15	-5	0	1617	1569
2-17	0	0	1158	1129	5-12	0	0	732	691	8	-9	0	2376	2178	1	-4	0	1923	1871
3-17	0	0	273	234	7-12	0	0	800	746	9	-8	0	382	353	2	-4	0	537	505
4-17	0	0	619	627	8-12	0	0	967	953	10	-8	0	846	769	3	-4	0	3117	2888
5-17	0	0	1062	1063	9-12	0	0	421	388	11	-8	0	809	738	4	-4	0	2951	2699
6-17	0	0	244	286	10-12	0	0	838	775	12	-8	0	988	896	5	-4	0	1192	1077
7-17	0	0	685	637	11-12	0	0	1287	1250	13	-8	0	1187	1114	6	-4	0	286	259
8-16	0	0	380	374	1-11	0	0	288	282	14	-8	0	368	304	7	-4	0	592	559
1-16	0	0	566	542	2-11	0	0	338	363	1	-7	0	1383	1315	8	-4	0	2148	1938
2-16	0	0	797	778	3-11	0	0	369	340	2	-7	0	2938	2792	9	-4	0	1709	1599
3-16	0	0	500	535	4-11	0	0	1081	1012	4	-7	0	2236	2149	10	-4	0	1875	1737
4-16	0	0	1270	1237	5-11	0	0	2065	1937	5	-7	0	2236	2149	11	-4	0	1875	1737
5-16	0	0	584	590	6-11	0	0	1928	1796	6	-7	0	543	479	12	-4	0	875	801
7-16	0	0	374	409	7-11	0	0	2379	2251	7	-7	0	2291	2109	13	-4	0	644	625
8-16	0	0	1048	995	8-11	0	0	721	706	8	-7	0	1459	1393	15	-4	0	888	877
1-15	0	0	996	1612	9-11	0	0	362	296	10	-7	0	1992	1867	1	-3	0	2094	1970
2-15	0	0	417	413	10-11	0	0	512	458	11	-7	0	1011	964	2	-3	0	4372	4061
3-15	0	0	1649	1619	11-11	0	0	700	393	13	-7	0	1257	1208	3	-3	0	1602	1466
4-15	0	0	336	336	1-10	0	0	3368	3401	14	-7	0	319	346	4	-3	0	1449	1336
5-15	0	0	226	174	2-10	0	0	1084	1011	15	-7	0	1197	1200	5	-3	0	1304	1198
9-15	0	0	772	753	3-10	0	0	494	495	6	-6	0	2087	1960	6	-3	0	1525	1550
10-15	0	0	523	477	4-10	0	0	691	638	7	-6	0	1891	1789	7	-3	0	970	935
0-14	0	0	682	643	5-10	0	0	556	511	8	-6	0	2090	1934	8	-3	0	1411	1366
2-14	0	0	745	720	6-10	0	0	936	869	9	-6	0	1451	1376	9	-3	0	857	818
3-14	0	0	1613	1599	8-10	0	0	577	568	10	-6	0	236	233	10	-3	0	474	458
4-14	0	0	362	360	10-10	0	0	1694	1629	11	-6	0	1077	1012	11	-3	0	1341	1281
5-14	0	0	1107	1057	12-10	0	0	414	454	12	-6	0	1628	1436	13	-3	0	799	771
6-14	0	0	217	84	13-10	0	0	606	562	14	-6	0	2382	2235	15	-3	0	728	665
7-14	0	0	855	822	1-9	0	0	1753	1689	16	-3	0	817	774	1	-2	0	491	516
8-14	0	0	327	307	2-9	0	0	1298	1235	9	-5	0	288	296	2	-2	0	5003	4614
9-14	0	0	1434	1369	3-9	0	0	1037	1006	10	-5	0	319	316	3	-2	0	1787	1582
10-14	0	0	425	444	4-9	0	0	1581	1492	11	-6	0	464	466	4	-2	0	2326	2132
11-14	0	0	298	333	5-9	0	0	3326	3167	14	-6	0	2511	2364	5	-2	0	213	178
1-13	0	0	611	610	6-9	0	0	1157	1093	15	-6	0	1758	1726	6	-2	0	662	586
2-13	0	0	1260	1229	7-9	0	0	2226	2122	16	-6	0	813	723	7	-2	0	353	350
3-13	0	0	784	739	8-9	0	0	598	579	17	-6	0	479	432	8	-2	0	223	2007
4-13	0	0	1020	981	9-9	0	0	1010	976	18	-6	0	253	194	9	-2	0	967	894
5-13	0	0	931	898	10-9	0	0	572	552	19	-6	0	878	796	10	-2	0	1813	1765
6-13	0	0	969	924	11-9	0	0	618	562	12	-5	0	2031	1910	11	-2	0	692	626
7-13	0	0	825	765	12-9	0	0	472	444	1	-5	0			13	-2	0		
8-13	0	0	680	641	1-8	0	0	2927	2918	2	-5	0			15	-2	0		
9-13	0	0	236	227	2	-8	0			3	-5	0			16	-2	0		
10-13	0	0	340	342	1	-8	0			4	-5	0			17	-2	0		

H3DEP+ REZ(CO)6CL3- NO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

PAGE 2

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-6-16	1	1	436	442	5-14	1	1	495	502	-7-11	1	1	354	325	-7-9	1	1	411	449	13-8	1	1	306	248
-5-16	1	1	212	276	6-14	1	1	521	488	-6-11	1	1	472	492	-6-9	1	1	1252	1284	14-8	1	1	830	817
-4-16	1	1	1330	1423	8-14	1	1	329	270	-5-11	1	1	850	872	-5-9	1	1	489	498	-15-7	1	1	384	407
-3-16	1	1	1205	1279	9-14	1	1	1409	1362	-4-11	1	1	615	633	-4-9	1	1	1128	1120	-13-7	1	1	903	957
-2-16	1	1	1442	1445	-12-13	1	1	668	659	-3-11	1	1	1036	1054	-3-9	1	1	707	730	-12-7	1	1	801	853
-1-16	1	1	530	526	-10-13	1	1	1088	1129	-2-11	1	1	974	1006	-2-9	1	1	2460	2459	-11-7	1	1	265	299
1-16	1	1	677	683	-9-13	1	1	754	783	-1-11	1	1	2775	2749	-1-9	1	1	1162	1116	-10-7	1	1	1935	2057
2-16	1	1	680	659	-8-13	1	1	956	962	0-11	1	1	1884	1828	0-9	1	1	3825	3762	-9-7	1	1	437	441
3-16	1	1	328	342	-7-13	1	1	268	206	1-11	1	1	1398	1373	1-9	1	1	1533	1564	-8-7	1	1	1782	1821
4-16	1	1	301	309	-5-13	1	1	1090	1144	3-11	1	1	535	561	2-9	1	1	897	892	-7-7	1	1	216	231
5-16	1	1	533	552	-4-13	1	1	605	632	4-11	1	1	574	548	3-9	1	1	1557	1495	-6-7	1	1	258	291
6-16	1	1	252	221	-3-13	1	1	451	455	6-11	1	1	1145	1120	4-9	1	1	796	781	-5-7	1	1	1373	1424
7-16	1	1	283	270	-2-13	1	1	867	942	7-11	1	1	1008	981	5-9	1	1	1357	1302	-4-7	1	1	892	956
8-16	1	1	811	743	-1-13	1	1	1405	1390	8-11	1	1	275	245	6-9	1	1	802	757	-3-7	1	1	234	258
-10-15	1	1	230	233	0-13	1	1	773	755	9-11	1	1	1008	981	7-9	1	1	356	383	-2-7	1	1	587	561
-9-15	1	1	1436	1489	1-13	1	1	612	623	10-11	1	1	1416	1334	8-9	1	1	1149	1086	-1-7	1	1	2750	2695
-8-15	1	1	336	350	2-13	1	1	1076	1068	11-11	1	1	828	809	9-9	1	1	679	699	0-7	1	1	469	466
-7-15	1	1	271	302	3-13	1	1	934	922	12-11	1	1	1416	1334	10-9	1	1	846	818	1-7	1	1	2257	2152
-6-15	1	1	359	406	4-13	1	1	1068	1027	-13-10	1	1	273	267	11-9	1	1	845	829	2-7	1	1	2682	2564
-5-15	1	1	1105	1120	6-13	1	1	1229	187	-12-10	1	1	747	779	12-9	1	1	1588	1479	3-7	1	1	961	870
-4-15	1	1	476	525	7-13	1	1	1221	1199	-11-10	1	1	416	409	13-9	1	1	440	418	4-7	1	1	2736	2613
-3-15	1	1	689	727	8-13	1	1	834	754	-8-10	1	1	1823	1879	-15-8	1	1	277	304	6-7	1	1	511	442
-1-15	1	1	298	293	10-13	1	1	649	614	-7-10	1	1	813	820	-14-8	1	1	692	687	7-7	1	1	930	851
0-15	1	1	224	193	11-13	1	1	838	767	-6-10	1	1	2458	2627	-12-8	1	1	653	692	8-7	1	1	1413	1334
1-15	1	1	498	491	-13-12	1	1	251	189	-5-10	1	1	535	542	-11-8	1	1	270	303	9-7	1	1	687	643
2-15	1	1	427	390	-11-12	1	1	696	691	-4-10	1	1	250	256	-10-8	1	1	1109	1170	10-7	1	1	668	591
3-15	1	1	1777	1774	-10-12	1	1	492	515	-3-10	1	1	570	578	-9-8	1	1	1164	1195	11-7	1	1	899	817
4-15	1	1	459	442	-9-12	1	1	519	536	-2-10	1	1	468	474	-8-8	1	1	2237	2307	13-7	1	1	747	768
5-15	1	1	695	677	-7-12	1	1	1833	1894	-1-10	1	1	227	234	-7-8	1	1	1164	1195	14-7	1	1	899	817
7-15	1	1	1115	1038	-5-12	1	1	1307	1348	0-10	1	1	1595	1569	-6-8	1	1	890	949	-15-6	1	1	1084	1135
8-15	1	1	371	371	-4-12	1	1	1121	1185	1-10	1	1	1095	1037	-5-8	1	1	2003	2093	-14-6	1	1	685	698
9-15	1	1	1063	1010	-3-12	1	1	359	377	2-10	1	1	525	529	-4-8	1	1	1163	1253	-13-6	1	1	219	202
-1-14	1	1	588	619	-2-12	1	1	1362	1373	3-10	1	1	567	525	-3-8	1	1	160	139	-12-6	1	1	575	503
-9-14	1	1	281	311	0-12	1	1	471	441	4-10	1	1	2371	2205	-2-8	1	1	2210	2259	-11-6	1	1	885	916
-8-14	1	1	405	424	1-12	1	1	1303	1292	5-10	1	1	661	645	-1-8	1	1	163	155	-10-6	1	1	1156	1184
-7-14	1	1	719	711	2-12	1	1	523	532	6-10	1	1	2847	2673	0-8	1	1	1081	1040	-9-6	1	1	341	371
-6-14	1	1	531	545	3-12	1	1	590	575	7-10	1	1	597	554	1-8	1	1	919	865	-8-6	1	1	1018	1015
-5-14	1	1	673	656	4-12	1	1	334	337	8-10	1	1	482	489	2-8	1	1	2389	2275	-7-6	1	1	1052	1069
-4-14	1	1	801	849	5-12	1	1	2205	2113	9-10	1	1	356	322	3-8	1	1	1135	1061	-6-6	1	1	985	1013
-3-14	1	1	2138	2209	7-12	1	1	1618	1456	12-10	1	1	1110	1195	4-8	1	1	1014	963	-5-6	1	1	844	873
-2-14	1	1	544	553	8-12	1	1	859	854	-14-9	1	1	1110	1195	5-8	1	1	2882	2742	-4-6	1	1	1620	1699
-1-14	1	1	605	625	10-12	1	1	841	790	-13-9	1	1	362	420	6-8	1	1	1632	1531	-3-6	1	1	2501	2745
0-14	1	1	247	221	12-12	1	1	291	261	-12-9	1	1	1086	1118	7-8	1	1	1805	1886	-2-6	1	1	1396	1405
1-14	1	1	331	329	-13-11	1	1	1160	1204	-11-9	1	1	955	975	8-8	1	1	886	811	-1-6	1	1	1739	1766
2-14	1	1	339	346	-12-11	1	1	812	863	-10-9	1	1	390	400	9-8	1	1	1131	1048	0-6	1	1	1266	1205
3-14	1	1	574	569	-11-11	1	1	553	619	-9-9	1	1	602	622	10-8	1	1	330	311	-6-6	1	1	2786	2594
4-14	1	1	532	490	-8-11	1	1	308	312	-8-9	1	1	468	485	12-8	1	1	274	308	1-6	1	1	1178	1109

H3DEP+ PE2(CO)SCL3- PD DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
5-13	2	2	1275	1206	12-11	2	2	563	558	12-9	2	2	869	820	5-7	2	2	2547	2485	5-5	2	2	993	982
6-13	2	2	1060	1017	-14-10	2	2	1241	1327	-15-8	2	2	585	568	6-7	2	2	437	417	5-5	2	2	244	276
7-13	2	2	438	453	-13-10	2	2	479	413	-13-8	2	2	594	727	7-7	2	2	302	308	5-5	2	2	1875	1795
8-13	2	2	1245	1237	-12-10	2	2	661	667	-11-8	2	2	1049	1134	8-7	2	2	1910	1847	5-5	2	2	3345	330
9-13	2	2	834	764	-11-10	2	2	215	270	-10-8	2	2	674	737	10-7	2	2	1409	1571	5-5	2	2	2349	2273
10-13	2	2	734	733	-8-10	2	2	477	613	-9-8	2	2	1712	1826	12-7	2	2	691	696	5-5	2	2	329	278
-13-12	2	2	915	949	-7-10	2	2	1503	494	-8-8	2	2	665	690	13-7	2	2	599	503	-12-5	2	2	1233	1216
-12-12	2	2	730	386	-6-10	2	2	1503	1653	-8-8	2	2	676	921	-15-6	2	2	541	503	-11-5	2	2	1813	1829
-11-12	2	2	271	239	-5-10	2	2	846	676	-7-8	2	2	1708	1338	-13-6	2	2	727	617	-10-4	2	2	1547	1629
-10-12	2	2	914	390	-4-10	2	2	210	217	-6-8	2	2	1153	1193	-12-6	2	2	1808	1906	-9-4	2	2	1243	1316
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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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0	-3	2	573	525	-11	-1	2	700	718	0	-17	3	266	244	-8	-13	3	778	857	0	-11	3	753	743
1	-3	2	1939	1998	-9	-1	2	805	829	1	-17	3	232	231	-7	-13	3	588	607	1	-11	3	583	607
2	-3	2	1106	1074	-8	-1	2	3004	2965	2	-17	3	1325	1329	-6	-13	3	339	396	2	-11	3	245	245
3	-3	2	1276	1197	-7	-1	2	2220	2215	3	-17	3	406	409	-5	-13	3	339	361	3	-11	3	722	722
4	-3	2	336	354	-6	-1	2	2229	2211	4	-17	3	705	689	-4	-13	3	381	367	4	-11	3	722	722
5	-3	2	2216	2237	-5	-1	2	3124	3061	5	-16	3	363	440	-3	-13	3	1333	1362	5	-11	3	1240	1204
6	-3	2	1225	1184	-3	-1	2	1621	1545	6	-16	3	786	813	-1	-13	3	759	762	6	-11	3	1234	1197
7	-3	2	658	652	-2	-1	2	160	25	7	-16	3	848	866	0	-13	3	737	745	7	-11	3	830	805
8	-3	2	2393	2328	-1	-1	2	1531	1515	8	-16	3	1553	1607	1	-13	3	1093	1085	8	-11	3	254	254
9	-3	2	512	550	0	-1	2	3454	3587	9	-16	3	765	806	2	-13	3	1496	1525	9	-11	3	553	575
10	-3	2	1040	998	1	-1	2	993	1046	10	-16	3	650	672	3	-13	3	563	516	10	-11	3	1206	1164
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12	-3	2	492	460	3	-1	2	791	793	12	-16	3	638	610	5	-13	3	835	796	12	-11	3	882	916
13	-3	2	1068	1015	4	-1	2	4289	4257	13	-16	3	381	392	6	-13	3	724	694	13	-11	3	220	250
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16	-3	2	624	627	7	-1	2	1800	1840	16	-16	3	354	358	9	-13	3	1014	1096	16	-11	3	725	750
17	-3	2	1005	1013	8	-1	2	1196	1187	17	-16	3	1675	1133	10	-13	3	545	57	17	-11	3	513	528
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19	-3	2	2679	2681	10	-1	2	909	928	19	-15	3	386	383	12	-12	3	1018	1041	19	-11	3	292	297
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21	-3	2	1531	1545	12	-1	2	859	862	21	-15	3	402	411	14	-12	3	1314	1356	21	-11	3	1613	1642
22	-3	2	1698	1702	13	-1	2	1506	1478	22	-15	3	1387	1372	15	-12	3	443	475	22	-11	3	826	870
23	-3	2	438	483	14	0	2	601	638	23	-15	3	1481	1475	16	-12	3	1786	1759	23	-11	3	2404	2420
24	-3	2	728	702	15	0	2	1129	1056	24	-15	3	368	397	17	-12	3	188	135	24	-11	3	253	238
25	-3	2	626	620	16	0	2	1143	1092	25	-15	3	229	236	18	-12	3	1034	1024	25	-11	3	443	443
26	-3	2	3369	3442	17	0	2	2560	3479	26	-15	3	276	270	19	-12	3	145	146	26	-11	3	2494	2404
27	-3	2	1798	1881	18	0	2	1107	1018	27	-15	3	576	607	20	-12	3	1145	1102	27	-11	3	751	733
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29	-3	2	601	582	20	0	2	421	366	29	-14	3	397	403	22	-12	3	1131	1064	29	-11	3	447	451
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31	-3	2	2553	2469	22	0	2	626	647	31	-14	3	1929	1987	24	-12	3	230	216	31	-11	3	613	517
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33	-3	2	1917	1917	24	0	2	1973	1949	33	-14	3	1776	1833	26	-12	3	289	279	33	-11	3	784	784
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35	-3	2	1102	1047	26	0	2	435	372	35	-14	3	238	240	28	-11	3	494	467	35	-11	3	424	440
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37	-3	2	508	492	28	0	2	849	859	37	-14	3	209	126	30	-11	3	513	486	37	-11	3	394	461
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39	-3	2	1754	1679	30	0	2	503	494	39	-14	3	403	437	32	-11	3	1731	1789	39	-11	3	296	240
40	-3	2	1257	1213	31	0	2	964	972	40	-14	3	1384	1330	33	-11	3	840	852	40	-11	3	463	469
41	-3	2	1088	1121	32	0	2	521	509	41	-14	3	632	649	34	-11	3	1160	1200	41	-11	3	816	856
42	-3	2	528	530	33	0	2	297	311	42	-14	3	322	268	35	-11	3	599	616	42	-11	3	1274	1274
43	-3	2	565	553	34	0	2	421	414	43	-14	3	460	481	36	-11	3	1038	1030	43	-11	3	1303	1274
44	-3	2	591	552	35	0	2	737	725	44	-14	3	1099	1162	37	-11	3	1607	1638	44	-11	3	1138	1103
45	-3	2	1271	1265	36	0	2			45	-14	3			38	-11	3			45	-11	3		

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0	0	3	4542	4714	0-14	4	4	344	324	-7-11	4	4	756	762	-4-9	4	4	427	443	-9-7	4	4	1073	1128
2	0	3	220	192	1-14	4	4	1877	1824	-6-11	4	4	525	553	-3-9	4	4	1180	1191	-6-7	4	4	1073	1128
4	0	3	4409	4455	2-14	4	4	527	486	-5-11	4	4	242	213	-2-9	4	4	1493	1557	-5-7	4	4	314	297
6	0	3	2607	2632	3-14	4	4	1209	1220	-4-11	4	4	246	291	-1-9	4	4	1469	1460	-4-7	4	4	2528	2658
8	0	3	949	917	4-14	4	4	564	565	-3-11	4	4	1174	1212	0-9	4	4	1948	1981	-3-7	4	4	318	353
10	0	3	1281	1259	5-14	4	4	518	517	-2-11	4	4	1502	1509	1-9	4	4	749	748	-2-7	4	4	660	687
12	0	3	1209	1234	6-14	4	4	323	269	-1-11	4	4	1851	1839	2-9	4	4	495	482	-1-7	4	4	1834	1844
-4-18	4	4	597	602	-12-13	4	4	339	372	0-11	4	4	1226	1240	4-9	4	4	1973	1962	1-7	4	4	579	613
-2-18	4	4	642	614	-10-13	4	4	505	502	1-11	4	4	798	793	5-9	4	4	479	470	2-7	4	4	1672	1692
-1-18	4	4	528	563	-9-13	4	4	595	642	2-11	4	4	819	816	6-9	4	4	262	236	3-7	4	4	1415	1360
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-1-17	4	4	461	438	-5-13	4	4	1085	1107	5-11	4	4	1009	995	9-9	4	4	1024	1030	6-7	4	4	1842	1824
0-17	4	4	277	250	-4-13	4	4	1198	1218	6-11	4	4	259	317	10-9	4	4	543	494	7-7	4	4	455	429
2-17	4	4	318	326	-2-13	4	4	1193	1177	7-11	4	4	475	479	11-9	4	4	293	311	8-7	4	4	568	582
-9-16	4	4	278	253	0-13	4	4	396	401	8-11	4	4	826	825	-12-8	4	4	1200	1264	9-7	4	4	846	853
-8-16	4	4	232	241	1-13	4	4	538	517	-14-10	4	4	438	488	-10-8	4	4	973	1006	-16-6	4	4	718	742
-5-16	4	4	427	389	2-13	4	4	1028	998	-11-10	4	4	397	391	-9-8	4	4	882	921	-13-6	4	4	726	746
-4-16	4	4	315	294	3-13	4	4	694	641	-10-10	4	4	373	348	-8-8	4	4	1000	1054	-11-6	4	4	1111	1153
-3-16	4	4	754	747	4-13	4	4	836	822	-9-10	4	4	334	340	-6-8	4	4	1288	1371	-10-6	4	4	2032	2095
0-16	4	4	841	842	5-13	4	4	765	754	-8-10	4	4	1701	1776	-5-8	4	4	872	864	-9-6	4	4	1218	1235
-2-16	4	4	342	337	6-13	4	4	867	867	-7-10	4	4	889	932	-4-8	4	4	235	243	-8-6	4	4	501	525
1-16	4	4	1055	1053	-11-12	4	4	239	183	-6-10	4	4	1060	1127	-3-8	4	4	1315	1346	-5-6	4	4	394	438
2-16	4	4	705	705	-10-12	4	4	1178	1189	-5-10	4	4	420	414	-2-8	4	4	1332	1339	-4-6	4	4	560	572
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-9-15	4	4	821	866	-7-12	4	4	601	627	-2-10	4	4	1687	1690	1-8	4	4	2052	2029	-1-6	4	4	2893	2698
-7-15	4	4	689	717	-6-12	4	4	353	369	-1-10	4	4	280	275	2-8	4	4	862	865	0-6	4	4	1871	1879
-6-15	4	4	347	380	-5-12	4	4	832	868	0-10	4	4	233	235	3-8	4	4	1553	1554	-3-6	4	4	1322	1329
-5-15	4	4	1654	1725	-4-12	4	4	1079	1073	1-10	4	4	431	417	4-8	4	4	389	354	-2-6	4	4	1922	1923
-4-15	4	4	401	436	-3-12	4	4	325	338	2-10	4	4	2133	2108	5-8	4	4	1553	1564	3-6	4	4	287	315
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1-15	4	4	215	208	1-12	4	4	1031	1036	8-10	4	4	956	941	8-8	4	4	494	481	6-6	4	4	944	965
3-15	4	4	859	843	3-12	4	4	528	568	9-10	4	4	443	443	9-8	4	4	460	448	8-6	4	4	303	315
6-15	4	4	252	276	4-12	4	4	1954	1941	10-10	4	4	1567	1625	10-8	4	4	868	836	11-6	4	4	505	550
-11-14	4	4	1260	1349	7-12	4	4	573	579	-14-9	4	4	798	719	-16-7	4	4	847	882	-15-5	4	4	275	278
-10-14	4	4	493	478	8-12	4	4	615	626	-13-9	4	4	899	925	-15-7	4	4	856	914	-13-5	4	4	785	802
-8-14	4	4	309	339	-14-11	4	4	645	658	-12-9	4	4	482	497	-14-7	4	4	323	282	-11-5	4	4	246	252
-6-14	4	4	390	420	-13-11	4	4	845	883	-10-9	4	4	921	982	-13-7	4	4	1192	1227	-12-5	4	4	700	742
-5-14	4	4	741	765	-12-11	4	4	1115	1169	-9-9	4	4	1307	1364	-12-7	4	4	289	295					
-3-14	4	4	970	1017	-9-11	4	4	663	681	-8-9	4	4	663	671	-11-7	4	4	191	160					

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-10	-5	4	264	308	-14	-3	4	322	337	7	-2	4	1173	1156	4	0	4	2739	2725	-8	-13	5	741	773
-9	-5	4	1306	1349	-13	-3	4	1058	1011	8	-2	4	1051	1087	6	0	4	2844	2919	-7	-13	5	563	553
-7	-5	4	1177	1183	-12	-3	4	605	605	9	-2	4	362	402	8	0	4	390	354	-6	-13	5	772	796
-6	-5	4	926	922	-10	-3	4	648	681	10	-2	4	1005	997	10	0	4	838	826	-5	-13	5	773	805
-5	-5	4	3530	3613	-9	-3	4	1091	1071	11	-2	4	941	943	12	0	4	272	325	-4	-13	5	898	893
-4	-5	4	1507	1495	-8	-3	4	361	357	12	-2	4	236	164	12	0	4	262	284	-3	-13	5	717	691
-3	-5	4	2213	2300	-7	-3	4	810	799	13	-2	4	484	460	13	0	4	230	204	-1	-13	5	782	748
-2	-5	4	565	577	-6	-3	4	2613	2677	17	-1	4	238	213	13	0	4	802	810	-1	-13	5	762	764
-1	-5	4	1014	990	-5	-3	4	2427	2442	15	-1	4	837	831	17	0	4	230	170	1	-13	5	1194	1204
0	-5	4	198	169	-4	-3	4	2559	2634	14	-1	4	1362	1346	17	0	4	289	283	1	-13	5	1120	1134
1	-5	4	1007	991	-2	-3	4	1450	1461	13	-1	4	1429	1395	17	0	4	899	864	3	-13	5	427	429
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3	-5	4	2342	2398	0	-3	4	1686	1684	11	-1	4	352	309	16	0	4	937	961	5	-13	5	936	923
4	-5	4	223	216	1	-3	4	172	154	10	-1	4	1607	1627	16	0	4	739	742	6	-13	5	759	763
5	-5	4	256	216	2	-3	4	1109	1134	9	-1	4	1066	1065	16	0	4	1035	1066	13	-12	5	861	887
6	-5	4	2642	2840	3	-3	4	2531	2593	8	-1	4	1450	1446	16	0	4	397	377	12	-12	5	310	295
7	-5	4	529	548	4	-3	4	1124	1086	7	-1	4	842	826	16	0	4	314	300	10	-12	5	416	441
8	-5	4	1237	1268	5	-3	4	1215	1232	6	-1	4	1673	1629	16	0	4	735	743	9	-12	5	531	517
9	-5	4	401	398	6	-3	4	1738	1783	5	-1	4	532	523	16	0	4	778	748	7	-12	5	362	400
-1	-4	4	792	790	7	-3	4	732	810	4	-1	4	1641	1608	15	0	4	289	252	6	-12	5	1092	1078
-13	-4	4	687	693	8	-3	4	2114	2161	3	-1	4	550	526	15	0	4	220	119	4	-12	5	1550	1601
-12	-4	4	1233	1233	9	-3	4	242	243	2	-1	4	2212	2246	15	0	4	927	957	3	-12	5	1677	1697
-11	-4	4	2091	2084	10	-3	4	554	568	1	-1	4	2356	2243	15	0	4	242	273	1	-12	5	1086	1103
-10	-4	4	1582	1603	11	-3	4	971	996	0	-1	4	1626	1729	15	0	4	952	966	0	-12	5	467	454
-9	-4	4	826	864	13	-3	4	495	500	1	-1	4	1494	1545	15	0	4	655	643	0	-12	5	1086	1103
-8	-4	4	891	916	15	-3	4	425	447	1	-1	4	1137	1145	15	0	4	655	643	0	-12	5	1086	1103
-7	-4	4	706	675	15	-2	4	372	308	3	-1	4	198	214	15	0	4	1519	1522	4	-12	5	283	242
-6	-4	4	1199	1203	14	-2	4	446	424	5	-1	4	1238	1229	15	0	4	312	314	6	-12	5	243	260
-5	-4	4	182	89	13	-2	4	361	350	6	-1	4	214	237	15	0	4	761	759	12	-11	5	860	894
-4	-4	4	352	392	12	-2	4	1103	1125	7	-1	4	233	286	14	0	4	723	747	11	-11	5	1417	1514
-3	-4	4	1916	1985	10	-2	4	1132	1100	8	-1	4	211	183	14	0	4	701	719	10	-11	5	979	1074
-2	-4	4	672	657	9	-2	4	1999	1981	9	-1	4	949	940	14	0	4	701	704	9	-11	5	1414	1474
0	-4	4	2631	2600	8	-2	4	3576	3515	10	-1	4	1104	1137	14	0	4	1297	1300	8	-11	5	547	569
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3	-4	4	1788	1808	5	-2	4	1867	1858	13	-1	4	351	355	14	0	4	530	550	5	-11	5	458	472
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8	-4	4	556	579	1	-2	4	1078	1135	10	0	4	535	556	14	0	4	295	295	1	-11	5	195	167
10	-4	4	1294	1288	0	-2	4	631	614	8	0	4	3737	3657	14	0	4	820	795	0	-11	5	1200	1207
12	-4	4	505	488	2	-2	4	1362	1413	6	0	4	2338	2254	14	0	4	445	436	0	-11	5	1385	1395
13	-4	4	1308	1360	3	-2	4	1666	1654	4	0	4	2660	2654	13	0	4	801	731	0	-11	5	532	536
16	-3	4	1121	1112	4	-2	4	2400	2387	0	0	4	891	802	13	0	4	883	925	0	-11	5	813	801
-15	-3	4	220	187	6	-2	4	813	859	2	0	4	813	802	13	0	4	533	554	0	-11	5	813	801

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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-12-10	5	5	751	739	-4-8	5	5	511	513	-6-6	5	5	1445	1496	-3-4	5	5	159	124	-9-2	5	5	536	497
-10-10	5	5	589	616	-3-8	5	5	2068	2122	-5-6	5	5	2393	2482	-2-4	5	5	1154	1161	-8-2	5	5	851	840
-8-10	5	5	259	223	-2-8	5	5	735	756	-4-6	5	5	1910	1922	-4-4	5	5	1661	1661	-7-2	5	5	519	532
-7-10	5	5	427	423	-1-8	5	5	1761	1789	-3-6	5	5	1271	1305	-4-4	5	5	2371	2350	-6-2	5	5	2268	2253
-6-10	5	5	705	722	-1-8	5	5	379	387	-3-6	5	5	2015	2065	-4-4	5	5	1887	1108	-5-2	5	5	1199	1199
-4-10	5	5	833	840	2-8	5	5	1200	1209	1-6	5	5	1860	1897	3-4	5	5	1911	1978	-4-2	5	5	338	356
-3-10	5	5	634	618	3-8	5	5	284	308	2-6	5	5	1490	1507	4-4	5	5	312	371	-3-2	5	5	1271	1250
-2-10	5	5	2779	2831	4-8	5	5	738	716	3-6	5	5	1595	1660	5-4	5	5	604	637	-1-2	5	5	2601	2701
-1-10	5	5	844	858	5-8	5	5	555	563	4-6	5	5	362	339	6-4	5	5	857	876	0-2	5	5	635	636
0-10	5	5	1306	1270	6-8	5	5	659	656	6-6	5	5	1545	1640	7-4	5	5	2169	2216	1-2	5	5	939	978
2-10	5	5	620	593	7-8	5	5	784	755	6-6	5	5	1289	1298	8-4	5	5	1098	1110	2-2	5	5	1512	1500
3-10	5	5	211	198	8-8	5	5	707	713	7-6	5	5	1421	1451	9-4	5	5	324	303	3-2	5	5	675	693
4-10	5	5	1049	1052	9-8	5	5	1162	1232	8-6	5	5	405	368	10-4	5	5	492	469	4-2	5	5	536	569
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6-10	5	5	308	312	11-8	5	5	710	714	10-6	5	5	338	344	12-4	5	5	317	331	6-2	5	5	1701	1633
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8-10	5	5	332	314	13-8	5	5	565	598	12-6	5	5	1098	1096	14-4	5	5	546	569	8-2	5	5	1149	1158
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-8-9	5	5	2170	2256	-9-7	5	5	1053	1067	-5-5	5	5	2077	2156	-11-3	5	5	1205	1284	-16-1	5	5	377	374
-7-9	5	5	525	504	-7-7	5	5	2197	2312	-4-5	5	5	371	413	-10-3	5	5	478	502	-14-1	5	5	1037	1021
-6-9	5	5	1463	1497	-6-7	5	5	1863	1993	-3-5	5	5	1775	1842	-9-3	5	5	1231	1194	-12-1	5	5	726	695
-5-9	5	5	363	316	-5-7	5	5	376	409	-4-5	5	5	1873	1867	-8-3	5	5	1232	1152	-11-1	5	5	956	938
-4-9	5	5	1157	1166	-4-7	5	5	2197	2272	-5-5	5	5	678	656	-7-3	5	5	2078	2033	-10-1	5	5	1671	1621
-3-9	5	5	280	271	-3-7	5	5	941	970	-6-5	5	5	2327	2457	-6-3	5	5	1474	1464	-9-1	5	5	2127	2070
-2-9	5	5	1106	1070	-2-7	5	5	372	412	-5-5	5	5	306	293	-5-3	5	5	834	845	-8-1	5	5	2907	2832
-1-9	5	5	186	229	-1-7	5	5	1929	1974	-4-5	5	5	915	926	-4-3	5	5	2492	2558	-6-1	5	5	1300	1309
0-9	5	5	674	653	0-7	5	5	788	747	-3-5	5	5	300	320	-3-3	5	5	1574	1620	-5-1	5	5	655	657
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2-9	5	5	359	369	2-7	5	5	676	680	-1-5	5	5	1416	1443	0-3	5	5	1353	1442	-3-1	5	5	910	936
3-9	5	5	453	423	3-7	5	5	227	260	0-5	5	5	439	487	1-3	5	5	1921	1964	-2-1	5	5	393	430
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5-9	5	5	655	640	5-7	5	5	324	313	2-5	5	5	326	307	3-3	5	5	1949	1972	-2-1	5	5	828	865
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7-9	5	5	341	359	7-7	5	5	738	717	4-5	5	5	346	304	5-3	5	5	952	848	0-1	5	5	697	687
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9-9	5	5	775	771	9-7	5	5	403	414	6-5	5	5	1092	1099	7-3	5	5	906	1206	2-1	5	5	2243	2265
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-13-8	5	5	1236	1205	-13-6	5	5	836	837	-12-4	5	5	549	573	-10-3	5	5	846	876	-7-1	5	5	1552	1589
-11-8	5	5	209	205	-11-6	5	5	1042	1046	-10-4	5	5	459	463	-9-3	5	5	300	300	-6-1	5	5	695	681
-10-8	5	5	1289	1294	-10-6	5	5	801	831	-9-4	5	5	1686	1726	-8-3	5	5	1410	1449	-5-1	5	5	453	441
-8-8	5	5	368	373	-8-6	5	5	803	796	-7-4	5	5	829	842	-6-3	5	5	1484	1439	-4-1	5	5	774	719
-7-8	5	5	1020	1000	-7-6	5	5	460	447	-6-4	5	5	2715	2790	-5-3	5	5	262	317	-4-1	5	5	2396	2346
-6-8	5	5	2255	2357	-6-6	5	5	460	447	-5-4	5	5	2715	2790	-4-3	5	5	262	317	-3-1	5	5	2396	2346

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-12	0	5	746	701	-4-13	6	6	562	573	-5-10	6	6	608	618
-10	0	5	829	754	-3-13	6	6	988	967	-4-10	6	6	280	275
-8	0	5	204	152	-2-13	6	6	894	924	-3-10	6	6	513	514
-6	0	5	1865	1770	0-13	6	6	1183	1200	-2-10	6	6	516	513
-4	0	5	202	155	1-13	6	6	1168	1246	0-10	6	6	886	920
-2	0	5	2639	2656	2-13	6	6	816	824	2-10	6	6	1138	1148
0	0	5	2109	2082	3-13	6	6	675	678	3-10	6	6	543	598
2	0	5	1632	1628	4-13	6	6	437	452	4-10	6	6	2012	2002
4	0	5	904	900	5-13	6	6	539	544	6-10	6	6	890	891
6	0	5	794	816	6-13	6	6	277	261	8-10	6	6	302	264
8	0	5	1564	1582	-13-12	6	6	478	496	-15	-9	6	365	375
10	0	5	859	931	-12-12	6	6	787	759	-14	-9	6	1263	1343
12	0	5	519	549	-9-12	6	6	1098	1146	-13	-9	6	614	607
-3-16	6	6	486	481	-7-12	6	6	883	918	-11	-9	6	416	425
-4-16	6	6	755	726	-6-12	6	6	653	664	-10	-9	6	766	761
-3-16	6	6	464	481	-4-12	6	6	672	696	-9	-9	6	452	481
-1-16	6	6	516	524	-2-12	6	6	573	594	-8	-9	6	742	777
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1-16	6	6	518	489	0-12	6	6	985	988	-4	-9	6	444	426
-9-15	6	6	568	594	2-12	6	6	479	457	-3	-9	6	1161	1212
-7-15	6	6	838	857	3-12	6	6	1404	1424	-2	-9	6	863	896
-6-15	6	6	367	363	5-12	6	6	1039	1016	-1	-9	6	1951	2043
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-4-15	6	6	239	272	-13-11	6	6	628	645	-1	-9	6	920	925
-3-15	6	6	318	305	-11-11	6	6	270	255	2	-9	6	427	405
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1-15	6	6	1066	1049	-7-11	6	6	845	884	8	-9	6	824	806
2-15	6	6	630	627	-6-11	6	6	182	217	9	-9	6	695	630
3-15	6	6	760	740	-5-11	6	6	531	544	-14	-8	6	216	177
-1-14	6	6	508	471	-4-11	6	6	1530	1599	-13	-8	6	894	899
-10-14	6	6	299	351	-3-11	6	6	1052	1064	-12	-8	6	270	236
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-7-14	6	6	257	303	-1-11	6	6	248	234	-10	-8	6	1764	1797
-6-14	6	6	229	249	0-11	6	6	366	408	-9	-8	6	750	792
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-12-13	6	6	656	708	-12-10	6	6	218	179	-3	-8	6	348	344
-11-13	6	6	604	694	-11-10	6	6	603	617	-1	-8	6	1608	1642
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-7-13	6	6	801	587	-8-10	6	6	621	622	3	-8	6	850	855
-6-13	6	6	292	329	-6-10	6	6			4	-8	6		

H30EP+ REZ(CO)6CL3- NO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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-7	-3	6	1969	1967	-11	-1	6	400	404	-5	-14	7	493	492	-2	-11	7	1280	1287	-8	-8	7	951	992
-6	-3	6	1223	1224	-10	-1	6	807	775	-4	-14	7	420	372	-1	-11	7	487	456	-7	-8	7	468	509
-5	-3	6	653	608	-8	-1	6	1252	1241	-2	-14	7	627	616	0	-11	7	566	539	-6	-8	7	710	729
-4	-3	6	1217	1225	-1	-1	6	463	464	-1	-14	7	788	806	1	-11	7	248	239	-5	-8	7	380	369
-3	-3	6	641	902	-1	-1	6	1630	1590	0	-14	7	586	595	2	-11	7	1173	1184	-4	-8	7	543	543
-2	-3	6	645	677	-1	-1	6	454	416	1	-14	7	1335	1350	3	-11	7	1121	1179	-3	-8	7	1231	1226
-1	-3	6	1343	1359	-4	-1	6	904	918	2	-14	7	294	264	4	-11	7	817	790	-2	-8	7	402	396
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1	-3	6	674	721	-2	-1	6	2681	2783	-1	-13	7	377	374	-1	-10	7	701	721	0	-8	7	1006	1020
2	-3	6	1783	1825	-1	-1	6	1849	1873	-9	-13	7	285	230	-1	-10	7	424	379	1	-8	7	477	448
3	-3	6	724	745	0	-1	6	423	404	-8	-13	7	723	750	-8	-10	7	256	318	2	-8	7	678	639
4	-3	6	295	256	1	-1	6	998	1068	-6	-13	7	825	870	-6	-10	7	1230	1314	3	-8	7	456	438
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6	-3	6	1093	1093	4	-1	6	359	363	-3	-13	7	783	803	-3	-10	7	1389	1445	5	-8	7	662	657
7	-3	6	385	382	6	-1	6	1088	1101	-4	-13	7	355	346	-2	-10	7	1463	1478	6	-8	7	339	331
8	-3	6	817	876	8	-1	6	585	590	-3	-13	7	355	346	-1	-10	7	1463	1478	7	-8	7	321	275
9	-3	6	745	771	9	-1	6	997	1045	-1	-13	7	1088	1083	-1	-10	7	694	690	8	-8	7	577	587
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13	-3	6	365	400	13	-1	6	964	971	5	-13	7	624	654	4	-10	7	300	329	12	-8	7	851	861
14	-3	6	815	804	14	0	6	842	832	6	-13	7	499	532	5	-10	7	761	770	13	-8	7	211	221
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19	-3	6	2168	2145	19	0	6	666	730	11	-13	7	537	562	10	-10	7	801	853	18	-8	7	241	267
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H3DEP+ REZ(CO)6CL3- MD DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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7	-7	8	419	422	5	-4	8	1340	1355	-15	-1	8	641	618	-11	-11	9	728	747	4	-8	9	516	515
-15	-6	8	320	301	6	-4	8	876	870	-14	-1	8	270	287	-10	-11	9	390	469	5	-8	9	782	767
-13	-6	8	379	365	7	-4	8	1502	1617	-13	-1	8	361	344	-9	-11	9	369	395	-12	-7	9	652	667
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-22	-3	6	303	262	16	-2	6	297	244	-6	-18	7	380	394	7	-14	7	428	464	-16	-7	7	384	382
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H30EP+ RE2(CO)6CL3- MD DATA 40-55 DEG 2THETA 10 FO AND 10FC

PAGE 9

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H3DEP+ REZ(CO)6CL3- 10 DATA 40-55 DEG 2THETA 10 FO AND 10FC										PAGE 10									
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Atom	X	Y	Z	U(1)	U(2)	U(3)	U(12)	U(13)	U(23)
B(1)	0.12959(1)	0.19521(1)	0.14057(2)	435(1)	517(1)	626(1)	-46(3)	299(2)	-21(3)
B(2)	0.29162(2)	0.09642(1)	0.21963(2)	486(1)	524(1)	542(1)	21(3)	165(2)	-99(3)
Cl(1)	0.2647(1)	0.2022(1)	0.3046(1)	51(1)	52(1)	57(1)	-17(1)	22(1)	-21(1)
Cl(2)	0.1539(1)	0.0741(1)	0.2135(1)	56(1)	49(1)	61(1)	-19(1)	31(1)	-6(1)
Cl(3)	0.2147(1)	0.1535(1)	0.0594(1)	56(1)	64(1)	52(1)	2(2)	75(1)	-2(2)
N(1)	0.2252(3)	0.0536(3)	0.6760(5)	37(3)	69(4)	60(4)	17(6)	-13(6)	-14(7)
N(2)	0.0901(3)	0.1398(1)	0.5997(4)	42(1)	85(4)	39(1)	15(6)	25(4)	-13(6)
N(3)	0.0159(3)	0.0529(3)	0.4024(4)	39(3)	64(4)	40(3)	-7(6)	5(5)	-7(6)
N(4)	0.1637(3)	-0.0275(3)	0.4853(5)	49(3)	43(4)	63(4)	9(6)	0(6)	-4(6)
C(1)	0.2486(4)	0.0107(4)	0.6951(4)	39(4)	63(5)	60(5)	18(8)	-8(7)	-7(8)
C(2)	0.3456(4)	0.0300(4)	0.7516(5)	32(3)	61(5)	65(5)	7(7)	4(7)	-10(7)
C(3)	0.2154(4)	0.0837(4)	0.8107(6)	37(3)	56(4)	46(4)	-20(7)	-2(6)	-4(8)
C(4)	0.2412(4)	0.0997(4)	0.7552(6)	52(4)	66(5)	49(4)	6(8)	24(6)	-4(8)
C(5)	0.1807(4)	0.1490(4)	0.7598(6)	47(4)	75(5)	43(4)	12(8)	10(6)	-17(8)
C(6)	0.1155(4)	0.1678(4)	0.6689(6)	45(4)	76(5)	49(4)	24(8)	24(6)	-6(8)
C(7)	0.0609(4)	0.2144(4)	0.7029(6)	53(4)	78(5)	46(4)	33(8)	34(6)	-21(8)
C(8)	0.0650(4)	0.1702(4)	0.5404(5)	35(3)	80(5)	57(4)	22(7)	26(6)	-10(8)
C(9)	-0.0447(4)	0.1512(4)	0.4424(6)	34(3)	71(5)	44(4)	25(7)	10(6)	0(8)
C(10)	-0.0477(4)	0.0997(4)	0.3756(4)	35(3)	60(4)	52(4)	13(7)	20(6)	0(7)
C(11)	-0.1022(4)	0.0403(4)	0.2782(5)	34(3)	67(5)	44(4)	1(7)	15(6)	4(7)
C(12)	-0.0799(4)	0.0244(4)	0.2242(5)	34(3)	55(4)	46(3)	-10(7)	16(6)	4(7)
C(13)	0.0015(4)	0.0073(3)	0.3225(5)	34(3)	44(4)	45(3)	0(7)	14(6)	0(7)
C(14)	0.0593(4)	-0.0445(4)	0.3189(6)	49(4)	44(4)	51(4)	-13(7)	11(7)	-3(7)
C(15)	0.1277(4)	-0.0607(4)	0.3919(6)	52(4)	42(4)	62(4)	0(7)	17(7)	-29(9)
C(16)	0.1741(5)	-0.1134(4)	0.3400(7)	52(4)	57(4)	77(5)	39(8)	-10(8)	-52(11)
C(17)	0.2404(5)	-0.1143(4)	0.5345(8)	65(5)	66(5)	111(7)	71(9)	-6(9)	-29(9)
C(18)	0.2916(5)	-0.0437(4)	0.5516(7)	49(4)	76(5)	91(6)	54(8)	-19(9)	-25(10)
C(19)	0.4371(5)	-0.0017(5)	0.4404(7)	52(4)	74(6)	90(5)	13(10)	-21(9)	-22(11)
C(20)	0.4853(6)	0.0320(7)	0.4082(13)	10(5)	110(9)	254(15)	24(13)	58(15)	-7(10)
C(21)	0.3477(5)	0.1142(5)	0.5733(10)	62(5)	97(7)	65(5)	41(10)	26(8)	-4(11)
C(22)	0.3914(7)	0.1944(6)	0.5233(10)	60(4)	102(8)	115(9)	-36(14)	-17(15)	-24(15)
C(23)	0.0749(5)	0.2522(5)	0.5054(7)	55(5)	96(6)	75(5)	15(10)	22(6)	4(11)
C(24)	0.1375(4)	0.3095(6)	0.6207(9)	92(7)	92(7)	114(8)	11(13)	37(13)	-24(13)
C(25)	-0.0751(5)	0.2425(5)	0.5872(7)	61(5)	90(6)	98(5)	27(9)	24(8)	-9(14)
C(26)	-0.0574(7)	0.3295(6)	0.5443(9)	91(7)	102(8)	102(4)	60(13)	-12(14)	-29(9)
C(27)	-0.1749(4)	0.1205(5)	0.5196(6)	33(3)	95(5)	60(4)	24(8)	7(7)	57(11)
C(28)	-0.1544(5)	0.1702(5)	0.1441(8)	67(5)	90(4)	90(6)	74(10)	38(9)	1(12)
C(29)	-0.1004(4)	-0.0114(4)	0.1401(6)	41(4)	63(5)	63(4)	-15(8)	8(7)	-47(10)
C(30)	-0.0744(5)	0.0064(5)	0.0620(8)	83(5)	82(6)	63(4)	-34(10)	77(8)	-23(10)
C(31)	0.1594(5)	-0.1551(4)	0.2225(8)	61(5)	63(5)	63(5)	20(9)	-7(10)	-39(12)
C(32)	0.1941(4)	-0.1190(5)	0.3052(8)	54(6)	64(6)	103(7)	23(11)	58(14)	-39(12)
C(33)	0.3077(4)	-0.1774(8)	0.5156(9)	163(10)	217(13)	91(7)	-190(19)	170(17)	17(17)
C(34)	0.3570(10)	-0.1500(7)	0.4439(11)	266(15)	115(11)	134(9)	4(22)	31(7)	14(9)
C(35)	0.0347(4)	0.1783(4)	0.0446(6)	54(4)	67(5)	70(5)	-3(8)	29(9)	-7(9)
C(36)	0.0775(4)	0.2119(4)	0.2474(7)	95(6)	53(5)	69(5)	-59(9)	62(7)	-34(10)
C(37)	0.1205(4)	0.2464(4)	0.1224(7)	45(3)	60(5)	101(5)	25(8)	22(5)	-28(9)
C(38)	0.1217(4)	0.2252(7)	0.2252(7)	55(3)	54(5)	78(6)	9(9)	7(8)	-26(9)
C(39)	0.2764(4)	0.0201(4)	0.1386(7)	49(4)	59(5)	83(5)	-11(8)	7(8)	-9(10)
C(40)	0.3400(4)	0.0454(4)	0.3457(8)	73(4)	56(5)	79(5)	-14(10)	8(10)	-14(9)
C(41)	-0.0212(3)	0.1470(3)	-0.0272(6)	61(4)	107(5)	107(5)	-34(8)	-36(8)	-5(8)
C(42)	0.0254(3)	0.2237(3)	0.3005(6)	103(5)	104(5)	114(4)	3(7)	142(5)	-25(8)
C(43)	0.1154(4)	0.3419(3)	0.0987(6)	103(4)	53(3)	154(5)	32(7)	47(8)	-34(10)
C(44)	0.4561(3)	0.1377(4)	0.2277(6)	56(3)	113(5)	163(6)	-44(7)	52(7)	-52(7)
C(45)	0.2907(3)	-0.0237(3)	0.0277(6)	45(4)	74(4)	121(4)	1(7)	36(10)	6(9)
C(46)	0.1407(3)	0.0150(4)	0.4191(6)	140(7)	99(5)	104(5)	29(11)	-36(10)	0(6)
C(47)	0.1407(3)	0.1234(3)	0.4704(4)	79(3)	79(4)	31(7)	-2(6)	73(5)	0(6)
C(48)	0.109(3)	0.049(3)	0.562(4)	40					
C(49)	0.100(3)	0.149(3)	0.544(4)	40					
C(50)	0.046(3)	0.052(3)	0.445(4)	49					

APPENDIX

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