Properties of Distorted Tetraphenylporphyrins

Thesis by
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Acknowledgments:

I owe a large debt of gratitude to my advisor, Harry B. Gray. Harry, thanks for your faith in and support of me. I will always look back on the time I have spent in your labs with gratitude for the learning I was allowed to do there. Additionally, I can't count the number of times I walked into your office demoralized only to emerge rejuvenated.

I have put off writing this part of my thesis for as long as possible as I know that I will not be able to do justice to my feelings for people at Caltech, both past and present, in print. Your friendship has been and continues to be a vital part of my life. I will see you all and tell you in person.

To all the people who I have had the pleasure to work with thank you for teaching me all the things you did and for making my graduate career relatively painless.

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Abstract:

X-ray crystallographic structure determinations reveal that tetrakis(pentafluorophenyl)-porphyrin derivatives substituted with bulky β-substituents undergo a tetrahedral distortion that reduces the macrocyclic symmetry from D_{4h} to D_2. The nickel complex of [2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin], $NiTFPPBr_8$, has nitrogen atoms displaced ±0.192 Å and *meso*-carbons ±0.211 Å from the plane of the porphyrin. Despite large conformational changes, bond distances and angles are essentially conserved for all tetraphenylporphyrins. Electrochemical and UV-vis spectroelectrochemical experiments revealed a novel, ligand-centered two-electron (2e) oxidation for Zn and Mg derivatives. Values for the 1e potentials were calculated from K_{disp}, the constant for the disproportionation of the singly oxidized product into the doubly oxidized and the neutral species, $E^{o'}_{2+/0}$, and the Nernst equation. The redox potentials are consistent with semiempirical AM1 calculations that indicate that $D_{4h} \rightarrow D_2$ distortion destabilizes the HOMOs (a_{1u}, $a_{2u} \rightarrow$ a, b_1) preferentially over the ($e_g \rightarrow b_2$, b_3) LUMOs whereas halogen substitution lowers the energy of both the HOMO and the LUMO approximately equally. Consistent with the *meso*-substituent influencing relative ordering, EPR spectra of $ZnTPP^+$, and $ZnTFPP^+$, and $ZnTFPPBr_8^+$ reveal a_{2u}, a_{1u}, and a(a_{1u}) HOMOs, respectively. Furthermore, the β-octaethyl and octamethyl tetrakis(pentafluorophenyl)porphyrins undergo a similar net 2e oxidation. Thus, the distortion observed in the neutral molecule appears to mirror an electronically favorable geometry for the doubly oxidized product. An understanding of the sterics and electronics that influence frontier orbital energy levels creates the possibility of tuning porphyrins for a variety of applications: light harvesting, electron transfer, and catalytic reactions involving 2e reductions.

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CHAPTER 1:

INTRODUCTION

Porphyrins and porphyrin-like species have been and continue to be the subjects of numerous studies stemming from their central roles in diverse biological reactions. They are light harvesters and reductants[1] in the photosynthetic reaction center, and ligands both in the catalytic sight in monooxygenase enzymes, such as cytochrome C and catalase, and in the center for reversible oxygen binding in hemoglobins and myoglobins.[2,3] They are the pigments that produce the green color in plants and the red and blue colors of blood. Symmetric porphyrins, such as 5,10,15,20-tetraphenylporphyrin TPP and octaethylporphyrin, OEP, have been synthesized. Figure 1 contains pictures of the various natural, with, in some cases, an indication of the enzyme or environment that they can be found in, and synthetic porphyrin derivatives. It is of interest to explore the properties of metalloporphyrins not only to gain insight into their biological functions, but also in order to exploit their catalytic and light-harvesting potential. In nature the functionality and effectiveness of the metalloporphyrin is dependent not only on environment, i.e., the size of enzyme pocket or availability of axially coordinating ligands, but also upon the nature of the substitution around the porphyrin macrocycle. The β-octaalkylated derivatives of TPP have been studied to understand the effects of changes in macrocyclic conformation on biological function.[4-10]

The studies presented here concern synthetic TPP derivatives, specifically the β-halogenated and alkylated derivatives of TFPP (TFPP = 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin),[11] $TFPPX_8$ (where X= H, Cl, Br, Me, Et). Figure 2 contains a picture of $TFPPX_8$ as well as an explanation of notation. The synthesis β-halogenated derivatives was first reported by Callot.[12-14] Lyons and Ellis exploited Fe, Mn, and Cr derivatives of these ligands as biomimetic catalysts for the selective oxidation of the tertiary and secondary positions of light alkanes.[15,16] Other workers had previously used the metalloporphyrins for biomimetic hydroxylation and epoxidation involving iodosylbenzene and H_2O_2.[13] Lyons and Ellis discovered that these catalysts can use dioxygen from the air and function for many turnovers without added coreductants. Recent mechanistic work indicates that the mechanism is probably not biomimetic, i.e., involving a $P^{+}Fe(IV)=O$ species (where P^{+} = a porphyrin cation radical) as the postulated oxidant,[17-19] at all, but is radical-based and Fenton-like in that the $FeTFPPX_8$ (X = Cl, Br) cycles between its Fe^{2+} and Fe^{3+} states splitting the alkylhydroperoxides (Haber-Weiss mechanism) formed from alkyl autooxidation.[20,21] The information reported here about the changes in electronics induced by halogenation is consistent with this mechanistic insight.

Chapter 2 presents crystallographically determined structures of the unmetallated and metallated derivatives of the completely halogenated porphyrin macrocycles, [2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin]M(II), $MTFPPCl_8$, (M = Cu) and [2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin]M(II) (M = Cu, Ni, Zn, and H_2), $MTFPPBr_8$. The structural consequences of the substitution of the periphery of the porphyrin with bulky electron-withdrawing substituents are a distortion that reduces the molecular symmetry from D_{4h} to D_2. Appendices 1-7 contain ORTEPs and supplementary material for the crystal structure determinations.

Gouterman's four orbital model is an extremely effective scheme for interpreting the electronic behavior of the porphyrin macrocycle.[22] The four frontier orbitals of D_{4h} symmetric porphyrins are divided into two nearly degenerate HOMO's of a_{1u} and a_{2u} symmetry and two LUMO's of e_g symmetry (a_{1u}, $a_{2u} \rightarrow$ a, b_1, $e_g \rightarrow b_2$, b_3 in D_2). The relative energies HOMO and LUMO orbitals as well as of the a_{1u} versus the a_{2u} are modulated by metal substitution and the placement and electronic nature of the substituents on the porphyrin ring.

Chapter 4 contains electronic spectra and Chapter 3 electrochemical data for the β-halogenated and alkylated TFPPs. The red-shifted UV-vis spectra for the distorted porphyrins reveal that the energy gap between the HOMO and LUMO orbitals has narrowed. Halogenation of the porphyrin makes the porphyrin macrocycle and any redox active metal center more difficult to oxidize and more easy to reduce. The effect of halogen substitution is larger on the ring redox potentials than on metal-based ones. Semiempirical AM1 calculations[23] and electrochemical data reveal that the HOMO orbitals are more sensitive to distortion than the LUMO. The observation of a two electron oxidation wave for the Zn and Mg derivatives of $TFPPX_8$ but not $TPPX_8$ (X = Cl, Br, Me, Et) illustrates the extreme sensitivity of the frontier orbitals to the nature of the substituent. Chapter 5 presents some conclusions and attempts to sort out the relative effects of substituents and distortion on the energies of the HOMOs and LUMOs through comparisons between porphyrins with varying substitution.

References and Notes:

(1) Dolphin, D.; Felton, R. H. *Acc. Chem. Res.* **1974**, *7*, 26-32.

(2) Lehninger, A. L. *Biochemistry;* 2nd ed.; Worth Publishers, Inc.: New York, 1975.

(3) Bertini, I.; Gray, H. B.; Lippard, S. J.; Valentine, J. S. *Bioinorganic Chemistry*; University Science Books: Mill Valley, CA, 1994.

(4) Barkigia, K. M.; Renner, M. W.; Furenlid, L. R.; Medforth, C. J.; Smith, K. M.; Fajer, J. *J. Am. Chem. Soc.* **1993**, *115*, 3627-3635.

(5) Barkigia, K. M.; Berber, M. D.; Fajer, J.; Medforth, C. J.; Renner, M. W.; Smith, K. M. *J. Am. Chem. Soc.* **1990**, *112*, 8851-8857.

(6) Czernuszewicz, R. S.; Li, X.-Y.; Spiro, T. G. *J. Am. Chem. Soc.* **1989**, *111*, 7024-7031.

(7) Shelnutt, J. A.; Medforth, C. J.; Berber, M. D.; Barkigia, K. M.; Smith, K. M. *J. Am. Chem. Soc.* **1991**, *113*, 407-4087.

(8) Sparks, L. D.; Medforth, C. J.; Park, M.-S.; Chamberlain, J. R.; Ondrias, M. R.; Senge, M. O.; Smith, K. M.; Shelnutt, J. A. *J. Am. Chem. Soc.* **1993**, *115*, 581-592.

(9) Medforth, C. J.; Senge, M. O.; Smith, K. M.; Sparks, L. D.; Shelnutt, J. A. *J. Am. Chem. Soc.* **1992**, *114*, 9859-9869.

(10) Takeda, J.; Ohya, T.; Sato, M. *Inorg. Chem.* **1992**, *31*, 2877-2880.

(11) Longo, F. R.; Finarelli, M. G.; Kim, J. B. *J. Heterocycl. Chem.* **1969**, *6*, 927-931.

(12) Wijesekera, T.; Matsumoto, A.; Dolphin, D.; Lexa, D. *Angew. Chem. Int. Ed. Engl.* **1990**, *29*, 1028-1030.

(13) Traylor, T. G.; Tsuchiya, S. *Inorg. Chem.* **1987**, *26*, 1338-1339.

(14) Callot, H. J. *Bull. Soc. Chim. Fr.* **1974**, 1492-1496.

(15) Ellis, P. E.; Lyons, J. E. *Catal. Lett.* **1991**, *8*, 45-52.

(16) Ellis, P. E.; Lyons, J. E. *Cataylsis Letters* **1989**, *3*, 389-398.

(17) Montellano, P. R. O. d. *Cytochrome P-450: Structure, Mechanism, and Biochemistry*; Plenum Press: New York, 1986.

(18) Paengand, K. J.; Kincaid, J. R. *J. Am. Chem. Soc.* **1988**, *110*, 7913.

(19) Leising, R. A.; Kojima, T.; Que, L. In *The Activation of Dioxygen and Homogeneous Catalytic Oxidation*; D. H. R. Barton, A. E. Maretell and D. T. Sawyer, Eds.; Plenum Press: New York, 1993; pp 321-331, and references therein.

(20) Labinger, J. A. *Catal. Lett.* **1994**, *26*, 95-99.

(21) Grinstaff, M. W.; Hill, M. G.; Labinger, J. A.; Gray, H. B. *Science* **1994**, *264*, 1311-1313.

(22) Gouterman, M. In *The Porphyrins*; D. Dolphin, Ed.; Academic Press: New York, 1978; Vol. III; pp 1-165.

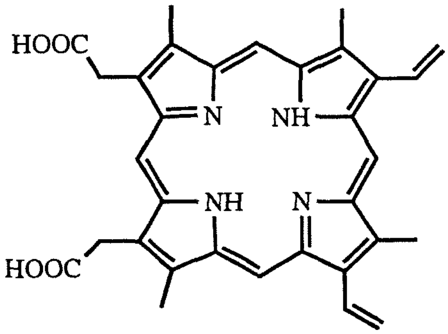
(23) Takeuchi, T.; Gray, H. B.; Goddard, W. A. *J. Am. Chem. Soc.* **1994**, *116*, 9730-9732.

Table 1.1. Abbreviations for Natural and Synthetic Porphyrins.

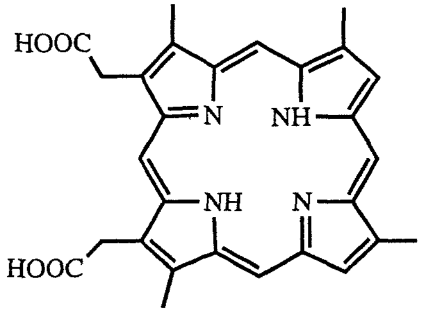
H_2Deut	2,4-diacetlydeuteroporphyrin
H_2P	porphyrin
H_2OEP	octaethylporphyrin
H_2TPP	5,10,15,20-tetraphenylporphyrin
H_2TPPBr_8	2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin
H_2TPPEt_8	2,3,7,8,12,13,17,18-octaethyl-5,10,15,20-tetraphenylporphyrin
H_2TPPMe_8	2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetraphenylporphyrin
H_2TFPP	5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
$H_2TFPPBr_8$	2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
$H_2TFPPCl_8$	2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
$H_2TFPPEt_8$	2,3,7,8,12,13,17,18-octaethyl-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
$H_2TFPPMe_8$	2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
H_2TMP	Tetramesitylporphyrin

Figure 1.1. Common natural and synthetic porphyrins.

Natural Porphyrins:

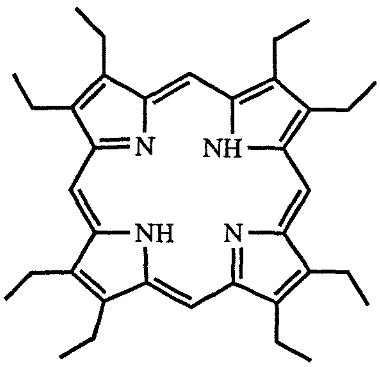


Protoporphyrin IX,
(hemoglobin, myoglobin, and
most cytochromes)

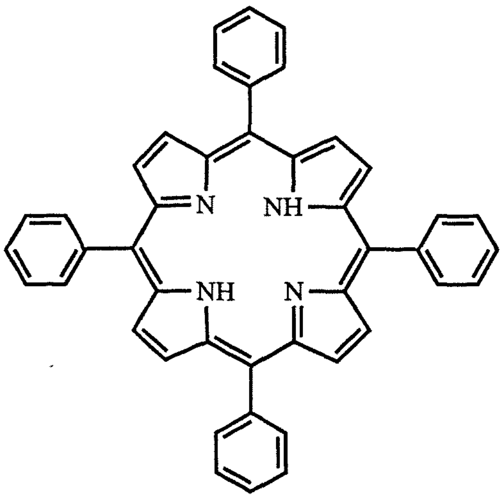


Deuteroporphyrin

Synthetic Porphyrins:

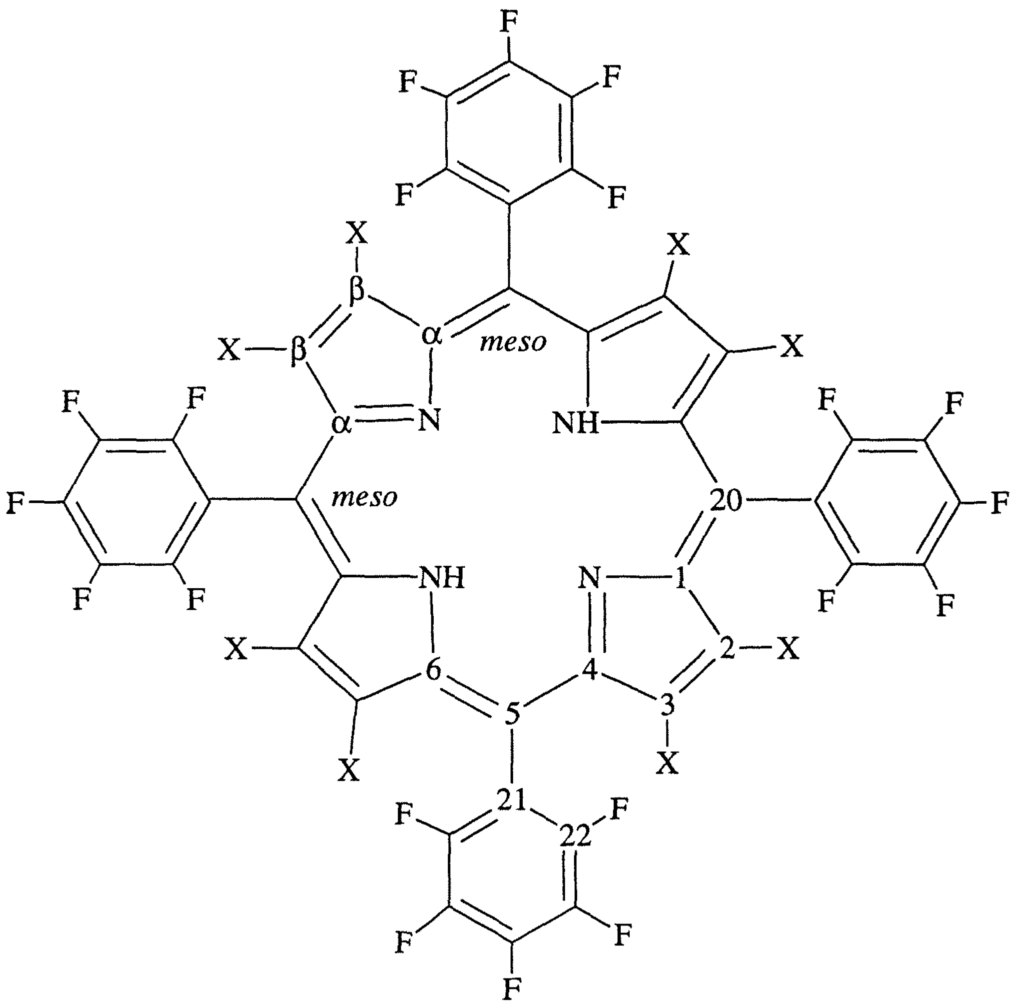


OEP



TPP

Figure 1.2. β-octasubstituted (H, Cl, Br, Me, Et) 5,10,15,20-tetrakis-(pentafluorophenyl)porphyrins with atomic numbering scheme and nomenclature.


F
F
F
F
F
X
X
β
X
β
α
meso
α
N
NH
meso
20
NH
N
1
2
X
6
5
4
3
X
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21
22
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CHAPTER 2:

SYNTHESIS AND X-RAY CRYSTAL STRUCTURES OF TETRAKIS(PENTAFLUOROPHENYL)PORPHYRINS

Introduction:

This chapter presents both the methods for the synthesis and metallation of tetrakis(pentafluorophenyl)porphyrin (TFPP) ligands substituted with either halogens or alkyl groups at the β-positions, and the structural consequences of β-substitution on the expected planarity of the macrocycle. Most syntheses presented are derived from standard procedures in porphyrin chemistry, with modifications. It was found that TFPP derivatives are less susceptible to chromatographic and light degradation than the tetraphenylporphyrin (TPP) derivatives and therefore are more easily studied. X-ray crystallographic structure determination revealed that the macrocycles with bulky β-substituents are highly nonplanar. Comparisons of the average displacements of the *meso-* and β- carbon atoms from a plane defined by the four nitrogen atoms indicates that the ruffling of the porphyrin macrocycle increases along the series: $H_2 \approx Zn < Cu < Ni$. Nonplanarity does not significantly alter the bond lengths in the porphyrin macrocycle, as compared to structures determined for planar tetraphenylporphyrins and to Hoard's 'average porphyrin'.[1,2] Resonance Raman data for the 'structural marker' bands, i.e., those bands that are sensitive to macrocyclic distortion, for the halogenated porphyrins are also discussed and compared to those for distorted β-octaalkylated TPPs.

Results and Discussion:

Synthesis:

The synthesis of perhalogenated tetraphenylporphyrins, $H_2TFPPCl_8$ and $H_2TFPPBr_8$, can be accomplished via two different routes in 2-3 hrs, starting with the commercially available compound, ZnTFPP. The free ligand is significantly more difficult to halogenate than the metallated porphyrin and it is therefore necessary to avoid demetallating reaction conditions, such as production of large quantities of HCl. Halogenation of the pyrrole positions can either be accomplished with $Cl_2(g)$ or $Br_2(l)$ in dry refluxing CCl_4[3,4] or with *N*-chlorosuccinimide (NCS) or *N*-bromosuccinimide (NBS) in refluxing CH_3OH.[5,6] Both methods produce material which is contaminated with partially halogenated products (determined through isolation of bands from a preparatory thin-layer chromatogram (tlc) and mass spectral analysis of the resulting products). Essentially pure perhalogenated porphyrin can be obtained via careful purification on flash silica gel.

Attempts to synthesize the perfluorinated derivative with a variety of fluorinating agents, such as F_2, CoF_3, AgF_2, and XeF_2 (starting with ZnTFPP),[7] and halogen exchange reagents, KF, $(CH_3)_4NF$, and HF (starting with $ZnTFPPBr_8$ or $ZnTFPPCl_8$),[8] proved unsuccessful. The fluorinating agents which reacted by radical mechanisms, F_2, CoF_3, AgF_2, and XeF_2 were found in general to produce highly fluorinated products (characterized by mass spec, UV-vis,[9] and ^{19}F NMR) in which the porphyrin had lost aromaticity. It was found in reactions with KF that despite the robust nature of the perhalogenated catalysts, high temperatures (> 100 °C) coupled with the presence of metal salts frequently cause dehalogenation of the β-positions.

$H_2TFPPMe_8$ can be synthesized according to the scheme shown in Figure 2.1. Ethyl-3,4-dimethylpyrrole-2-carboxylate was synthesized by the method of Barton and Zard[10] and decarboxylated in refluxing ethylene glycol/NaOH solution.[11] The resulting 3,4-dimethyl pyrrole was condensed with pentafluorobenzaldehyde to generate the octamethylporphyrin according to the procedure of Lindsey et al.[12,13] $H_2TFPPEt_8$ can be synthesized in a similar manner, coupling the 3,4-diethyl pyrrole with pentafluorobenzaldehyde. The methodology for the synthesis of the β-ocaalkylated TFPPs is similar to that employed in the synthesis of β-ocaalkylated TPPs. This represents one of the first, if not the first report of the synthesis of the these TFPP derivatives.

The synthesis of the related tetraphenylporphyrins was found to be less facile.[12,14,15] The tetraphenylporphyrins, especially the Zn derivatives, are unstable on various chromatographic material (alumina and silica gel). Typically, Zn derivatives of porphyrins are known to be photosensitive, although the tetrakis(pentafluorophenyl) derivatives are not. It would appear that substitution of the *meso* position of the porphyrin with a perfluorophenyl group confers stability to the macrocycle.

Distorted porphyrins are easily demetallated by bubbling $HCl_{(g)}$ through a room temperature $CHCl_3$ solution for 3-5 min. Other acids, such as HF and HBr, are also capable of demetallating the porphyrin. A short alumina column is used to separate the porphyrin from the metal salt and any remaining Zn porphyrin. The zinc, magnesium, copper, nickel, palladium and cobalt derivatives can be synthesized from the corresponding metal acetates in $CH_3OH/CHCl_3$ solutions.[16] Distorted porphyrins are easier to metallate than planar ones.[17,18] More difficult metallations, such as for Fe, can be accomplished in 120 °C dimethylformamide (DMF).[19] Care must be taken because decomposition of DMF leads to substitution of the para fluorine of the phenyl ring by dimethylamine.[20]

The progress of the halogenation reaction can be followed both by tlc and UV-vis. The UV-vis bands of ZnTFPP red-shift and broaden. Due to the sensitivity of the fluorine nucleus to environment and the large spectral window for fluorine shifts, ^{19}F NMR has proven to be a useful technique for determining the degree of contamination with the 5, 6, and 7- halogenated derivatives.[5]

Structural Characterization:

Crystals were grown and structures determined for the following derivatives: H_2TFPP, CuTFPP,[5] $CuTFPPCl_8$,[21] $H_2TFPPBr_8$,[5] $NiTFPPBr_8$,[22,23] $CuTFPPBr_8$[23] and $ZnTFPPBr_8$.[24] ORTEPs for the structures can be found in Figure 1 of Appendixes 1-7 (supplementary material for the X-ray crystal structure determinations). Structures for $H_2TFPPCl_8$, $ZnTFPPCl_8$,[5] $[RuTFPPCl_8](CO)H_2O$,[25] $[FeTFPPBr_8]Cl$, and $[FeTFPPBr_8]Py_2$ (where Py = pyridine)[26-28] have also been obtained by coworkers.

H_2TFPP and CuTFPP both crystallized in spacegroup $R\bar{3}$ without solvent molecules in the lattice. $CuTFPPCl_8$ crystallized with one molecule of CH_2Cl_2 per porphyrin. Although the N atoms of the core are slightly (± 0.076 Å) tetrahedrally distorted, the copper ion has approximately square-planar coordination as is typical for Cu(II) porphyrins,[1] with a Cl from the dichloromethane at 3.51 Å as the closest axial neighbor to the copper. $H_2TFPPBr_8$ crystallized with molecules of *o*-dichlorobenzene stacked between the porphyrins. A view of this stacking can be seen in Figure A4.2. The crystals of $NiTFPPBr_8$ and $CuTFPPBr_8$ are isostructural (spacegroup C2/c). The unit cell contains eight porphyrins and four molecules of CH_2Cl_2. The Ni(II) and Cu(II) ions are four-coordinate; the nearest axial neighbors, Br atoms from adjacent molecules, at 3.42 and 3.53 Å in $NiTFPPBr_8$ and 3.36 and 3.48 Å in $CuTFPPBr_8$, are too distant to bond formally. The metal-nitrogen bond distances observed in these structures are within the typical range observed for M(II) ions coordinated to porphyrin ligands.[1] Typical closest porphyrin-porphyrin distances within the macrocycle are 3.9 Å for $NiTFPPBr_8$, thus precluding the possibility of π-π interactions between the porphyrin molecules.

The $ZnTFPPBr_8$ molecule crystallized from a complex mixture of solvents. The unit cell contains both a CCl_4 and *o*-dichlorobenzene molecule per $ZnTFPPBr_8$ molecule. The zinc ion is five-coordinate and has an axially coordinated oxygen atom from either a methanol half of the time or an acetone half of the time. Figure A7.2 contains an ORTEP projection of the unit cell. There is a crystallographic mirror plane through N1, Zn and N3, perpendicular to the porphyrin plane. The zinc ion sits 0.180 Å above the plane of the porphyrin (toward the coordinated oxygen atom). The Zn-O bond length, 2.16 Å, is similar to the Zn-O bond length of 2.22(5) Å for $ZnTMPP(H_2O)$.[29] In contrast, the structures determined for ZnTFPP and $ZnTFPPCl_8$ show the zinc atom to be four-coordinate and inside the porphyrin core. Reports of both in and above-the-plane zinc coordination exist for a variety of zinc porphyrin complexes.[1,30,31] In general, it is not unusual for porphyrins to include a variety of solvents within the crystal lattice, a property that has led to them being called 'porphyrin sponges'.[32] The inefficiency of recrystallization as a method for purification is perhaps explained.

Tables 2.1 and 2.2 contains a selection of average bond lengths; and Tables 2.3 and 2.4 list average angles determined for all the structures and a comparison to Hoard's 'average porphyrin'. X-ray crystallographically determined structures for H_2TFPP, $H_2TFPPCl_8$, and $H_2TFPPBr_8$ are shown in Figure 2.2. Figure 2.3 contains representations of the structures for the copper derivatives of the halogenated series.

The porphyrin macrocycle, which is essentially planar in TFPP (D_{4h} symmetry), appears increasingly more tetrahedrally distorted in $TFPPCl_8$ and $TFPPBr_8$ (D_2 symmetry) (Figs. 2.2 and 2.3). The individual pyrrole rings are essentially planar. The distortion of the porphyrin can be viewed as follows: pairs of bromines are alternately above and below the plane of the macrocycle as are the *meso*-carbons. The macrocyclic distortions can be quantified as the average displacements of the relevant atoms from a plane defined by the four N atoms (Tables 2.5 and 2.6). The two types of distortion observed, manifested in the nonplanarity of the *meso*- and β-carbons, have been termed 'ruffle' (or a twist distortion) and 'saddle', respectively.[33] The distortion minimizes the sterically unfavorable (short) interatomic contacts between the β-substituents and the ortho-carbon of the phenyl rings.

Despite these large changes in macrocyclic conformation, bond distances are essentially conserved (see the resonance Raman section for further discussion; also, it is difficult to determine trends since differences between bond lengths and angles are usually within the error associated with the determination of the bond length or angle) for all the halogenated and unhalogenated copper derivatives. Within experimental error, the values observed for the bond lengths and angles are within the 'average' range reported by Hoard[2] for planar porphyrins with varying metal substitutions and substituents (Tables 2.1, 2.2, 2.3 and 2.4). The distortion of the macrocycle appears to be accomplished through the adjustment of bond angles and bond torsion angles. The halogenated derivatives appear to be slightly more structurally amorphous, i.e., they exhibit more variation in chemically equivalent bond lengths within a single molecule than do their unhalogenated counterparts; this can be seen in the deviation in the crystallographically different bonds for the N-C_α and

C_α-C_β bonds (Table 2.2). Although the phenyl rings are rotated into the plane of the porphyrin in the distorted derivatives, C_{Ph}-C_{meso} distances indicate negligible double bond character between the phenyl group and the porphyrin.

The free ligand contains less twist distortion than do the metallated derivatives (except $CuTFPPCl_8$). This difference can be viewed in Figures 2.4 and 2.5, which contain simplified representations of the unmetallated and metallated porphyrin macrocycles. The most distorted macrocycle is that of $NiTFPPBr_8$, consistent with ruffling contracting the core of the porphyrin (as measured by the shorter M-N bond lengths for Ni as compared to Cu and Zn). For the $NiTFPPBr_8$ macrocycle, nitrogen atoms are displaced alternately ±0.192 Å, *meso*-carbons ±0.211 Å, β-carbons ±1.31 Å, and bromine atoms ±2.05 Å from the plane of the porphyrin. The Zn(II) and the H_2 derivatives are the least distorted (in the Zn(II) structure the metal atom is sitting slightly above the porphyrin core).

The metal-induced structural changes for the perhalogenated TPPs are qualitatively similar to those observed for metallosubstitution in OEP and β-octaalkyl TPPs. C_α-C_{meso} bond lengths and C_α-C_{meso}-C_α bond angles increase, and N-C_α and C_α-N-C_α bond angles decrease with increasing size of the metal.[5,34]

Resonance Raman Spectroscopy:

The resonance Raman spectra of porphyrins contain two relatively intense bands, associated with in-plane skeletal modes, that have been observed to shift with porphyrin macrocyclic distortion.[35] These bands, ν_2 and ν_4, are primarily associated with C_β-C_β stretching modes (calculated to be 60 % of ν_2 with an additional 19% associated with C_β-Et vibrations) and C_α-N and C_α-C_{meso} stretching modes (53 % and 24% of ν_4, respectively), respectively.[36] These polarized peaks are found in the resonance Raman spectra that arise from excitation near the B absorption band. Table 2.8 contains values for ν_2 and ν_4 for halogenated and unhalogenated Ni(II)tetraphenylporphyrins; the spectra are given in Appendix 8.[37,38] Although ν_2 and ν_4 are primarily skeletal modes, ν_2 also contains some phenyl character, as can be seen from the shift observed from NiTPP to NiTFPP of -4 cm^{-1}, as well as the C_β-substituent (and perhaps c_{meso}-substituent) character that is observed in the +28 cm^{-1} shift from NiTPP to NiOEP; ν_4 is less perturbed in a similar comparison: +1 cm^{-1} and +9 cm^{-1}. Both bands shift to lower energy (-10 cm^{-1}) with increasing distortion of the macrocycle; and these shifts are within the range reported by Shelnutt et al.[35] for the similarly distorted β-octaalkyltetraphenylporphyrins. Although the effects of changes in reduced mass and altered electronics (i.e., electron-withdrawing versus electron-donating substituents) on the frequencies of the observed skeletal modes are not entirely clear, in a comparison between NiP and NiOEP the effect of β-alkyl substitution is not to *lower* the frequency of ν_4 and ν_2.

Conclusions:

The $TFPPCl_8$ derivatives are about two-thirds as distorted as the $TFPPBr_8$ derivatives, consistent with the chlorine atom having a smaller van der Waals radius than bromine. Although no structure was determined for $NiTFPPCl_8$, the metal effects found for the other derivatives of the $TFPPCl_8$ ligand mirror those determined for the $TFPPBr_8$ derivatives, such that the free ligand and Zn are less distorted than the Cu derivatives and this distortion approximately correlates with M-N bond lengths. A dampening of ruffling with increasing M-N bond length has been observed in β-octaalkyltetraphenylporphyrins.[34] Although the porphyrin is extremely sterically crowded, it is still relatively flexible. This flexibility has previously been observed; in fact, two crystalline forms exist for NiOEP (OEP = octaethylporphyrin): one that is essentially planar (triclinic crystals)[39] and one that is twist-distorted (tetragonal crystals).[40] In the more ruffled structure, M-N bond lengths are contracted from 1.958(2) Å (planar) to 1.929(3) Å (ruffled). Resonance Raman experiments indicate that a solution of NiOEP contains a variety of flat and ruffled structural polymorphs.[41] For the $NiTPPR_8$ molecules M-N bond lengths have been used in EXAFS studies to judge the degree of distortion of the porphyrins.[42]

The distortions observed in these perhalogenated tetraphenylporphyrins are analogous to those observed in the β-octaalkyl-substituted derivatives.[12] Table 2.7 contains out-of-plane values for distorted β-alkylated porphyrins. It can be seen that the structure determined for $ZnTPPEt_8$ is more distorted than that for $ZnTFPPBr_8$. The structure determined for $NiTFPPBr_8$ is more twist-distorted than that determined for $NiTPPEt_8$, although the $NiTPPEt_8$ structure is more saddled. It may be possible to obtain structures for Ni derivatives with varying degrees of twist-distortion, analogous to the situation observed in NiOEP. Consistent with the $NiTFPPBr_8$ derivative being less distorted than the $NiTPPEt_8$, the resonance Raman band is observed at higher energy for $NiTFPPBr_8$. The only crystallographic observation of a planar persubstituted tetraphenylporphyrin is one in which the β-alkylsubstituents are constrained into a 5-membered ring, copper β-tetrapropanotetrakis(3,4,5-trimethoxyphenyl)porphyrin, resulting in a molecule in which the b-substituents are essentially smaller (C_β-C_β-CH_2 angle is 13° smaller than in the octaethyl derivative),[43] consistent with the idea that macrocyclic nonplanarity relieves $C_{Ph_{ortho}}$ - β-X (X = R, Br, Cl) steric strain. Thus, distortion is a steric effect in β-substituted TPPs.

The interporphyrin distances, 3.9 Å, indicate that the distortions do not arise from π-π interactions. Resonance Raman spectroscopy of the halogenated TFPPs is consistent with the maintenance of distorted structures in solution. The $TFPPBr_8$ derivatives are very slightly less distorted than the $TPPEt_8$ ligands.

Experimental:

Porphyrins. ZnTPP (Aldrich) was used as received. ZnTFPP (Porphyrin Products) was purified on flash silica gel ('Baker', 40μm), eluting with CH_2Cl_2/hexane. The middle fraction of the pink band was isolated. H_2TFPP (Aldrich) was used as received. CuTFPP was synthesized from H_2TFPP and excess $CuCl_2$ by stirring in 100 °C DMF according to the Alder method[19] and purified on flash silica gel eluting with CH_2Cl_2/hexane.

ZnTFPPCl$_8$. ZnTFPPCl$_8$ was prepared from purified ZnTFPP and Cl_2(g) in refluxing CCl_4 under a steady stream of Ar(g).[3,4] The halogenated porphyrin is chromatographically purified initially on a short column of neutral alumina, eluting with $CHCl_3$. The porphyrin runs as a tightly loaded green band with a r_f of about 0.5. The porphyrin is then further purified on flash silica gel, eluting with a gradient (10:1 to 1:1) of CH_2Cl_2/hexane ($r_f \approx 0.5$ in 1:1 CH_2Cl_2/hexane). It is also possible to synthesize the porphyrin from *N*-chlorosuccimimide in methanol, in a procedure similar to that used for the preparation of ZnTFPPBr$_8$. Mass spectral analysis revealed a set of peaks (reflecting the relative abundances of the isotopes of Zn and Cl) centered at mass 1313.8. λ_{max} (CH_2Cl_2): nm (ε x 10^{-3}), 364 (34), 442(200), 574(20). ^{19}F NMR ($CDCl_3$, 500 MHz, vs. $CFCl_3$ = 0 ppm): δ -137.8 (q, 2 F, *o*-Ar-F), δ -150.7 (t, 1 F, *p*-Ar-F), δ -162.7 (sextuplet, 2 F, *m*-Ar-F).

ZnTFPPBr$_8$. ZnTFPPBr$_8$ was synthesized from purified ZnTFPP and 5 equiv (per β-hydrogen) *N*-bromosuccinimide in refluxing methanol (3 hrs).[5,6] The porphyrin is purified in the same manner as ZnTFPPCl$_8$. It is possible to synthesize the porphyrin from about 10 equiv (per β-hydrogen) of Br_2 in dry refluxing CCl_4. The Br_2 is added slowly through an addition funnel and the reaction is complete in about 4 hrs. Mass spectral analysis revealed a set of peaks (reflecting the isotope abundances for Zn and Br) centered at mass 1670.1. λ_{max} (CH_2Cl_2): nm (ε x 10^{-3}), 360(34), 460(200), 594(20). ^{19}F NMR ($CDCl_3$, 500 MHz, vs. $CFCl_3$ = 0 ppm): δ -137.7 (q, 2 F, *o*-Ar-F), δ -150.6 (t, 1 F, *p*-Ar-F), δ -162.3 (sextuplet, 2 F, *m*-Ar-F).

ZnTFPPMe$_8$. H_2TFPPMe$_8$ was synthesized via the condensation of 3,4-dimethylpyrrole and pentafluorobenzaldehyde.[12,13] 3,4-Dimethylpyrrole was prepared from ethyl-3,4-dimethylpyrrole-2-carboxylate.[11] Ethyl-3,4-dimethylpyrrole-2-carboxylate was prepared as follows:[10] a solution of 40 g 2-acetoxy-3-nitrobutane in 250 mL of a 1:1 solution of isopropyl alcohol (IPA) and tetrahydrofuran (THF) was added slowly over a 1 h period to a solution of ethyl isocyanoacetate (0.8 equiv) and 1,1,3,3-tetramethylguanidine

(1.7 equiv) in 500 mL 1:1 IPA:THF. The resulting pyrrole (70% yield) was purified on silica gel, eluting with CH_2Cl_2, and sublimed in vacuo at 80°C. Ethyl-3,4-dimethylpyrrole-2-carboxylate (20 g) was decarboxylated with 7.5 g of NaOH in 100 mL refluxing ethylene glycol. The reaction solution was poured into water, and the pyrrole was extracted with hexane, dried over $MgSO_4$, and purified by passing through a pad of silica gel. The resulting pyrrole, a white crystalline solid that melted near room temperature to form a stinky yellow oil (25% yield), was used immediately in the next reaction. A solution of 0.5 g 3,4-dimethylpyrrole and 1 equiv pentafluorobenzaldehyde (Aldrich) in 500 mL freshly distilled CH_2Cl_2 with 0.1 equivalent boron trifluoride etherate (Aldrich) was stirred at room temperature under Ar for 1 h. Four equiv (per porphyrinogen) of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone were added and the solution was refluxed for 30 min. $H_2TFPPMe_8$ was partially purified on a short column of neutral alumina, eluting with $CHCl_3$. $H_2TFPPMe_8$ was metallated in 10 min at room temperature in $CHCl_3$ by addition of a solution of $Zn(OAc)_2{\cdot}(H_2O)_2$ in methanol. Flash chromatography (silica gel), eluting with CH_2Cl_2/hexane, yielded $ZnTFPPMe_8$ as a green band (35% yield). Mass spectral analysis revealed a single peak at mass 1148.09. λ_{max} (CH_2Cl_2): nm (ε x 10^{-3}), 352 (35), 434 (200), 570 (20), 602 (15). ^1H NMR ($CDCl_3$, 500 MHz): δ 2.30(s). ^{19}F NMR ($CDCl_3$, 500 MHz, vs. $CFCl_3$ = 0 ppm): δ -137.7 (q, 2 F, *o*-Ar-F), δ -152.4 (t, 1 F, *p*-Ar-F), δ -162.1 (sextuplet, 2 F, *m*-Ar-F).

ZnT(2,6)FPPMe$_8$. $H_2T(2,6)FPPMe_8$ was synthesized, via the condensation of 3,4-diethylpyrrole and 2,6-difluorobenzaldehyde, a methodology similar to that employed in the synthesis of $H_2TFPPMe_8$.[12,13] Mass spectral analysis revealed a single peak at mass 1148.09. λ_{max} (CH_2Cl_2): nm (ε x 10^{-3}), 352 (35), 434 (200), 570 (20), 602 (15). ^1H NMR ($CDCl_3$, 500 MHz): δ 2.30(s). ^{19}F NMR ($CDCl_3$, 500 MHz, vs. $CFCl_3$ = 0 ppm): δ -137.7 (q, 2 F, *o*-Ar-F), δ -152.4 (t, 1 F, *p*-Ar-F), δ -162.1 (sextuplet, 2 F, *m*-Ar-F).

ZnTFPPEt$_8$. $H_2TFPPEt_8$ was synthesized, via the condensation of 3,4-diethylpyrrole and pentafluorobenzaldehyde, a methodology similar to that employed in the synthesis of $H_2TFPPMe_8$.[12,13] The starting material, 4-nitro-3-hexanol, was synthesized from 1-nitropropane and propionaldehyde.[10] $H_2TFPPEt_8$ was partially purified on a short column of neutral alumina, eluting with $CHCl_3$. $H_2TFPPEt_8$ was metallated in 10 min at room temperature in $CHCl_3$ by addition of a solution of $Zn(OAc)_2{\cdot}(H_2O)_2$ in methanol. Flash chromatography (silica gel), eluting with CH_2Cl_2/hexane, yielded $ZnTFPPEt_8$ as a green band (35% yield). Mass spectral analysis revealed a single peak at mass 1261. λ_{max} (CH_2Cl_2): nm (ε x 10^{-3}), 354 (34), 450 (200), 585 (20), 620 (15). ^1H NMR ($CDCl_3$, 500 MHz): δ . ^{19}F NMR ($CDCl_3$, 500 MHz, vs. $CFCl_3$ = 0 ppm): δ -137.7 (q, 2 F, *o*-Ar-F), δ -152.4 (t, 1 F, *p*-Ar-F), δ -162.1 (sextuplet, 2 F, *m*-Ar-F).[44]

H_2TFPPX_8 (X = Cl, Br, Me, Et). The distorted porphyrins were demetallated by bubbling HCl(g) through a stirred, room temperature $CHCl_3$ solution for 3-5 min. The resulting free ligand can be purified on a short column of acidic or neutral alumina. The free ligand runs as a dark brown band near the solvent front. A small green band ($ZnTFPPX_8$) can frequently be seen running behind the product. Care must be taken at this stage in order not to have a large percentage of the product remain bound (most likely as an ion pair between the protonated porphyrin and the oxygen of the alumina) to the top of the column. Acidic alumina is a better choice to avoid product loss on the column.

$MTFPPX_8$ (X = Cl, Br, Me, Et; M = Co, Ni, Pd, Cu, Zn, Mg). The metallated derivatives (M = Cu, Co, Ni) of $TFPPX_8$ were synthesized by the addition of a CH_3OH solution of the corresponding metal acetate, $M(OAc)_2{\cdot}(H_2O)_X$, to a CH_3Cl solution of H_2TFPPX_8. Typical reactions were complete in 5-10 min as monitored by UV-vis and tlc. Significantly longer reaction times (> 2 hr) led to porphyrin degradation. If metallation was slow, as for $TFPPCl_8$, reactions were gently heated. Products were purified by flash silica gel chromatography, eluting with CH_2Cl_2/hexane.

^1H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker AM-500.

Crystal Structure Determination. Crystals of the octabromo and octachloro derivatives were grown in some cases simply from the slow (3-4 days) evaporation of room temperature CH_2Cl_2 solutions (CuTFPP, H_2TFPP, CuTFPPCl$_8$, CuTFPPBr$_8$, NiTFPPBr$_8$). Crystals of H_2TFPPBr$_8$ and ZnTFPPBr$_8$ were grown from 9:1 solutions of CH_2Cl_2 : *o*-dichlorobenzene (ODCB). The porphyrin presumably crystallized from a concentrated ODCB solution. In general, it was observed that more highly purified porphyrins crystallized more easily. Structures were solved on a Enraf-Nonius CAD-4 diffractometer using Mo Kα radiation. Atomic scattering factors and values for f' and f'' were taken from Cromer and Waber[45] and Cromer.[46] Calculations were performed using programs of the CRYM Crystallographic Computing System,[47] MULTAN88,[48] and ORTEPII.[49] Parameters are reported in Appendices 1-7, Tables 1-4.

Resonance Raman. Resonance Raman spectra were recorded at 25 °C in a CH_2Cl_2 solution. The excitation source was the 441.6 nm line of a LiConix He-Cd laser (7 mW). The absorbance solutions at 442 nm were 0.5 per mm. Data were collected using a Spex 1403 monochromator.

References and Notes:

(1) Scheidt, W. R. In *The Porphyrins*; D. Dolphin, Ed.; Academic Press: New York, 1978; Vol. III; pp 463-511.

(2) Hoard, J. L. *Ann. N.Y. Acad. Sci.* **1973**, *206*, 18-31.

(3) Wijesekera, T.; Matsumoto, A.; Dolphin, D.; Lexa, D. *Angew. Chem. Int. Ed. Engl.* **1990**, *29*, 1028-1030.

(4) J. E. Lyons and P. E. Ellis, private communication.

(5) Birnbaum, E. R.; Hodge, J. A.; Grinstaff, M. W.; Schaefer, W. P.; Henling, L.; Labinger, J. A.; Bercaw, J. E.; Gray, H. B. *Inorg. Chem.* submitted 11/2/94.

(6) Hoffmann, P.; Labat, G.; Robert, A.; Meunier, B. *Tetrahedron Lett.* **1990**, *31*, 1991-1994.

(7) The preparation of the fully fluorinated *meso*-tetraphenylporphyrin has been reported in the literature (Tsuchiya, S.; Seno, M. *Chem. Lett.* **1989**, 236-266), but attempts to repeat this synthesis failed.

(8) Typical reaction conditions: dry refluxing acetonitrile or dry dimethylsulfoxide (100 °C) and from 1 hr to several days.

(9) The UV-vis spectra of porphyrin-like molecules with reduced aromaticity, chlorins and bacteriochlorins, typically exhibit low energy bands (700 nm) with extinction coefficients intermediate between the B and Q bands of typical porphyrins.

(10) Barton, D. H. R.; Kervagoret, J.; Zard, S. Z. *Tetrahedron* **1990**, *46*, 7587-7598.

(11) K. Smith and T. Forsyth, personal communication.

(12) Barkigia, K. M.; Berber, M. D.; Fajer, J.; Medforth, C. J.; Renner, M. W.; Smith, K. M. *J. Am. Chem. Soc.* **1990**, *112*, 8851-8857.

(13) Lindsey, J. S.; Wagner, R. W. *J. Org. Chem.* **1989**, *54*, 828-836.

(14) The $TPPX_8$ compounds were not pursued further due to the difficulty in obtaining a pure sample and the existence of previous work (in the case of the alkyl derivatives). Although it was possible to reproduce the UV-vis spectrum of $ZnTPPBr_8$ reported in the

literature (Bhyrappa, P.; Krishnan, V. *Inorg. Chem.* **1991**, *30*, 239-245), the Q-bands were broadened, more intense, and more separated than usually observed for porphyrins. Inability to purify the compound led to difficulty obtaining mass spectra, NMR and CV data. In fact, a low-energy band was observed to grow into the UV-vis spectrum of $ZnTPPMe_8$ as the compound decomposed. The spectrum of the decomposed $ZnTPPMe_8$ looked similar to that of $ZnTPPBr_8$, raising some doubt about the purity of the $ZnTPPBr_8$ sample used for studies reported in the literature.

(15) The synthesis of $TFPPBr_8$ ligand can be accomplished by refluxing $CoTPPBr_8$ with NBS in CH_2Cl_2 (D'Souza, F.; Villard, A.; Van Caemelbecke, E.; Franzen, M.; Boschi, T.; Tagliatesta, P.; Kadish, K. M. *Inorg. Chem.* **1993**, *32*, 4042-4048).

(16) EPR (Cu, Co), electrochemical, and NMR results indicate that the air-stable oxidation states of these metals (+2) are those typically seen for porphyrins.

(17) Takeda, J.; Ohya, T.; Sato, M. *Inorg. Chem.* **1992**, *31*, 2877-2880.

(18) Bhyrappa, P.; Nethaji, M.; Krishnan, V. *Chem. Lett.* **1993**, 869-872.

(19) Adler, A. D.; Longo, F. R.; Kampas, F.; Kim, J. *J. Inorg. Nucl. Chem.* **1970**, *32*, 2443-2445.

(20) Battioni, P.; Brigaud, O.; Desvaux, H.; Mansuy, D.; Traylor, T. G. *Tetrahedron Lett.* **1991**, *32*, 2893-2896.

(21) Schaefer, W. P.; Hodge, J. A.; Hughes, M. E.; Gray, H. B. *Acta Crystallogr.* **1993**, *C49*, 1342-1345.

(22) While the *Acta Cryst.* manuscript was in review, a structure was reported for $NiTFPPBr_8$: Mandon, D.; Ochsenbein, P.; Fischer, J.; Weiss, R.; Jayaraj, K.; Austin, R. N.; Gold, A.; White, P. S.; Brigaud, O.; Battioni, P.; Mansuy, D. *Inorg. Chem.* **1992**, *31*, 2044-2049. The structure reported is in agreement with ours.

(23) Henling, L. M.; Schaefer, W. P.; Hodge, J. A.; Hughes, M. E.; Gray, H. B.; Lyons, J. E.; Ellis, P. E. *Acta Crystallogr.* **1993**, *C49*, 1743-1747.

(24) Marsh, R. E.; Schaefer, W. P.; Hodge, J. A.; Hughes, M. E.; Gray, H. B. *Acta Crystallogr.* **1993**, *C49*, 1339-1342.

(25) Birnbaum, E. R.; Schaefer, W. P.; Labinger, J. A.; Bercaw, J. E.; Gray, H. B. *Inorg. Chem.* submitted.

(26) Grinstaff, M. W.; Hill, M. G.; Birnbaum, E. R.; Schaefer, W. P.; Labinger, J. A.; Gray, H. B. *Inorg. Chem.* in preparation.

(27) Grinstaff, M. W.; Hill, M. G.; Labinger, J. A.; Gray, H. B. *Science* **1994**, *264*, 1311-1313.

(28) Structures have also been reported for the Fe^{3+} derivatives of β-octahalogenated tetramesitylporphyrins (Ochsenbein, P.; Mandon, D.; Fischer, J.; Weiss, R.; Austin, R.; Jayaraj, K.; Gold, A.; Terner, J.; Bill, E.; Muther, M.; Trautwein, A. X. *Angew. Chem. Int. Ed. Engl.* **1993**, *32*, 1437-1439).

(29) Song, H.; Scheidt, W. R. *Inorg. Chim. Acta* **1990**, *173*, 3-41.

(30) Schauer, C. K.; Anderson, O. P.; Eaton, S. S.; Eaton, G. R. *Inorg. Chem.* **1985**, *24*, 4082-4086.

(31) Golder, A. J.; Povey, D. C.; Silver, J.; Jassim, Q. A. A. *Acta Crystallogr.* **1990**, *C46*, 1210-1212.

(32) Byrn, M. P.; Curtis, C. J.; Goldberg, I.; Hsiou, Y.; Khan, S. I.; Sawin, P. A.; Tendick, S. K.; Strouse, C. E. *J. Am. Chem. Soc.* **1991**, *113*, 6549-6557.

(33) Scheidt, W. R.; Lee, Y. J. *Struct. Bonding* **1987**, *64*, 1-70.

(34) Sparks, L. D.; Medforth, C. J.; Park, M.-S.; Chamberlain, J. R.; Ondrias, M. R.; Senge, M. O.; Smith, K. M.; Shelnutt, J. A. *J. Am. Chem. Soc.* **1993**, *115*, 581-592.

(35) Shelnutt, J. A.; Medforth, C. J.; Berber, M. D.; Barkigia, K. M.; Smith, K. M. *J. Am. Chem. Soc.* **1991**, *113*, 407-4087.

(36) These potential energy distributions were calculated for NiOEP (Kitagawa, T.; Ozaki, Y. *Struct. Bonding* **1987**, *64*, 71-114).

(37) M. E. Hughes, unpublished results.

(38) Lyons, J. E.; Ellis, P. E.; Wagner, R. W.; Thompson, P. B.; Gray, H. B.; Hughes, M. E.; Hodge, J. A. *Symposium on Natural Gas Upgrading II, Division of Petroleum Chemsitry, American Chemical Society, San Francisco Meeting, April* **1992**, 307-317.

(39) Cullen, D. L.; Meyer, E. F. *J. Am. Chem. Soc.* **1974**, *96*, 2095-2102.

(40) Meyer, E. F. *Acta Crystallogr.* **1972**, *B28*, 2162-2167.

(41) Czernuszewicz, R. S.; Li, X.-Y.; Spiro, T. G. *J. Am. Chem. Soc.* **1989**, *111*, 7024-7031.

(42) Barkigia, K. M.; Renner, M. W.; Furenlid, L. R.; Medforth, C. J.; Smith, K. M.; Fajer, J. *J. Am. Chem. Soc.* **1993**, *115*, 3627-3635.

(43) Senge, M. O.; Medforth, C. J.; Sparks, L. D.; Shelnutt, J. A.; Smith, K. M. *Inorg. Chem.* **1993**, *32*, 1716-1723.

(44) A. Eckermann, unpublished results.

(45) Cromer, D. T.; Waber, J. T. In *International Tables for X-ray Crystallography*; Kluwer Academic Publishers: Dordrecht, 1974; Vol. IV; pp 99-101.

(46) Cromer, D. T. In *International Tables for X-ray Crystallography*; Kluwer Academic Publishers: Dordrecht, 1974; Vol. IV; pp 149-151.

(47) Duchamp, D. J. *Am. Crystallogr. Assoc. Meet., Bozeman, Montana, Paper B14* **1964**, 29-30.

(48) Debaerdemaeker, T.; Germain, G.; Main, P.; Refaat, L. S.; Tate, C.; Woolfson, M. M. *MULTAN88. Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*; Univs. of York, England and Louvain, Belgium: 1988.

(49) Johnson, C. K. "*ORTEP*II.," Oak Ridge National Laboratory, Oak Ridge, TN, USA, 1976.

(50) Medforth, C. J.; Senge, M. O.; Smith, K. M.; Sparks, L. D.; Shelnutt, J. A. *J. Am. Chem. Soc.* **1992**, *114*, 9859-9869.

(51) Spiro, T. G.; Czernuszewicz, R. S.; Li, X.-Y. *Coord. Chem. Rev.* **1990**, *100*, 541-571.

Table 2.1. Selected Average Bond Lengths (Å) for Planar Porphyrins.[a]

Bond	H_2TFPP	CuTFPP	ZnTFPP[5]	Hoard's 'Average Porphyrin'[b]
N - C_α	1.369(4)	1.376(3,2)	1.371	1.383-1.370
C_α - C_β	1.438(5)	1.437(4,5)	1.438	1.446
C_β - C_β	1.329(5)	1.334(4,2)	1.339	1.350-1.380
C_α - C_m	1.393(4)	1.387(4,4)	1.398	1.375-1.407
C_m - C_{Ph}	1.500(5)	1.494(4,1)	—	—
H - N	0.91(4)	—	—	—
M - N	—	1.996(2,2)	2.036	1.960-2.098
Ct - N[c]	2.0166 2.0882	1.996	2.036	1.960-2.098

[a] The numbers in parentheses represent the average error in individual bond lengths and the magnitude of the deviation observed in the crystallographically different bonds (calculated as $[(X_{av} - X^-) - (X_{av} - X^+)]/2$, where X_{av} = the average of the crystallographically different bonds and X^- and X^+ are the maximum negative and positive deviations from the average, respectively), respectively.

[b] The numbers shown are for NiDeut (Deut = 2,4-Diacetyldeuteroporphyrin) and $SnTPPCl_2$, respectively. These two porphyrins represent a contracted and an expanded core, respectively. Sn(IV) is the largest metal ion that has been observed to bind in the center of the macrocycle.[1,2]

[c] Core size is defined as the distance between the center of the molecule (Ct) and a projection of the nitrogen atoms into the porphyrin plane.

Table 2.2. Selected Average Bond Lengths (Å) for Distorted TFPP Derivatives.[a]

Bond	$CuTFPPCl_8$	$H_2TFPPBr_8$	$NiTFPPBr_8$	$CuTFPPBr_8$	$ZnTFPPBr_8$[b]
$N - C_\alpha$	1.376(5,8)	1.368(10,35)	1.387(7,9)	1.380(10,10)	1.37(3)
$C_\alpha - C_\beta$	1.449(5,9)	1.456(11,18)	1.444(8,13)	1.440(11,20)	1.45(3)
$C_\beta - C_\beta$	1.346(6,4)	1.348(11,6)	1.341(8,3)	1.333(11,24)	1.35(3)
$C_\alpha - C_m$	1.396(5,8)	1.411(11,11)	1.384(8,8)	1.396(11,13)	1.39(3)
$C_m - C_{Ph}$	1.501(6,4)	1.481(11,8)	1.493(9,6)	1.496(11,10)	1.48(3)
M - N	2.007(3,4)	—	1.902(4,4)	1.971(6,4)	2.042(13,10)
Ct - N[c]	2.007	2.0252 2.0602	1.902	1.971	2.033

[a] The numbers in parentheses represent the average error in individual bond lengths and the magnitude of the deviation observed in the crystallographically different bonds, respectively.
[b] The Zn atom is displaced 0.180 Å from the plane of the porphyrin.
[c] Core size is defined as the distance between the center of the molecule (Ct) and a projection of the nitrogen atoms into the porphyrin plane.

Table 2.3. Selected Average Angles (°) for Planar Porphyrins.[a]

Angles	H_2TFPP	CuTFPP	ZnTFPP[5]	Hoard's 'Average Porphyrin'[b]
N1 - M- N2	—	90.0(1,4)	89.8	—
N1- M - N3	—	180.0	179.6	—
C_α - N - C_α	107.4(3)	105.2(2,3)	106.2	104.4-109.2
N - C_α - C_m	125.4(3)	125.2(2,2)	125.1	125.3-126.4
N - C_α - C_β	108.5(3)	110.2(2,2)	109.6	111.0-108.2
C_α - C_β - C_β	107.2(3)	107.2(2,2)	107.3	106.8-107.2
C_α - C_m - C_α	127.2(3)	124.7(2,1)	126.1	123.8-126.4
C_m - C_α - C_β	126.4(3)	124.6(2,2)	125.4	123.7-125.4
C_6F_5 dihedral[c]	79(3)	78(3)	72.6	—

[a] The numbers in parentheses represent the average error in individual bond lengths and the magnitude of the deviation observed in the crystallographically different bonds (calculated as $[(X_{av} - X^-) - (X_{av} - X^+)]/2$, where X_{av} = the average of the crystallographically different bonds and X^- and X^+ are the maximum negative and positive deviations from the average, respectively), respectively.

[b] The numbers shown are for NiDeut and $SnTPPCl_2$, respectively. Both metals are sitting in the plane of the porphyrin.[1,2]

[c] The dihedral angle refers to the angle between the plane of the porphyrin and the plane of the C_6F_5 group.

Table 2.4. Selected Average Angles (°) for Distorted TFPP Derivatives.[a]

Angles	$CuTFPPCl_8$	$H_2TFPPBr_8$	$NiTFPPBr_8$	$CuTFPPBr_8$	$ZnTFPPBr_8$[b]
N1 - M- N2	90.2(1,4)	—	90.6(2,2)	90.4(2,6)	89.6(7,2)
N1- M - N3	173.0(1,7)	—	168.4(2,.5)	171.2(2,2)	169.4(8,1)
C_α - N - C_α	107.3(3,2)	108.8(6,10)	106.6(4,4)	107.6(6,8)	108.7(17)
N - C_α - C_m	124.9(3,6)	124.0(7,4)	121.9(5,9)	122.1(7,11)	124.6(17)
N - C_α - C_β	108.7(3,3)	108.1(6,22)	108.4(5,7)	107.8(6,10)	107.7(16)
C_α - C_β - C_β	107.5(3,4)	107.4(7,12)	107.8(5,7)	108.1(7,2)	107.7(17)
C_α - C_m - C_α	123.8(4,2)	124.6(7,-)	121.4(5,6)	123.0(7)	124.0(17)
C_m - C_α - C_β	126.2(3,5)	127.6(7,3)	129.0(5,7)	129.5(7,8)	127.6(17)
C_6F_5 dihedral[c]	68.4	54.3	45.4	45.7	54.6

[a] The numbers in parentheses represent the average error in individual bond lengths and the magnitude of the deviation observed in the crystallographically different bonds, respectively.
[b] The Zn atom is displaced 0.180 Å from the plane of the porphyrin.
[c] The dihedral angle refers to the angle formed between the plane of the porphyrin and the plane of the C_6F_5 group.

Table 2.5. Average Deviations (±Å) of Atoms from Porphyrin Plane (defined by four N atoms) and Core Sizes for TFPP and $TFPPCl_8$ Derivatives.

Atom	H_2TFPP	CuTFPP	ZnTFPP[5]	$H_2TFPPCl_8$[5]	$CuTFPPCl_8$	$ZnTFPPCl_8$[5]
N	0.00	0.00	0.00	0.088	0.122	0.10
C_m	0.039	0.026	0.040	0.023	0.033	0.13
$C_ß$	0.071	0.051	0.074	0.625	0.701	0.79, 0.68
Cl 1	—	—	—	1.06	1.128	1.17
Cl 2	—	—	—	1.06	1.352	1.48
Ct - N[a]	2.0166 2.0882	1.996	2.036	2.075	2.007	2.029

[a] Core size is defined as the distance between the center of the molecule (Ct) and a projection of the nitrogen atoms into the porphyrin plane.

Table 2.6. Average Deviation (±Å) of atoms from Porphyrin Plane (defined by four N atoms) and Core Sizes for Distorted $TFPPBr_8$ Derivatives.

Atom	$H_2TFPPBr_8$	$NiTFPPBr_8$	$CuTFPPBr_8$	$ZnTFPPBr_8$
N	0.076	0.192	0.149	0.082[a]
C_m	0.091	0.187	0.163	0.021
$C_ß$	0.903	1.175	1.12	0.971
Br 1	1.587	1.855	1.82	1.33
Br 2	1.851	2.249	2.16	1.71
Ct - N[b]	2.0252 2.0602	1.902	1.971	2.033

[a] Metal atom is 0.180 Å above the porphyrin plane.
[b] Core size is defined as the distance between the center of the molecule (Ct) and a projection of the nitrogen atoms into the porphyrin plane.

Table 2.7. Average Deviation (±Å) of atoms from Porphyrin Plane and Core Sizes for Distorted Octaalkyl Porphyrins.

Atom	NiOEP (ruffled)[a]	$NiTPPEt_8$[b]	$NiTPPPr_8$[b]	$ZnTPPEt_8$[c]	H_2TPPPh_8[d]
N	< 0.01	0.19	0.019	0.063	0.08
C_m	0.51	0.03	0.06	0.050	0.00
$C_β$	0.21	1.24	1.29	1.079	0.99
Ct - N[e]	1.929(3)	1.906(3)	1.901(2)	2.048	–

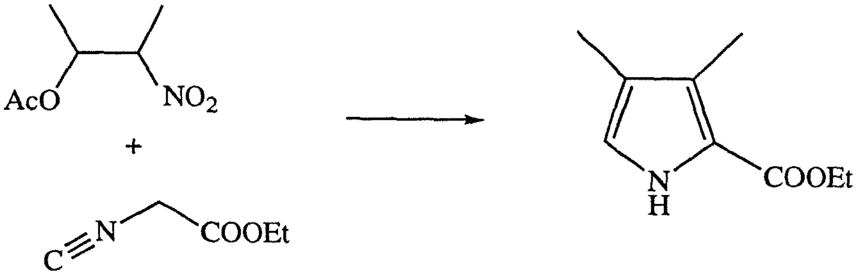
[a] From reference 40.
[b] From reference 42.
[c] Metal atom is 0.240 Å above the porphyrin plane. From references 12,34.
[d] From reference 50. Ct-N not reported.
[e] Core size is defined as the distance between the center of the molecule (Ct) and a projection of the nitrogen atoms into the porphyrin plane.

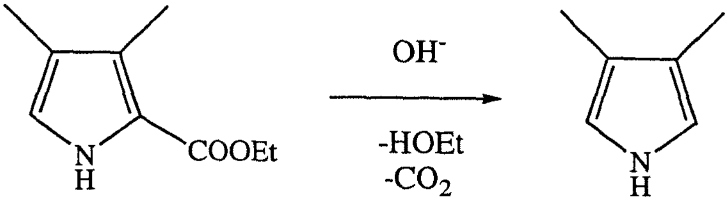
Table 2.8. Structure-Sensitive Resonance Raman Marker Bands (25 °C, CH_2Cl_2, 442 nm excitation) for Planar and Distorted Ni(II)Tetraphenylporphyrins.[37,38]

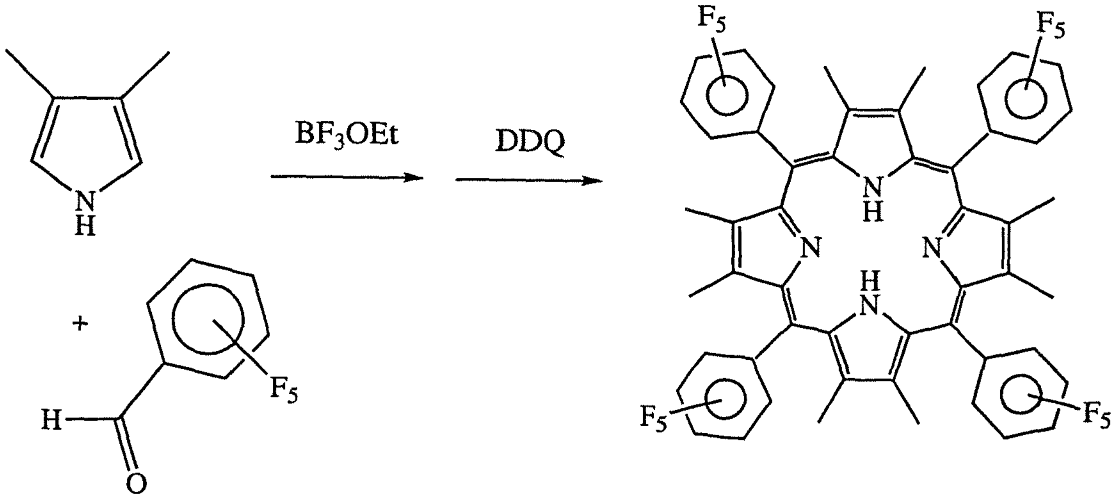
Compound	ν_4 (cm^{-1})	ν_2 (cm^{-1})
NiTFPP	1375	1568
$NiTFPPCl_8$	1363	1557
$NiTFPPBr_8$	1354	1542
NiP[a]	1376	1575
NiOEP[a]	1383	1600
NiTPP[b]	1374	1572
$NiTPPMe_8$[b]	1362	1574
$NiTPPEt_8$[b]	1350	1562
$NiTPPPr_8$[b]	1360	1560
$NiTPPPh_8$[b]	1353	1545

[a] From reference 51. Recorded in CH_2Cl_2, excitation at 406.7 nm.
[b] From reference 35. Recorded in CS_2, excitation at 457.9 nm.

Figure 2.1. Scheme for synthesis of β-octamethyltetraphenylporphyrins. With minor modifications, the reaction can be generalized to the synthesis of most β-alkylated and *meso*-tetraphenylporphyrins.

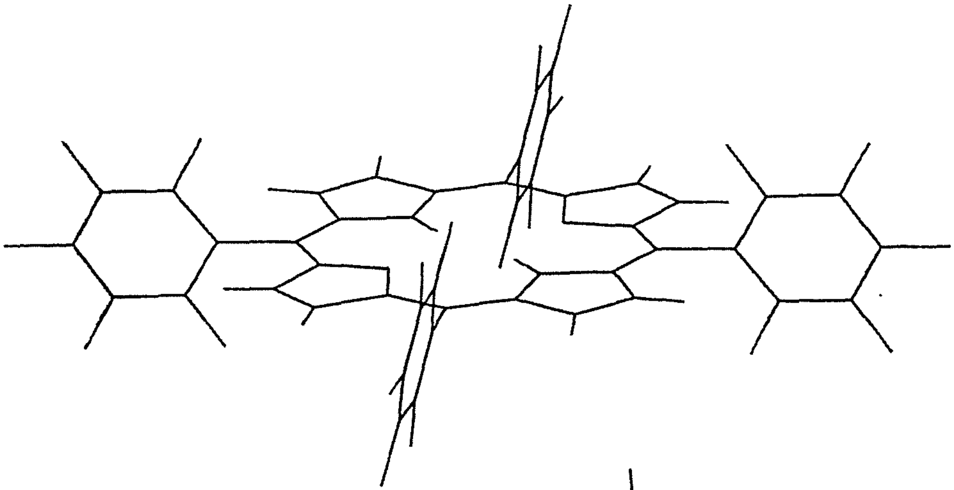




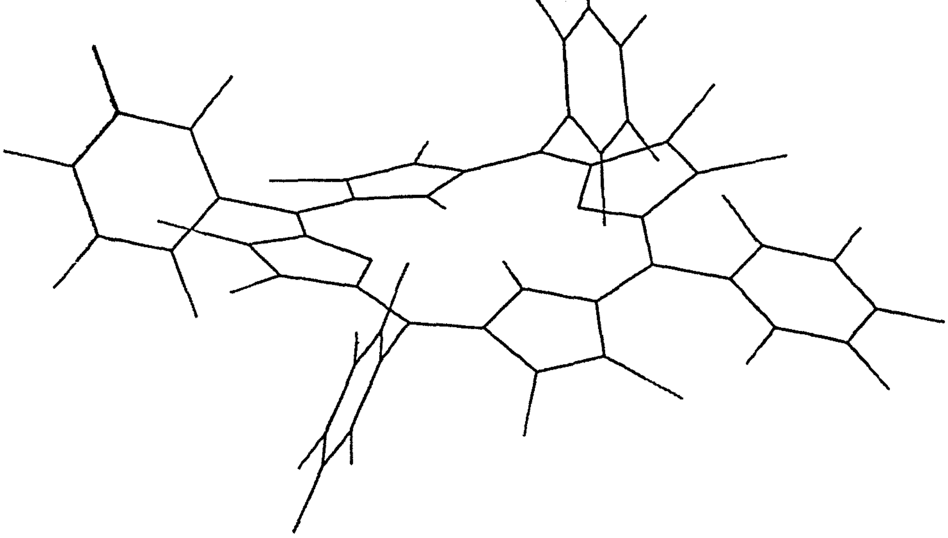


$H_2TFPPMe_8$

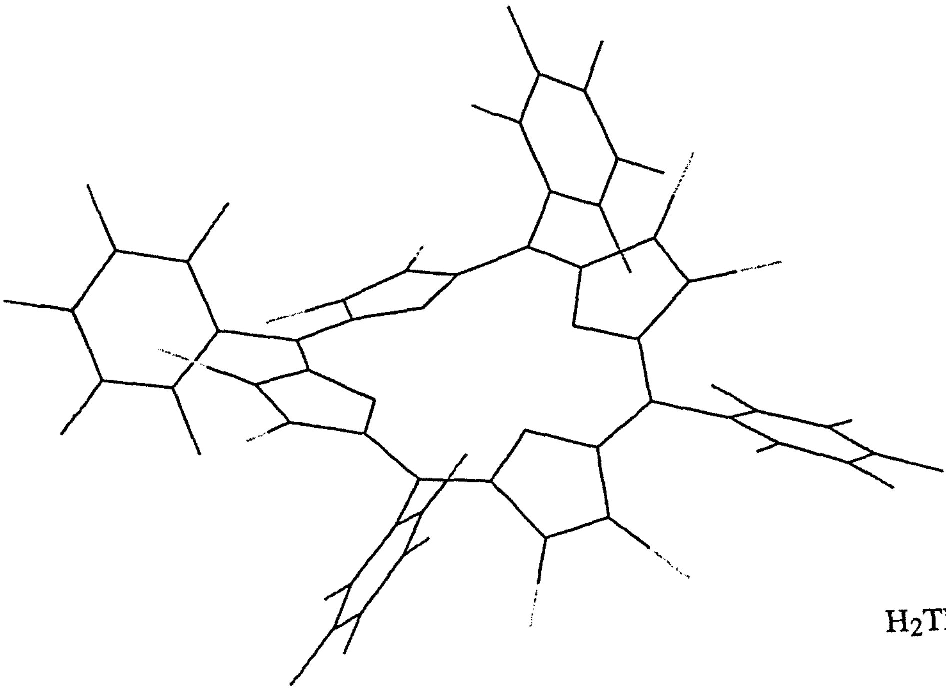
Figure 2.2. X-ray crystallographically determined structures for H_2TFPP, $H_2TFPPCl_8$, and $H_2TFPPBr_8$.



H_2TFPP

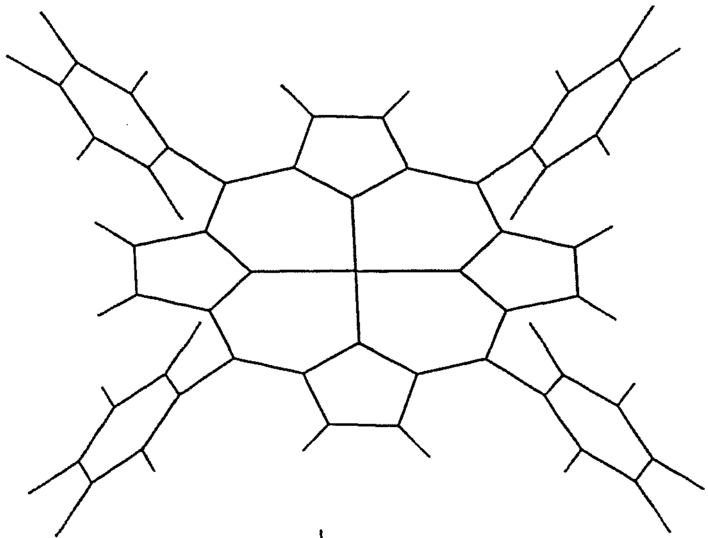


$H_2TFPPCl_8$

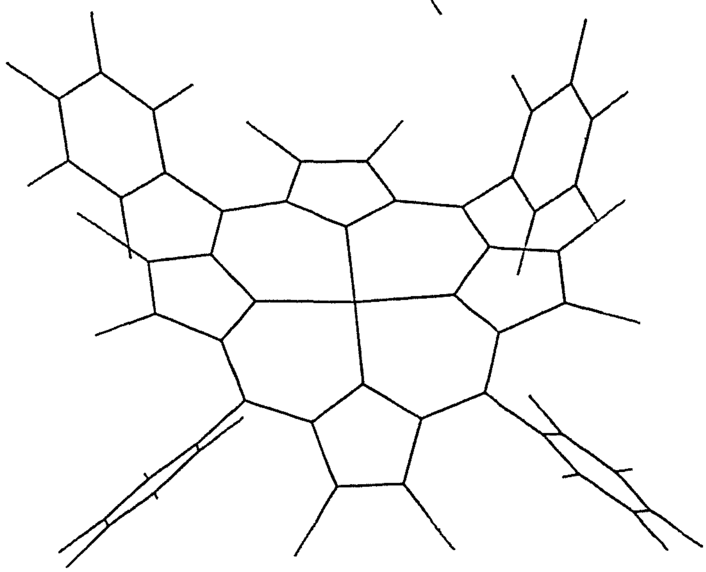


$H_2TFPPBr_8$

Figure 2.3. X-ray crystallographically determined structures for CuTFPP, $CuTFPPCl_8$, and $CuTFPPBr_8$.



CuTFPP



$CuTFPPCl_8$

$CuTFPPBr_8$

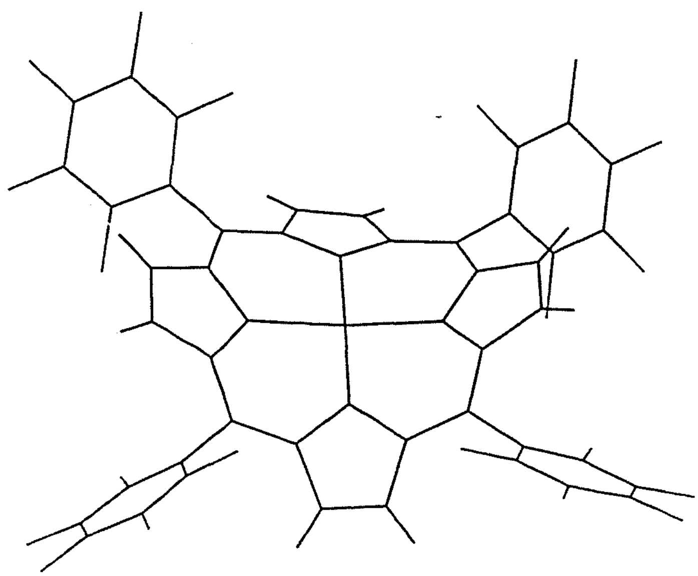
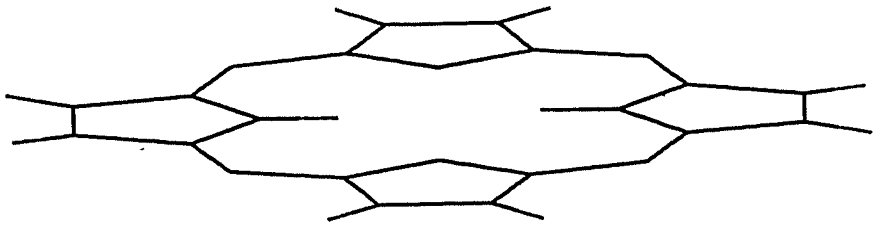
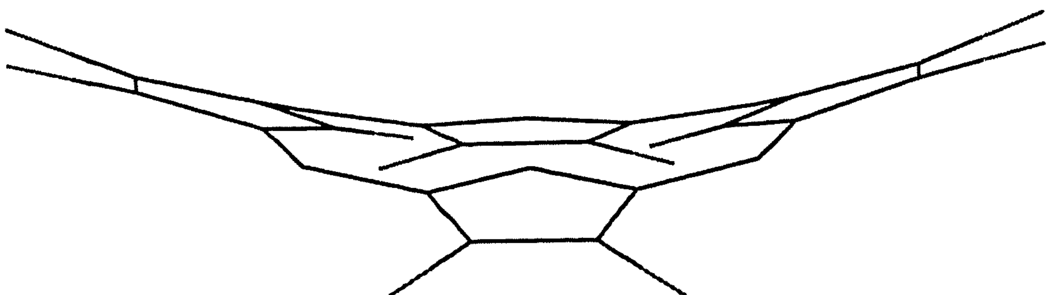


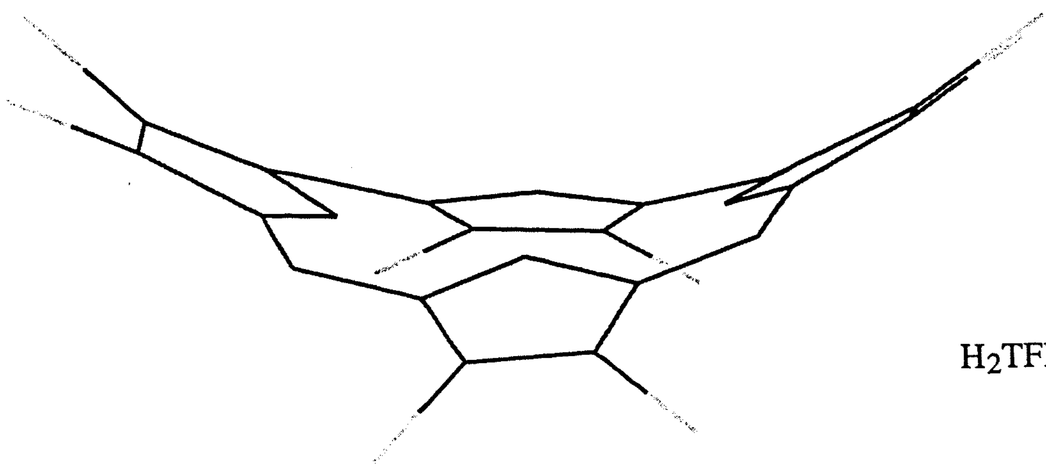
Figure 2.4. X-ray crystallographically determined structures for H_2TFPP, $H_2TFPPCl_8$, and $H_2TFPPBr_8$ with β-substituents and pentafluorophenyl groups removed. The side-view shows the slight twist-distortion of the $H_2TFPPCl_8$ and $H_2TFPPBr_8$.



H_2TFPP

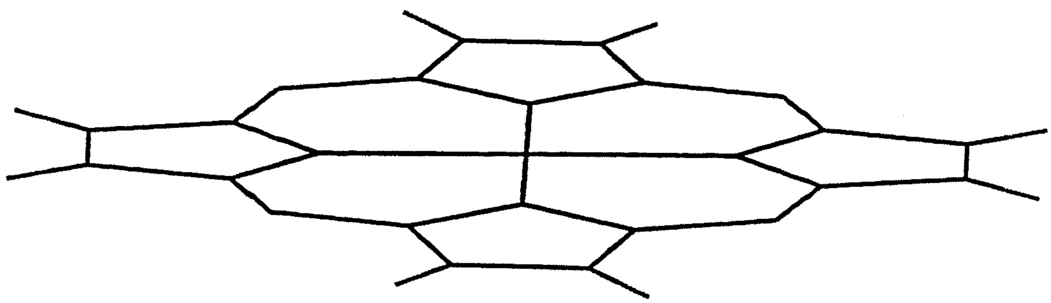


$H_2TFPPCl_8$

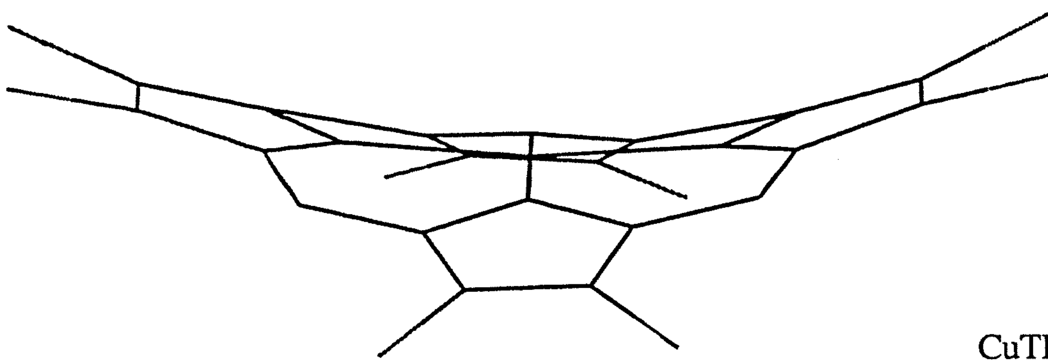


$H_2TFPPBr_8$

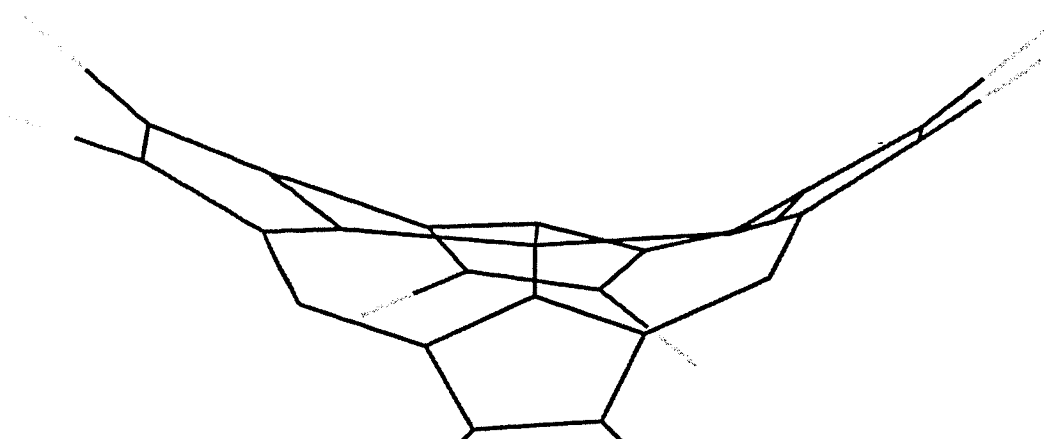
Figure 2.5. X-ray crystallographically determined structures for CuTFPP, $CuTFPPCl_8$, and $CuTFPPBr_8$ with β-substituents and pentafluorophenyl groups removed. The side view shows the large twist-distortion in the $CuTFPPCl_8$ and $CuTFPPBr_8$ derivatives.



CuTFPP

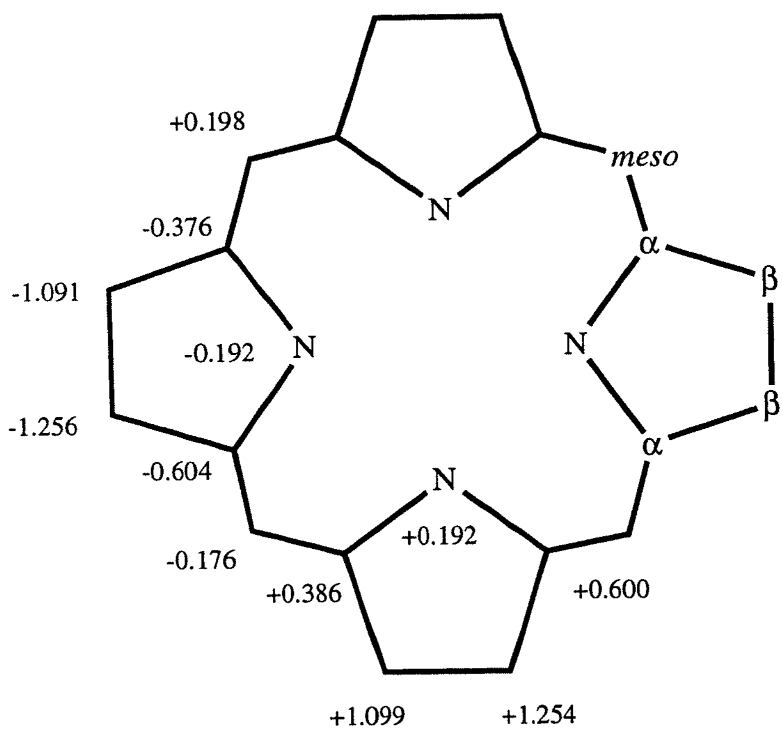


$CuTFPPCl_8$



$CuTFPPBr_8$

Figure 2.6. Geometry of distortion. Displacements of selected atoms (Å) from the average porphyrin plane for $NiTFPPBr_8$.



+0.198
meso
-0.376
N
α
β
-1.091
-0.192
N
N
β
-1.256
α
-0.604
N
+0.192
-0.176
+0.386
+0.600
+1.099
+1.254

CHAPTER 3:

ELECTROCHEMISTRY

Introduction:

Porphyrin macrocycles, containing nonredox-active metals, such as Zn and Mg, typically undergo two reversible one-electron (1e) oxidations and two reversible 1e reductions in nonaqueous media.[1] The products of 1e oxidations are π-cation radicals whose electronic structures have been studied extensively, due to their central role in biological processes such as photosynthesis and other oxidation-reduction reactions.[2,3] Oxidation and reduction waves for redox-active metals, such as Co(II), Fe(III), Mn(II), and Cr(II) are frequently observable within the confines of the four ligand-centered waves. The cobalt porphyrin is unique, among these metals, in its ability to be reversibly reduced to a M^+ oxidation state. The origin of redox processes can be identified through EPR and spectroelectrochemical experiments.[4] The UV-vis spectra of ligand-centered π-cation radicals and doubly oxidized species are quite distinctive.[5]

Results and Discussion:

Non-redox Active Metals:

The cyclic voltammograms of ZnTFPP and ZnTFPPX_8 (X = Cl, Br, Me) are shown in Figure 3.1. The reduction potentials are compared with that of ZnTPP in Table 3.1. Halogenation of the porphyrin causes a positive shift in the reduction potentials, as well as a merging of the two 1e oxidations into a single 2e response. The UV-vis spectral changes accompanying the oxidations of ZnTFPP are shown in Figure 3.2. As the potential is slowly cycled between 1.0 and 1.5 V, the initial absorptions of ZnTFPP decrease, giving rise to features at 390, 413, 625, and 695 nm. Further oxidation results in the appearance of a broad, sloping system with a maximum at 342 nm. Analogous spectral changes are observed during the oxidation of ZnTFPPBr_8. As the potential is swept through the 2e wave, the two prominent absorption bands in the spectrum of ZnTFPPBr_8 (455, 585 nm) lose intensity, giving way to a band at 363 nm. However, these changes do not occur isosbestically; absorptions at 420 and 450 nm maximize midway through the electrolysis, indicating that a radical-disproportionation reaction is occurring.[6]

The UV-vis spectra of the singly and doubly oxidized species of both ZnTFPP and $ZnTFPPBr_8$ (Figure 3.3) establish that the oxidations are localized on the porphyrin ring. The spectrum of each singly oxidized species is that of a π-cation radical, featuring a characteristically broad, split absorption system in the Soret region (the low-energy band, at 700 nm, is difficult to see for $ZnTFPPBr_8$); the principal absorption of each doubly oxidized complex, as expected for a porphyrin dication, is a broad, blue-shifted band.[5] The appearance of these spectra rule out the formation of isoporphyrins (i.e., porphyrins that are reduced/substituted at the *meso* position), because isoporphyrins are characterized by relatively intense ($\varepsilon = 2 \times 10^4$ $\underline{M}^{-1}cm^{-1}$) bands that fall between 750 and 950 nm (spectra were observed to 1000 nm).[7] One-electron couples can be extracted from the two-electron potentials, according to the following scheme:[8]

$K_{disp}=[P][P^{2+}]/[P^+]$,

$E = E^0{}_{+/0} + 0.059\log([P^+]/[P]) = E^0{}_{2+/+} + 0.059\log([P^{2+}]/[P^+])$,

$\log(K_{disp})= (E^0{}_{+/0} - E^0{}_{2+/+})/0.059$,

$E^0{}_{2+/0} = (E^0{}_{2+/+} + E^0{}_{+/0})/2$.

Equilibrium constants for the disproportionation of the singly oxidized porphyrin into the neutral and doubly oxidized forms (K_{disp}) are 12±5 and 5±3 for $ZnTFPPCl_8^+$ and $ZnTFPPBr_8^+$, respectively.[9]

The cyclic voltammogram of $ZnTFPPMe_8$ is similar to those of the perhalogenated porphyrins; two 1e reductions and one 2e oxidation are observed (Figure 3.1). Methylation of ZnTFPP results in a porphyrin that is easier to oxidize and harder to reduce. Slow cycling of the potential between 0.75 and 1.25 V yields spectral changes (Figure 3.4) comparable to the oxidation processes seen for $ZnTFPPBr_8$ and $ZnTFPPCl_8$. The initial absorptions of $ZnTFPPMe_8$ (434, 570, 602 nm) decrease and ultimately yield the spectrum of $ZnTFPPMe_8^{2+}$ (327 nm). Again, absorptions (650-750 nm) attributable to a cation radical are observed midway through the electrolysis. K_{disp} for $ZnTFPPMe_8^{+}$ is 0.4±1.[9]

In contrast, the cyclic voltammograms (Figure 3.6) observed for Cu(II) derivatives of TFPP and $TFPPMe_8$, clearly show two 1e oxidations. Data for the ligand-centered oxidation and reduction processes are shown in Table 3.2. The Cu(II) metal induces essentially equivalent positive shifts (average shifts = 0.04 V) in the reduction potentials for both the oxidations and reductions as compared to the Zinc(II) derivatives.

Several exceptions to the characteristic1e transfers observed for porphyrins have been reported: Murray observed a net 2e oxidation of CuTPP and H_2TPP in toluene with perchlorate as the supporting electrolyte, and attributed the multielectron response to specific metal-binding and acid-base properties of the medium;[10,11] Kadish observed a similar 2e wave for CoTPP in toluene;[12] and Saveant observed a 2e process that led to the formation of an isoporphyrin (with the accompanying loss of a proton).[13] Two groups have worked on the electrochemistry of $CoTPPBr_8$: for experiments in benzonitrile, it was found that two 1e oxidation waves merge, but the identity of the 2e oxidized product was not established;[14] for experiments in CH_2Cl_2, two 1e oxidations were observed.

Redox-Active Metals:

The data for the redox processes observed for Cobalt complexes of the halogenated and non-halogenated tetraphenyl porphyrins is collected in Table 3.3. Figure 3.7 contains the UV-vis spectroelectrochemical data that clearly indicate that the redox processes observed at -0.11 V and -0.08 V, for the $Co^{2+/+}$, couple of $TFPPBr_8$ and $TFPPCl_8$, respectively, are metal-centered. The double-Soret observed in the Co(I) species is typical of Co(I) porphyrins although its origin has not been conclusively identified.[15] Similarly, the sharp UV-vis bands generated by the first oxidation identify the process as metal-centered.[15] The $Co^{3+/2+}$ oxidation process was not reversible, consistent with $Co^{3+/2+}$ couples typically being kinetically slow and extremely ligand-dependent.

Conclusions:

Despite the changes induced in the tetraphenylporphyrin ligand by the substitution of bulky electron-withdrawing ligands, their electrochemical properties are similar to those observed for the metalloderivatives of OEP, TPP, and TFPP: the stable oxidation states observed for the metallo-derivatives are similar (exception = Fe(II)) and the ligand can undergo two reversible oxidations and reductions. The observed merging of the two 1e electron oxidations into a single electron response is shown to be dependent on the macrocycle being substituted with a perfluorophenyl group at the meso position and upon its being distorted. The effect was shown not to be a product of the electronic interaction of the halogen substituents with the oxidized species by the fact that the same phenomenon is observed for the octamethylated TFPP derivative. Porphyrins substituted with perfluorophenyl groups at the *meso* positions give $^2A_{1u}$ cation radicals.[16] (See Chapter 4 for a further discussion.) Resonance Raman and IR spectra of the $^2A_{1u}$ and $^2A_{2u}$ cation radicals reveal distinctly different vibrational characteristics for the two types of cations.[17,18]

For tetraphenylporphyrins the observed β-substituent-induced redox potential shifts are not equivalent for ring reduction and ring oxidation. The reduction potentials for oxidations typically are less positively shifted than the potentials for reductions in the case of the β-halogenated porphyrins, and are more positively shifted than the potentials for reductions in the case of β-alkylated tetraphenylporphyrins.[19-22] In a comparison between $ZnTFPPEt_8$ and $ZnTFPPMe_8$, the change in potential for reductions is negligible (0.04 V), the oxidation potential is shifted at least 0.20 V more negative. These shifts have been attributed to distortion effects that raise the energy of the HOMO preferentially over the LUMO (see Chapter 4 for more complete discussion).[23]

Reports for the metalloderivatives of the $TPPBr_8$ ligand show large positive shifts in reduction potentials for the substitution of Cu(II) for Zn(II). Shifts of 0.22 V for oxidations and 0.34 V for reductions were reported.[21] The large shift appears to correlate with having phenyl groups as opposed to a perfluorophenyl groups in the *meso* position.

Experimental:

Electrochemistry. All electrochemical experiments were performed with either a Bioanalytical Systems (BAS) Model 100 electrochemical analyzer or an EG&G Princeton Applied Research Model 173 Potentiostat/Galvanostat driven by a Model 175 Universal Programmer. Cyclic voltammetry was performed at room temperature with a normal three-electrode configuration consisting of a highly polished glassy carbon disk working electrode ($A = 0.07$ cm^2) 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, high purity) and tetrabutylammonium hexafluorophosphate ($TBAPF_6$) (Southwestern Analytical) were used as received. Electrolyte solutions were passed through activated alumina prior to use. Typical reactant concentrations for cyclic voltammetry were in the range of 10^{-3}-10^{-4} M.

Potentials are reported vs. aqueous AgCl/Ag and are not corrected for the junction potential. Under conditions identical with those employed here, the ferrocenium/ferrocene couple has $E°' = 0.48$ V.

Spectroelectrochemistry. Thin-layer UV-vis spectroelectrochemistry employed an optically transparent platinum working electrode.[8] Spectral changes were monitored either by a Tracor Northern TN-6500 diode array apparatus employing a Xe arc lamp as the light source, or a Hewlett-Packard 8452A diode array spectrophotometer.

EPR. EPR spectra were recorded at -50 °C in CH_2Cl_2/ 0.1 M $TBAClO_4$ (Southwestern analytical) solution. Solutions of oxidized species were prepared via the bulk electrochemical oxidation in some cases in situ and in some cases on the bench top and transferred to an EPR tube via syringe.

Porphyrin syntheses and purification procedures are reported in Chapter 2.

References and Notes:

(1) Kadish, K. M. *Prog. in Inorganic Chem.* **1986**, *34*, 435-605.

(2) Davis, D. G. In *The Porphyrins*; D. Dolphin, Ed.; Academic Press, Inc.: New York, 1979; Vol. V; pp 127-152.

(3) Dolphin, D.; Felton, R. H. *Acc. Chem. Res.* **1974**, *7*, 26-32.

(4) Grinstaff, M. W.; Hill, M. G.; Labinger, J. A.; Gray, H. B. *Science* **1994**, *264*, 1311-1313.

(5) Fajer, J.; Borg, D. C.; Forman, A.; Dolphin, D.; Felton, R. H. *J. Am. Chem. Soc.* **1970**, *92*, 3451-3459.

(6) Traylor, T. G.; Tsuchiya, S. *Inorg. Chem.* **1987**, *26*, 1338-1339.

(7) Dolphin, D.; Felton, R. H.; Borg, D. C.; Fajer, J. *J. Am. Chem. Soc.* **1970**, *92*, 743-745.

(8) Hill, M. G.; Mann, K. R. *Inorg. Chem.* **1991**, *30*, 1429-1431.

(9) Hodge, J. A.; Hill, M. G.; Gray, H. B. *Inorg. Chem.* in press.

(10) Geng, L.; Murray, R. W. *Inorg. Chem.* **1986**, *25*, 3115-3120.

(11) Geng, L.; Ewing, A. G.; Jernigan, J. C.; Murray, R. W. *Anal. Chem.* **1986**, *58*, 852-860.

(12) Mu, X. H.; Lin, X. Q.; Kadish, K. M. *Electroananylsis* **1989**, *1*, 113-116.

(13) El-Kasmi, A.; Lexa, D.; Maillard, P.; Momenteau, M.; Saveant, J.-M. *J. Am. Chem. Soc.* **1991**, *113*, 1586-1595.

(14) D'Souza, F.; Villard, A.; VanCaemelbecke, E.; Franzen, M.; Boschi, T.; Tagliatesta, P.; Kadish, K. M. *Inorg. Chem.* **1993**, *32*, 4042-4048.

(15) Gouterman, M. In *The Porphyrins*; D. Dolphin, Ed.; Academic Press: New York, 1978; Vol. III; pp 1-165.

(16) Gross, Z.; Barzilay, C. *Angew. Chem.* **1992**, *31*, 1615-1617.

(17) Czernuszewicz, R. S.; Macor, K. A.; Li, X.-Y.; Kincaid, J. R.; Spiro, T. G. *J. Am. Chem. Soc.* **1989**, *111*, 3860-3869.

(18) Prendergast, K.; Spiro, T. G. *J. Phys. Chem.* **1991**, *95*, 9728-9736.

(19) Kadish, K. M.; D'Souza, F.; Villard, A.; Autret, M.; Caemelbecke, E. V.; Bianco, P.; Antonini, A.; Tagliatesta, P. *Inorg. Chem.* **1994**, *33*, 5169-5170.

(20) Ochsenbein, P.; Ayougou, K.; Mandon, D.; Fischer, J.; Weiss, R.; Austin, R. N.; Jayaraj, K.; Gold, A.; Terner, J.; Fajer, J. *Angew. Chem.* **1994**, *33*, 348-350.

(21) Bhyrappa, P.; Krishnan, V. *Inorg. Chem.* **1991**, *30*, 239-245.

(22) Bhyrappa, P.; Nethaji, M.; Krishnan, V. *Chem. Lett.* **1993**, 869-872.

(23) Takeuchi, T.; Gray, H. B.; Goddard, W. A. *J. Am. Chem. Soc.* **1994**, *116*, 9730-9732.

(24) Felton, R. H.; Linschitz, H. *J. Am. Chem. Soc.* **1966**, *88*, 1113-1116.

Table 3.1. Reduction Potentials of Zinc(II) and Mg(II) Porphyrins.[a]

Porphyrin	$E^{o'}_{2+/0}$	$E^{o'}_{2+/+}$	$E^{o'}_{+/0}$	$E^{o'}_{0/-}$	$E^{o'}_{-/2-}$
ZnTPP[b]	–	1.16	0.80	-1.33	-1.66
ZnTFPP	–	1.58	1.37	-0.95	-1.37
$ZnTFPPBr_8$	1.55	1.53[c]	1.57[c]	-0.48	-0.76
$MgTFPPBr_8$	1.54	–[e]	–[e]	-0.47	-0.76
$ZnTFPPCl_8$	1.60	1.57[c]	1.63[c]	-0.47	-0.75
$ZnTFPPMe_8$	0.98	0.99[c]	0.97[c]	-1.14	-1.52[d]
$ZnT(2,6)FPPMe_8$	0.80	–[e]	–[e]	-1.36	-1.66
$ZnTFPPEt_8$	0.77	–[e]	–[e]	-1.18	-1.56

[a] V vs. AgCl/Ag in 1.0 M KCl; $Fc^{+/0}$ = 0.48 V; 0.1 M $TBAPF_6/CH_2Cl_2$.
[b] Potentials are in good agreement with literature values.[1]
[c] Calculated from the respective K_{disp} and $E^{o'}_{2+/0}$ couples, and the expressions $\ln K_{disp}=nF(E^o_{+/0}-E^o_{2+/+})/RT$ and $E_{2+/0}=(E^o_{+/0} + E^o_{2+/+})/2$.
[d] E_{pc}.
[e] Not determined.

Table 3.2. Reduction Potentials of Copper(II) and Palladium(II) Porphyrins.[a]

Porphyrin	$E^{o'}_{2+/+}$	$E^{o'}_{+/0}$	$E^{o'}_{0/-}$	$E^{o'}_{-/2-}$
CuTPP	1.33[b]	0.99[b]	-1.20[c]	-1.68[c]
CuTFPP	1.63 (1.75)	1.39 (1.42)	-0.86 (-0.92)	-1.32 (-1.36)
$CuTFPPBr_8$	1.77	1.51 (1.56)	-0.43 (-0.44)	-0.80 (-0.77)
$CuTFPPCl_8$	≈1.80	1.58	-0.36 (-0.41)	-0.68 (-0.76)
$PdTFPPCl_8$	–	–	(-0.43)	(-0.78)
$CuTFPPMe_8$	1.22(1.37)	0.97(1.01)	-1.02 (-1.10)	-1.38 (-1.47)

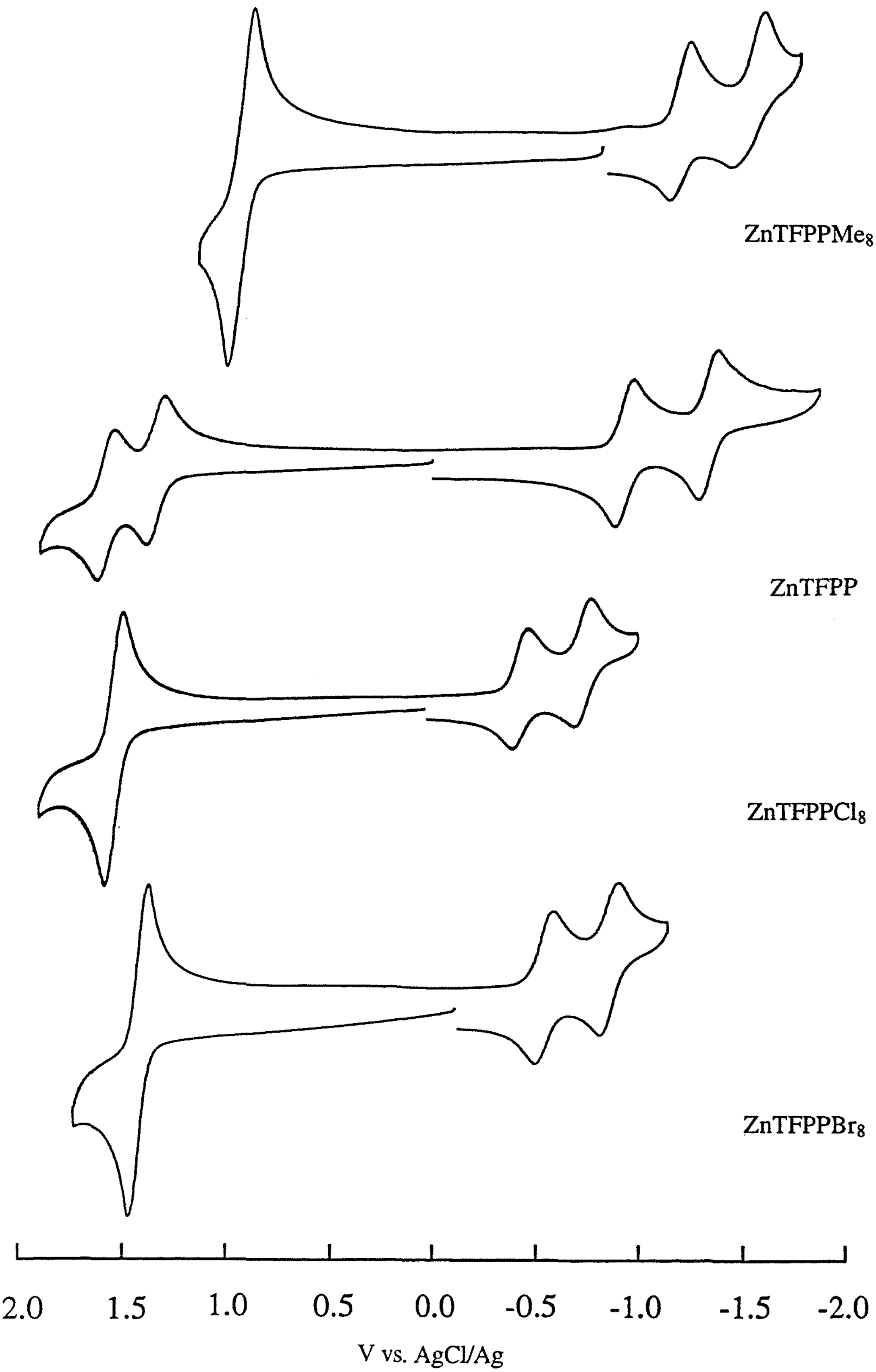
[a] V vs. AgCl/Ag in 1.0 M KCl; $Fc^{+/0}$ = 0.44 V; 0.1 M $TBAPF_6/CH_3CN$. Potentials in ( ) are recorded in 0.1 M $TBAPF_6/CH_2Cl_2$; $Fc^{+/0}$ = 0.48 V. Oxidations were not observed for $CuTFPPCl_8$ and $PdTFPPCl_8$ in CH_2Cl_2, in a potential sweep to 1.8 V.
[b] Recorded in benzonitrile. V vs SCE.[24]
[c] Recorded in DMSO. V vs SCE.[24]

Table 3.3. Reduction Potentials of Cobalt Porphyrins.[a]

Porphyrin	$E^{o'}_{2+/+}$	$E^{o'}_{+/0}$	$M^{o'}_{3+/2+}$	$M^{o'}_{2+/+}$	$E^{o'}_{0/-}$
CoTPP[b]	1.25	1.11	0.89	-0.98	-1.49[c]
CoTFPP	1.77	1.54	1.24	-0.56	-1.59
$CoTFPPBr_8$		1.75	1.21[c],0.30[c]	-0.11	-1.01
$CoTFPPCl_8$		1.70	1.55,0.63[d]	-0.08	-1.11

[a] V vs. AgCl/Ag in 1.0 M KCl; $Fc^{+/0}$ = 0.48 V; 0.1 M $TBAPF_6/CH_2Cl_2$,.
[b] Potentials are in good agreement with literature values; ref. [1].
[c] E_{pc}. Perhaps reflecting the oxidation of a unligated cobalt(II) and the reduction of a ligated cobalt(III) center.
[d] Waves corresponded to less than 1e, yet unlike the $CoTFPPBr_8$ case, exhibited reverse waves as well.

Figure 3.1. Cyclic voltammograms of ZnTFPP and $ZnTFPPX_8$ (X = Me, Cl, Br) in 0.1 M $TBAPF_6/CH_2Cl_2$..



ZnTFPPMe$_8$
ZnTFPP
ZnTFPPCl$_8$
ZnTFPPBr$_8$
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
V vs. AgCl/Ag

Figure 3.2. Changes in the absorption spectrum of ZnTFPP in 0.1 M $TBAPF_6/CH_2Cl_2$ recorded during a slow (4 mV/s) cyclic potential sweep.

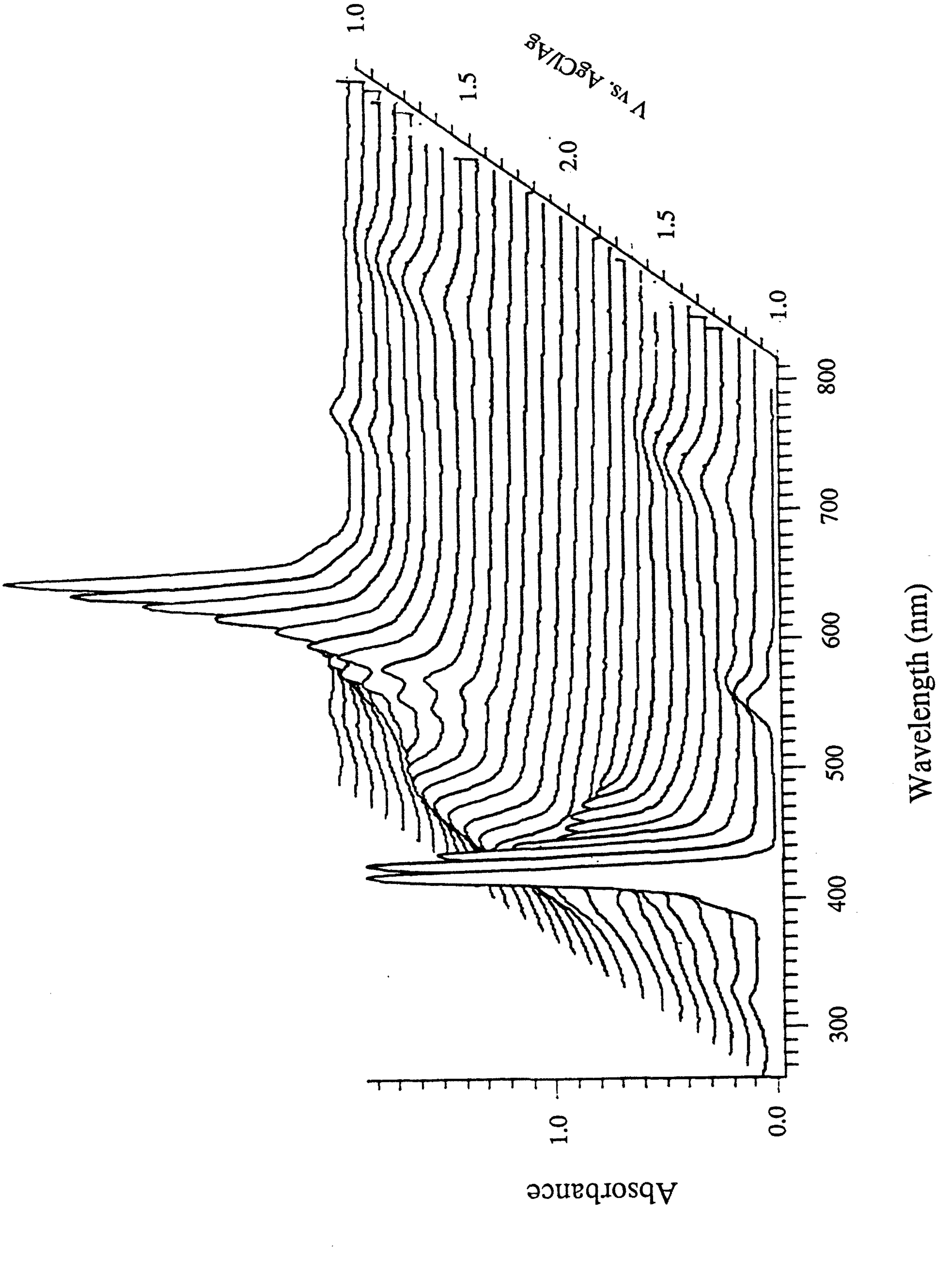

Absorbance
0.0
1.0
300
400
500
600
700
800
Wavelength (nm)
V vs. AgCl/Ag
1.0
1.5
2.0
1.5
1.0

Figure 3.3. (a) Electronic spectra of ZnTFPP (— • —), $ZnTFPP^+$ (———), and $ZnTFPP^{2+}$ (- - -) in 0.1 M $TBAPF_6/CH_2Cl_2$. (b) Electronic spectra of $ZnTFPPBr_8$ (— • —), $ZnTFPPBr_8^+$ (———), and $ZnTFPPBr_8^{2+}$ (- - -) in 0.1 M $TBAPF_6/CH_2Cl_2$. The spectrum of $ZnTFPPBr_8^+$ was extracted from the measured value of K_{disp}.

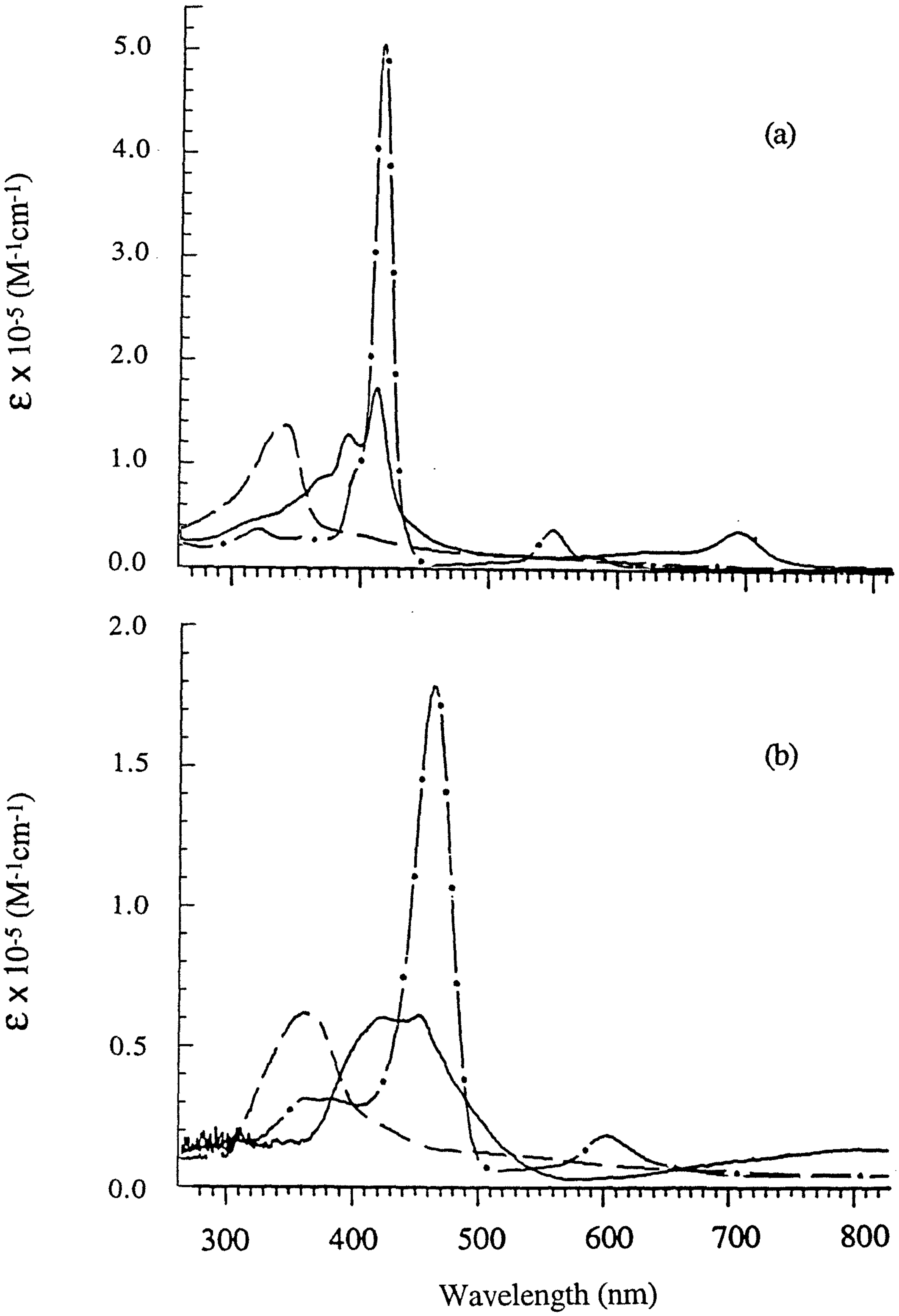

5.0
4.0
3.0
2.0
1.0
0.0
(a)
ε x 10-5 (M-1cm-1)
2.0
1.5
1.0
0.5
0.0
(b)
ε x 10-5 (M-1cm-1)
300
400
500
600
700
800
Wavelength (nm)

Figure 3.4. Changes in the absorption spectrum of $ZnTFPPMe_8$ in 0.1 M $/CH_2Cl_2$ recorded during a slow (4 mV/s) cyclic potential sweep.

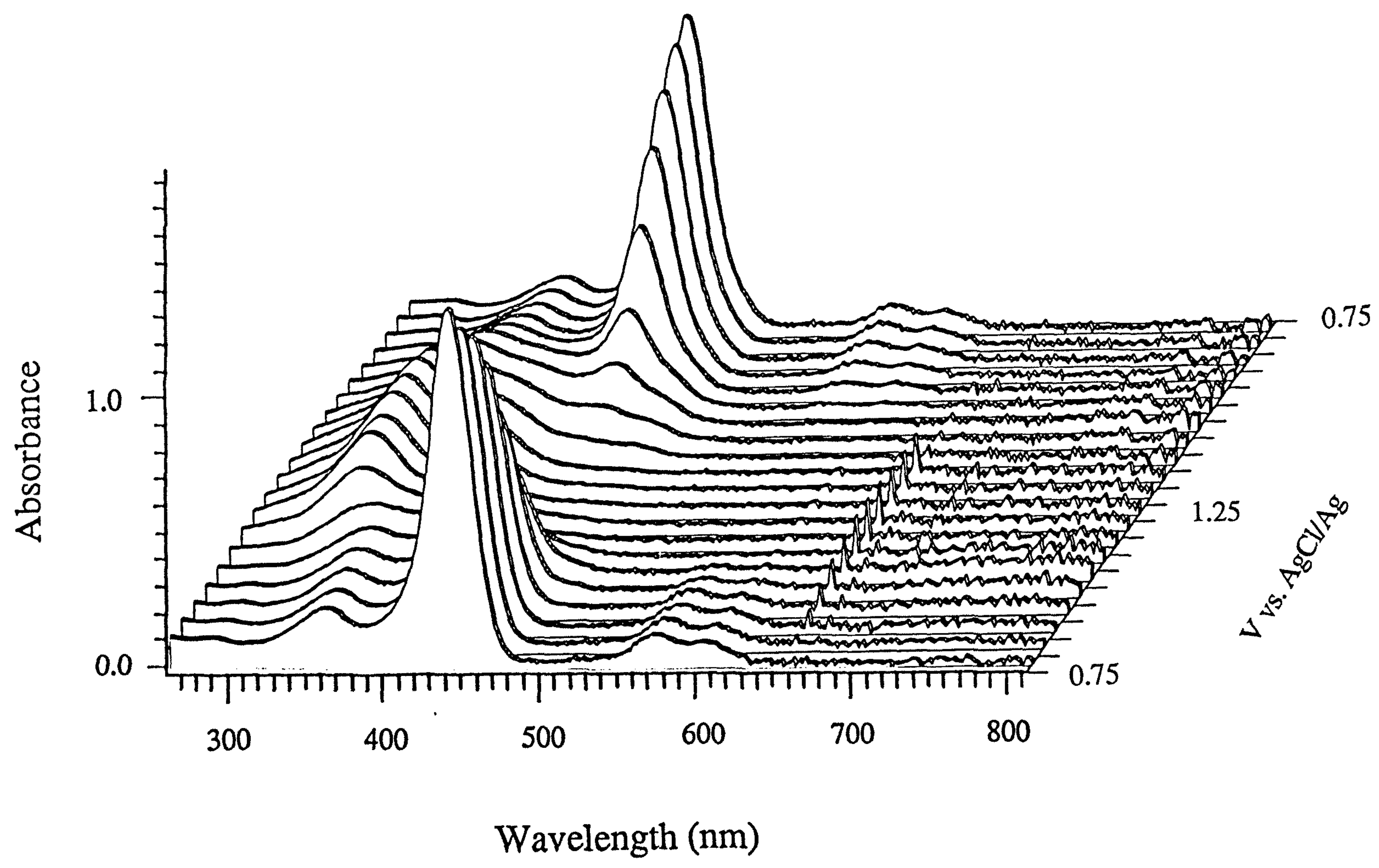

Absorbance
1.0
0.0
300
400
500
600
700
800
Wavelength (nm)
0.75
1.25
0.75
V vs. AgCl/Ag

Figure 3.5. EPR spectra for the electrochemically generated π-cation radicals of ZnTPP ($^2A_{1u}$)(g = 2.03), ZnTFPP ($^2A_{1u}$)(g = 2.05), and $ZnTFPPBr_8$ ($^2A(^2A_{1u})$)(g = 2.015) (top to bottom). Recorded in $TBAPF_6/CH_2Cl_2$, at -50 °C. See Chapter 4 for corresponding orbital density maps.

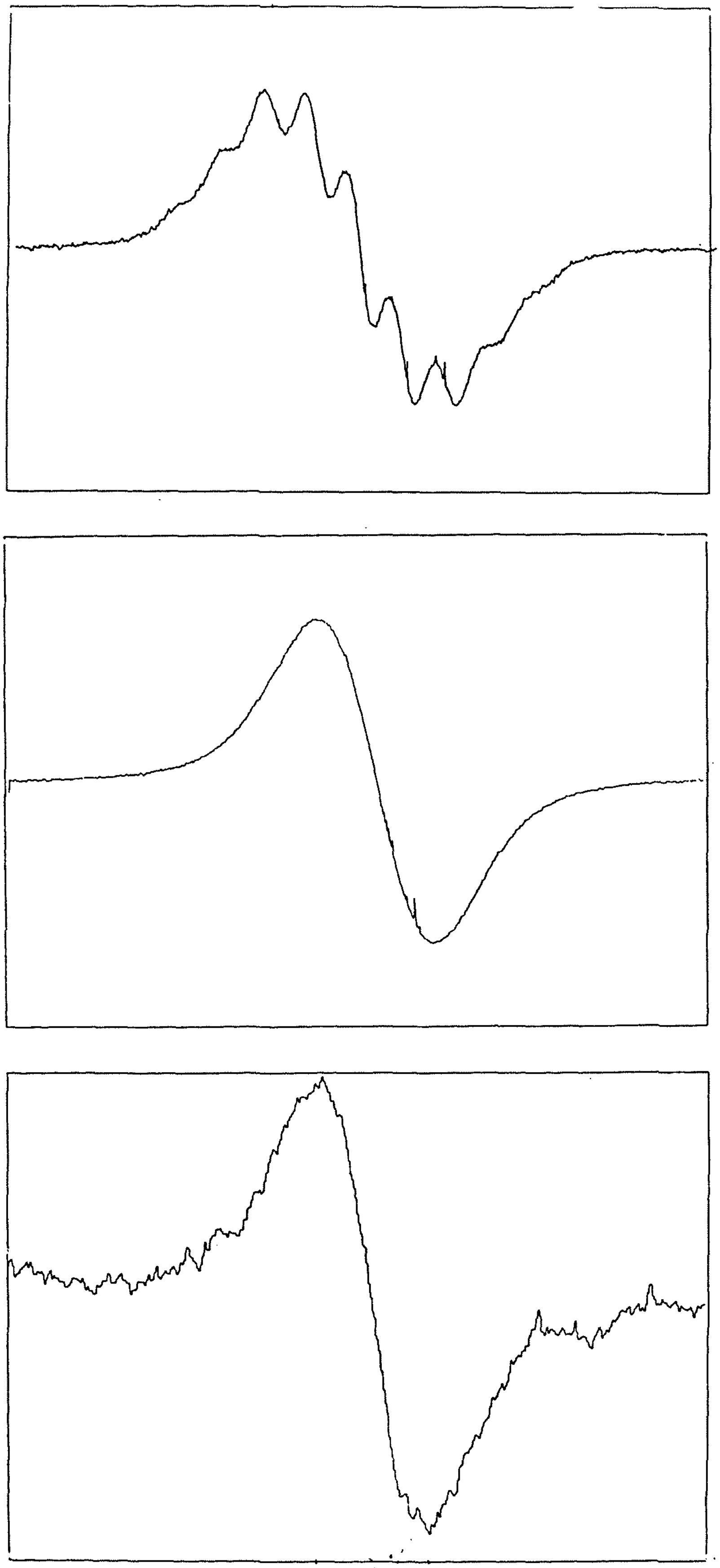


Figure 3.6. Cyclic voltammograms of CuTFPP and $CuTFPPMe_8$ in 0.1 M $TBAPF_6/CH_2Cl_2$..

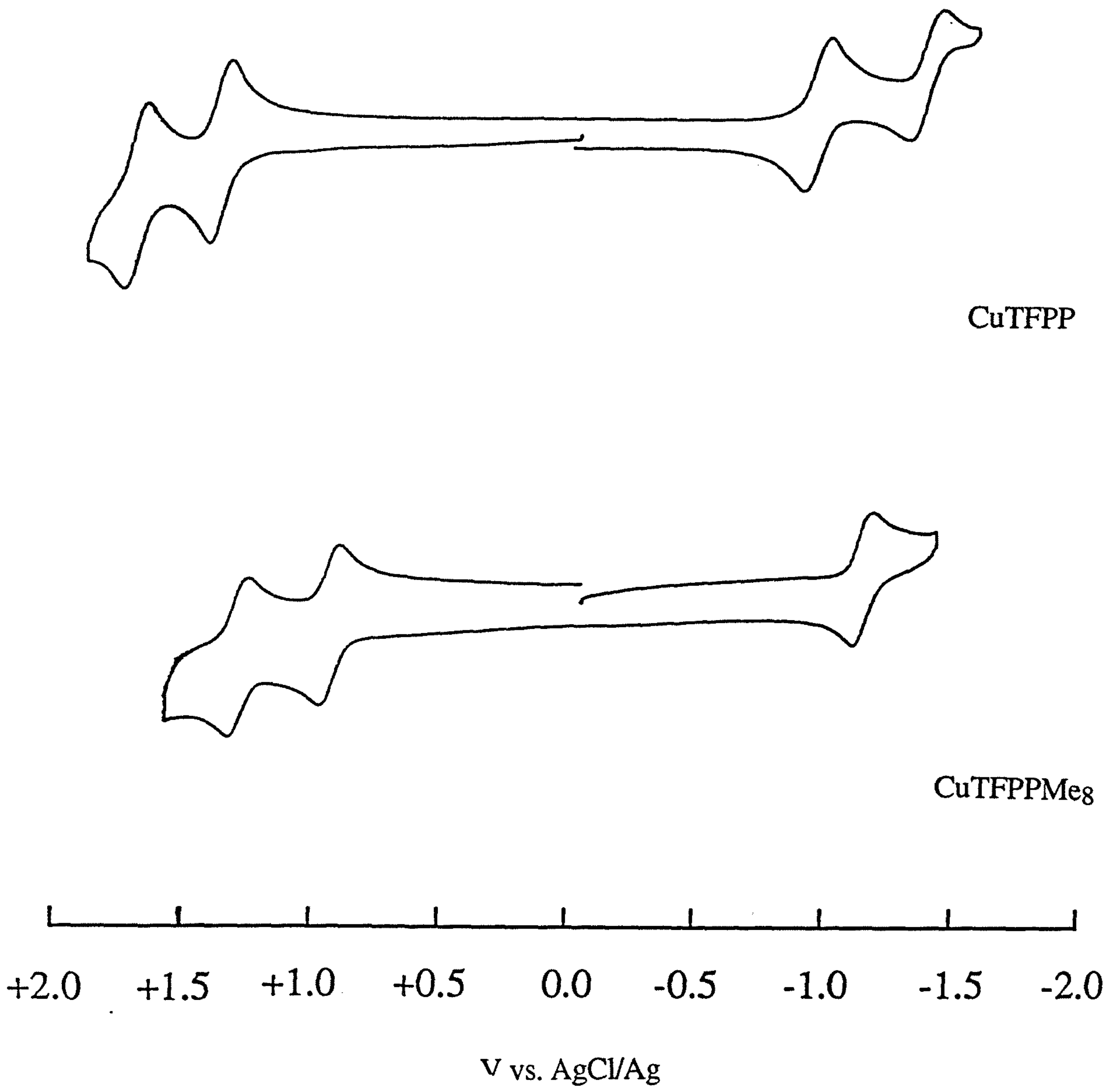
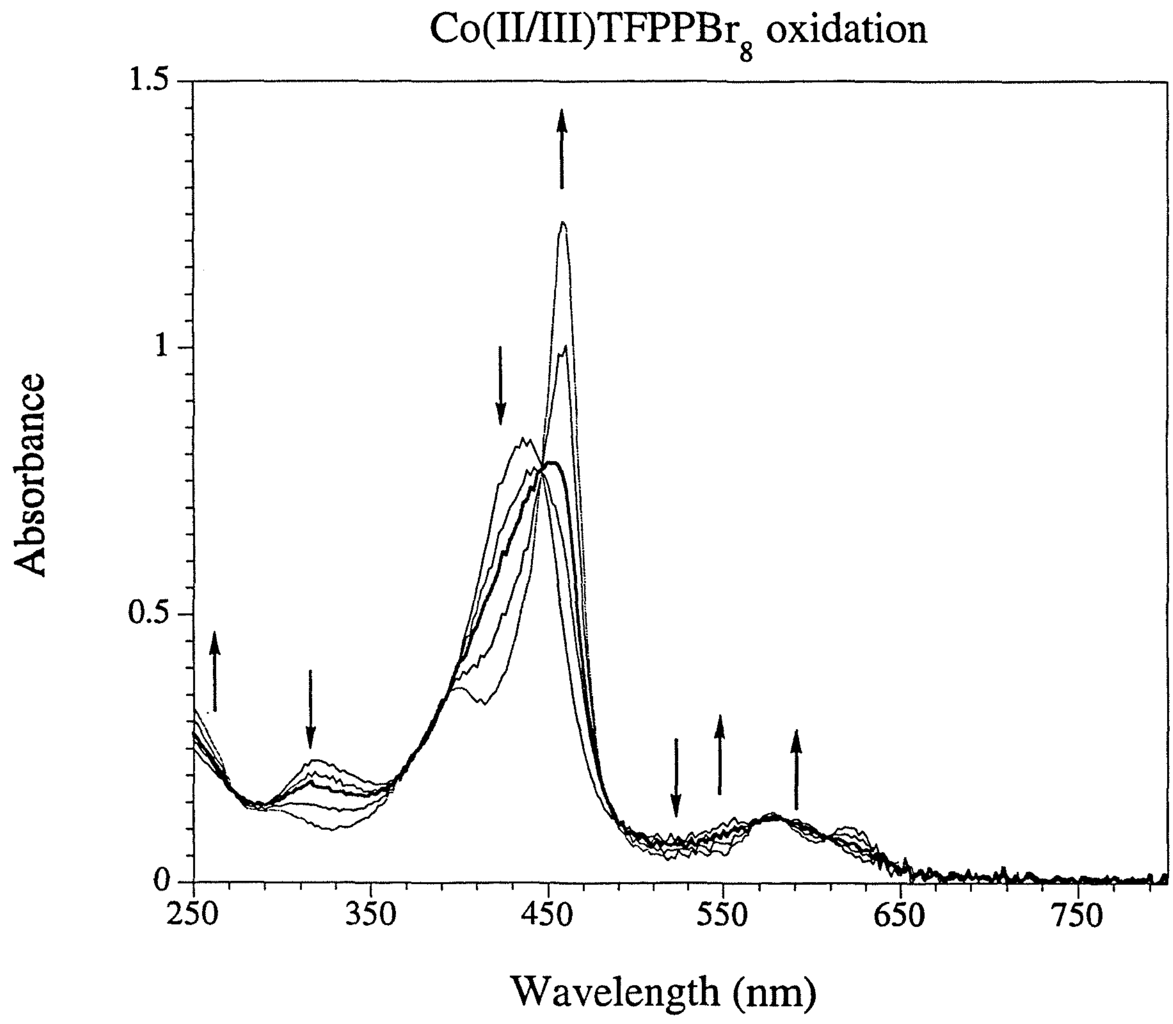
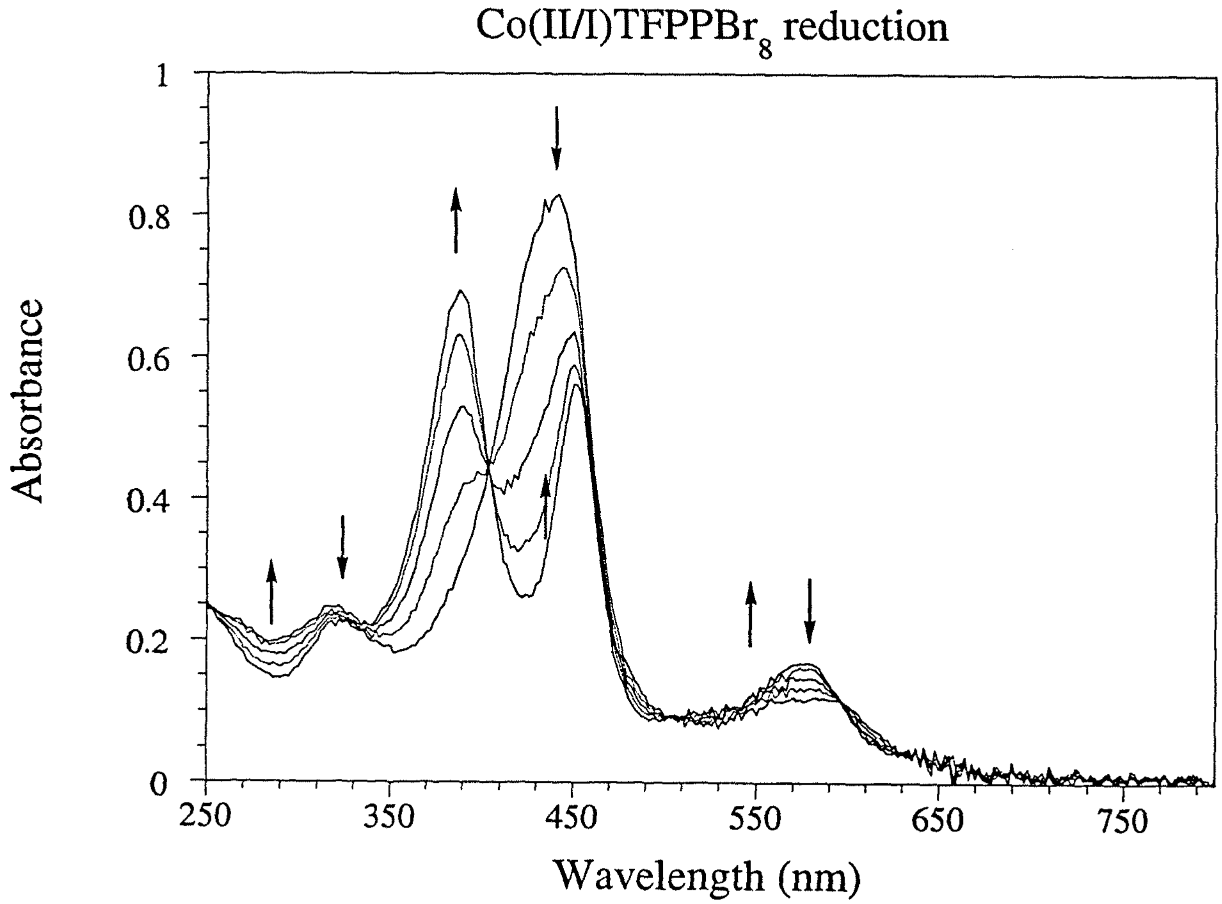

CuTFPP
CuTFPPMe8
+2.0
+1.5
+1.0
+0.5
0.0
-0.5
-1.0
-1.5
-2.0
V vs. AgCl/Ag

Figure 3.7. Changes in the absorption spectrum of $CoTFPPBr_8$ in 0.1 M $TBAPF_6/CH_2Cl_2$ recorded during a slow (4 mV/s) cyclic potential sweep showing (a.) the oxidation of Co(II) to Co(III) (occurring at approximately 0.5 V) and (b.) the reduction of Co(II) to Co(I) (occurring at approximately -0.1 V).



Co(II/III)TFPPBr$_8$ oxidation
1.5
1
0.5
0
250
350
450
550
650
750
Absorbance
Wavelength (nm)



Co(II/I)TFPPBr$_8$ reduction
Absorbance
Wavelength (nm)
0
0.2
0.4
0.6
0.8
1
250
350
450
550
650
750

CHAPTER 4:

ELECTRONIC STRUCTURE

Introduction:

In 1956, when R. J. P. Williams published a review entitled, "The Properties of Metalloporphyrins,"[1] the UV and visible absorption spectra of naturally occurring porphyrins and their metallo-derivatives (especially Fe(III)) were well-documented. Although it was generally accepted that the optical absorption spectra were π-π^* or possibly N-π^* in origin, questions remained about the number of bands, the relative intensities of the bands, the shifts observed with metallo- and peripheral substitution, and changes in axial ligation at the metal-center. Figure 4.1 shows the spectrum for a typical metalloporphyrin derivative, ZnOEP. Although OEP is a synthetic porphyrin, its spectral properties closely mimic those of most natural porphyrins.

Molecular orbital calculations were reported as early as 1949, but their 'necessarily crude' nature precluded truly meaningful insight.[2] Most naturally occurring porphyrins are essentially planar and highly conjugated, therefore it was assumed that most electronic spectral properties originate with the π-electrons. Simple Hückel calculations, in which molecular orbitals are generated from linear combinations of atomic orbitals, generate the result that there are two nearly, yet accidentally, degenerate filled orbitals of a_{1u} and a_{2u} symmetry for the D_{4h} porphyrin and two degenerate π orbitals of e_g symmetry that are next in energy and unfilled.[3] Later semi-empirical self-consistent-field,[4] modified and extended Hückel,[5] and complete neglect of differential overlap methods reproduced the spirit of the simple Hückel calculations.[2] The labels B and Q refer to one and nine units of angular momentum in the excited state configurations, generated from transitions between the molecular orbitals.[3]

Gouterman proposed that the observed Q and B bands were the result of the interaction of the $(a_{2u}e_g)$ and the $(a_{1u}e_g)$ configurations rather than individual transitions between molecular orbitals.[6] Figure 4.2 shows the molecular orbitals and the states resulting from the mixing of configurations. Thus, although $a_{1u}\rightarrow e_g$ and $a_{2u}\rightarrow e_g$

transitions would be expected to yield bands of relatively equal intensity, a spectrum resulting from the interaction of the configurations would not. This type of configuration interaction had been used previously to explain the electronic spectra of polyenes.[3,7] Gouterman qualitatively explained metallo- and peripheral substitution induced changes in porphyrin electronic spectra as resulting from the interaction of the metal d_π and p_π orbitals with the porphyrin e_g and a_{2u} orbitals. He made the empirical observation that the metal d orbitals had less effect on the spectra than the p_z orbital. The increasing electronegativity of the central metal atom acts inductively to lower the energies of the e_g and a_{2u} orbitals.[6]

Results and Discussion:

The UV-vis spectra of porphyrins and metalloporphyrins are dominated by two relatively intense singlet π-π^* transitions, termed the B bands ($\varepsilon \approx 10^5$ M^{-1} cm^{-1}) (or Soret band) and the lower energy Q bands ($\varepsilon \approx 10^4$ M^{-1} cm^{-1}). Figure 4.1 contains a UV-vis spectrum of ZnOEP with the B and Q bands marked. These transitions are quite adequately explained by Gouterman's four orbital model. The HOMOs consist of two nearly degenerate orbitals of a_{1u} and a_{2u} symmetry and the LUMOs of two degenerate orbitals of e_g symmetry (in D_{4h} symmetry) and configuration interaction between ($a_{1u}e_g$) and ($a_{2u}e_g$) generates the Q and the B states (Figure 4.2).[6] Two bands are frequently observed in the visible region, the Q(0,0) and the higher energy Q(1,0). The spectra of the free ligands (H_2Ps) frequently show four distinct Q bands: the $Q_x(0,1)$, $Q_x(0,0)$, $Q_y(0,1)$, and $Q_y(0,0)$, produced by the reduction of symmetry from D_{4h} to D_{2h}.[8]

The energies of the π-π^* transitions are affected by substituents around the ring, metal-substitution (and ligand-substitution on the metal), and distortion of the macrocycle from planarity. From the calculated orbital electron-density maps (Figure 4.3) it is possible to see that the energy of the a_{2u} orbital should be affected both by metallosubstitution and by the electron-donating or withdrawing ability of the *meso*-substituent, since it has density concentrated at the Ns and the *meso*-carbons. The calculated electron density on the nitrogens is in accord with EPR spin-density mappings for the porphyrin cation radical of ZnTPP in which hyperfine structure produced by coupling to the nitrogens is clearly visible.[9] In comparison, the a_{1u} orbital is relatively unaffected by *meso*- and metallosubstitution since electron density is concentrated at the α-carbon. The a_{1u} orbital has density at the β-positions. Furthermore, the e_g orbitals are predicted to have density at the Ns and β-positions. Metal effects on the π-π* transitions take the form of metal interaction with the a_{2u} orbital (lowering the energy) and electron donation from the d_{xz}, d_{yz} orbitals to the e_g orbitals (an interaction that raises the energies of the e_g orbitals). The (d_{xz}, d_{yz}) - e_g interaction is commonly referred to as metal-ligand backbonding. Additionally, it is possible to observe extra bands in the UV-vis spectra of metalloporphyrins arising from metal-to-ligand and ligand-to-metal charge transfers.

The UV-vis absorption bands of distorted β-substituted tetraphenylporphyrins have been observed to shift to lower energy with increasing distortion of the macrocycle. Semiempirical AM1 calculations on $TFPPX_8$ (X = H, Cl, Br) reveal that, although the distortion destabilizes both the HOMO and LUMO, the effect is greater on the HOMO. Furthermore, it was predicted that halogenation of the macrocycle lowers the energy of the HOMOs and LUMOs approximately equally.[10] Electrochemical data (Chapter 3) are consistent with these predictions. Relative to the flat ZnTFPP complex, $ZnTFPPCl_8$ and $ZnTFPPBr_8$ are, respectively, 0.47 and 0.48 V easier to reduce, but only 0.26 and 0.20 V harder to oxidize. In the case of $ZnTFPPMe_8$, the macrocycle is 0.4 V easier to oxidize and only 0.19 V harder to reduce than ZnTFPP. The effect is especially evident in a comparison of $ZnTFPPMe_8$ to $ZnTFPPEt_8$: the octaethyl macrocycle is at least 0.20V easier to oxidize, and only 0.04V harder to reduce. Electronic structure calculations show that the electron-density patterns of the D_{4h} HOMOs and LUMOs are maintained in the D_2 system (a_{1u}, a_{2u} $\rightarrow$ a, b_1, $e_g \rightarrow b_2$, b_3).[10] Figure 4.3 contains a picture of the calculated energy distributions of the $a(a_{1u})$, $b_1(a_{2u})$, and b_2, $b_3(e_g)$ orbitals. ZINDO calculations performed on $ZnTPPEt_8$ give similar results: HOMOs are raised in energy by 0.12 eV, whereas LUMOs are relatively insensitive to distortion.[11]

The relative extinction coefficients for the distorted porphyrins relative to the flat TFPP are shown in Figure 4.4. Although the bands for the distorted porphyrins appear to be less than half as intense as the planar one, oscillator strength estimates show that the bands are actually closer in intensity than first appearances would indicate.[12] Oscillator strengths for the spectra shown were calculated to be 1.82, 1.55, and 1.96 $M^{-1}cm^{-2}$ for CuTFPP, $CuTFPPCl_8$ and $CuTFPPBr_8$, respectively. This trend of wider bands accompanied by decreased extinction coefficients is true for all distorted tetraphenylporphyrin derivatives and is consistent with the large Stokes shift observed for the $H_2TFPPEt_8$ fluorescence, suggesting that the singlet excited state is distorted relative to the ground state.[13,14]

Tables 4.1 and 4.2 contain UV-vis data for metalloderivatives of various tetraphenylporphyrins and other common porphyrins. In general, metallation causes a large energy shifts for distorted porphyrins. The directions (either red or blue compared to the free ligand) are similar to those observed for TPP and OEP derivatives. Q and B bands are observed to shift in energy approximately equally. An exception is the Pd(II) derivatives in which the Q-bands are more red-shifted by metal substitution than the Soret. The shifts in Soret energy with metal-substitution observed (0.142 eV for $ZnTFPPBr_8$ to $CuTFPPBr_8$) are larger than for the planar porphyrins (0.044 eV for ZnTFPP to CuTFPP). The perhalogenated tetraphenyl porphyrins also exhibit an accessible higher protonation state in which the Soret is red-shifted (to 490 nm in the case $H_4TFPPBr_8^{++}$). The accessibility of higher protonation states is typical of distorted halogenated porphyrins.[13]

Typically, a red emission is observable for the free ligands of planar porphyrins. This emission is visible under a hand-held UV lamp and can be used to follow the progress of metallation reactions by the disappearance of the red emission. This emission was not observable for the perhalogenated metalloporphyrins, although an emission could be seen in the intense laser beam during the collection of resonance Raman data. It has been reported that weaker emission is observed for distorted octaalkylporphyrins than for planar porphyrins.[14]

The HOMO energy order is $a_{1u} > a_{2u}$ for TFPP derivatives. The increasing absorption intensity of Q(0,0) relative to Q(1,0) for the series $ZnTFPPX_8 < CuTFPPX_8 < PdTFPPX_8$ (X = Cl, Br, Me) (Figures 4.5 and 4.6) is consistent with this assignment.[15] The relative intensities of the two Q bands are dependent on the energy difference between the $a(a_{1u})$ and the $b_1(a_{2u})$ orbitals. The intensity of the Q(1,0) is relatively constant. The qualitative MO energy level scheme shown in Figure 4.9 is derived from this observation. $ZnTPP^+$ and $ZnTFPP^+$ have been assigned to $^2A_{1u}$ and $^2A_{1u}$ radical cations, respectively, from EPR measurements.[9,16] The almost complete absence of the Q (0,0) band for $ZnTFPPBr_8$ is indicative of the closeness of the energy levels of the a_{1u} and a_{2u} orbitals. When the ligand is metallated with copper, the Cu(II) ion interacts with the a_{2u} orbital, lowering it in energy, and increasing the gap between the a_{1u} and a_{2u} orbitals, thus the (0,0) band is observable in the spectrum of $CuTFPPBr_8$. Furthermore, the EPR spectrum of $ZnTFPPBr_8^+$ (recorded at -50°C in $CH_2Cl_2/TBAClO_4$) reveals a broad, structureless signal at g = 2.015, consistent with a $^2A(^2A_{1u})$ ground state (see Chapter 3).

Figure 4.7 shows the spectra of $ZnTFPPMe_8$, $ZnTFPPEt_8$, and $ZnTFPPBr_8$. Consistent with $TFPPMe_8$ being less distorted than $TFPPEt_8$, $ZnTFPPMe_8$ is blue-shifted relative to $ZnTFPPEt_8$. Inconsistent with distortion as the only effect on the energy of the Soret transition, $ZnTFPPBr_8$ is significantly red-shifted as compared to $ZnTFPPEt_8$. $ZnTFPPEt_8$ should be more distorted than $ZnTFPPBr_8$, therefore it would seem that the energy of the Soret band is also affected by the substituent. It appears that β-substitution has a larger effect on the LUMOs than the HOMOs.

Metal- and distortion-induced shifts in the absorption energies, similar to $TFPPBr_8$, are observed for the $TPPBr_8$ metalloderivatives (Table 4.2).[13] A large Q(0,0) band is observed for $ZnTPPBr_8$ and it decreases in intensity along the series Zn > Cu > Pd. The authors assign the HOMO as a_{2u}.

A further substituent effect can be seen comparing the spectra of $CuT(2,6)FPPMe_8$ and $CuTFPPMe_8$ (Figure 4.8). The Q(0,0) band has less intensity for the $T(2,6)FPPMe_8$ derivative, implying the a_{1u} and a_{2u} orbitals are closer in energy in the $T(2,6)FPPMe_8$ derivative, consistent with the a_{2u} orbital being lowered in energy by halogenation of the phenyl ring.

Conclusions:

The electronic behavior of distorted metalloporphyrins is adequately explained in terms of Gouterman's four orbital model. Although the observed shifts are similar to those for planar porphyrins, the reason for the magnitude of the metal-induced shifts is unresolved. Using the predictions of Gouterman's calculations it is possible to determine the HOMO for the porphyrin. (It is not possible to predict this calculationally.) It was determined that porphyrins substituted with as few as two fluorines on the phenyl groups have $^2A_{1u}$ cation radicals. Figure 4.9 shows a diagram of the relative a_{1u} and a_{2u} energy levels for a series of tetraphenyl porphyrins. It can be seen that *meso*-substitution is the important factor in determining the HOMO.

Metal effects determined from cyclic voltammetric measurements (Chapter 3) are far less interesting than those seen in the UV-vis spectra. Cu(II) substitution shifts both the HOMOs and LUMOs to lower energy (by only about 0.04 V) approximately equally, as compared to the Zn(II) porphyrins. Thus, it is not possible to explain the observed red-shift in the UV-vis spectra from these measurements. Furthermore, although the observed red-shift in the Pd(II) spectrum is attributed to metal-to-ligand back-bonding to the unfilled porphyrin e_g orbitals, it is not possible to observe the expected increase in LUMO energy electrochemically. Metal-to-ligand back-bonding has been observed electrochemically and UV-vis spectroscopically in the case of the Ru derivatives of $TFPPPCl_8$.[17] Furthermore, the energy gap between the first oxidation and the first reduction of the porphyrin ligands for the distorted porphyrins at around 2.0 eV. This energy falls between the energies of the B and Q bands, but corresponds most closely to that of the Q band.

Experimental:

UV-vis spectra were recorded on either a Hewlett-Packard 8452A diode array spectrophotometer or a Cary-14 retrofitted with an OLIS 3820 operating system. Solvents were EM Science Omnisolve grade or Burdick and Jackson, high purity. Porphyrin syntheses and purification procedures are reported in Chapter 2.

References and Notes:

(1) Williams, R. J. P. *Chem. Rev.* **1956**, *56*, 299-328.

(2) Chantrell, S. J.; McAuliffe, C. A.; Munn, R. W.; Pratt, A. C. *Coord. Chem. Rev.* **1974**, *16*, 259-284, and references therein.

(3) Platt, J. R. In *Radiation Biology*; A. Hollaender, Ed.; McGraw-Hill: New York, 1956; Vol. III; pp 71-123.

(4) Weiss, C.; Kobayashi, H.; Gouterman, M. *J. Mol. Spectrosc.* **1965**, *16*, 415-450.

(5) Zerner, M.; Gouterman, M. *Theoret. Chim. Acta (Berl.)* **1966**, *4*, 44-63.

(6) Gouterman, M. *J. Chem. Phys.* **1959**, *30*, 1139-1161.

(7) Moffitt, W. *J. Chem. Phys.* **1954**, *22*, 1820-1829.

(8) Gouterman, M. In *The Porphyrins*; D. Dolphin, Ed.; Academic Press: New York, 1978; Vol. III; pp 1-165.

(9) Fajer, J.; Borg, D. C.; Forman, A.; Dolphin, D.; Felton, R. H. *J. Am. Chem. Soc.* **1970**, *92*, 3451-3459.

(10) Takeuchi, T.; Gray, H. B.; Goddard, W. A. *J. Am. Chem. Soc.* **1994**, *116*, 9730-9732.

(11) Barkigia, K. M.; Chantranupong, L.; Smith, K. M.; Fajer, J. *J. Am. Chem. Soc.* **1988**, *110*, 7566-7567.

(12) Oscillator strenghts were estimated according to $f = 4.60x10^{-9}\varepsilon_{max}\upsilon_{1/2}$. Values of extinction coefficents were taken to be 540,000, 200,000, and 200,000 $M^{-1}cm^{-1}$ for CuTFPP, $CuTFPPCl_8$ and $CuTFPPBr_8$, respectively.

(13) Bhyrappa, P.; Krishnan, V. *Inorg. Chem.* **1991**, *30*, 239-245.

(14) Regev, A.; Galili, T.; Medforth, C. J.; Smith, K. M.; Barkigia, K. M.; Fajer, J.; Levanon, H. *J. Phys. Chem.* **1994**, *98*, 2520-2526.

(15) Spellane, P. J.; Gouterman, M.; Antipas, A.; Kim, S.; Liu, Y. C. *Inorg. Chem.* **1980**, *19*, 386-391.

(16) Gross, Z.; Barzilay, C. *Angew. Chem.* **1992**, *31*, 1615-1617.

(17) Birnbaum, E. R.; Schaefer, W. P.; Labinger, J. A.; Bercaw, J. E.; Gray, H. B. *Inorg. Chem.* submitted.

(18) Grinstaff, M. W.; Hill, M. G.; Birnbaum, E. R.; Schaefer, W. P.; Labinger, J. A.; Gray, H. B. *Inorg. Chem.* in preparation.

(19) Sparks, L. D.; Medforth, C. J.; Park, M.-S.; Chamberlain, J. R.; Ondrias, M. R.; Senge, M. O.; Smith, K. M.; Shelnutt, J. A. *J. Am. Chem. Soc.* **1993**, *115*, 581-592.

(20) Barkigia, K. M.; Berber, M. D.; Fajer, J.; Medforth, C. J.; Renner, M. W.; Smith, K. M. *J. Am. Chem. Soc.* **1990**, *112*, 8851-8857.

(21) Skillman, A. G.; Collins, J. R.; Loew, G. H. *J. Am. Chem. Soc.* **1992**, *114*, 9538-9544.

Table 4.1. Soret Bands of Metallotetraphenylporphyrins (λ_{max} /nm in CH_2Cl_2).[a]

Metal	TPP[b]	TFPP	$TFPPCl_8$	$TFPPBr_8$	$TFPPMe_8$	$TFPPEt_8$
Fe(III)Cl	416[c]	418[c]		440[c]		384,436
Co	410	404(554)	430	438(600)	–[d]	–[d]
Ni	404[e,f]	406(560)	430(594)	436(600)	–[d]	–[d]
Pd			423(580)	434(592)	420(581)	–[d]
Cu	405[e,f]	408(570)	430(602)	438(613)	424(601)	–[d]
Zn	418	414(580)	442[f]	464[f]	434(603)	450(619)
Mg	400(600)[e]		–[d]	460[f]	–[d]	–[d]
H_2	418	412	436	454	434	450

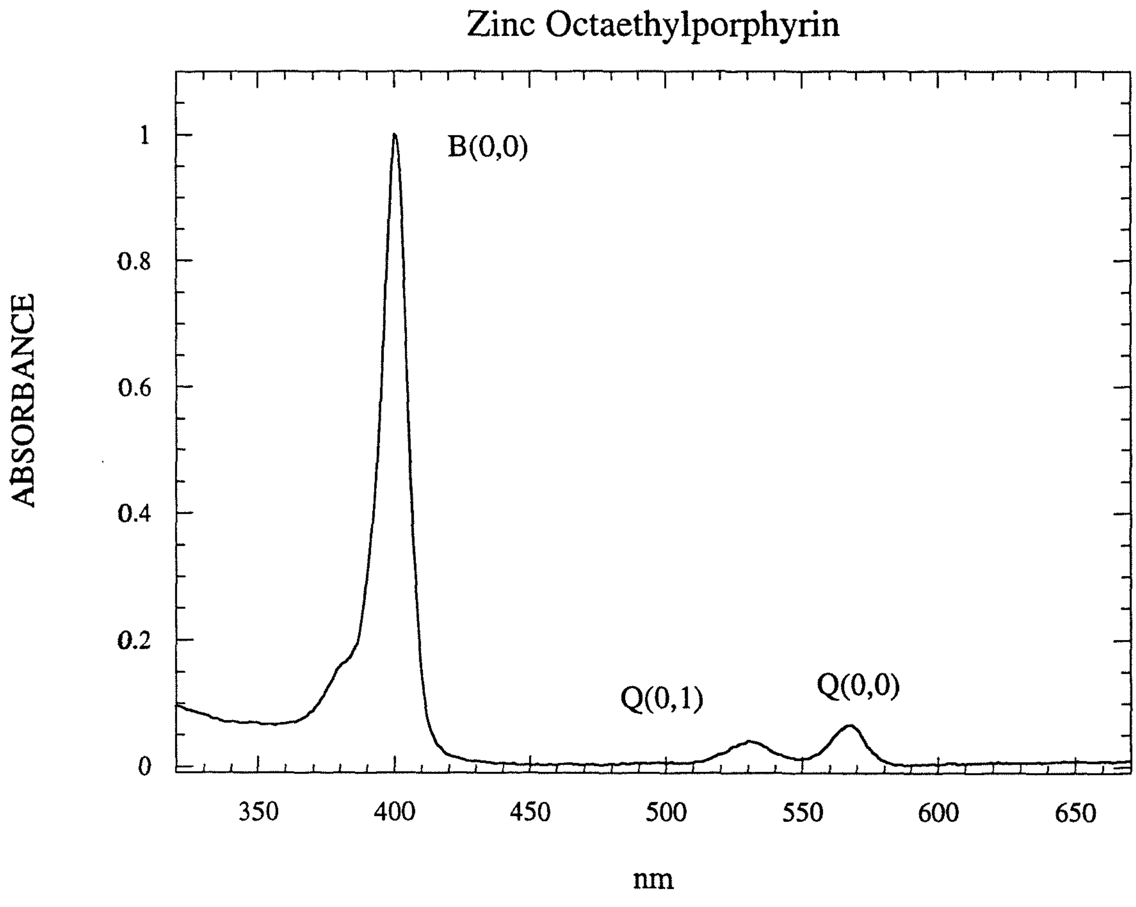
[a] Q(0,0) in ( ).
[b] Data is in agreement with literature reports.
[c] From reference 18.
[d] Not determined.
[e] From reference 8 and references therein. Recorded in the vapor phase.
[f] Q(0,0) not observed.

Table 4.2. Soret Bands of Related Metalloporphyrins (λ_{max} /nm in CH_2Cl_2).[a]

Metal	OEP[b]	$TPPBr_8$[c]	$TPPEt_8$	$T(2,6)FPPMe_8$
Fe(III)Cl			399, 442[d]	–[f]
Co	382(554)	446	432[d]	–[f]
Ni	384(558)	448		–[f]
Cu	388(566)	466	430[d]	423
Zn	386(572)	466	454[e]	434
H_2		469		434

[a] Q(0,0) in ( ).
[b] From reference 8 and references therein. Recorded in the vapor phase.
[c] From reference 13. Recorded in CH_2Cl_2.
[d] From reference 19. The solvent was not reported
[e] From reference 20. Recorded in CH_2Cl_2.
[f] Not determined.

Figure 4.1. Typical UV-vis spectrum of planar porphyrin (ZnOEP) showing B (Soret) and Q bands. Recorded in CH_2Cl_2.



Zinc Octaethylporphyrin
ABSORBANCE
1
0.8
0.6
0.4
0.2
0
B(0,0)
Q(0,1)
Q(0,0)
350
400
450
500
550
600
650
nm

Figure 4.2. Gouterman's Four Orbital Model. Configuration interaction between ($a_{1u}e_g$) and ($a_{2u}e_g$) produces excited Q and B states corresponding to observed Q and B transitions in electronic spectra of porphyrins.

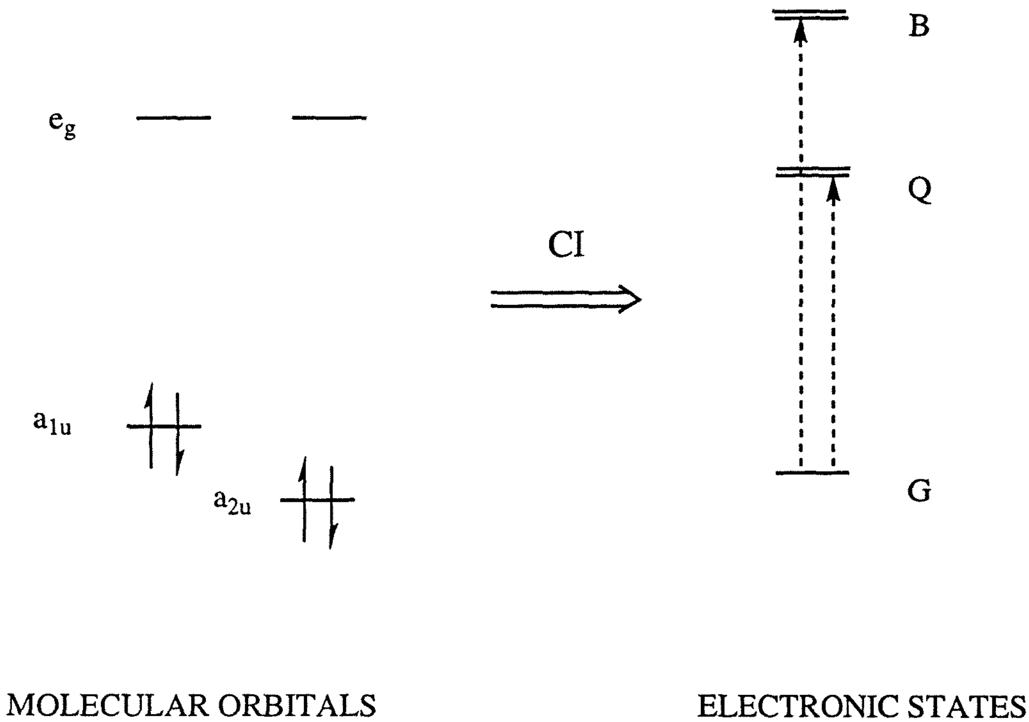
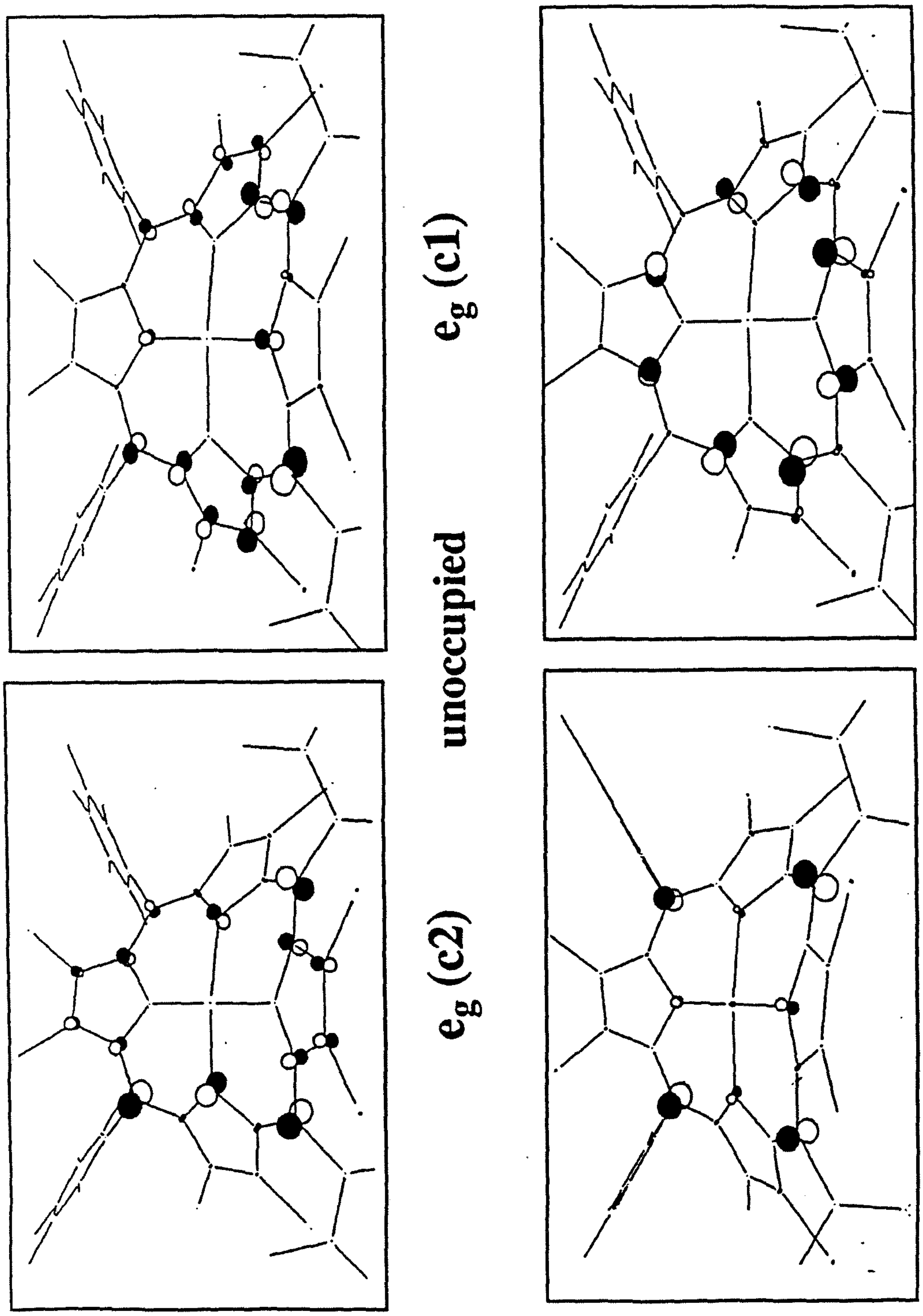
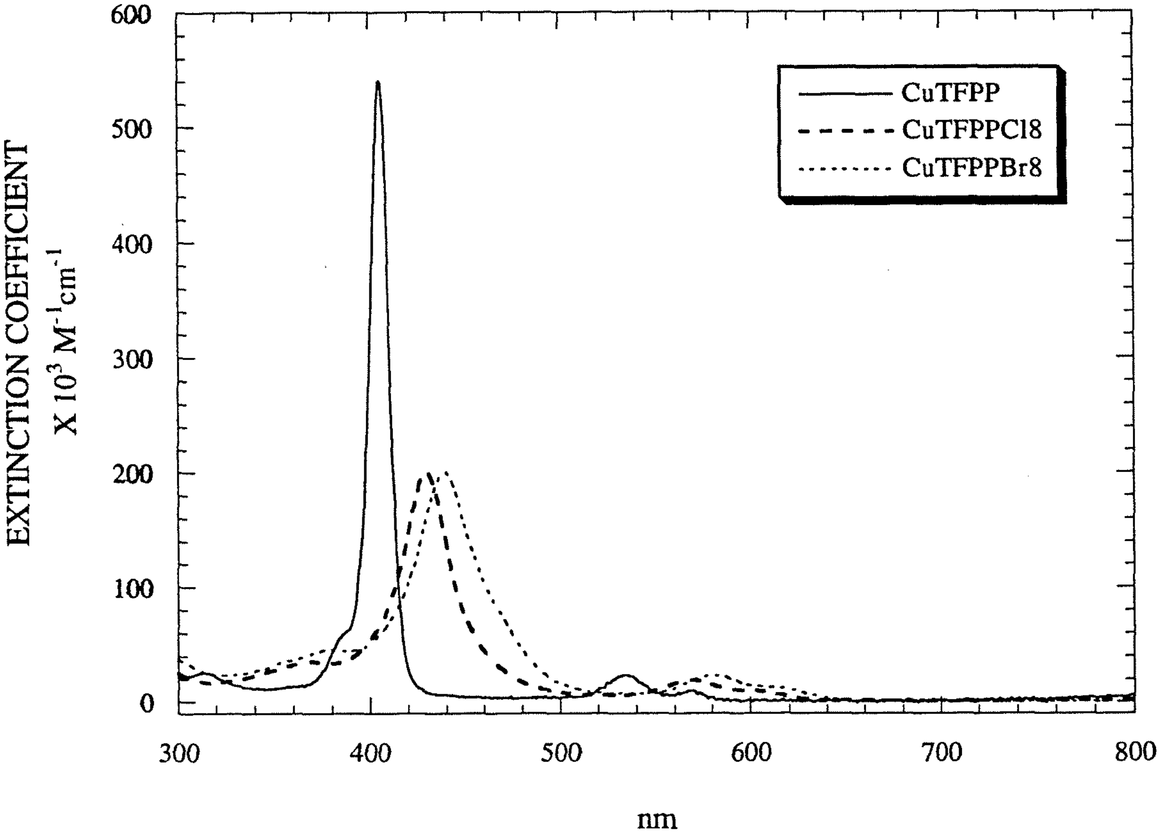

e$_g$
a$_{1u}$
a$_{2u}$
CI
B
Q
G
MOLECULAR ORBITALS
ELECTRONIC STATES

Figure 4.3. Pictures of calculated electron probability distributions for the frontier orbitals of D_2 porphyrins. From reference 10 .



e_g (c1)
unoccupied
e_g (c2)
a_{1u} (b2)
occupied
a_{2u} (b1)

Figure 4.4. UV-vis spectra of CuTFPP, $CuTFPPCl_8$, and $CuTFPPBr_8$ showing (a.) relative extinction coefficients and (b.) normalized spectra. Recorded in acetonitrile.



600
500
400
300
200
100
0
300
400
500
600
700
800
EXTINCTION COEFFICIENT
X 10^3 $M^{-1}cm^{-1}$
nm
CuTFPP
CuTFPPCl8
CuTFPPBr8

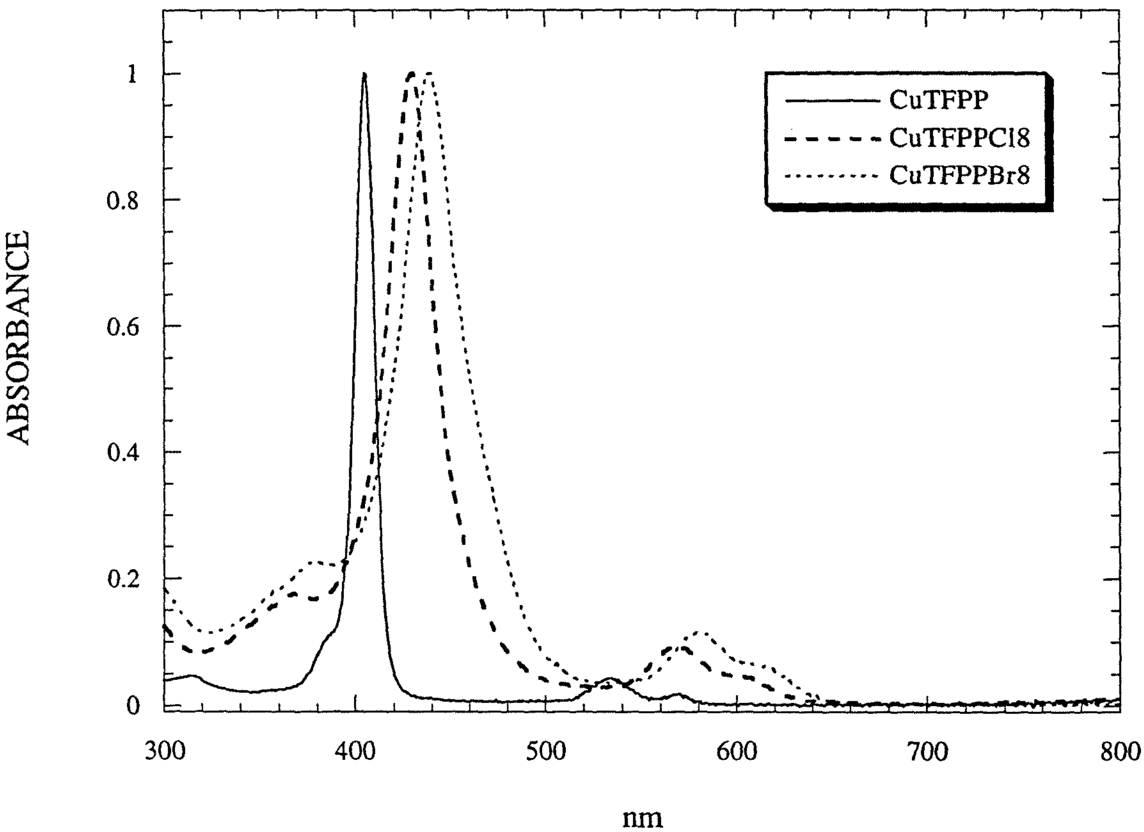
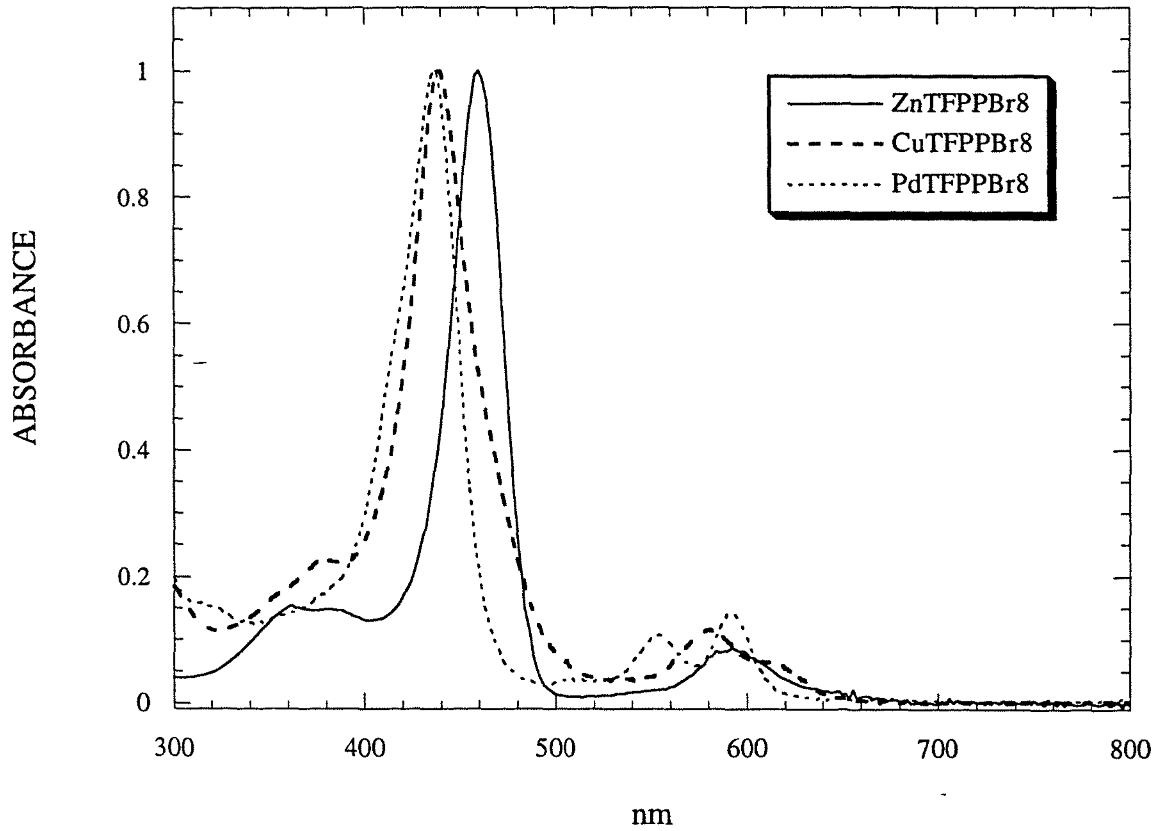
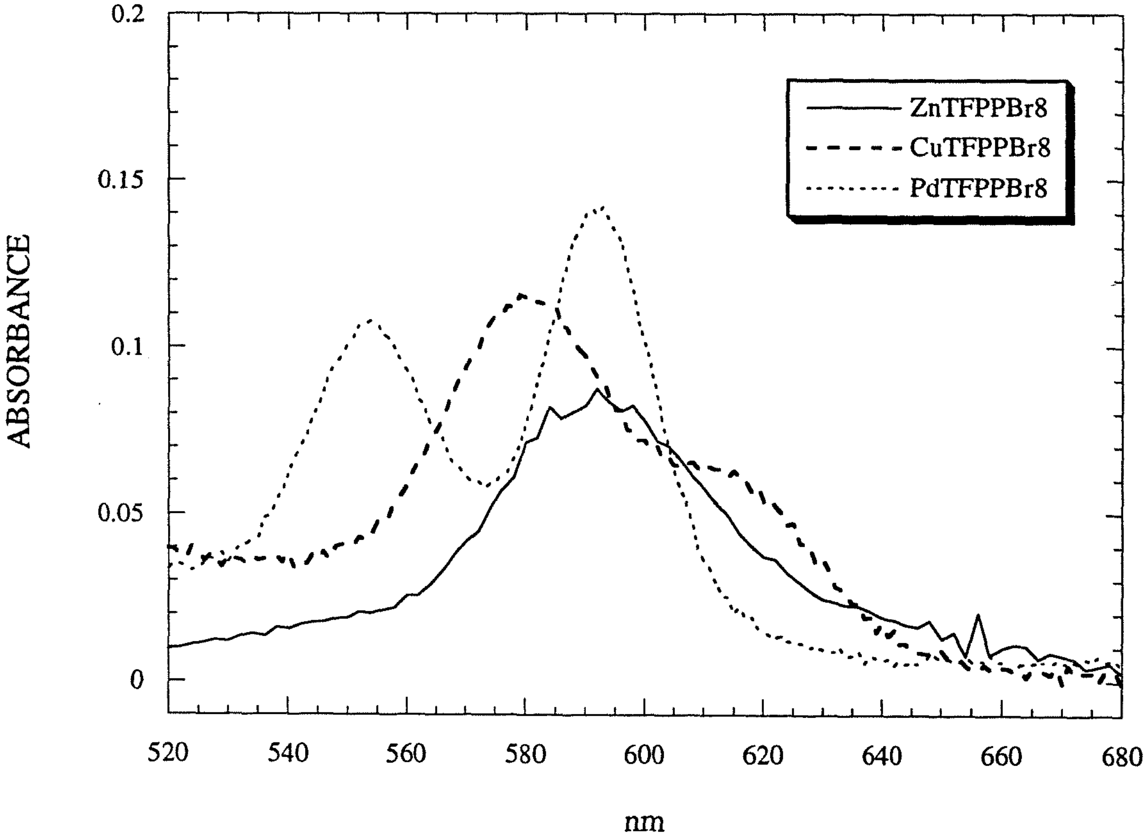

CuTFPP
CuTFPPCl8
CuTFPPBr8
ABSORBANCE
0
0.2
0.4
0.6
0.8
1
300
400
500
600
700
800
nm

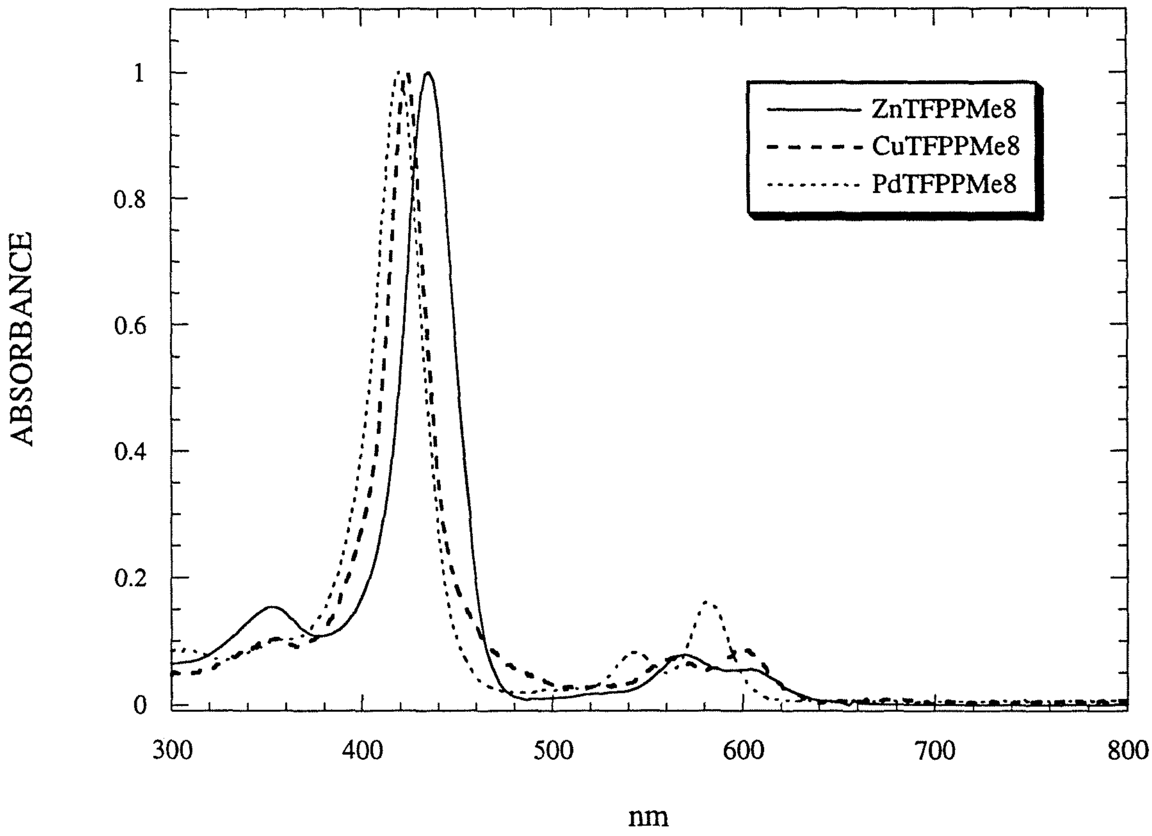
Figure 4.5. UV-vis spectra of $PdTFPPBr_8$, $CuTFPPBr_8$, and $ZnTFPPBr_8$, demonstrating metal effects. Recorded in CH_2Cl_2.


ZnTFPPBr8
CuTFPPBr8
PdTFPPBr8
ABSORBANCE
nm
0
0.2
0.4
0.6
0.8
1
300
400
500
600
700
800



ABSORBANCE
0.2
0.15
0.1
0.05
0
520
540
560
580
600
620
640
660
680
nm
ZnTFPPBr8
CuTFPPBr8
PdTFPPBr8

Figure 4.6. UV-vis spectra of $PdTFPPMe_8$, $CuTFPPMe_8$ and $ZnTFPPMe_8$. Recorded in CH_2Cl_2.


ZnTFPPMe8
CuTFPPMe8
PdTFPPMe8
ABSORBANCE
nm
0
0.2
0.4
0.6
0.8
1
300
400
500
600
700
800

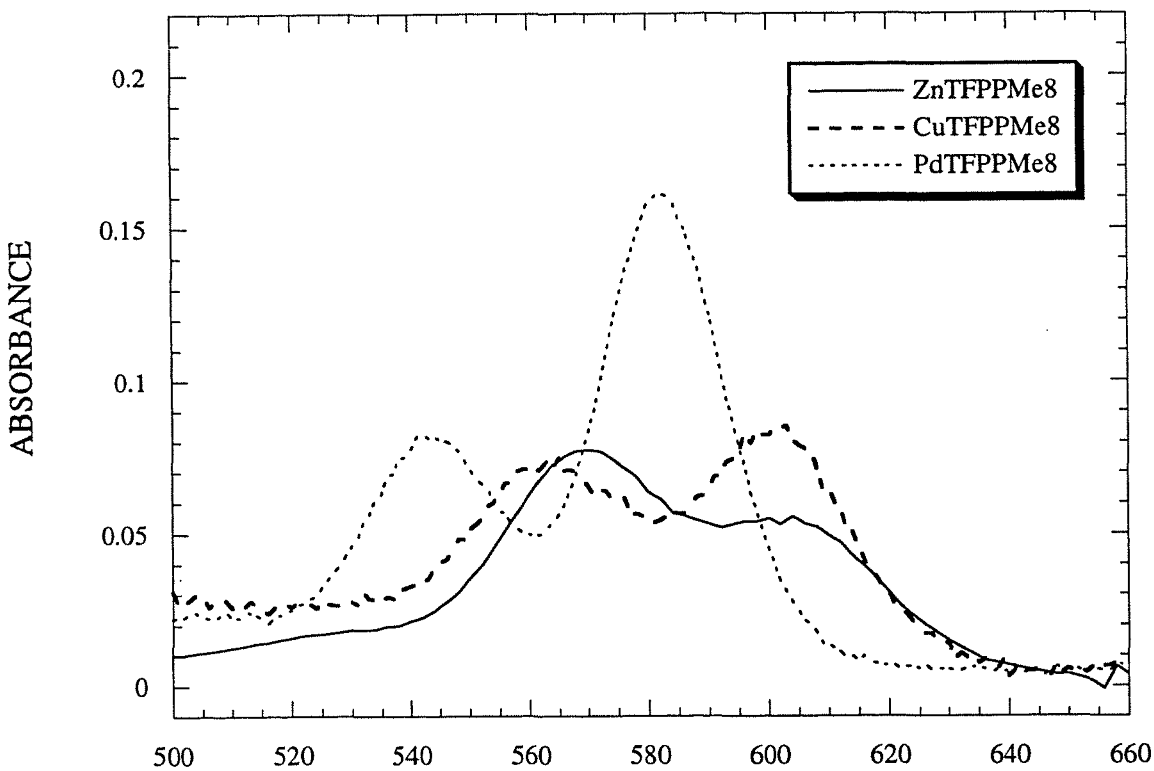
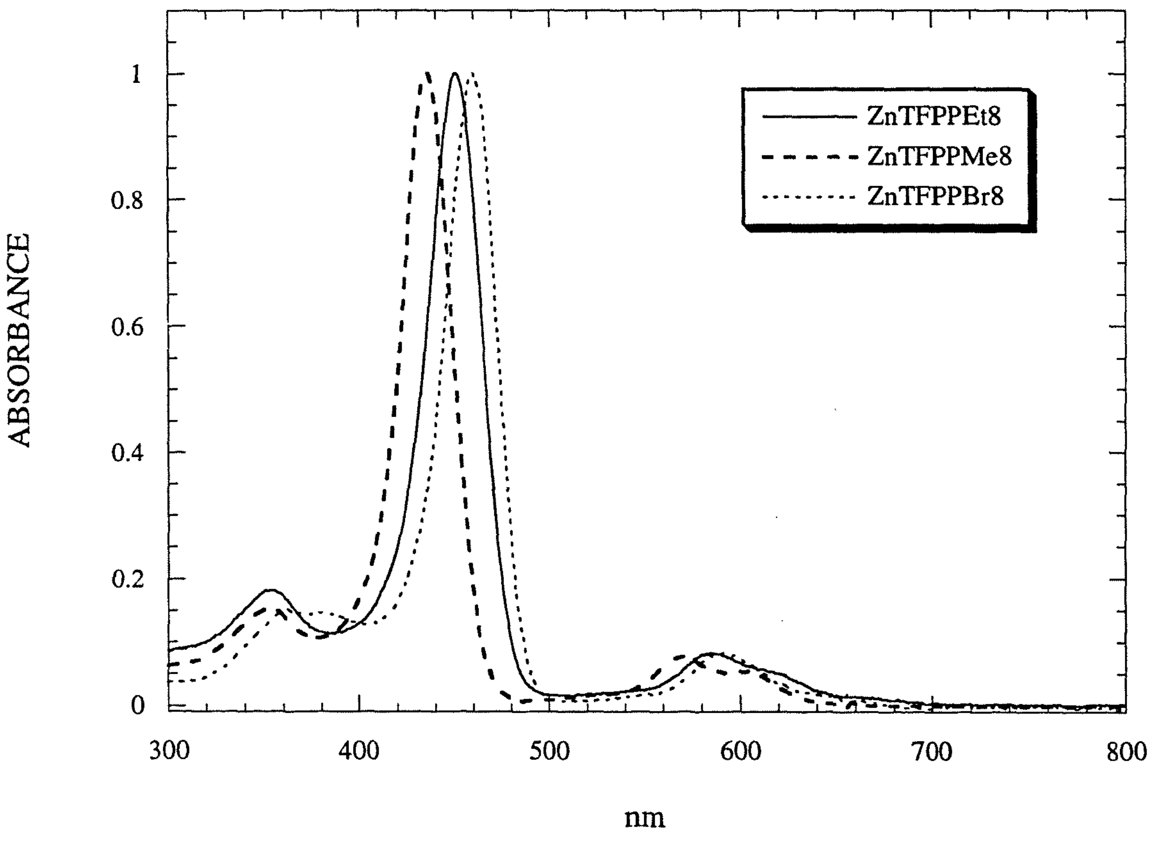
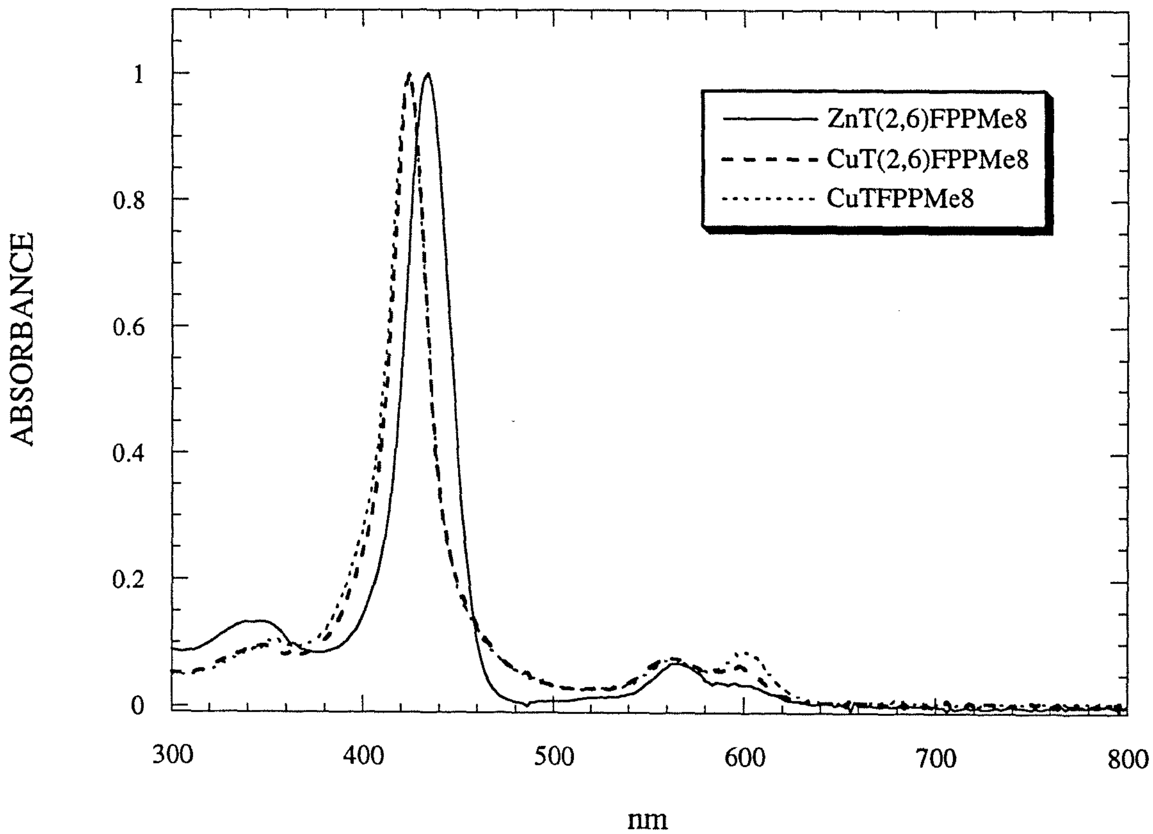

ZnTFPPMe8
CuTFPPMe8
PdTFPPMe8
ABSORBANCE
0.2
0.15
0.1
0.05
0
500
520
540
560
580
600
620
640
660
nm

Figure 4.7. UV-vis spectra of $ZnTFPPMe_8$, $ZnTFPPEt_8$, and $ZnTFPPBr_8$. Recorded in CH_2Cl_2.



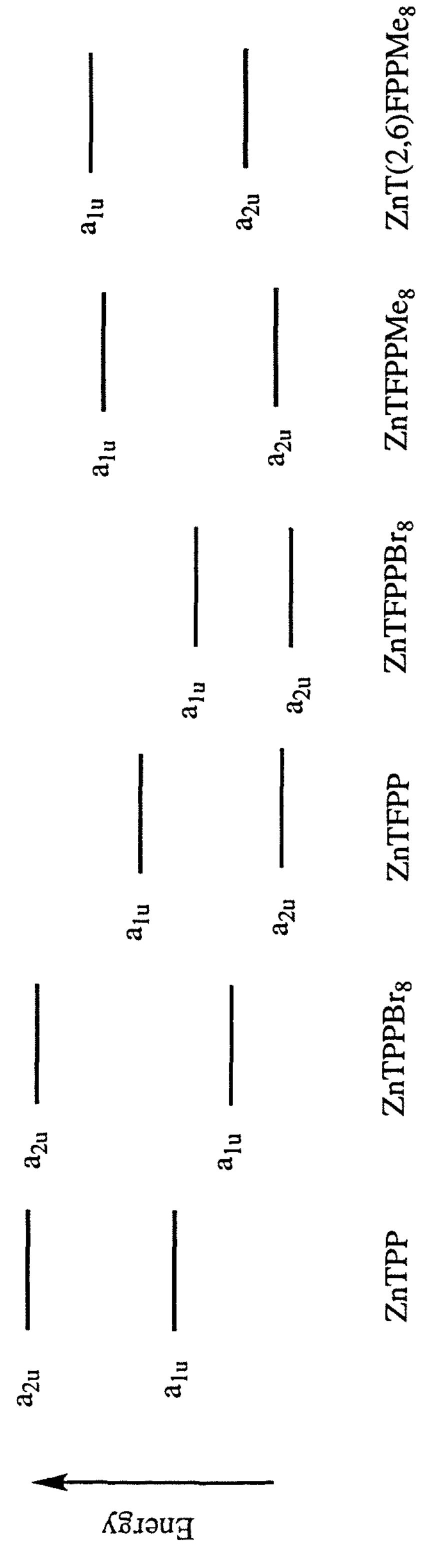
ZnTFPPEt8
ZnTFPPMe8
ZnTFPPBr8
ABSORBANCE
0
0.2
0.4
0.6
0.8
1
300
400
500
600
700
800
nm

Figure 4.8. UV-vis spectra of CuT(2,6)FPPPMe$_8$ and ZnT(2,6)FPPMe$_8$, and CuTFPPMe$_8$. Recorded in CH_2Cl_2.



ABSORBANCE
0
0.2
0.4
0.6
0.8
1
300
400
500
600
700
800
nm
ZnT(2,6)FPPMe8
CuT(2,6)FPPMe8
CuTFPPMe8

Figure 4.9. Qualitative MO scheme showing effects of substituents on the relative energies of the $a(a_{1u})$ and the $b_1(a_{2u})$ orbitals for a series of tetraphenylporphyrins.



ZnT(2,6)FPPMe$_8$
a$_{1u}$
a$_{2u}$
ZnTFPPMe$_8$
a$_{1u}$
a$_{2u}$
ZnTFPPBr$_8$
a$_{1u}$
a$_{2u}$
ZnTFPP
a$_{1u}$
a$_{2u}$
ZnTPPBr$_8$
a$_{2u}$
a$_{1u}$
ZnTPP
a$_{2u}$
a$_{1u}$
Energy

CHAPTER 5:

REVELATIONS

Crystal structures of tetraphenylporphyrins substituted with both alkyl groups and halogens in the β-pyrrole positions reveal a two-fold distortion that reduces the molecular symmetry to D_2: there is a saddling (in which the pyrrole β-carbons are alternately above and below the mean porphyrin plane) and a smaller ruffling (in which the *meso* carbons are above and below the mean plane). The distortion reduces the repulsions attributable to the short interatomic contacts between the β-substituents and the ortho-carbons of the phenyl groups by twisting the phenyl ring from an approximately perpendicular orientation to a more nearly coplanar one (a difference of about 15°). The distortion can be quantified as the average displacement of the *meso* and β- atoms from an average plane defined by the four N atoms (the N atoms are not coplanar: a tetrahedral distortion (±0.082 Å) is observed): $ZnTFPPBr_8$ C_{meso}, ±0.021 Å, C_β ±0.971 Å. Comparing the structures of $CuTFPPX_8$, displacements from planarity for X = Cl are about 70% of those for X = Br.[1-7]

Theoretical[8] and experimental work on tetraphenylporphyrins has shown that a $D_{4h} \rightarrow D_2$ distortion destabilizes the HOMOs (a_{1u}, a_{2u} in D_{4h} to a, b_1 in D_2) preferentially over the LUMOs (e_g in D_{4h} to b_2, b_3 in D_2). Substituent effects on the LUMOs are larger than on those observed on the HOMOs, thus β-halogenation also causes a slight red-shift in the observed UV-vis spectra and β-alkylation a slight blue-shift. Gouterman's four orbital model performs well for distorted porphyrins.[9]

Electronic structure calculations show that the electron-density patterns of the D_{4h} HOMOs and LUMOs are maintained in the D_2 system.[8] The relative ordering of the a(a_{1u}) and b_1(a_{2u}) orbitals is particularly sensitive to *meso* substitution, in accord with calculations and EPR spin-density mappings that indicate that the a(a_{1u}) orbital localizes electron density predominantly on C_α, whereas a b_1(a_{2u}) electron is concentrated on the *meso* position. Absorption, emission, and EPR spectra demonstrate that the ground state of $ZnTPP^+$ is $^2A_{2u}$, whereas that of $ZnTFPP^+$ or $ZnTFPPX_8^+$ is $^2A_{1u}$ or $^2A(^2A_{1u})$.[10-12] An electron-withdrawing group at the *meso* position lowers the energy of the b_1(a_{2u}) orbital relative to the a(a_{1u}). Since neither orbital places a significant amount of density at the β-positions, the HOMO for porphyrins with perfluorophenyl groups in the *meso* position is a or a_{1u}.

The results of electrochemical and spectroelectrochemical experiments that show that the π-cation radicals derived from the highly distorted (nonplanar) $ZnTFPPX_8$ (X = Cl, Br, Me) complexes are kinetically unstable, disproportionating rapidly to $ZnTFPPX_8^{2+}$ and the corresponding neutral species. We have found that *both* fluorophenyl substitution at the *meso* position and macrocyclic nonplanarity are required for π-cation radical disproportionation; the electronic nature of the β- substituent appears to be unimportant. Depopulation of the a(a_{1u}) orbital lowers the electronic barrier to saddling of the porphyrin structure, particularly if there are electron-withdrawing groups at the *meso* position. We propose that the requirement for a net 2e oxidation is then met in a porphyrin whose structure is distorted toward the geometrical configuration of the ground state of the doubly oxidized species.[13]

It should be possible to use these distorted zinc tetrakis(pentafluorophenyl)porphyrins as donors or acceptors in reactions requiring 2e steps. A 2e donor with a potential as low as 0.77 V vs AgCl/Ag ($ZnTFPPEt_8$) has been synthesized. It should be possible to further tune the potential positively 0.19 V with the $MgT(2,6)FPPEt_8$ derivative. Furthermore it has been shown that light-absorbing properties can be modulated through distortion, metal- and substituent effects. The $ZnTFPPMe_8$ porphyrin represents a molecule able to absorb over a wide range of wavelengths. In addition, the distorted octaalkyl tetrakis(pentafluorophenyl)porphyrins exhibit redox potentials similar to TPPs; therefore, it should be possible to test further the importance of distortion versus $Fe^{2+/3+}$ redox potential on catalytic activity for the $[FeTFPPX_8]Cl$ (X= Me, Et) derivatives. Furthermore, the low oxidation potential exhibited by $ZnTFPPEt_8$ provides the possibility that a crystal of the doubly oxidized porphyrin may be grown in order to test the theory that the a_{1u} dication is distorted.[14-16]

References and Notes:

(1) Birnbaum, E. R.; Hodge, J. A.; Grinstaff, M. W.; Schaefer, W. P.; Henling, L.; Labinger, J. A.; Bercaw, J. E.; Gray, H. B. *Inorg. Chem.* submitted 11/2/94.

(2) Henling, L. M.; Schaefer, W. P.; Hodge, J. A.; Hughes, M. E.; Gray, H. B.; Lyons, J. E.; Ellis, P. E. *Acta Crystallogr.* **1993**, *C49*, 1743-1747.

(3) Marsh, R. E.; Schaefer, W. P.; Hodge, J. A.; Hughes, M. E.; Gray, H. B. *Acta Crystallogr.* **1993**, *C49*, 1339-1342.

(4) Schaefer, W. P.; Hodge, J. A.; Hughes, M. E.; Gray, H. B. *Acta Crystallogr.* **1993**, *C49*, 1342-1345.

(5) Barkigia, K. M.; Berber, M. D.; Fajer, J.; Medforth, C. J.; Renner, M. W.; Smith, K. M. *J. Am. Chem. Soc.* **1990**, *112*, 8851-8857.

(6) Barkigia, K. M.; Renner, M. W.; Furenlid, L. R.; Medforth, C. J.; Smith, K. M.; Fajer, J. *J. Am. Chem. Soc.* **1993**, *115*, 3627-3635.

(7) Medforth, C. J.; Senge, M. O.; Smith, K. M.; Sparks, L. D.; Shelnutt, J. A. *J. Am. Chem. Soc.* **1992**, *114*, 9859-9869.

(8) Takeuchi, T.; Gray, H. B.; Goddard, W. A. *J. Am. Chem. Soc.* **1994**, *116*, 9730-9732.

(9) Gouterman, M. *Journal of Chemical Physics* **1959**, *30*, 1139-1161.

(10) Gross, Z.; Barzilay, C. *Angew. Chem.* **1992**, *31*, 1615-1617.

(11) Fajer, J.; Borg, D. C.; Forman, A.; Dolphin, D.; Felton, R. H. *J. Am. Chem. Soc.* **1970**, *92*, 3451-3459.

(12) Spellane, P. J.; Gouterman, M.; Antipas, A.; Kim, S.; Liu, Y. C. *Inorg. Chem.* **1980**, *19*, 386-391.

(13) Hodge, J. A.; Hill, M. G.; Gray, H. B. *Inorg. Chem.* in press.

(14) Initial attempts to grow a crystal using chemical oxidants such as, Ce^{4+} (in the form of cerium ammonium nitrate) and tris(*p*-bromophenyl)amminium Hexachloroantimonate, met with failure, at least partially due to the ease with which the porphyrin is demetallated.

Spaulding et al. reported the generation of crystals of $[ZnTPP^{+}]ClO_4$ via bulk electrochemical oxidation.[16] (This necessitated the removal of the electrolyte before the crystal could be grown.)

(15) Scholz, W. F.; Reed, C. A.; Lee, Y. J.; Scheidt, W. R.; Lang, G. *J. Am. Chem. Soc.* **1982**, *104*, 6791-6793.

(16) Spaulding, L. D.; Eller, P. G.; Bertrand, J. A.; Felton, R. H. *J. Am. Chem. Soc.* **1974**, *96*, 982-987.

Appendix 1. Supplimentary Material for
the X-ray Crystal Structure Determination of H_2TFPP.

Figure A1.1. ORTEP diagram for H_2TFPP (50% probability ellipsoids) and numbering scheme for macrocycle.

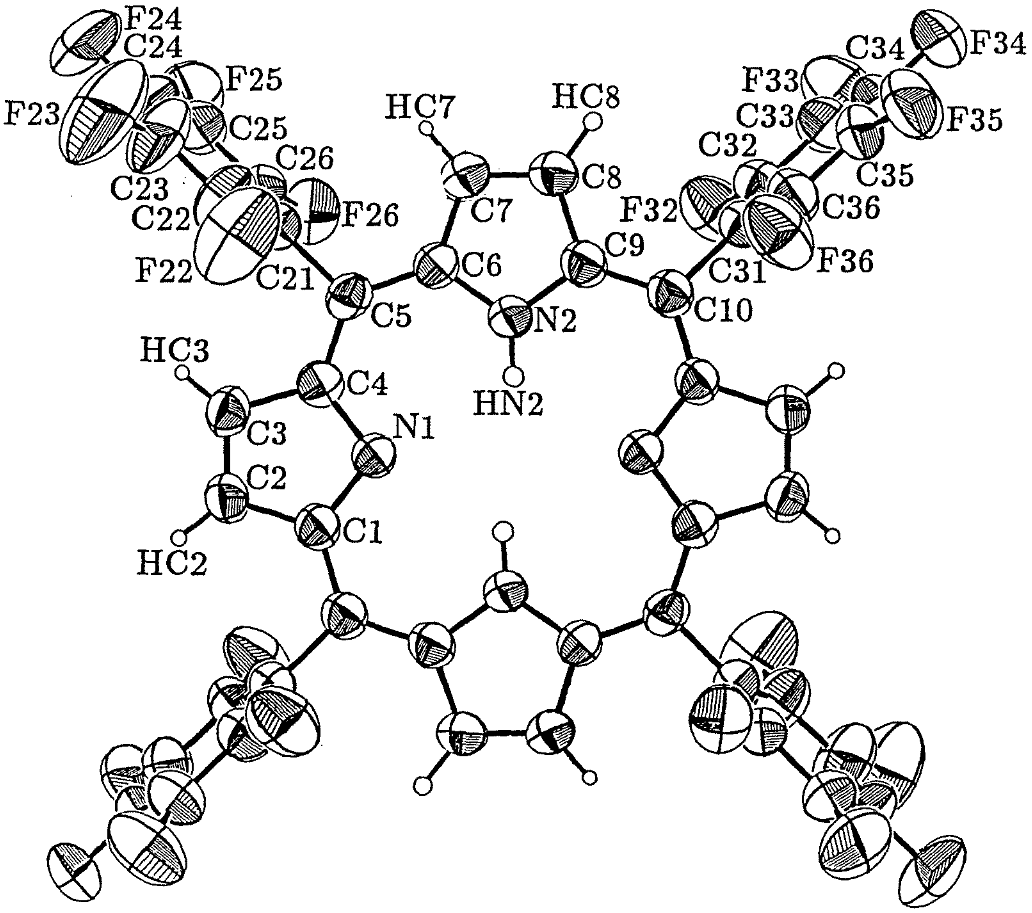


Table A1.1. Crystal and Intensity Collection Data for H_2TFPP.

Formula: $C_{44}H_{10}N_4F_{20}$	Formula Weight: 982.57
Crystal Color: dark red	Habit: plate
Crystal Size: 0.19 x 0.35 x 0.36 mm	
Crystal System: rhombohedral	Space Group: $R\bar{3}$
a = 20.327(4) Å	$\alpha = 90$
b = 20.327(4) Å	$\beta = 90$
c = 24.368(5) Å	$\gamma = 120$
V = 8720(3) $Å^3$	Z = 9
D = 1.67 g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 1.60$ cm^{-1}	T = 295 K
Enraf-Nonius Cad-4 diffractometer	ω scan
Transmission coeff. = -	range for data collection: 1 - 25
$\pm h = 24, \pm k = 24, \pm l = 28$	
Number of reflections measured: 7209	
Number of independent reflections: 3403	
Goodness of fit for merging data: 0.94	
R = 0.081 on F for 2821 reflections with $F_o^2 > 0$	
R = 0.047 on F for 1805 reflections with $F_o^2 > 3\sigma(F_o^2)$	
wR = 0.011 on F^2 for 3403 reflections	
Final goodness of fit: 1.78 for 327 parameters and 3403 reflections	

Table A1.2. Final Refined Heavy Atom Parameters x 10^4 for H_2TFPP.

Atom	x	y	z	U_{eq}
N1	4289(1)	−1048(1)	−295(1)	503(6)
N2	5808(1)	189(1)	−601(1)	529(7)
C1	3576(2)	−1569(2)	−116(1)	534(8)
C2	3255(2)	−2234(2)	−461(1)	611(10)
C3	3759(2)	−2117(2)	−846(1)	590(9)
C4	4412(2)	−1370(2)	−747(1)	502(7)
C5	5071(2)	−1039(2)	−1069(1)	515(7)
C6	5706(2)	−322(2)	−1005(1)	517(8)
C7	6369(2)	25(2)	−1341(1)	621(9)
C8	6849(2)	714(2)	−1139(1)	632(9)
C9	6503(2)	832(2)	−666(1)	560(8)
C10	6795(2)	1470(2)	−332(1)	560(8)
C21	5116(2)	−1512(2)	−1526(1)	553(8)
C22	4751(2)	−1615(2)	−2016(2)	899(12)
C23	4772(3)	−2072(3)	−2422(2)	1153(17)
C24	5185(3)	−2420(2)	−2341(2)	1040(15)
C25	5555(2)	−2336(2)	−1867(2)	845(12)
C26	5518(2)	−1881(2)	−1464(1)	614(9)
C31	7578(2)	2104(2)	−465(1)	595(9)
C32	8214(2)	2074(2)	−305(1)	736(11)

Atom	x	y	z	U_{eq}
C33	8938(2)	2658(3)	−411(2)	882(14)
C34	9027(2)	3280(2)	−690(2)	829(13)
C35	8419(2)	3322(2)	−864(2)	813(12)
C36	7701(2)	2740(2)	−750(1)	734(11)
F22	4344(2)	−1270(2)	−2100(1)	1461(9)
F23	4392(2)	−2170(2)	−2886(1)	2011(14)
F24	5221(2)	−2869(2)	−2732(1)	1675(10)
F25	5943(1)	−2695(1)	−1775(1)	1431(9)
F26	5897(1)	−1801(1)	−995(1)	900(6)
F32	8135(1)	1469(1)	−30(1)	1064(7)
F33	9544(1)	2619(2)	−252(1)	1385(10)
F34	9732(1)	3852(1)	−805(1)	1215(8)
F35	8515(1)	3932(1)	−1146(1)	1198(8)
F36	7105(1)	2794(1)	−921(1)	1081(7)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table A1.3. Complete Distances and Angles for H_2TFPP.

	Distance(Å)		Distance(Å)
N1 –C1	1.371(4)	C10 –C31	1.499(5)
N1 –C4	1.365(4)	C21 –C22	1.367(5)
N2 –C6	1.369(4)	C21 –C26	1.367(5)
N2 –C9	1.372(4)	C22 –C23	1.372(7)
N2 –HN2	0.91(4)	C22 –F22	1.343(5)
C1 –C2	1.441(5)	C23 –C24	1.354(7)
C1 –C10′	1.398(4)	C23 –F23	1.326(6)
C2 –C3	1.320(5)	C24 –C25	1.342(7)
C2 –HC2	0.94(3)	C24 –F24	1.348(6)
C3 –C4	1.453(5)	C25 –C26	1.375(5)
C3 –HC3	0.92(3)	C25 –F25	1.334(5)
C4 –C5	1.400(4)	C26 –F26	1.342(4)
C5 –C6	1.391(4)	C31 –C32	1.379(5)
C5 –C21	1.502(4)	C31 –C36	1.376(5)
C6 –C7	1.424(5)	C32 –C33	1.376(6)
C7 –C8	1.338(5)	C32 –F32	1.339(4)
C7 –HC7	0.93(3)	C33 –C34	1.366(6)
C8 –C9	1.433(5)	C33 –F33	1.332(5)
C8 –HC8	0.99(3)	C34 –C35	1.350(6)
C9 –C10	1.387(4)	C34 –F34	1.347(5)

Distance(Å)		Angle(°)	
C35 –C36	1.372(5)	C4 –N1 –C1	105.3(2)
C35 –F35	1.344(5)	C9 –N2 –C6	109.5(3)
C36 –F36	1.336(4)	HN2 –N2 –C6	127.6(22)
		HN2 –N2 –C9	123.0(22)
		C2 –C1 –N1	110.3(3)
		C10′ –C1 –N1	125.2(3)
		C10′ –C1 –C2	124.5(3)
		C3 –C2 –C1	107.4(3)
		HC2 –C2 –C1	122.4(17)
		HC2 –C2 –C3	130.2(17)
		C4 –C3 –C2	106.9(3)
		HC3 –C3 –C2	130.0(17)
		HC3 –C3 –C4	123.0(17)
		C3 –C4 –N1	110.1(3)
		C5 –C4 –N1	125.6(3)
		C5 –C4 –C3	124.3(3)
		C6 –C5 –C4	127.2(3)
		C21 –C5 –C4	117.2(3)
		C21 –C5 –C6	115.6(3)
		C5 –C6 –N2	125.8(3)

Angle(°)		Angle(°)	
C7 –C6 –N2	106.9(3)	C24 –C23 –C22	118.9(5)
C7 –C6 –C5	127.3(3)	F23 –C23 –C22	120.2(5)
C8 –C7 –C6	108.8(3)	F23 –C23 –C24	120.8(5)
HC7 –C7 –C6	121.9(16)	C25 –C24 –C23	121.0(5)
HC7 –C7 –C8	129.2(16)	F24 –C24 –C23	120.4(5)
C9 –C8 –C7	107.9(3)	F24 –C24 –C25	118.6(4)
HC8 –C8 –C7	127.5(18)	C26 –C25 –C24	118.9(4)
HC8 –C8 –C9	124.6(18)	F25 –C25 –C24	121.4(4)
C8 –C9 –N2	106.9(3)	F25 –C25 –C26	119.7(4)
C10 –C9 –N2	125.3(3)	C25 –C26 –C21	122.7(3)
C10 –C9 –C8	127.7(3)	F26 –C26 –C21	119.4(3)
C9 –C10 –C1′	125.7(3)	F26 –C26 –C25	117.9(3)
C31 –C10 –C1′	117.5(3)	C32 –C31 –C10	121.2(3)
C31 –C10 –C9	116.8(3)	C36 –C31 –C10	122.1(3)
C22 –C21 –C5	123.0(3)	C36 –C31 –C32	116.7(3)
C26 –C21 –C5	121.0(3)	C33 –C32 –C31	122.1(4)
C26 –C21 –C22	116.0(3)	F32 –C32 –C31	119.8(3)
C23 –C22 –C21	122.5(4)	F32 –C32 –C33	118.1(3)
F22 –C22 –C21	118.8(4)	C34 –C33 –C32	118.8(4)
F22 –C22 –C23	118.7(4)	F33 –C33 –C32	121.1(4)

	Angle(°)
F33 –C33 –C34	120.1(4)
C35 –C34 –C33	120.8(4)
F34 –C34 –C33	119.6(4)
F34 –C34 –C35	119.6(4)
C36 –C35 –C34	119.7(4)
F35 –C35 –C34	120.2(4)
F35 –C35 –C36	120.1(4)
C35 –C36 –C31	121.8(3)
F36 –C36 –C31	119.3(3)
F36 –C36 –C35	118.8(3)

′ indicates atom related by inversion

Table A1.4. Final Refined Hydrogen Atom Parameters for H_2TFPP.

x, y and $z \times 10^4$

Atom	x	y	z	B
HC2	2775(15)	−2661(14)	−392(10)	4.9(7)
HC3	3736(14)	−2423(14)	−1131(10)	4.2(7)
HC7	6409(13)	−207(13)	−1659(10)	3.8(6)
HC8	7357(16)	1084(16)	−1280(11)	6.3(8)
HN2	5483(18)	129(18)	−323(13)	7.9(10)

Table A1.5. Observed and Calculated Structure Factors for H_2TFPP. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\dfrac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

Tetra(pentafluorophenyl)porphyrin Page 1

0 0 1			
3	1213	1203	9
6	5602	5624	-4
9	101	135	-18
12	439	454	-15
15	689	677	9
18	262	288	-17
21	340	325	9
24	107	69	7
27	139	143	-1
1 -1 1			
2	572	575	-3
5	2381	2379	0
8	221	234	-11
11	1057	1072	-12
14	581	593	-10
17	417	435	-14
20	129	157	-10
23	-69	122	-25
26	177	130	14
1 0 1			
1	452	415	73
4	2440	2463	-12
7	2012	2035	-14
10	1053	1074	-21
13	303	317	-17
16	528	503	28
19	-69	38	-13
22	590	579	10
25	-15	71	-9
28	132	42	23
1 1 1			
0	176	67	63
3	875	895	-18
6	713	689	26
9	666	680	-13
12	554	544	9
15	240	219	13
18	-123	28	-28
21	98	118	-5
24	206	227	-9
27	-44	112	-17
2 -3 1			
2	1808	1780	19
5	2189	2159	12
8	262	271	-8
11	1234	1239	-4
14	210	215	-3
17	-74	12	-9
20	-35	0	-1
23	128	131	0
26	-76	89	-16
2 -2 1			
1	59	11	19
4	1514	1497	10
7	145	134	6
10	1132	1120	9
13	633	647	-12
16	216	209	4
19	252	252	0
22	529	493	24
25	152	143	2
28	142	82	14
2 -1 1			
3	348	398	-52
6	4242	4226	5
9	164	177	-9
12	666	675	-8
15	785	789	-3
18	223	235	-6
21	647	649	-1
24	235	210	10
27	168	190	-8
2 0 1			
2	1158	1184	-26
5	4787	4946	-42
8	2756	2790	-15
11	1163	1185	-20
14	531	504	31
17	148	185	-25
20	-64	15	-9
23	132	113	7
26	195	180	8
2 1 1			
1	2529	2572	-16
4	-107	74	-32
7	573	569	5
10	188	120	40
13	157	236	-54
16	1185	1188	-1
19	-45	105	-20
22	170	154	5
25	-83	29	-9
28	-97	20	-11
2 2 1			
0	3543	3481	17
3	3172	3204	-13
6	811	806	4
9	675	614	58
12	1174	1161	9
15	385	385	0
18	515	526	-8
21	326	342	-9
24	318	297	11
27	101	71	5
3 -5 1			
2	938	941	-3
5	823	809	13
8	1106	1102	2
11	390	402	-10
14	153	202	-28
17	-71	16	-8
20	155	117	12
23	109	111	0
26	140	112	7
3 -4 1			
1	3222	3233	-3
4	2054	2070	-8
7	311	360	-38
10	2200	2188	5
13	738	736	1
16	79	107	-8
19	280	284	-2
22	840	792	31
25	262	234	12
28	150	166	-5
3 -3 1			
3	2092	2073	10
6	3862	3816	11
9	242	215	21
12	231	280	-40
15	221	239	-11
18	391	403	-8
21	46	33	1
24	201	146	19
27	137	47	17
3 -2 1			
2	345	351	-9
5	1595	1615	-10
8	670	676	-5
11	345	337	6
14	529	498	26
17	111	107	1
20	479	496	-12
23	170	210	-16
26	120	128	-2
3 -1 1			
1	841	804	32
4	3380	3434	-16
7	412	415	-3
10	2145	2152	-3
13	1053	1083	-23
16	341	327	10
19	250	252	-1
22	-81	18	-9
25	147	131	5
28	82	59	3
3 0 1			
0	3476	3410	23
3	2327	2345	-9
6	2831	2878	-21
9	611	612	-1
12	94	55	15
15	905	861	43
18	239	229	8
21	-16	124	-30
24	179	137	20
27	159	150	3
3 1 1			
2	2058	2080	-10
5	3151	3166	-4
8	526	498	29
11	345	376	-27
14	437	444	-6
17	378	372	3
20	632	634	-1
23	94	12	10
26	164	119	13
3 2 1			
1	1438	1442	-2
4	2158	2162	-2
7	46	99	-13
10	909	930	-18
13	1347	1323	16
16	399	407	-5
19	202	220	-9
22	357	309	26
25	182	179	1
28	25	94	-9
3 3 1			
0	1789	1707	39
3	255	304	-49
6	1182	1152	23
9	1663	1623	19
12	884	854	24
15	63	96	-9
18	730	713	12
21	397	393	2
24	148	97	13
27	237	165	26
4 -7 1			
2	1491	1499	-5
5	180	204	-26
8	786	791	-5
11	89	84	1
14	537	519	14
17	88	130	-13
20	565	595	-21
23	102	23	11
26	122	113	2
4 -6 1			
1	102	152	-29
4	1326	1312	12
7	920	898	19
10	-87	11	-11
13	645	634	9
16	614	644	-25
19	418	396	14
22	106	33	12
25	114	85	6
28	161	160	0
4 -5 1			
3	635	647	-16
6	637	624	13
9	924	936	-8
12	314	311	2
15	409	427	-14
18	379	368	7
21	183	99	26
24	129	118	3
27	61	67	0
4 -4 1			
2	1053	1074	-25
5	3413	3390	7
8	1637	1644	-3
11	786	771	12
14	367	333	26
17	485	481	3
20	61	99	-8
23	373	326	26
26	-153	13	-31
4 -3 1			
1	444	450	-7
4	4295	4294	0
7	1263	1285	-14
10	270	255	12
13	827	861	-29
16	490	487	1
19	169	167	0
22	267	238	14
25	215	160	20
28	72	88	-2
4 -2 1			
3	419	439	-34
6	2565	2566	0
9	1047	1046	0
12	380	333	39
15	103	102	0
18	79	7	9
21	444	452	-5
24	422	417	2
27	125	93	7

4 -1 1

2	668	624	39
5	1840	1883	-21
8	2361	2403	-19
11	629	629	0
14	113	79	11
17	-26	0	-1
20	334	295	22
23	126	105	5
26	111	47	11

4 0 1

1	4053	3993	18
4	1130	1118	11
7	544	559	-20
10	293	309	-19
13	804	804	0
16	804	772	32
19	308	327	-17
22	432	422	8
25	86	81	1
28	159	80	26

4 1 1

0	435	436	0
3	1297	1336	-25
6	1067	1059	5
9	2516	2541	-10
12	287	298	-9
15	411	438	-21
18	152	175	-10
21	-54	121	-23
24	43	2	2
27	223	194	11

4 2 1

2	1280	1287	-4
5	1346	1352	-5
8	1748	1723	11
11	772	746	22
14	165	150	6
17	382	384	-1
20	119	153	-11
23	243	229	6
26	196	209	-5

4 3 1

1	354	384	-23
4	276	261	13
7	257	272	-12
10	554	600	-31
13	231	250	-12
16	84	85	0
19	106	137	-9
22	42	110	-12
25	218	197	8

4 4 1

0	87	133	-16
3	335	404	-75
6	1205	1166	34
9	739	729	8
12	109	80	6
15	244	263	-12
18	96	32	11
21	141	179	-14
24	124	107	4
27	-14	7	0

5 -9 1

2	605	576	28
5	941	890	42
8	1086	1052	25
11	498	495	2
14	521	525	-2
17	146	129	5
20	279	331	-30
23	-123	24	-20
26	71	68	0

5 -8 1

1	205	224	-15
4	1918	1855	34
7	1520	1493	17
10	227	237	-7
13	471	506	-21
16	366	359	4
19	114	150	-12
22	139	151	-4
25	86	47	5

5 -7 1

3	728	705	22
6	976	1014	-33
9	699	658	36
12	211	217	-2
15	430	391	29
18	732	725	5
21	281	310	-16
24	92	67	4
27	135	29	18

5 -6 1

2	390	390	0
5	2085	2102	-9
8	210	188	15
11	360	365	-3
14	493	475	14
17	-68	8	-7
20	501	517	-10
23	-45	71	-8
26	71	100	-5

5 -5 1

1	2222	2296	-41
4	2435	2409	11
7	1228	1197	23
10	812	856	-29
13	478	479	-1
16	279	278	0
19	188	143	18
22	428	464	-23
25	66	83	-2
28	104	84	3

5 -4 1

3	5541	5484	12
6	563	586	-25
9	2281	2217	25
12	-72	29	-12
15	826	770	42
18	458	437	15
21	394	380	9
24	368	336	17
27	84	71	2

5 -3 1

2	3115	3075	14
5	1873	1841	18
8	736	722	10
11	468	441	24
14	956	930	19
17	691	699	-6
20	84	72	2
23	281	273	3
26	77	139	-15

5 -2 1

1	865	876	-9
4	1097	1121	-24
7	2078	2118	-17
10	1380	1367	8
13	1128	1143	-11
16	320	327	-5
19	425	398	18
22	302	272	15
25	222	234	-5
28	-41	76	-8

5 -1 1

0	2310	2318	-4
3	401	380	16
6	510	491	15
9	2251	2249	0
12	172	178	-3
15	632	652	-16
18	-72	78	-18
21	200	267	-34
24	200	194	2
27	50	76	-3

5 0 1

2	218	239	-27
5	421	430	-10
8	1026	1043	-17
11	586	578	10
14	208	196	10
17	-47	62	-14
20	183	230	-32
23	-67	75	-18
26	214	195	10

5 1 1

1	379	388	-9
4	529	517	9
7	215	282	-44
10	163	172	-5
13	121	84	12
16	387	378	6
19	-98	18	-14
22	90	101	-2
25	-115	43	-19

5 2 1

0	1374	1357	12
3	1232	1295	-39
6	913	880	35
9	372	331	24
12	1748	1750	-1
15	672	670	1
18	167	220	-26
21	233	263	-15
24	-92	21	-11
27	-39	15	-2

5 3 1

2	104	68	10
5	712	722	-9
8	1093	1109	-12
11	208	175	13
14	-59	68	-14
17	718	703	11
20	145	193	-19
23	429	412	10
26	106	49	9

5 4 1

1	1111	1119	-4
4	1561	1572	-6
7	145	4	54
10	78	59	4
13	515	468	26
16	115	121	-1
19	379	390	-7
22	-133	34	-25
25	89	69	3

5 5 1

0	259	268	-5
3	107	95	4
6	1356	1421	-45
9	153	183	-16
12	690	691	0
15	350	391	-21
18	264	272	-4
21	-127	33	-23
24	38	55	-1

6 -11 1

2	1376	1340	24
5	1207	1121	59
8	622	590	36
11	663	638	20
14	146	158	-5
17	724	704	10
20	198	228	-13
23	159	139	6

6 -10 1

1	384	383	0
4	922	924	-1
7	1581	1583	-1
10	670	674	-3
13	392	404	-8
16	296	277	7
19	-59	64	-9
22	-32	55	-5
25	75	37	4

6 -9 1

3	1058	1055	1
6	133	170	-29
9	390	427	-33
12	467	445	17
15	266	228	15
18	399	407	-5
21	-38	61	-6
24	49	30	1

6 -8 1

2	63	61	0
5	622	627	-6
8	797	781	13
11	156	158	-1
14	643	607	20
17	671	655	11
20	-71	96	-18
23	110	56	10
26	15	74	-6

6 -7 1

1	2184	2197	-6
4	1396	1412	-13
7	585	502	74
10	590	611	-19

Tetra(pentafluorophenyl)porphyrin

13	111	90	5
16	291	313	-14
19	-94	50	-16
22	287	327	-22
25	46	69	-3

6 -6 1

3	382	388	-10
6	5406	5321	18
9	1240	1255	-11
12	375	349	15
15	600	589	9
18	-109	15	-19
21	75	18	6
24	-64	48	-8
27	-55	83	-11

6 -5 1

2	1719	1737	-11
5	1717	1725	-4
8	1265	1265	0
11	259	253	3
14	938	905	25
17	163	100	22
20	675	687	-8
23	154	146	2
26	63	36	3

6 -4 1

1	121	114	3
4	2704	2717	-5
7	299	292	6
10	2706	2688	6
13	167	94	30
16	868	878	-7
19	521	524	-2
22	57	149	-23
25	227	227	0
28	31	9	0

6 -3 1

3	3881	3868	3
6	533	525	8
9	160	184	-10
12	1173	1179	-4
15	86	26	11
18	187	171	7
21	-26	129	-23
24	56	3	3
27	-50	70	-8

6 -2 1

2	4504	4459	13
5	931	909	24
8	671	596	51
11	118	101	6
14	643	630	10
17	198	235	-20
20	-81	165	-47
23	-69	12	-6
26	56	87	-5

6 -1 1

1	132	129	1
4	1391	1415	-14
7	431	419	8
10	1274	1286	-8
13	1257	1199	39
16	197	205	-4
19	158	168	-3
22	-41	40	-4
25	30	8	0

6 0 1

0	755	762	-9
3	1587	1601	-10
6	768	755	13
9	218	166	46
12	1198	1198	0
15	353	348	5
18	329	354	-23
21	-119	73	-37
24	173	190	-9
27	-83	5	-11

6 1 1

2	1568	1580	-8
5	605	644	-30
8	929	970	-27
11	272	308	-29
14	102	67	9
17	359	348	6
20	-138	58	-32
23	230	275	-22
26	24	11	0

6 2 1

1	233	233	0
4	310	308	1
7	641	654	-16
10	283	220	31
13	235	259	-16
16	128	135	-2
19	-95	37	-14
22	255	239	7
25	-87	14	-9

6 3 1

0	2426	2405	9
3	1149	1129	11
6	447	490	-42
9	284	259	18
12	63	51	1
15	-76	54	-14
18	-112	64	-24
21	82	3	8
24	-148	0	-29

6 4 1

2	52	44	1
5	347	299	38
8	381	388	-8
11	-17	46	-4
14	-21	14	0
17	318	345	-16
20	129	145	-4
23	107	80	5
26	-60	42	-6

6 5 1

1	911	850	37
4	1279	1324	-32
7	770	726	36
10	364	354	7
13	245	224	11
16	535	579	-23
19	50	178	-36
22	-115	24	-17
25	40	45	0

6 6 1

0	1796	1861	-30
3	571	566	4
6	144	99	17
9	-91	51	-27
12	430	442	-8
15	-97	49	-17
18	-35	34	-2
21	188	200	-4
24	120	75	9

7 -13 1

2	777	763	11
5	706	716	-8
8	561	555	5
11	-58	98	-20
14	-79	96	-21
17	385	409	-15
20	141	127	3
23	168	211	-16

7 -12 1

1	759	761	-1
4	440	433	5
7	503	487	13
10	135	180	-21
13	172	172	0
16	1056	1009	30
19	-20	18	0
22	181	194	-4
25	41	1	1

7 -11 1

3	1542	1531	6
6	1041	1042	-1
9	569	557	10
12	419	439	-15
15	147	153	-2
18	139	150	-2
21	-41	14	-2
24	-98	10	-11

7 -10 1

2	644	645	-1
5	928	895	26
8	299	277	16
11	-28	34	-3
14	200	177	11
17	431	437	-3
20	154	136	5
23	84	128	-10
26	-89	63	-13

7 -9 1

1	1429	1415	9
4	796	832	-33
7	813	787	21
10	264	224	26
13	-63	19	-7
16	844	828	8
19	-14	86	-10
22	344	363	-10
25	86	73	2

7 -8 1

3	341	331	9
6	171	135	19
9	1461	1448	7
12	648	655	-6
15	56	151	-22
18	83	151	-21
21	224	255	-14
24	260	255	1
27	57	55	0

7 -7 1

2	1357	1367	-8
5	884	898	-13
8	1803	1800	1
11	724	728	-3
14	243	305	-30
17	435	436	0
20	156	133	7
23	58	38	2
26	194	178	5

7 -6 1

1	734	745	-11
4	879	904	-28
7	1060	1101	-33
10	534	558	-22
13	209	230	-9
16	53	50	0
19	190	161	12
22	404	378	15
25	71	120	-10

7 -5 1

3	917	908	7
6	1170	1148	17
9	1029	1023	4
12	357	362	-3
15	199	118	35
18	712	713	0
21	260	281	-11
24	174	118	17
27	200	95	29

7 -4 1

2	2511	2447	28
5	2155	2185	-17
8	2496	2452	19
11	524	527	-2
14	1050	1044	4
17	299	287	7
20	184	190	-2
23	-76	41	-9
26	110	65	8

7 -3 1

1	1646	1592	27
4	1599	1602	-2
7	1596	1609	-8
10	1191	1264	-43
13	200	198	1
16	233	220	7
19	-121	64	-28
22	146	182	-13
25	131	85	10

7 -2 1

0	594	576	18
3	1019	1063	-30
6	625	618	8
9	155	134	7
12	1640	1660	-11
15	232	244	-7
18	-47	60	-8
21	37	96	-9
24	147	152	-1
27	106	96	2

7 -1 1

2	1473	1508	-24
5	365	367	-1
8	900	833	42

11	99	98	0
14	39	10	2
17	66	103	-9
20	254	276	-12
23	-92	11	-11
26	41	21	1
	7 0 1		
1	1370	1417	-39
4	444	465	-28
7	486	485	1
10	162	158	3
13	214	203	8
16	33	82	-12
19	-163	21	-59
22	-77	18	-11
25	95	82	3
	7 1 1		
0	1172	1190	-14
3	919	923	-3
6	763	737	17
9	123	113	2
12	742	717	20
15	861	886	-19
18	-154	27	-38
21	191	252	-28
24	23	55	-2
	7 2 1		
2	104	173	-38
5	1199	1102	54
8	298	324	-30
11	119	159	-12
14	-71	25	-9
17	510	511	-1
20	114	189	-27
23	-138	40	-27
26	-91	60	-14
	7 3 1		
1	1446	1387	38
4	594	590	2
7	851	846	4
10	417	409	6
13	429	432	-1
16	311	321	-6
19	248	243	2
22	236	287	-26
25	-106	40	-15
	7 4 1		
0	349	339	8
3	846	782	39
6	548	508	34
9	120	153	-20
12	72	83	-2
15	118	141	-5
18	289	304	-8
21	-145	2	-29
24	123	4	16
	7 5 1		
2	853	826	16
5	392	432	-34
8	353	368	-11
11	323	321	1
14	-70	113	-26
17	117	202	-23
20	-104	46	-17
23	197	125	22
	7 6 1		
1	420	470	-31
4	329	371	-33
7	74	84	-2
10	205	208	-2
13	-144	42	-35
16	-90	97	-23
19	329	299	11
22	109	81	5
	7 7 1		
0	162	235	-30
3	561	550	9
6	275	307	-21
9	42	99	-12
12	-139	107	-48
15	85	12	8
18	279	298	-10
21	202	211	-2
	8 -15 1		
2	646	642	3
5	-79	51	-14
8	-109	125	-43
11	71	144	-29
14	338	323	8
17	120	82	8
20	31	42	0
	8 -14 1		
1	294	296	-1
4	285	268	10
7	457	469	-9
10	170	187	-11
13	-55	122	-24
16	302	322	-11
19	17	55	-3
22	158	164	-1
	8 -13 1		
3	554	519	27
6	523	525	-1
9	627	627	0
12	126	173	-19
15	629	556	48
18	255	257	-1
21	61	126	-10
24	-133	3	-21
	8 -12 1		
2	157	179	-12
5	403	376	21
8	584	581	3
11	274	295	-13
14	164	182	-7
17	90	47	7
20	218	219	0
23	-71	11	-6
	8 -11 1		
1	565	570	-4
4	660	675	-13
7	287	293	-6
10	1247	1259	-7
13	533	518	11
16	612	595	12
19	131	223	-26
22	-36	98	-13
25	-80	49	-10
	8 -10 1		
3	216	259	-32
6	240	176	56
9	997	962	26
12	170	108	24
15	106	131	-8
18	468	467	0
21	-33	104	-14
24	120	154	-10
	8 -9 1		
2	1321	1315	4
5	1172	1177	-4
8	1685	1711	-15
11	144	102	16
14	140	163	-10
17	254	265	-4
20	144	206	-24
23	78	53	3
26	80	57	3
	8 -8 1		
1	329	349	-26
4	-70	33	-21
7	496	492	3
10	520	511	8
13	487	463	18
16	318	298	8
19	396	378	11
22	161	151	3
25	244	193	20
	8 -7 1		
3	400	364	33
6	389	371	16
9	837	842	-4
12	357	387	-24
15	656	650	3
18	195	176	8
21	57	32	2
24	124	48	14
27	138	26	18
	8 -6 1		
2	544	556	-12
5	145	50	51
8	503	528	-23
11	188	195	-4
14	132	82	11
17	64	143	-23
20	-67	67	-11
23	202	73	36
26	110	83	5
	8 -5 1		
1	426	447	-22
4	766	784	-17
7	516	490	23
10	792	760	26
13	175	155	7
16	211	225	-7
19	473	462	7
22	215	231	-7
25	141	27	20
	8 -4 1		
3	1653	1640	7
6	2251	2170	42
9	116	164	-25
12	732	682	29
15	1195	1169	17
18	325	338	-8
21	424	394	18
24	194	200	-2
27	177	107	19
	8 -3 1		
2	331	238	57
5	636	624	11
8	1338	1308	20
11	330	352	-13
14	247	236	6
17	67	5	6
20	-127	89	-34
23	52	26	2
26	158	99	15
	8 -2 1		
1	1603	1590	8
4	3521	3517	1
7	1231	1174	48
10	1196	1177	10
13	722	689	26
16	444	440	3
19	-145	37	-33
22	-37	62	-6
25	127	74	11
	8 -1 1		
0	2115	2107	3
3	1254	1248	4
6	310	295	8
9	223	285	-35
12	415	389	20
15	385	394	-6
18	322	360	-24
21	-147	78	-38
24	100	67	6
27	50	56	0
	8 0 1		
2	1482	1506	-18
5	951	927	23
8	426	421	6
11	1066	1056	9
14	501	512	-11
17	166	191	-15
20	241	285	-33
23	-129	31	-33
26	-103	66	-25
	8 1 1		
1	-78	138	-51
4	382	417	-33
7	94	110	-4
10	382	351	17
13	88	17	11
16	326	346	-13
19	221	255	-17
22	-113	44	-19
25	142	10	21
	8 2 1		
0	234	218	10
3	549	563	-13
6	2392	2394	0
9	356	368	-13
12	580	587	-3
15	-111	0	-19
18	133	175	-15
21	146	172	-9
24	122	127	-1
	8 3 1		

Tetra(pentafluorophenyl)porphyrin

2	86	125	-16
5	310	319	-5
8	117	87	10
11	332	334	0
14	626	656	-16
17	141	164	-8
20	299	323	-13
23	-45	17	-2

8 4 1

1	1369	1362	4
4	813	814	0
7	695	637	46
10	195	188	5
13	420	418	1
16	60	62	0
19	-127	81	-30
22	254	211	18

8 5 1

0	184	225	-25
3	309	352	-23
6	698	698	0
9	604	599	3
12	81	152	-23
15	355	438	-57
18	85	81	0
21	77	21	6
24	71	50	2

8 6 1

2	648	673	-14
5	270	269	0
8	301	269	19
11	-129	83	-52
14	-93	94	-24
17	338	287	27
20	-83	62	-9
23	-148	17	-28

8 7 1

1	785	774	6
4	361	364	-2
7	-21	88	-12
10	91	154	-20
13	61	137	-19
16	273	262	5
19	86	103	-3
22	211	66	26

8 8 1

0	259	256	1
3	13	13	0
6	188	238	-26
9	221	253	-16
12	566	537	26
15	131	160	-9
18	121	26	15
21	45	73	-3

9 -17 1

2	-147	38	-36
5	394	389	3
8	556	562	-4
11	456	442	8
14	205	128	26
17	248	195	21
20	196	178	6

9 -16 1

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9 -15 1

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9 -14 1

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9 -13 1

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9 -12 1

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9 -11 1

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9 -10 1

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9 -9 1

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9 -8 1

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9 -7 1

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9 -6 1

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9 -5 1

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9 -4 1

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9 -3 1

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9 -2 1

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9 -1 1

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9 2 1

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9 3 1

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9 4 1

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Tetra(pentafluorophenyl)porphyrin

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Tetra(pentafluorophenyl)porphyrin

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4	462	465	-1
7	164	95	18
10	67	40	2
13	-80	76	-14
20 -4 1			
0	106	156	-15
3	587	554	20
6	482	448	20
9	241	255	-6
12	-99	38	-9
20 -3 1			
2	175	119	17
5	306	224	36
8	96	62	5
11	152	105	12
20 -2 1			
1	108	126	-4
4	-68	77	-12
7	159	132	8
10	47	118	-12
20 -1 1			
0	-33	65	-6
3	169	106	17
6	299	283	8
9	-105	7	-13
20 0 1			
2	152	117	13
5	162	139	9
8	170	170	0
20 1 1			
1	-36	77	-8
4	-106	27	-14
21 -20 1			
2	87	20	7
5	191	170	7
21 -19 1			
1	62	98	-6
4	78	23	6
7	23	63	-3
21 -18 1			
3	148	1	23
6	50	19	2
9	126	22	16
21 -17 1			

2	114	37	12
5	102	105	0
8	-47	3	-2
11	107	137	-7
21	-16	1	
1	-36	32	-2
4	75	49	3
7	123	75	10
10	-76	52	-10
21	-15	1	
3	348	266	39
6	71	24	5
9	-104	33	-14
12	17	32	0
21	-14	1	
2	478	467	6
5	108	85	5
8	192	248	-24
11	-57	80	-11
21	-13	1	
1	814	771	26
4	-52	30	-4
7	143	123	5
10	111	136	-6
13	39	13	1
21	-12	1	
3	54	137	-18
6	213	199	5
9	159	71	21
12	116	112	0
21	-11	1	
2	336	326	5
5	123	139	-4
8	-40	85	-10
11	33	5	1
14	130	172	-12
21	-10	1	
1	520	459	26
4	-81	49	-11
7	156	192	-13
10	-69	49	-8
13	234	165	25
21	-9	1	
0	78	5	7
3	-119	8	-13
6	184	211	-10
9	42	36	0
12	77	8	6
21	-8	1	
2	-79	40	-9
5	249	214	10
8	197	154	15
11	206	207	0
21	-7	1	
1	70	56	2
4	-110	37	-17
7	320	289	11
10	163	185	-7
13	-74	10	-6
21	-6	1	
0	-112	5	-16
3	368	343	13
6	137	52	17
9	49	2	1
12	20	49	-2
21	-5	1	
2	96	53	7
5	241	200	16
8	223	205	7
11	-128	9	-14
21	-4	1	
1	131	120	3
4	303	261	19
7	79	10	6
10	251	245	2
21	-3	1	
0	106	97	1
3	-33	14	-1
6	119	102	4
9	175	70	24
21	-2	1	
2	-82	96	-18
5	176	171	1
8	151	75	17
21	-1	1	
1	-41	6	-1
4	82	5	7
22	-19	1	
2	-93	49	-12
22	-18	1	
1	131	120	2
4	-97	58	-15
22	-17	1	
3	320	301	9
6	145	132	3
22	-16	1	
2	176	68	26
5	99	68	5
8	55	22	2
22	-15	1	
1	110	26	12
4	129	87	9
7	113	82	6
10	-73	3	-6
22	-14	1	
3	41	103	-10
6	143	156	-4
9	-97	45	-13
22	-13	1	
2	308	347	-21
5	-43	92	-12
8	234	220	6
11	108	124	-3
22	-12	1	
1	-107	23	-15
4	-68	47	-8
7	151	200	-17
10	-62	72	-10
22	-11	1	
3	-33	117	-17
6	131	200	-24
9	93	73	3
22	-10	1	
2	357	310	16
5	-94	82	-19
8	-99	23	-12
11	121	189	-21
22	-9	1	
1	146	42	20
4	118	43	9
7	-109	37	-16
10	68	3	5
22	-8	1	
0	-106	15	-14
3	261	245	6
6	-125	39	-15
9	-120	6	-17
22	-7	1	
2	-86	54	-12
5	122	108	3
8	340	322	6
22	-6	1	
1	-70	95	-16
4	72	8	5
7	157	139	5
22	-5	1	
0	-96	40	-13
3	342	316	12
6	78	40	5
22	-4	1	
2	143	90	12
5	191	101	25
22	-3	1	
1	203	98	29
4	132	2	17
23	-17	1	
1	145	126	5
4	27	81	-6
23	-16	1	
3	67	97	-5
6	139	104	8
23	-15	1	
2	164	148	5
5	72	150	-19
23	-14	1	
1	75	89	-2
4	-106	52	-16
7	92	48	6
23	-13	1	
3	116	77	7
6	272	242	13
23	-12	1	
2	90	79	2
5	159	127	9
8	-83	78	-14
23	-11	1	
1	135	2	13
4	134	156	-6
7	133	188	-18
23	-10	1	
0	-112	40	-17
3	145	121	4
6	115	80	7
23	-9	1	
2	32	53	-2
5	-68	33	-4
8	119	96	5
23	-8	1	
1	-72	53	-9
4	100	95	0
7	109	52	6
23	-7	1	
0	-105	6	-13
3	58	46	1
6	110	94	3
23	-6	1	
2	197	62	32
24	-13	1	
1	-29	45	-3
24	-12	1	
3	169	128	11
24	-11	1	
2	101	47	5
24	-10	1	
1	147	154	-2

Appendix 2. Supplimentary Material for the X-ray Crystal Structure Determination of CuTFPP.

Figure A2.1. ORTEP diagram for CuTFPP (50% probability ellipsoids) and numbering scheme for macrocycle.

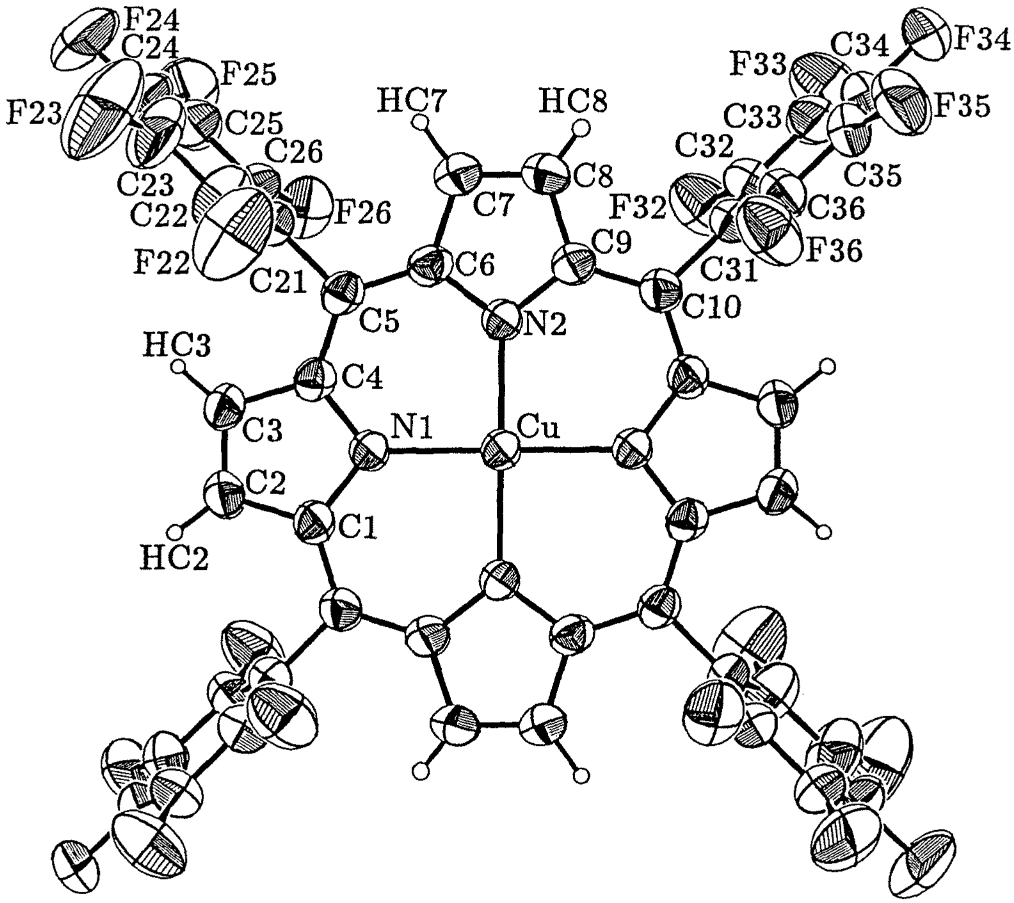

Table A2.1. Crystal and Intensity Collection Data for CuTFPP.

Formula: $CuC_{44}H_8N_4F_{20}$	Formula Weight: 1044.10
Crystal Color: ruby red	Habit: plate
Crystal Size: 0.28 x 0.52 x 0.54 mm	
Crystal System: rhombohedral	Space Group: $R\bar{3}$
$a = 20.358(5)$ Å	$\alpha = 90$
$b = 20.358(5)$ Å	$\beta = 90$
$c = 24.347(6)$ Å	$\gamma = 120$
$V = 8739(4)$ Å^3	$Z = 9$
$D = 1.77$ g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 6.96$ cm^{-1}	$T = 298$ K
Enraf-Nonius Cad-4 diffractometer	ω scan
Transmission coeff. = 0.75 - 0.84	range for data collection: 1-25
$\pm h = 28, \pm k = 28, \pm l = 34$	
Number of reflections measured: 12512	
Number of independent reflections: 5651	
Goodness of fit for merging data: 0.95	
$R = 0.0791$ on F for 4625 reflections with $F_o^2 > 0$	
$R = 0.0491$ on F for 3104 reflections with $F_o^2 > 3\sigma(F_o^2)$	
$wR = 0.009$ on F^2 for 5651 reflections	
Final goodness of fit: 1.99 for 329 parameters and 5651 reflections	

Table A2.2. Final Refined Heavy Atom Parameters x 10^4 for CuTFPP.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
Cu	5000	0	0	417(1)
N1	4300(1)	−1035(1)	−296(1)	429(4)
N2	5763(1)	163(1)	−576(1)	446(4)
C1	3587(1)	−1551(1)	−107(1)	470(6)
C2	3266(2)	−2221(1)	−439(1)	563(7)
C3	3772(1)	−2114(1)	−830(1)	532(6)
C4	4420(1)	−1373(1)	−743(1)	439(5)
C5	5069(1)	−1051(1)	−1066(1)	457(5)
C6	5690(1)	−330(1)	−990(1)	465(6)
C7	6354(2)	7(2)	−1336(1)	570(7)
C8	6826(2)	691(2)	−1130(1)	593(7)
C9	6463(1)	796(1)	−661(1)	487(6)
C10	6775(1)	1441(1)	−338(1)	494(6)
C21	5112(1)	−1524(1)	−1518(1)	506(6)
C22	4748(2)	−1627(2)	−2009(1)	816(9)
C23	4780(3)	−2081(2)	−2417(1)	1074(14)
C24	5193(3)	−2436(2)	−2330(2)	961(12)
C25	5552(2)	−2348(2)	−1854(2)	803(9)
C26	5516(1)	−1892(1)	−1454(1)	575(7)
C31	7558(1)	2065(1)	−472(1)	556(7)

Atom	x	y	z	U_{eq}
C32	8192(2)	2032(2)	−313(1)	671(8)
C33	8919(2)	2615(2)	−430(1)	775(10)
C34	9011(2)	3233(2)	−711(1)	753(10)
C35	8403(2)	3286(2)	−878(1)	758(10)
C36	7680(2)	2702(2)	−758(1)	667(8)
F22	4345(2)	−1282(1)	−2098(1)	1347(8)
F23	4398(2)	−2179(2)	−2884(1)	1876(12)
F24	5223(2)	−2877(1)	−2727(1)	1580(9)
F25	5944(1)	−2703(1)	−1767(1)	1386(8)
F26	5893(.9)	−1810(.9)	−986(.8)	844(5)
F32	8107(1)	1429(1)	−40(1)	975(6)
F33	9522(1)	2566(1)	−271(1)	1252(8)
F34	9719(1)	3800(1)	−823(1)	1056(7)
F35	8505(1)	3896(1)	−1158(1)	1112(7)
F36	7092(1)	2767(1)	−926(1)	997(6)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table A2.3. Complete Distances and Angles for CuTFPP.

	Distance(Å)		Distance(Å)
Cu –N1	1.997(2)	C9 –C10	1.383(4)
Cu –N2	1.994(2)	C10 –C31	1.495(4)
N1 –C1	1.377(3)	C21 –C22	1.367(4)
N1 –C4	1.373(3)	C21 –C26	1.371(4)
N2 –C6	1.375(3)	C22 –C23	1.379(6)
N2 –C9	1.378(3)	C22 –F22	1.339(4)
C1 –C2	1.432(4)	C23 –C24	1.371(6)
C1 –C10′	1.388(4)	C23 –F23	1.335(5)
C2 –C3	1.337(4)	C24 –C25	1.334(6)
C2 –HC2	0.96(3)	C24 –F24	1.341(5)
C3 –C4	1.439(4)	C25 –C26	1.372(5)
C3 –HC3	0.95(2)	C25 –F25	1.334(4)
C4 –C5	1.388(4)	C26 –F26	1.337(3)
C5 –C6	1.390(4)	C31 –C32	1.382(4)
C5 –C21	1.493(4)	C31 –C36	1.380(4)
C6 –C7	1.442(4)	C32 –C33	1.387(5)
C7 –C8	1.332(4)	C32 –F32	1.329(4)
C7 –HC7	0.99(3)	C33 –C34	1.360(5)
C8 –C9	1.434(4)	C33 –F33	1.339(4)
C8 –HC8	0.88(3)	C34 –C35	1.357(5)

	Distance(Å)		Angle(°)
C34 –F34	1.348(4)	N1 –Cu –N2	90.4(1)
C35 –C36	1.383(5)	N1 –Cu –N2′	89.6(1)
C35 –F35	1.339(4)	N1 –Cu –N1′	180.0
C36 –F36	1.333(4)	N2 –Cu –N2′	180.0
		Cu –N1 –C1	127.4(2)
		Cu –N1 –C4	127.1(2)
		Cu –N2 –C6	127.1(2)
		Cu –N2 –C9	128.0(2)
		C4 –N1 –C1	105.5(2)
		C9 –N2 –C6	104.9(2)
		C2 –C1 –N1	110.0(2)
		C10′ –C1 –N1	125.4(2)
		C10′ –C1 –C2	124.6(2)
		C3 –C2 –C1	107.4(2)
		HC2 –C2 –C1	125.1(16)
		HC2 –C2 –C3	127.4(16)
		C4 –C3 –C2	107.1(2)
		HC3 –C3 –C2	131.4(15)
		HC3 –C3 –C4	121.5(15)
		C3 –C4 –N1	110.0(2)

			Angle(°)				Angle(°)
C5	–C4	–N1	125.3(2)	C22	–C21	–C5	122.8(3)
C5	–C4	–C3	124.7(2)	C26	–C21	–C5	120.9(2)
C6	–C5	–C4	124.8(2)	C26	–C21	–C22	116.3(3)
C21	–C5	–C4	117.5(2)	C23	–C22	–C21	121.9(3)
C21	–C5	–C6	117.7(2)	F22	–C22	–C21	119.2(3)
C5	–C6	–N2	125.3(2)	F22	–C22	–C23	118.8(3)
C7	–C6	–N2	110.3(2)	C24	–C23	–C22	119.2(4)
C7	–C6	–C5	124.4(2)	F23	–C23	–C22	119.6(4)
C8	–C7	–C6	107.0(3)	F23	–C23	–C24	121.1(4)
HC7	–C7	–C6	126.8(15)	C25	–C24	–C23	120.2(4)
HC7	–C7	–C8	126.2(15)	F24	–C24	–C23	119.1(4)
C9	–C8	–C7	107.4(3)	F24	–C24	–C25	120.6(4)
HC8	–C8	–C7	126.8(19)	C26	–C25	–C24	119.7(3)
HC8	–C8	–C9	125.7(19)	F25	–C25	–C24	120.1(3)
C8	–C9	–N2	110.4(2)	F25	–C25	–C26	120.1(3)
C10	–C9	–N2	124.9(2)	C25	–C26	–C21	122.6(3)
C10	–C9	–C8	124.7(2)	F26	–C26	–C21	119.5(3)
C9	–C10	–C1′	124.6(2)	F26	–C26	–C25	117.9(3)
C31	–C10	–C1′	117.4(2)	C32	–C31	–C10	121.5(2)
C31	–C10	–C9	118.1(2)	C36	–C31	–C10	121.6(2)

	Angle(°)
C36 –C31 –C32	116.9(3)
C33 –C32 –C31	121.6(3)
F32 –C32 –C31	119.5(3)
F32 –C32 –C33	118.9(3)
C34 –C33 –C32	119.4(3)
F33 –C33 –C32	120.1(3)
F33 –C33 –C34	120.5(3)
C35 –C34 –C33	120.9(3)
F34 –C34 –C33	119.2(3)
F34 –C34 –C35	119.9(3)
C36 –C35 –C34	119.4(3)
F35 –C35 –C34	120.1(3)
F35 –C35 –C36	120.6(3)
C35 –C36 –C31	121.9(3)
F36 –C36 –C31	119.8(3)
F36 –C36 –C35	118.3(3)

′ indicates atom related by inversion

Table A2.4. Final Refined Hydrogen Atom Parameters for CuTFPP.

x, y and $z \times 10^4$

Atom	x	y	z	B
HC2	2778(14)	−2659(13)	−384(9)	4.6(6)
HC3	3752(12)	−2425(12)	−1128(9)	3.9(5)
HC7	6435(12)	−214(13)	−1674(10)	4.4(5)
HC8	7270(16)	1026(15)	−1263(10)	5.7(7)

Table A2.5. Anisotropic Displacement Parameters for CuTFPP.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	406(2)	366(2)	518(2)	223(2)	26(2)	−12(2)
N1	416(11)	365(10)	523(12)	209(9)	39(9)	−15(9)
N2	435(11)	378(10)	538(12)	212(9)	54(9)	−13(9)
C1	440(13)	392(13)	603(16)	226(11)	5(12)	−31(11)
C2	456(15)	413(15)	740(19)	158(13)	18(14)	−83(13)
C3	523(15)	441(14)	630(18)	239(13)	−17(13)	−135(13)
C4	472(14)	416(13)	519(14)	289(12)	−21(11)	−28(11)
C5	496(14)	446(13)	505(15)	292(12)	−5(11)	−28(11)
C6	498(14)	466(14)	493(15)	287(12)	50(11)	−4(11)
C7	586(17)	540(16)	583(17)	281(14)	120(14)	−33(14)
C8	501(16)	539(17)	692(19)	224(14)	180(14)	19(14)
C9	452(14)	450(14)	580(16)	241(12)	62(12)	−22(12)
C10	425(13)	428(13)	619(16)	205(11)	48(12)	−24(12)
C21	539(15)	435(14)	521(16)	226(12)	49(12)	−60(11)
C22	1094(26)	878(23)	640(21)	616(21)	−133(19)	−125(18)
C23	1566(39)	1028(29)	537(22)	580(29)	−184(23)	−241(20)
C24	1233(33)	726(23)	788(26)	388(23)	287(23)	−217(20)
C25	727(21)	627(19)	1097(28)	371(17)	207(20)	−146(19)
C26	514(16)	504(15)	696(18)	246(13)	82(14)	−71(13)
C31	461(14)	465(15)	678(18)	183(12)	94(13)	−63(13)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C32	505(17)	658(19)	770(21)	231(15)	65(14)	−62(16)
C33	455(17)	862(24)	885(24)	236(17)	42(16)	−178(19)
C34	504(18)	618(20)	824(23)	46(16)	145(16)	−248(17)
C35	700(21)	450(17)	927(24)	139(16)	184(17)	−65(16)
C36	502(16)	512(17)	905(22)	191(14)	115(15)	−50(15)
F22	1931(24)	1634(21)	1016(16)	1296(21)	−617(16)	−273(15)
F23	3015(39)	2059(29)	736(15)	1405(29)	−657(20)	−547(18)
F24	2070(26)	1255(19)	1242(19)	701(19)	455(18)	−551(15)
F25	1185(17)	1168(17)	2184(25)	872(15)	165(17)	−444(16)
F26	791(12)	864(12)	1074(14)	562(10)	−190(10)	−147(10)
F32	691(12)	1006(14)	1277(16)	461(11)	22(10)	219(12)
F33	486(11)	1475(20)	1654(21)	385(12)	−58(12)	13(16)
F34	584(11)	814(12)	1186(15)	−89(9)	229(10)	−323(11)
F35	1001(14)	574(11)	1501(19)	199(11)	352(13)	202(11)
F36	729(12)	710(12)	1552(18)	359(10)	143(12)	300(11)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table A2.6. Observed and Calculated Structure Factors for CuTFPP. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F_{obs}^2 - F_{calc}^2}{\sigma F_{obs}^2}\right)$. A minus sign preceeding F_{obs} indicates that F_{obs}^2 is negative.

Tetra(pentafluorophenyl)porphinato Copper(II) Page 1

0 0 1			
3	3351	3507	-54
6	3661	3813	-48
9	1742	1757	-9
12	1032	1053	-19
15	379	407	-27
18	513	519	-5
21	1173	1169	3
24	528	478	35
27	529	498	20
30	380	338	19
33	222	132	20
1 -1 1			
2	1357	1337	16
5	1613	1583	20
8	1001	1031	-29
11	1622	1655	-21
14	1073	1052	17
17	-27	89	-15
20	135	65	18
23	-26	48	-3
26	260	247	5
29	261	226	12
32	-78	18	-4
1 0 1			
4	3045	3232	-79
7	1431	1414	14
10	1762	1776	-9
13	834	859	-30
16	271	245	27
19	251	267	-14
22	318	379	-60
25	266	259	4
28	179	143	14
31	-92	2	-9
34	-17	59	-3
1 1 1			
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3	1695	1673	15
6	80	78	0
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15	-39	69	-12
18	350	341	7
21	437	421	12
24	130	53	15
27	-75	78	-11
30	147	154	-1
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2 -3 1			
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5	1799	1752	29
8	274	279	-6
11	716	703	14
14	734	742	-8
17	281	292	-7
20	279	261	11
23	66	22	4
26	180	216	-13
29	157	110	10
32	63	19	2
2 -2 1			
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4	3854	4043	-57
7	2438	2450	-5
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25	199	221	-9
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34	151	114	6
2 -1 1			
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27	314	312	1
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17	823	814	9
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26	101	124	-7
29	306	247	32
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7	1379	1392	-9
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23	176	24	32
26	140	49	16
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14	314	240	61
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31	120	89	4
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21	298	313	-13
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3 2 1			
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16	69	50	3
19	531	510	17
22	575	515	44
25	350	334	9
28	134	234	-32
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15	445	439	5
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21	727	731	-3
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27	108	81	4
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4 -7 1			
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14	964	982	-15
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26	-118	18	-14
29	-105	76	-13
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9	441	465	-29
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18	673	679	-5
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33	143	52	12
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27	141	119	5
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4 2 1			
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5 -8 1			
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7	1067	1028	33
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5 0 1			
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26	387	369	14
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6 -7 1			
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7 -13 1			
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17	495	539	-34
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7 -12 1			
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25	78	73	0
28	-95	85	-12
31	195	157	8
7 -11 1			
3	2102	2067	18

Tetra(pentafluorophenyl)porphinato Copper(II)

6	1544	1528	10
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12	42	34	0
15	404	400	2
18	283	304	-12
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7 -10 1

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14	33	2	1
17	256	268	-6
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26	145	128	4
29	106	75	4

7 -9 1

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13	338	358	-17
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22	549	576	-20
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28	115	134	-3
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7 -8 1

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21	-51	77	-10
24	140	158	-5
27	109	134	-5
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7 -7 1

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17	703	745	-38
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7 -6 1

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4	319	334	-24
7	1615	1593	14
10	1098	1109	-10
13	-73	45	-14
16	137	122	5
19	481	448	26
22	94	181	-27
25	124	32	14
28	76	13	4
31	-44	11	-1

7 -5 1

3	1686	1678	5
6	1826	1808	10
9	1775	1733	25
12	934	930	3
15	182	93	37
18	604	622	-15
21	195	213	-8
24	220	217	0
27	267	225	17
30	-139	51	-17
33	-140	29	-14

7 -4 1

2	1665	1547	74
5	2927	2927	0
8	2050	1958	48
11	109	0	24
14	1538	1502	23
17	528	512	14
20	107	81	6
23	189	190	0
26	274	224	21
29	64	76	-1
32	-65	26	-3

7 -3 1

1	1069	965	93
4	2431	2405	12
7	1269	1284	-12
10	878	902	-24
13	540	514	25
16	190	159	15
19	212	259	-26
22	344	361	-11
25	239	207	13
28	319	268	21
31	203	19	28

7 -2 1

0	16	105	-32
3	1598	1616	-12
6	1090	1098	-8
9	243	240	3
12	1281	1280	1
15	245	207	24
18	255	235	11
21	188	202	-5
24	291	297	-3
27	326	268	27
30	254	189	19
33	-127	17	-11

7 -1 1

2	2165	2173	-4
5	1009	1007	1
8	1478	1348	88
11	239	223	12
14	392	320	60
17	58	101	-10
20	476	507	-25
23	187	167	7
26	64	131	-12
29	211	169	11
32	129	9	11

7 0 1

1	531	532	-1
4	1059	1070	-12
7	918	933	-18
10	357	344	18
13	645	656	-13
16	361	378	-19
19	173	226	-36
22	126	143	-7
25	67	24	5
28	-56	47	-6
31	98	14	9

7 1 1

0	710	713	-3
3	330	323	7
6	1280	1277	2
9	505	527	-23
12	1115	1108	5
15	1275	1309	-24
18	346	365	-14
21	-40	148	-26
24	-172	18	-32
27	-19	89	-7
30	51	30	1

7 2 1

2	790	804	-14
5	1791	1669	70
8	303	278	30
11	675	698	-22
14	344	390	-38
17	283	294	-6
20	361	388	-17
23	130	178	-14
26	-167	9	-27
29	-206	1	-34
32	-5	74	-3

7 3 1

1	862	765	91
4	139	48	36
7	693	656	37
10	232	218	9
13	123	214	-45
16	512	554	-36
19	-144	28	-26
22	-99	191	-49
25	-87	139	-25
28	-42	138	-16
31	130	24	11

7 4 1

0	591	573	19
3	529	496	34
6	1112	1095	14
9	473	500	-35
12	-93	121	-37
15	-40	96	-14
18	162	216	-22
21	-149	96	-35
24	117	119	0
27	111	92	2
30	164	152	2

7 5 1

2	1524	1498	16
5	808	815	-6
8	611	649	-39
11	29	72	-6
14	380	417	-28
17	393	453	-44
20	-147	89	-33
23	187	204	-5
26	-147	51	-20
29	154	116	7

7 6 1

1	217	185	20
4	932	972	-35
7	300	349	-42
10	468	481	-15
13	246	295	-31
16	40	123	-15
19	36	153	-23
22	177	210	-11
25	157	161	-1
28	-90	21	-6

7 7 1

0	594	623	-28
3	955	959	-3
6	655	661	-5
9	450	439	9
12	336	381	-33
15	187	223	-15
18	142	212	-25
21	339	332	3
24	127	133	-1
27	-43	110	-10

8 -15 1

2	233	244	-7
5	511	492	16
8	189	179	4
11	-118	108	-50
14	542	568	-20
17	266	245	10
20	257	255	0
23	-176	39	-28
26	-112	36	-10
29	137	6	12

8 -14 1

1	1374	1376	-1
4	860	892	-28
7	1654	1685	-19
10	1189	1188	0
13	750	732	15
16	229	152	30
19	486	512	-18
22	627	597	19
25	172	152	4
28	111	89	3

8 -13 1

3	1166	1119	36
6	936	935	0
9	886	922	-39
12	483	454	23
15	472	479	-5
18	518	522	-3
21	293	316	-12
24	-59	108	-14
27	-66	86	-9
30	-120	15	-10

8 -12 1

2	1548	1558	-6
5	732	753	-20
8	513	521	-10
11	1430	1475	-30
14	637	640	-3
17	584	568	12
20	763	751	9
23	399	392	4
26	-68	138	-19
29	153	145	1

8 -11 1

1	1110	1122	-10
4	90	105	-5
7	841	846	-5
10	1644	1714	-44
13	890	893	-1
16	366	405	-30
19	369	393	-16
22	296	284	6
25	162	196	-10
28	-170	22	-23
31	157	19	16

8 -10 l

3	1787	1815	-17
6	1099	1159	-61
9	2195	2215	-9
12	1172	1181	-7
15	658	647	9
18	1084	1065	14
21	566	554	9
24	594	566	18
27	231	248	-6
30	99	52	5

8 -9 l

2	786	752	34
5	1809	1780	19
8	1218	1241	-18
11	344	380	-33
14	547	572	-23
17	476	495	-15
20	-77	112	-22
23	-46	49	-4
26	36	58	-1
29	76	39	3
32	-187	9	-25

8 -8 l

1	2134	2149	-8
4	1526	1566	-33
7	2044	2049	-2
10	1920	1941	-12
13	1615	1624	-6
16	528	518	8
19	181	178	1
22	665	637	21
25	635	598	25
28	166	174	-1
31	-58	70	-5

8 -7 l

3	996	953	40
6	165	184	-14
9	435	418	17
12	744	793	-49
15	1117	1158	-32
18	566	539	22
21	215	175	16
24	171	183	-3
27	169	157	3
30	-28	54	-2

8 -6 l

2	2512	2487	11
5	1576	1578	-1
8	1070	1069	0
11	1117	1121	-3
14	1019	974	36
17	952	986	-28
20	578	579	0
23	418	365	33
26	450	403	27
29	288	245	15
32	70	27	2

8 -5 l

1	1026	1025	0
4	1642	1662	-13
7	122	7	35
10	1231	1154	59
13	319	308	9
16	753	764	-9
19	887	892	-4
22	432	422	6
25	189	87	26
28	231	119	29
31	126	95	4

8 -4 l

3	3595	3528	21
6	781	655	150
9	1560	1662	-70
12	2132	2145	-6
15	2252	2241	5
18	1001	1020	-15
21	-117	26	-18
24	679	614	46
27	453	420	19
30	327	307	8

8 -3 l

2	324	348	-28
5	166	121	28
8	924	851	67
11	723	726	-3
14	161	30	40
17	331	313	13
20	421	417	3
23	145	101	11
26	169	195	-9
29	149	31	16
32	92	51	4

8 -2 l

1	3782	3745	10
4	1924	1863	33
7	286	335	-74
10	2634	2626	3
13	1959	1969	-4
16	462	511	-45
19	574	586	-9
22	541	540	0
25	472	406	41
28	383	356	13
31	388	318	29

8 -1 l

0	2842	2805	14
3	736	714	24
6	186	214	-21
9	705	752	-50
12	87	32	12
15	70	32	6
18	103	145	-14
21	318	302	9
24	211	223	-4
27	127	116	2
30	232	182	14

8 0 l

2	410	415	-7
5	626	667	-60
8	1871	1828	29
11	114	175	-44
14	543	531	14
17	1129	1125	4
20	893	913	-20
23	454	455	-1
26	221	221	0
29	287	253	17
32	-6	99	-9

8 1 l

1	439	422	19
4	167	121	28
7	815	827	-12
10	946	928	15
13	352	379	-22
16	605	638	-29
19	494	516	-16
22	274	261	6
25	149	177	-8
28	149	183	-8
31	135	127	1

8 2 l

0	1160	1202	-36
3	2095	2154	-31
6	3817	3879	-18
9	815	823	-9
12	403	399	3
15	790	776	11
18	772	798	-21
21	669	681	-9
24	529	516	8
27	242	248	-1
30	183	220	-10

8 3 l

2	583	600	-18
5	702	699	2
8	563	540	23
11	-150	29	-40
14	414	461	-39
17	-157	36	-34
20	514	544	-22
23	44	147	-19
26	-129	28	-14
29	36	128	-10

8 4 l

1	99	7	18
4	2176	2191	-7
7	570	566	4
10	787	792	-6
13	368	394	-20
16	600	597	1
19	452	430	15
22	-42	149	-24
25	537	501	20
28	280	236	14

8 5 l

0	416	389	25
3	785	833	-47
6	1111	1135	-19
9	258	184	44
12	-79	167	-48
15	137	273	-65
18	200	235	-15
21	213	233	-8
24	82	65	2
27	41	111	-7
30	-108	71	-11

8 6 l

2	1929	1936	-4
5	817	822	-4
8	1449	1467	-12
11	827	825	2
14	549	577	-22
17	217	198	7
20	371	348	13
23	378	351	14
26	184	190	-1
29	153	138	2

8 7 l

1	1190	1189	0
4	640	666	-24
7	449	451	-1
10	427	454	-22
13	281	355	-48
16	497	494	1
19	89	69	3
22	-108	68	-15
25	150	124	5
28	-130	19	-12

8 8 l

0	1188	1160	20
3	751	782	-28
6	742	717	21
9	551	570	-17
12	1169	1157	10
15	634	643	-7
18	478	484	-4
21	204	240	-13
24	170	206	-9
27	-110	118	-18

9 -17 l

2	358	364	-4
5	859	876	-14
8	943	949	-4
11	675	657	14
14	78	13	6
17	-39	71	-6
20	-158	34	-25
23	70	125	-8
26	-157	87	-23

9 -16 l

1	354	377	-17
4	526	567	-36
7	136	126	3
10	-85	4	-9
13	304	280	13
16	198	224	-10
19	-50	25	-3
22	-9	148	-18
25	-131	116	-23
28	-66	3	-3

9 -15 l

3	325	298	20
6	857	842	13
9	465	488	-19
12	-85	51	-12
15	702	759	-46
18	135	95	9
21	216	173	14
24	-156	58	-23
27	-153	26	-18

9 -14 l

2	66	115	-14
5	858	827	27
8	293	288	3

11	575	624	-44
14	391	370	14
17	176	192	-5
20	273	264	4
23	105	132	-5
26	-110	86	-15
29	-137	61	-16
	9	-13	1
1	1031	999	26
4	150	120	13
7	156	134	10
10	579	626	-43
13	415	475	-49
16	277	318	-24
19	290	292	0
22	52	116	-10
25	56	87	-3
28	-165	8	-20
	9	-12	1
3	97	19	16
6	-68	118	-35
9	446	463	-15
12	547	570	-21
15	435	420	12
18	281	260	11
21	217	229	-5
24	114	157	-10
27	118	136	-3
30	150	138	2
	9	-11	1
2	529	492	37
5	584	509	72
8	732	733	0
11	301	279	16
14	453	443	7
17	132	116	4
20	339	346	-4
23	196	222	-10
26	143	84	10
29	-122	30	-11
	9	-10	1
1	456	500	-49
4	197	203	-4
7	293	275	15
10	261	239	15
13	-40	84	-13
16	274	271	2
19	212	247	-17
22	213	182	11
25	263	182	29
28	-108	76	-13
31	-94	36	-7
	9	-9	1
3	421	415	7
6	943	912	28
9	1307	1289	13
12	1411	1472	-43
15	-83	6	-10
18	88	128	-11
21	330	292	21
24	124	43	13
27	-118	61	-14
30	-78	31	-5
	9	-8	1
2	3129	3019	39
5	1150	1110	37
8	1127	1122	4
11	374	396	-20
14	276	256	13
17	306	313	-5
20	134	152	-5
23	132	179	-15
26	-5	36	-1
29	196	158	9
32	-37	23	-1
	9	-7	1
1	1011	937	66
4	3113	2913	70
7	1207	1221	-11
10	1574	1577	-1
13	88	83	1
16	351	359	-6
19	410	421	-8
22	481	452	20
25	172	50	25
28	148	9	17
31	-101	25	-7
	9	-6	1
3	1301	1210	68
6	48	23	5
9	840	854	-14
12	584	575	9
15	156	82	25
18	200	169	13
21	93	82	2
24	-64	11	-4
27	242	147	28
30	89	75	1
	9	-5	1
2	213	197	13
5	175	128	29
8	647	610	39
11	31	32	0
14	282	290	-6
17	330	351	-15
20	275	305	-17
23	473	444	19
26	386	359	14
29	248	173	22
32	98	93	0
	9	-4	1
1	1149	1125	19
4	458	394	69
7	1297	1264	28
10	570	553	18
13	854	845	7
16	577	590	-11
19	76	71	0
22	-133	114	-36
25	48	25	1
28	228	156	20
31	196	108	18
	9	-3	1
0	1574	1591	-11
3	721	735	-15
6	1211	1170	32
9	112	150	-19
12	170	64	41
15	622	590	28
18	639	648	-7
21	226	266	-20
24	133	57	14
27	266	225	14
30	123	17	10
	9	-2	1
2	1350	1283	49
5	-25	61	-9
8	232	257	-28
11	967	976	-8
14	386	389	-2
17	481	499	-16
20	-59	19	-4
23	298	278	10
26	78	91	-2
29	150	90	10
32	-103	57	-9
	9	-1	1
1	529	513	18
4	-89	13	-18
7	336	312	21
10	218	172	29
13	403	421	-15
16	476	479	-2
19	87	118	-7
22	199	164	12
25	-134	0	-18
28	146	0	16
31	-139	83	-19
	9	0	1
0	247	180	73
3	74	22	15
6	-113	15	-39
9	1652	1652	0
12	806	803	3
15	411	392	21
18	224	264	-30
21	-96	94	-29
24	-87	10	-10
27	-15	62	-4
30	-35	40	-3
	9	1	1
2	726	727	-1
5	605	618	-14
8	472	456	16
11	287	312	-19
14	416	422	-4
17	93	188	-32
20	-71	73	-11
23	-93	32	-9
26	-135	19	-15
29	73	33	3
	9	2	1
1	181	120	33
4	515	505	10
7	1355	1337	13
10	-95	77	-37
13	-88	143	-41
16	568	605	-31
19	465	465	0
22	-160	28	-28
25	90	83	1
28	-42	134	-14
31	48	45	0
	9	3	1
0	175	125	26
3	457	492	-36
6	1709	1667	24
9	70	56	2
12	173	207	-16
15	603	628	-20
18	-104	51	-15
21	-147	42	-25
24	286	302	-7
27	133	132	0
30	162	33	16
	9	4	1
2	177	176	0
5	509	511	-1
8	1290	1265	18
11	791	796	-5
14	-141	108	-43
17	206	217	-4
20	-89	154	-33
23	84	181	-23
26	50	139	-12
29	282	182	29
	9	5	1
1	315	336	-18
4	26	46	-2
7	120	17	21
10	169	91	27
13	409	438	-22
16	-153	21	-28
19	68	137	-14
22	58	46	1
25	139	169	-7
28	148	79	10
	9	6	1
0	112	87	7
3	542	526	14
6	267	270	-2
9	167	192	-11
12	-140	59	-44
15	332	339	-4
18	361	375	-8
21	-129	86	-23
24	150	102	9
27	-42	10	-1
	9	7	1
2	346	358	-9
5	109	151	-15
8	349	355	-4
11	129	177	-18
14	197	191	2
17	58	30	2
20	-64	9	-3
23	-131	37	-15
26	-89	124	-17
	9	8	1
1	360	357	2
4	496	510	-11
7	323	377	-39
10	78	43	5
13	567	570	-3
16	745	775	-22
19	202	224	-8
22	-147	35	-18
25	-182	41	-26
	9	9	1
0	178	183	-1
3	151	159	-2
6	273	327	-33
9	163	50	27
12	630	590	29
15	-110	42	-14
18	159	194	-11

21	160	141	4
24	79	101	-2

10 -19 1

2	560	522	28
5	300	309	-5
8	135	90	11
11	277	208	31
14	133	15	24
17	439	398	23
20	-70	80	-9
23	-77	74	-8

10 -18 1

1	801	826	-21
4	786	836	-41
7	465	438	19
10	732	721	8
13	393	385	6
16	503	477	16
19	460	428	18
22	203	166	9
25	163	200	-8

10 -17 1

3	63	49	2
6	112	85	7
9	-87	79	-17
12	454	447	7
15	261	320	-30
18	198	187	4
21	-51	125	-15
24	-97	37	-8
27	-54	54	-3

10 -16 1

2	572	566	5
5	1286	1315	-20
8	1115	1105	7
11	810	829	-19
14	448	404	29
17	689	656	23
20	381	381	0
23	196	226	-9
26	162	182	-4

10 -15 1

1	117	151	-13
4	358	345	9
7	491	440	41
10	-103	26	-22
13	267	334	-41
16	471	458	9
19	242	222	8
22	126	122	0
25	-161	74	-25
28	119	133	-2

10 -14 1

3	1373	1387	-10
6	1147	1143	3
9	1449	1459	-7
12	527	464	48
15	712	678	26
18	270	271	0
21	521	522	0
24	362	360	0
27	142	99	7

10 -13 1

2	768	765	2
5	424	420	3
8	432	424	9
11	-61	46	-8
14	437	453	-12
17	572	628	-44
20	262	253	4
23	126	143	-4
26	-35	53	-3
29	-119	59	-12

10 -12 1

1	1229	1229	0
4	965	990	-22
7	625	644	-24
10	820	780	34
13	540	523	15
16	716	741	-20
19	865	848	12
22	494	456	24
25	349	316	15
28	281	231	16

10 -11 1

3	1266	1280	-10
6	589	620	-41
9	148	136	5
12	225	236	-6
15	687	690	-2
18	243	202	19
21	232	246	-6
24	225	218	2
27	221	111	26
30	-129	42	-13

10 -10 1

2	1058	1086	-28
5	171	145	25
8	1936	2007	-39
11	1691	1758	-41
14	296	269	18
17	668	624	35
20	493	504	-7
23	436	452	-10
26	319	278	17
29	140	176	-8

10 -9 1

1	248	289	-39
4	1824	1818	4
7	166	146	10
10	1150	1173	-18
13	533	553	-18
16	295	350	-39
19	245	232	6
22	367	342	14
25	162	167	-1
28	256	187	21
31	-30	4	0

10 -8 1

3	1384	1431	-34
6	2116	2105	6
9	1291	1279	8
12	827	816	9
15	500	513	-11
18	580	537	33
21	711	709	2
24	140	106	8
27	356	327	13
30	211	147	15

10 -7 1

2	180	120	37
5	650	620	31
8	2218	2223	-2
11	187	243	-39
14	170	176	-3
17	222	226	-2
20	192	221	-13
23	167	69	23
26	116	44	10
29	246	182	19

10 -6 1

1	637	657	-22
4	2656	2702	-19
7	1008	1008	0
10	1789	1801	-6
13	389	403	-11
16	585	577	7
19	695	676	14
22	184	140	14
25	451	418	20
28	425	330	43
31	269	144	32

10 -5 1

3	900	875	23
6	160	248	-66
9	344	356	-11
12	379	370	8
15	1066	1092	-21
18	1054	1098	-34
21	147	154	-2
24	116	30	12
27	152	28	18
30	155	10	17

10 -4 1

2	910	756	135
5	376	484	-127
8	1071	1068	2
11	1636	1600	22
14	1621	1626	-3
17	964	976	-9
20	119	12	16
23	355	323	17
26	396	366	16
29	326	261	24
32	318	234	27

10 -3 1

1	1090	1070	16
4	486	447	40
7	879	922	-40
10	1244	1269	-19
13	111	74	10
16	63	72	-1
19	497	458	29
22	241	190	21
25	144	140	1
28	282	208	25
31	195	44	24

10 -2 1

0	2642	2667	-10
3	2704	2723	-7
6	257	299	-36
9	1084	1080	3
12	1350	1322	19
15	887	894	-5
18	545	516	23
21	573	590	-13
24	273	250	10
27	379	315	29
30	225	190	9

10 -1 1

2	1083	1023	49
5	-65	30	-10
8	666	608	54
11	365	319	38
14	298	271	18
17	106	135	-9
20	133	104	7
23	100	162	-16
26	165	123	9
29	211	188	6

10 0 1

1	1801	1805	-2
4	559	600	-57
7	845	847	-2
10	1161	1159	2
13	560	603	-52
16	545	557	-13
19	740	763	-23
22	373	346	22
25	123	173	-18
28	316	265	27
31	139	107	7

10 1 1

0	161	151	6
3	1163	1170	-4
6	152	180	-15
9	211	220	-5
12	593	584	7
15	103	207	-40
18	386	359	16
21	241	258	-7
24	-100	106	-20
27	81	5	4
30	-114	74	-13

10 2 1

2	3330	3289	13
5	2124	2111	6
8	461	500	-37
11	277	331	-56
14	662	643	15
17	1192	1183	5
20	309	304	2
23	172	236	-23
26	256	245	3
29	146	154	-1

10 3 1

1	631	637	-5
4	601	602	-1
7	587	576	10
10	361	321	30
13	469	520	-42
16	-43	160	-32
19	502	511	-6
22	246	289	-19
25	114	59	7
28	132	69	8

10 4 1

0	1969	1985	-8
3	759	791	-29
6	1086	1114	-22
9	1683	1675	4
12	247	266	-15
15	405	390	9
18	515	498	11

Tetra(pentafluorophenyl)porphinato Copper(II) Page 8

21	231	240	-3
24	301	282	7
27	292	274	6
10	5	1	
2	377	361	13
5	259	280	-14
8	867	905	-32
11	333	356	-16
14	-125	151	-45
17	343	322	11
20	140	220	-26
23	86	96	-1
26	-123	43	-12
10	6	1	
1	219	235	-9
4	290	304	-9
7	918	901	13
10	733	685	39
13	183	141	20
16	679	652	19
19	256	261	-2
22	325	344	-8
25	-119	102	-18
28	24	119	-9
10	7	1	
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3	-106	36	-18
6	385	448	-50
9	974	997	-17
12	-30	33	-2
15	78	64	2
18	49	26	1
21	-50	24	-2
24	-149	49	-19
27	-211	9	-32
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2	704	711	-6
5	697	674	18
8	770	745	19
11	765	748	12
14	955	951	3
17	152	209	-18
20	200	240	-13
23	128	143	-2
26	144	181	-7
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7	407	441	-24
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16	-97	87	-16
19	-49	96	-9
22	-116	146	-26
25	-112	69	-12
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3	926	941	-11
6	639	607	24
9	622	594	20
12	456	407	30
15	679	626	47
18	421	426	-2
21	-76	121	-15
24	-148	118	-25
11	-21	1	
2	108	132	-5
5	264	206	25
8	276	250	12
11	191	76	28
14	503	460	26
17	-42	14	-1
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23	-108	64	-10
11	-20	1	
1	382	417	-23
4	591	568	17
7	316	370	-33
10	200	9	39
13	187	110	21
16	-114	15	-12
19	107	109	0
22	-99	35	-8
11	-19	1	
3	31	88	-8
6	70	64	0
9	155	132	7
12	721	701	14
15	263	197	25
18	238	189	16
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11	-18	1	
2	193	223	-14
5	915	904	8
8	1036	1066	-22
11	298	227	35
14	122	103	4
17	29	29	0
20	-120	3	-12
23	105	152	-8
26	-108	3	-8
11	-17	1	
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4	853	847	5
7	151	154	0
10	382	391	-6
13	409	422	-8
16	143	60	16
19	301	299	0
22	-22	85	-6
25	147	116	5
11	-16	1	
3	-62	76	-14
6	572	585	-11
9	1130	1137	-4
12	241	245	-1
15	184	117	20
18	72	137	-13
21	100	39	7
24	-95	148	-24
27	-160	1	-18
11	-15	1	
2	613	618	-4
5	280	335	-41
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14	159	142	5
17	351	428	-51
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23	109	189	-19
26	-53	20	-2
11	-14	1	
1	33	72	-6
4	290	298	-5
7	537	513	20
10	194	245	-28
13	368	408	-29
16	84	39	6
19	154	168	-4
22	-80	79	-12
25	-88	101	-14
28	145	141	0
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3	216	180	20
6	167	164	1
9	-30	100	-16
12	125	66	14
15	234	152	33
18	95	76	3
21	96	115	-3
24	233	225	2
27	-69	9	-3
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8	746	750	-3
11	960	966	-4
14	917	929	-10
17	145	79	16
20	-77	67	-11
23	-84	94	-15
26	136	114	4
29	122	167	-9
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7	418	411	6
10	1110	1134	-19
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16	264	276	-6
19	184	90	27
22	-126	46	-19
25	251	211	13
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9	1138	1131	5
12	832	841	-7
15	590	610	-17
18	379	349	19
21	194	129	20
24	93	56	5
27	154	22	17
30	136	75	8
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11	642	653	-10
14	160	209	-24
17	87	10	9
20	276	298	-12
23	177	136	12
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13	59	103	-10
16	29	92	-10
19	219	243	-12
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25	165	78	18
28	143	25	15
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6	495	491	4
9	-108	40	-26
12	383	392	-7
15	332	310	16
18	266	273	-4
21	64	59	0
24	242	143	33
27	218	27	35
30	286	271	5
11	-6	1	
2	705	722	-18
5	1197	1201	-3
8	505	515	-12
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14	678	668	8
17	596	659	-56
20	700	712	-10
23	133	106	6
26	133	67	11
29	135	23	13
11	-5	1	
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4	374	403	-29
7	-23	60	-7
10	246	178	43
13	251	231	12
16	412	439	-21
19	182	157	9
22	32	3	1
25	283	272	5
28	142	108	6
31	189	63	21
11	-4	1	
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3	200	176	15
6	148	164	-8
9	440	462	-29
12	459	478	-18
15	252	256	-2
18	510	489	16
21	434	395	25
24	278	318	-20
27	114	78	5
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11	-3	1	
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5	732	726	6
8	701	745	-43
11	372	389	-15
14	499	514	-12
17	487	502	-12

20	169	175	-2
23	-70	121	-20
26	107	95	1
29	29	4	0
11 -2 l			
1	219	247	-21
4	605	549	54
7	383	443	-57
10	1242	1248	-5
13	315	293	16
16	48	94	-8
19	164	57	26
22	417	420	-2
25	261	197	24
28	144	51	13
31	-94	18	-6
11 -1 l			
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3	568	615	-49
6	184	203	-11
9	442	451	-7
12	859	849	8
15	377	376	1
18	-63	83	-13
21	-103	64	-16
24	-85	125	-22
27	158	81	14
30	221	138	19
11 0 l			
2	483	493	-13
5	102	175	-49
8	224	272	-48
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14	-61	105	-28
17	473	468	4
20	284	339	-44
23	-126	50	-26
26	208	223	-6
29	-117	69	-19
11 1 l			
1	118	113	2
4	167	204	-22
7	-32	36	-4
10	136	79	18
13	171	217	-22
16	115	91	5
19	128	201	-24
22	-55	131	-19
25	-122	73	-16
28	-167	14	-21
11 2 l			
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3	695	690	5
6	140	144	-1
9	337	318	14
12	247	272	-21
15	339	390	-33
18	350	414	-41
21	-119	106	-25
24	-173	70	-30
27	287	287	0
11 3 l			
2	69	49	3
5	783	783	0
8	210	169	20
11	776	792	-13
14	148	276	-60
17	-87	37	-10
20	-145	73	-27
23	-187	11	-31
26	31	23	0
29	160	117	7
11 4 l			
1	539	545	-5
4	498	489	7
7	174	198	-12
10	322	329	-5
13	145	120	10
16	-128	65	-23
19	-156	5	-25
22	-118	30	-13
25	228	204	6
28	206	170	8
11 5 l			
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3	619	623	-4
6	229	246	-9
9	136	129	2
12	624	649	-20
15	374	411	-23
18	447	421	15
21	64	87	-3
24	-154	66	-22
27	142	47	12
11 6 l			
2	321	365	-32
5	179	160	7
8	229	280	-29
11	530	550	-15
14	244	214	18
17	82	138	-11
20	305	329	-11
23	-149	98	-25
26	-114	21	-9
11 7 l			
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7	187	199	-5
10	291	268	12
13	271	150	48
16	66	39	2
19	-102	96	-18
22	100	147	-8
25	205	145	13
11 8 l			
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6	648	638	7
9	183	174	3
12	612	613	0
15	301	265	23
18	-54	38	-3
21	101	151	-9
24	-42	35	-2
11 9 l			
2	329	336	-4
5	564	586	-16
8	50	6	2
11	167	126	11
14	361	316	24
17	246	237	3
20	117	142	-4
23	-153	38	-18
11 10 l			
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7	361	323	21
10	215	188	10
13	302	267	15
16	246	205	18
19	182	166	3
22	41	20	0
11 11 l			
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9	121	151	-7
12	164	85	17
15	250	144	30
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12 -23 l			
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8	308	324	-7
11	209	96	26
14	28	9	0
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20	107	67	4
12 -22 l			
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4	327	295	16
7	246	251	-2
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13	510	436	40
16	336	310	15
19	-71	67	-6
12 -21 l			
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9	502	535	-23
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15	269	207	30
18	-203	1	-33
21	-50	96	-8
12 -20 l			
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5	536	509	19
8	854	833	15
11	706	708	-1
14	474	463	9
17	392	366	12
20	55	70	-1
23	-71	112	-12
12 -19 l			
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13	356	308	35
16	49	17	2
19	-80	120	-17
22	-156	55	-21
25	160	102	9
12 -18 l			
3	185	125	21
6	537	529	6
9	831	807	18
12	874	871	3
15	558	596	-27
18	447	411	20
21	219	265	-16
24	170	139	6
12 -17 l			
2	396	424	-21
5	800	809	-7
8	176	112	21
11	234	252	-13
14	654	692	-29
17	-129	7	-17
20	107	179	-17
23	65	70	0
26	100	62	4
12 -16 l			
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7	140	93	14
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13	649	662	-10
16	431	435	-2
19	379	387	-4
22	328	328	0
25	75	188	-21
12 -15 l			
3	175	200	-12
6	289	252	23
9	153	172	-11
12	245	285	-22
15	247	296	-26
18	216	232	-6
21	168	176	-2
24	-32	48	-2
27	-118	59	-12
12 -14 l			
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8	398	405	-7
11	302	347	-31
14	360	342	11
17	533	533	0
20	414	427	-7
23	326	328	0
26	336	284	20
29	230	173	14
12 -13 l			
1	1364	1375	-7
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7	606	600	7
10	657	686	-26
13	787	836	-41
16	830	807	17
19	346	370	-14
22	-79	128	-22
25	164	145	4
28	-89	37	-6
12 -12 l			
3	1381	1382	0
6	1405	1394	9
9	753	730	20
12	1042	1073	-25

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15	861	830	24
18	753	754	0
21	406	356	29
24	323	283	17
27	306	259	17

12 -11 l

2	283	282	0
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8	45	111	-17
11	1053	1114	-49
14	348	302	30
17	104	104	0
20	229	248	-8
23	32	103	-9
26	245	230	4
29	-35	4	0

12 -10 l

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7	1330	1363	-27
10	525	520	5
13	153	110	15
16	393	334	39
19	663	642	15
22	592	584	5
25	141	139	0
28	-64	120	-14

12 -9 l

3	91	16	14
6	1330	1285	31
9	487	494	-6
12	194	154	18
15	120	108	3
18	-79	2	-7
21	389	376	8
24	278	245	14
27	153	113	8
30	-86	98	-12

12 -8 l

2	2234	2163	34
5	1872	1847	14
8	1163	1183	-18
11	259	285	-18
14	366	385	-14
17	206	188	7
20	458	384	47
23	336	294	21
26	301	204	34
29	195	162	8

12 -7 l

1	1740	1675	38
4	1651	1579	44
7	-95	79	-28
10	553	598	-44
13	365	352	10
16	-61	48	-8
19	372	419	-33
22	322	302	10
25	417	415	1
28	155	20	17
31	118	66	6

12 -6 l

3	495	539	-46
6	1930	1981	-28
9	1483	1460	17
12	1459	1445	8
15	433	418	11
18	-77	9	-7
21	431	386	28
24	587	544	28
27	299	246	19
30	165	126	7

12 -5 l

2	437	454	-17
5	110	110	0
8	513	503	9
11	617	620	-2
14	433	438	-3
17	264	265	0
20	240	234	3
23	-49	69	-7
26	88	85	0
29	-85	66	-8

12 -4 l

1	1331	1386	-41
4	942	953	-9
7	1536	1513	14
10	2069	2067	1
13	1564	1544	12
16	716	664	42
19	158	54	24
22	346	306	21
25	222	231	-3
28	248	254	-2

12 -3 l

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3	1080	1111	-26
6	790	789	0
9	1226	1220	4
12	1065	1078	-10
15	160	158	1
18	292	353	-39
21	161	116	12
24	84	31	5
27	186	180	1
30	80	99	-2

12 -2 l

2	460	467	-6
5	473	480	-6
8	1414	1434	-13
11	1716	1758	-28
14	303	279	15
17	184	184	0
20	626	580	33
23	115	163	-13
26	280	229	18
29	158	155	0

12 -1 l

1	271	328	-48
4	218	275	-41
7	784	784	0
10	382	391	-6
13	280	280	0
16	457	455	1
19	250	255	-2
22	-113	19	-13
25	56	86	-3
28	121	40	9

12 0 l

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3	828	836	-9
6	427	459	-41
9	1312	1331	-15
12	1241	1272	-29
15	880	910	-30
18	541	521	20
21	387	379	6
24	132	99	8
27	160	165	-1

12 1 l

2	185	189	-2
5	357	345	10
8	738	747	-7
11	108	39	13
14	351	404	-37
17	151	229	-30
20	103	173	-18
23	55	171	-23
26	71	74	0
29	-116	82	-14

12 2 l

1	1370	1374	-3
4	993	973	16
7	1542	1553	-7
10	191	162	13
13	976	978	-1
16	980	964	11
19	499	474	16
22	-81	36	-7
25	-27	151	-18
28	172	159	2

12 3 l

0	237	231	3
3	910	920	-8
6	422	389	25
9	66	17	5
12	187	136	18
15	401	406	-3
18	274	294	-9
21	146	155	-2
24	72	65	0
27	202	111	18

12 4 l

2	837	839	-1
5	872	906	-29
8	332	297	22
11	117	8	16
14	727	697	29
17	750	721	20
20	302	337	-17
23	225	267	-14
26	275	255	6

12 5 l

1	564	617	-47
4	341	359	-13
7	777	811	-29
10	97	117	-4
13	667	663	3
16	192	230	-14
19	-118	44	-15
22	-172	20	-24
25	-34	84	-5

12 6 l

0	755	759	-2
3	909	932	-17
6	796	801	-3
9	256	175	35
12	818	800	13
15	373	328	34
18	430	429	0
21	292	314	-8
24	77	185	-20

12 7 l

2	-119	92	-28
5	141	51	19
8	-95	22	-11
11	487	497	-7
14	137	89	10
17	62	110	-7
20	218	233	-4
23	16	10	0

12 8 l

1	1077	1049	19
4	759	740	14
7	641	655	-10
10	711	706	3
13	589	594	-4
16	336	313	15
19	292	251	15
22	184	207	-5

12 9 l

0	188	124	19
3	279	293	-7
6	102	101	0
9	479	439	25
12	187	126	17
15	136	65	11
18	137	88	8
21	180	161	4

12 10 l

2	515	510	3
5	768	717	35
8	442	420	13
11	548	516	20
14	354	327	12
17	365	344	13
20	84	171	-15

12 11 l

1	-94	130	-25
4	223	169	18
7	296	294	0
10	191	152	10
13	214	242	-9
16	125	85	6
19	-167	68	-23

12 12 l

0	-71	57	-7
3	204	152	-16
6	472	450	12
9	428	448	-10
12	291	266	9
15	190	187	0
18	66	132	-12

13 -25 l

2	-35	163	-22
5	208	220	-3
8	269	258	4
11	201	215	-4
14	53	64	0

13 -24 l

1	-89	109	-18
4	80	78	0
7	194	164	8
10	-134	55	-17
13	-92	51	-8
16	-62	59	-5

13 -23 l

3	-127	22	-16
6	217	202	5
9	163	3	21
12	262	254	2
15	206	199	1
18	-53	95	-8

13 -22 l

2	218	281	-29
5	311	297	7
8	-40	65	-5
11	181	97	20
14	298	250	18
17	-150	149	-34
20	-137	34	-14

13 -21 l

1	-188	83	-48
4	147	205	-20
7	82	53	3
10	340	337	1
13	192	112	21
16	223	236	-4
19	-154	32	-19
22	92	109	-2

13 -20 l

3	550	540	7
6	327	329	-1
9	377	402	-15
12	288	267	9
15	259	311	-24
18	-152	11	-19
21	-59	73	-6
24	136	91	6

13 -19 l

2	409	443	-24
5	482	499	-12
8	294	245	24
11	-78	24	-7
14	137	178	-12
17	41	159	-21
20	-146	10	-17
23	-154	7	-17

13 -18 l

1	162	129	11
4	352	362	-6
7	273	253	10
10	151	185	-12
13	406	402	2
16	-22	4	0
19	-96	42	-9
22	6	100	-7
25	185	106	15

13 -17 l

3	260	226	18
6	248	204	21
9	97	111	-3
12	-133	44	-22
15	198	209	-4
18	-136	110	-30
21	-125	43	-14
24	-150	23	-17

13 -16 l

2	724	697	22
5	493	470	18
8	117	91	6
11	354	373	-12
14	-15	72	-6
17	-104	54	-14
20	-70	50	-7
23	-38	52	-3
26	188	163	5

13 -15 l

1	592	615	-21
4	422	418	2
7	440	456	-13
10	143	176	-12
13	131	132	0
16	199	281	-39
19	217	261	-18
22	148	147	0
25	151	57	14
28	-111	95	-14

13 -14 l

3	268	258	6
6	512	489	19
9	622	594	23
12	225	159	28
15	567	556	8
18	316	306	5
21	-93	21	-8
24	-26	136	-15
27	116	131	-2

13 -13 l

2	376	374	2
5	143	161	-10
8	144	149	-2
11	874	874	0
14	782	788	-4
17	94	17	9
20	106	103	0
23	248	217	10
26	170	92	14
29	-143	27	-14

13 -12 l

1	857	802	47
4	816	794	19
7	527	558	-38
10	821	842	-18
13	784	800	-12
16	682	694	-9
19	-64	2	-4
22	90	106	-2
25	160	130	6
28	100	105	0

13 -11 l

3	680	705	-24
6	106	113	-2
9	304	274	20
12	626	569	47
15	557	594	-30
18	-75	62	-10
21	121	156	-9
24	-111	13	-10
27	151	49	14

13 -10 l

2	103	8	18
5	518	555	-36
8	545	553	-10
11	681	635	39
14	78	95	-3
17	150	145	1
20	226	180	17
23	-107	61	-14
26	172	124	10
29	123	28	9

13 -9 l

1	1258	1236	16
4	819	799	17
7	174	129	20
10	542	525	15
13	144	173	-12
16	272	340	-43
19	142	41	19
22	131	76	11
25	74	21	4
28	137	189	-12

13 -8 l

3	270	306	-29
6	579	561	17
9	-93	29	-21
12	197	225	-15
15	473	487	-11
18	-98	34	-13
21	-89	14	-8
24	-111	7	-12
27	79	40	3
30	230	142	21

13 -7 l

2	189	190	0
5	1893	1859	19
8	709	702	6
11	58	34	3
14	320	354	-25
17	635	641	-4
20	517	474	29
23	145	90	11
26	118	39	9
29	-72	95	-10

13 -6 l

1	872	849	20
4	815	825	-9
7	745	734	10
10	631	637	-7
13	1024	1064	-32
16	217	207	4
19	212	178	14
22	302	271	15
25	-89	52	-9
28	-99	59	-10

13 -5 l

0	177	190	-7
3	417	416	0
6	128	52	21
9	146	126	7
12	421	392	23
15	461	437	18
18	577	578	0
21	386	372	8
24	139	181	-12
27	142	74	11
30	191	74	20

13 -4 l

2	435	421	12
5	503	462	36
8	595	566	25
11	781	811	-33
14	946	962	-12
17	48	53	0
20	228	193	14
23	-14	122	-14
26	201	137	16
29	-138	22	-14

13 -3 l

1	577	534	40
4	-102	7	-18
7	359	337	16
10	801	799	1
13	-71	14	-7
16	-95	22	-12
19	215	177	15
22	78	111	-6
25	137	72	10
28	-86	21	-5

13 -2 l

0	146	153	-3
3	139	196	-29
6	362	349	9
9	391	429	-30
12	80	24	11
15	70	145	-19
18	152	148	1
21	312	354	-23
24	164	149	4
27	-107	70	-12

13 -1 l

2	835	839	-4
5	374	390	-13
8	583	593	-8
11	796	781	12
14	237	242	-2
17	44	42	0
20	265	212	23
23	152	7	21
26	59	74	-1
29	205	163	10

13 0 l

1	879	881	-1
4	774	757	18
7	618	623	-5
10	128	140	-6
13	299	278	21
16	-50	16	-4
19	325	362	-29
22	-67	21	-6
25	-65	64	-9
28	113	107	1

13 1 l

0	876	866	8
3	352	323	21
6	181	74	37
9	1139	1162	-17
12	391	392	0
15	254	272	-9
18	-141	122	-37
21	-153	6	-22
24	-139	106	-24

Tetra(pentafluorophenyl)porphinato Copper(II)

27	-129	66	-15
13	2	l	
2	227	204	12
5	31	85	-9
8	619	650	-27
11	604	599	3
14	440	422	17
17	307	309	-1
20	-109	83	-18
23	-103	92	-15
26	139	124	2
13	3	l	
1	-52	71	-11
4	138	133	1
7	100	97	0
10	218	247	-14
13	209	155	20
16	250	269	-8
19	36	156	-21
22	189	98	19
25	66	52	1
13	4	l	
0	145	213	-30
3	199	257	-31
6	324	318	3
9	440	451	-7
12	232	246	-6
15	103	108	-1
18	-75	13	-5
21	273	215	19
24	151	174	-5
13	5	l	
2	290	305	-9
5	278	282	-2
8	554	575	-16
11	182	182	0
14	367	368	-1
17	149	182	-9
20	140	163	-5
23	-156	27	-19
26	127	31	9
13	6	l	
1	192	233	-19
4	542	513	21
7	114	4	14
10	157	108	13
13	223	167	20
16	307	289	12
19	98	62	4
22	98	49	5
25	-81	11	-4
13	7	l	
0	536	515	15
3	184	109	23
6	521	544	-16
9	244	280	-17
12	58	2	3
15	117	54	10
18	198	149	12
21	389	387	1
24	99	100	0
13	8	l	
2	375	346	17
5	186	153	10
8	113	93	4
11	205	230	-9
14	129	102	5
17	32	73	-4
20	135	56	10
13	9	l	
1	9	94	-9
4	223	242	-8
7	177	153	7
10	35	30	0
13	-108	53	-12
16	57	109	-6
19	-83	80	-9
13	10	l	
0	198	185	4
3	116	160	-11
6	154	102	12
9	168	99	15
12	87	86	0
15	87	116	-4
18	33	9	1
13	11	l	
2	-46	57	-4
5	102	46	6
8	-34	64	-4
11	160	130	6
14	104	0	8
17	152	86	10
13	12	l	
1	236	239	-1
4	265	209	18
7	148	36	15
10	82	99	-2
13	137	7	13
16	-123	5	-10
13	13	l	
0	190	270	-26
3	-157	39	-21
6	66	53	1
9	149	88	10
12	125	32	10
14	-27	l	
2	187	172	3
5	277	234	14
8	115	33	8
11	-122	107	-18
14	-26	l	
1	373	309	27
4	223	206	5
7	343	325	7
10	92	120	-4
13	91	141	-8
14	-25	l	
3	224	209	4
6	65	87	-2
9	56	122	-9
12	138	60	11
15	51	4	1
14	-24	l	
2	354	315	19
5	458	416	22
8	392	382	4
11	189	144	10
14	146	167	-4
17	113	140	-6
14	-23	l	
1	254	254	0
4	140	188	-14
7	204	152	16
10	-156	2	-21
13	-103	18	-8
16	171	126	13
19	99	64	3
14	-22	l	
3	562	540	14
6	422	415	4
9	334	311	11
12	543	527	9
15	346	355	-6
18	-189	72	-31
21	138	188	-10
14	-21	l	
2	-171	62	-37
5	153	160	-1
8	23	94	-8
11	198	156	13
14	161	57	25
17	-37	94	-7
20	-149	4	-16
14	-20	l	
1	667	667	0
4	830	819	8
7	527	484	29
10	346	344	1
13	635	608	24
16	221	220	0
19	104	180	-16
22	-143	78	-19
14	-19	l	
3	454	455	0
6	319	335	-10
9	50	63	-1
12	188	179	4
15	-91	100	-17
18	-39	9	-1
21	-146	15	-16
24	-104	137	-20
14	-18	l	
2	703	665	29
5	699	656	33
8	784	762	16
11	593	579	14
14	351	356	-3
17	127	238	-36
20	14	127	-12
23	193	159	8
14	-17	l	
1	563	552	8
4	565	536	23
7	696	661	27
10	598	624	-27
13	150	213	-23
16	-83	140	-27
19	149	156	-2
22	-154	19	-19
25	138	101	6
14	-16	l	
3	1238	1231	5
6	1302	1289	9
9	789	801	-12
12	711	698	10
15	701	682	14
18	313	361	-26
21	10	55	-2
24	199	155	11
27	196	157	8
14	-15	l	
2	651	620	26
5	345	335	6
8	135	181	-25
11	271	254	8
14	238	124	41
17	-74	33	-6
20	77	17	5
23	-182	23	-28
26	100	40	6
14	-14	l	
1	971	952	18
4	593	578	17
7	359	339	23
10	323	291	20
13	927	907	15
16	1046	1040	4
19	383	368	8
22	201	196	1
25	238	221	5
28	72	117	-5
14	-13	l	
3	545	529	13
6	-74	25	-8
9	110	128	-5
12	333	287	28
15	278	165	49
18	304	356	-30
21	47	134	-15
24	236	138	26
27	-97	12	-7
14	-12	l	
2	1525	1532	-5
5	1428	1403	16
8	714	694	23
11	464	454	8
14	1354	1376	-14
17	474	428	30
20	261	259	0
23	319	299	9
26	231	207	7
29	62	88	-2
14	-11	l	
1	415	419	-3
4	1168	1189	-15
7	228	242	-8
10	561	583	-19
13	275	291	-10
16	431	434	-1
19	299	336	-21
22	139	120	4
25	119	173	-12
28	111	143	-5

14 -10 l

3	1315	1300	10
6	530	507	20
9	256	273	-15
12	843	850	-5
15	765	709	43
18	727	695	24
21	481	446	22
24	250	222	10
27	-66	11	-3

14 -9 l

2	400	420	-18
5	279	225	35
8	502	469	28
11	178	109	25
14	247	300	-32
17	24	146	-24
20	-50	24	-3
23	-132	78	-23
26	-92	19	-7
29	-106	18	-8

14 -8 l

1	1524	1494	19
4	1488	1427	39
7	1590	1602	-7
10	849	869	-22
13	206	138	28
16	620	587	26
19	598	591	5
22	203	190	4
25	297	239	21
28	250	168	22

14 -7 l

3	781	773	7
6	1320	1302	12
9	90	56	7
12	63	171	-35
15	387	391	-2
18	239	195	19
21	151	99	12
24	223	137	23
27	-21	9	0

14 -6 l

2	844	856	-10
5	1113	1144	-24
8	1506	1493	8
11	367	345	22
14	1378	1377	0
17	590	552	28
20	448	472	-16
23	349	308	20
26	107	84	3
29	190	147	9

14 -5 l

1	402	410	-6
4	912	870	35
7	906	917	-9
10	763	831	-59
13	677	662	12
16	353	312	25
19	232	221	4
22	119	95	4
25	100	124	-4
28	168	143	5

14 -4 l

0	20	82	-10
3	756	782	-23
6	1668	1656	7
9	968	922	35
12	1206	1203	2
15	455	476	-15
18	803	761	31
21	436	403	20
24	324	340	-7
27	254	197	17

14 -3 l

2	340	336	3
5	1498	1522	-15
8	-147	95	-45
11	120	53	14
14	384	342	27
17	180	177	1
20	114	113	0
23	182	130	13
26	157	201	-11
29	-126	24	-11

14 -2 l

1	1544	1524	12
4	1836	1847	-6
7	959	989	-24
10	570	536	27
13	464	457	7
16	365	366	0
19	474	456	12
22	534	494	25
25	412	343	32
28	117	76	5

14 -1 l

0	524	541	-14
3	-81	57	-14
6	389	296	62
9	288	317	-18
12	436	391	31
15	227	216	4
18	219	160	21
21	161	110	12
24	401	365	17
27	142	96	7

14 0 l

2	761	774	-14
5	1316	1333	-14
8	417	385	32
11	1385	1396	-9
14	1161	1156	4
17	418	413	4
20	306	278	19
23	298	286	6
26	128	129	0

14 1 l

1	245	208	20
4	851	862	-9
7	483	499	-12
10	688	677	9
13	339	301	22
16	419	455	-23
19	-117	7	-13
22	116	154	-7
25	145	178	-7

14 2 l

0	1369	1401	-21
3	1163	1172	-6
6	411	407	3
9	296	277	11
12	318	257	33
15	702	697	5
18	461	492	-20
21	257	286	-11
24	240	266	-8
27	276	219	16

14 3 l

2	791	825	-28
5	337	359	-15
8	718	741	-18
11	460	486	-18
14	746	758	-9
17	329	330	0
20	-107	3	-9
23	-159	80	-24
26	187	132	11

14 4 l

1	570	572	-2
4	993	965	20
7	343	293	29
10	494	449	31
13	516	464	35
16	538	513	22
19	391	430	-19
22	177	171	1
25	335	252	28

14 5 l

0	524	527	-2
3	627	614	9
6	97	48	7
9	-85	47	-10
12	-25	72	-6
15	133	89	9
18	161	115	9
21	54	146	-13
24	87	97	-1

14 6 l

2	754	760	-5
5	701	706	-3
8	699	673	19
11	365	335	16
14	353	322	16
17	374	380	-3
20	470	444	13
23	177	194	-4

14 7 l

1	154	138	4
4	386	384	0
7	302	304	-1
10	184	181	0
13	23	120	-13
16	139	187	-12
19	131	48	10
22	-87	22	-5

14 8 l

0	365	352	7
3	558	569	-7
6	638	637	0
9	574	578	-2
12	304	266	15
15	234	186	14
18	203	161	15
21	149	183	-7

14 9 l

2	194	194	0
5	293	334	-21
8	370	366	2
11	219	222	-1
14	111	52	7
17	178	107	14
20	-45	107	-9

14 10 l

1	236	182	18
4	429	419	5
7	457	471	-7
10	301	292	3
13	345	304	17
16	97	112	-2

14 11 l

0	171	224	-15
3	105	48	6
6	225	254	-10
9	182	164	4
12	288	210	25
15	253	113	33

14 12 l

2	256	252	1
5	384	340	19
8	349	309	16
11	340	281	22
14	194	169	6

14 13 l

1	115	110	0
4	-84	14	-5
7	89	7	5
10	189	156	7

14 14 l

0	238	254	-4
3	175	192	-4
6	227	176	13

15 -28 l

1	53	126	-9
4	207	112	19

15 -27 l

3	-32	80	-5
6	100	81	2
9	236	221	4

15 -26 l

2	106	24	8
5	-109	64	-12
8	47	101	-5
11	238	118	28
14	-83	73	-8

15 -25 l

1	283	297	-5
4	82	1	5
7	176	184	-2
10	149	99	9
13	88	41	4
16	62	48	1

15 -24 l

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26	174	107	12
17 -8 l			
1	347	390	-32
4	466	510	-37
7	581	583	-1
10	188	191	-1
13	-65	81	-17
16	203	217	-5
19	233	202	11
22	36	55	-1
25	139	42	12
17 -7 l			
0	219	243	-13
3	236	275	-23
6	167	257	-45
9	369	396	-19
12	92	183	-27
15	284	254	15
18	221	214	3
21	155	81	14
24	126	120	0
27	-96	64	-9
17 -6 l			
2	894	874	15
5	26	34	0
8	1081	1128	-35
11	-89	84	-17
14	193	224	-18
17	-48	57	-5
20	-88	12	-7
23	-164	7	-22
26	173	68	17
17 -5 l			
1	84	58	4
4	576	579	-2
7	486	464	16
10	143	208	-24
13	343	399	-35
16	250	238	5
19	-78	7	-6
22	128	57	10
25	100	89	1
17 -4 l			
0	-58	25	-5
3	290	295	-3
6	698	679	14
9	496	487	6
12	-114	97	-25
15	-67	138	-35
18	240	270	-13
21	-97	96	-15
24	208	140	16
17 -3 l			
2	316	249	37
5	705	680	19
8	174	264	-41
11	233	281	-23
14	125	205	-26
17	80	70	1
20	188	108	18
23	119	9	10
26	141	65	10
17 -2 l			
1	1259	1279	-13
4	387	338	30
7	236	211	10
10	143	198	-19
13	35	130	-15
16	223	221	1
19	294	247	18
22	245	188	17
25	148	59	12
17 -1 l			
0	494	507	-10
3	291	246	22
6	367	411	-29
9	273	326	-28
12	-46	130	-19
15	79	84	0
18	-80	14	-6
21	132	54	11
24	80	129	-7
17 0 l			
2	570	600	-31
5	124	124	0
8	-9	122	-23
11	335	374	-32
14	-70	66	-13
17	62	145	-25
20	256	239	8
23	33	78	-5
17 1 l			
1	108	31	12
4	61	151	-21
7	-106	87	-21
10	224	177	18
13	131	125	1
16	116	44	9
19	119	106	2
22	-197	26	-29
17 2 l			
0	-81	108	-20
3	-117	151	-41
6	130	129	0
9	515	503	8
12	426	373	31
15	119	111	1
18	-36	6	-1
21	238	189	13
17 3 l			
2	84	132	-10
5	-84	5	-7
8	168	88	19
11	226	155	23
14	16	78	-4
17	144	167	-5
20	152	33	15
17 4 l			
1	38	3	1
4	220	231	-4
7	211	202	3
10	271	245	11
13	170	103	14
16	145	137	1
19	207	144	21
17 5 l			
0	192	75	28
3	454	459	-3
6	145	201	-17
9	103	9	9
12	-34	38	-2
15	-107	4	-9
18	23	16	0
17 6 l			
2	158	89	15
5	-96	44	-9
8	351	321	13
11	111	122	-1
14	115	129	-2
17	105	61	5
17 7 l			
1	199	123	18
4	275	202	25
7	99	55	5
10	-16	98	-7
13	85	85	0
16	167	69	15
17 8 l			
0	165	95	13
3	145	103	7
6	192	109	18
9	146	178	-7
12	125	118	1
15	156	39	15
17 9 l			
2	152	184	-7
5	44	115	-8
8	144	119	4
11	-71	32	-4
17 10 l			
1	67	54	1
4	-103	38	-8
7	74	48	2
10	202	187	3

17 11 l

0	95	58	3
3	-49	6	-1

18 -28 l

1	373	319	21
4	157	138	3

18 -27 l

3	60	120	-7
6	17	3	0
9	113	69	5

18 -26 l

2	315	228	30
5	113	128	-2
8	386	299	34
11	294	190	31

18 -25 l

1	-56	95	-9
4	-99	59	-10
7	-77	39	-5
10	81	27	4
13	123	30	9

18 -24 l

3	317	323	-2
6	226	226	0
9	135	151	-3
12	170	203	-8
15	-108	110	-24

18 -23 l

2	133	36	13
5	-155	20	-21
8	-133	1	-14
11	-93	21	-7
14	-106	31	-13
17	125	49	9

18 -22 l

1	547	572	-17
4	505	498	4
7	349	328	10
10	292	254	15
13	50	162	-26
16	124	131	-1
19	-111	69	-11

18 -21 l

3	145	103	9
6	269	265	1
9	260	253	2
12	-93	53	-13
15	-136	94	-22
18	-158	8	-19

18 -20 l

2	532	489	28
5	565	551	10
8	527	470	36
11	424	431	-6
14	178	173	1
17	60	120	-8
20	179	124	11

18 -19 l

1	108	222	-38
4	670	662	6
7	154	100	13
10	47	66	-3
13	-115	108	-24
16	71	133	-10
19	40	96	-5
22	162	23	17

18 -18 l

3	438	403	31
6	509	521	-10
9	561	562	-2
12	277	265	5
15	299	291	3
18	440	426	7
21	392	338	23

18 -17 l

2	-62	18	-4
5	433	426	4
8	527	517	7
11	86	131	-10
14	-142	69	-25
17	62	98	-4
20	125	26	11
23	-114	6	-9

18 -16 l

1	783	790	-5
4	1065	1055	7
7	745	727	13
10	627	618	8
13	323	332	-4
16	322	333	-5
19	331	300	12
22	146	79	10

18 -15 l

3	-117	86	-25
6	-114	42	-17
9	330	297	18
12	253	243	4
15	223	255	-14
18	-39	73	-5
21	287	247	14
24	61	53	0

18 -14 l

2	789	760	22
5	-158	59	-35
8	319	320	0
11	839	845	-5
14	563	528	24
17	231	201	11
20	281	258	9
23	199	176	6

18 -13 l

1	427	430	-1
4	-88	97	-20
7	338	383	-29
10	687	673	10
13	412	404	5
16	-104	117	-25
19	151	133	4
22	180	152	6
25	-96	44	-8

18 -12 l

3	820	861	-33
6	470	465	3
9	825	783	31
12	610	603	7
15	402	394	4
18	349	302	24
21	401	417	-8
24	266	250	5

18 -11 l

2	523	534	-8
5	348	426	-57
8	215	265	-25
11	172	227	-22
14	404	414	-7
17	96	107	-2
20	60	100	-5
23	130	57	10
26	90	14	5

18 -10 l

1	1162	1150	8
4	352	284	41
7	707	735	-23
10	445	389	36
13	882	868	13
16	419	444	-16
19	332	309	11
22	233	201	9
25	247	185	17

18 -9 l

3	230	164	28
6	495	448	33
9	516	539	-17
12	-134	59	-23
15	251	215	15
18	47	48	0
21	132	143	-2
24	45	59	-1

18 -8 l

2	966	935	24
5	531	515	12
8	222	179	18
11	48	171	-29
14	358	362	-3
17	569	565	3
20	279	275	1
23	127	136	-1
26	208	174	8

18 -7 l

1	727	712	12
4	135	139	-1
7	167	280	-54
10	74	119	-9
13	-173	11	-33
16	111	119	-1
19	299	317	-8
22	27	54	-1
25	-131	4	-12

18 -6 l

0	665	674	-7
3	551	570	-15
6	942	899	32
9	538	547	-6
12	459	482	-15
15	281	270	7
18	444	431	7
21	180	214	-10
24	163	163	0

18 -5 l

2	561	562	-1
5	232	148	33
8	137	136	0
11	272	261	5
14	-131	58	-21
17	104	68	5
20	68	115	-7
23	-129	41	-14
26	46	48	0

18 -4 l

1	1410	1380	19
4	1436	1403	20
7	725	718	5
10	551	576	-18
13	370	374	-2
16	368	361	5
19	232	239	-2
22	339	303	14
25	204	173	7

18 -3 l

0	540	489	37
3	274	158	48
6	170	126	13
9	88	137	-11
12	60	148	-18
15	105	197	-25
18	-128	9	-14
21	258	231	9
24	-76	76	-8

18 -2 l

2	927	918	7
5	778	810	-25
8	280	277	1
11	228	224	1
14	448	466	-11
17	215	203	5
20	385	343	19
23	121	176	-11

18 -1 l

1	306	294	6
4	407	425	-11
7	61	194	-34
10	117	230	-38
13	290	327	-18
16	207	239	-11
19	268	178	28
22	143	1	14

18 0 l

0	761	767	-5
3	501	503	-2
6	261	309	-35
9	615	608	7
12	401	392	7
15	153	159	-2
18	255	231	14
21	154	169	-4

18 1 l

2	242	240	1
5	-111	21	-13
8	426	441	-10
11	202	162	13

14	106	15	9
17	79	97	-2
20	204	92	22
18 2 1			
1	498	460	24
4	130	70	11
7	537	530	4
10	824	804	13
13	467	468	0
16	159	155	0
19	341	327	7
18 3 1			
0	530	522	5
3	146	112	8
6	-56	39	-4
9	391	374	9
12	225	159	19
15	-134	9	-14
18	223	118	24
18 4 1			
2	559	572	-8
5	103	78	4
8	391	346	21
11	448	437	6
14	221	211	3
17	229	219	2
18 5 1			
1	194	193	0
4	90	24	6
7	-70	29	-4
10	173	176	0
13	166	175	-2
16	111	74	4
18 6 1			
0	489	446	23
3	363	310	23
6	399	372	12
9	215	153	16
12	269	212	18
15	254	221	10
18 7 1			
2	232	70	35
5	202	175	7
8	121	101	3
11	58	0	2
14	269	184	24
18 8 1			
1	407	407	0
4	498	455	21
7	417	387	14
10	262	189	20
18 9 1			
0	123	112	1
3	350	307	16
6	247	257	-3
9	117	39	8
18 10 1			
2	191	249	-16
19 -27 1			

1	160	97	10
4	145	45	12
7	-77	105	-11
19 -26 1			
3	-46	71	-5
6	-41	75	-5
9	-63	65	-5
19 -25 1			
2	191	203	-3
5	207	223	-5
8	125	130	0
11	229	142	21
14	153	22	15
19 -24 1			
1	262	222	13
4	236	227	2
7	-97	46	-9
10	116	23	9
13	151	25	15
19 -23 1			
3	207	221	-4
6	-117	68	-15
9	-121	17	-12
12	138	135	0
15	-36	90	-6
19 -22 1			
2	149	105	9
5	60	160	-18
8	197	151	12
11	140	73	11
14	-94	23	-7
17	103	70	3
19 -21 1			
1	350	311	19
4	376	387	-6
7	34	63	-2
10	40	27	0
13	104	133	-5
16	97	108	-1
19	-98	38	-7
19 -20 1			
3	113	114	0
6	353	278	36
9	352	295	28
12	-118	67	-16
15	-39	49	-3
18	154	38	15
21	231	217	3
19 -19 1			
2	114	102	3
5	11	92	-11
8	223	235	-6
11	381	376	3
14	-177	14	-27
17	158	123	7
20	170	168	0
19 -18 1			
1	517	538	-15
4	106	93	2

7	55	105	-8
10	369	367	1
13	94	93	0
16	136	87	8
19	353	292	24
22	239	184	14
19 -17 1			
3	156	102	14
6	121	88	7
9	108	102	1
12	-106	110	-23
15	-74	4	-4
18	173	194	-5
21	122	21	10
19 -16 1			
2	481	469	8
5	535	555	-14
8	43	112	-11
11	-131	61	-31
14	196	197	0
17	-76	104	-14
20	-70	1	-3
23	-104	11	-7
19 -15 1			
1	235	256	-10
4	297	331	-20
7	404	409	-3
10	241	281	-19
13	-138	26	-20
16	106	73	5
19	-92	42	-8
22	136	84	8
19 -14 1			
3	392	429	-25
6	-136	76	-28
9	188	116	21
12	311	288	16
15	-77	89	-13
18	-87	77	-11
21	-42	88	-7
24	100	33	6
19 -13 1			
2	-112	27	-16
5	440	432	5
8	213	232	-8
11	248	241	3
14	78	83	0
17	148	173	-7
20	-88	16	-6
23	174	106	13
19 -12 1			
1	781	762	14
4	79	148	-17
7	691	720	-23
10	343	347	-2
13	-151	105	-52
16	155	146	2
19	308	244	25
22	196	245	-15
25	102	19	6
19 -11 1			
3	333	321	7
6	173	264	-42
9	225	285	-29

12	-57	2	-3
15	-28	9	0
18	145	10	17
21	-113	65	-13
24	116	96	3
19 -10 1			
2	173	271	-48
5	835	854	-14
8	-151	48	-29
11	177	277	-44
14	56	42	1
17	-39	24	-2
20	170	154	4
23	-27	57	-3
19 -9 1			
1	233	287	-29
4	382	401	-13
7	-163	71	-37
10	94	175	-22
13	-145	8	-22
16	177	163	4
19	41	58	-1
22	-50	35	-2
25	80	16	4
19 -8 1			
0	222	201	9
3	-107	143	-38
6	140	230	-35
9	220	244	-10
12	198	235	-14
15	127	109	5
18	108	96	2
21	-113	2	-10
24	-54	27	-2
19 -7 1			
2	498	487	8
5	-72	109	-19
8	404	434	-19
11	-114	63	-18
14	139	242	-36
17	169	172	0
20	82	47	3
23	153	112	7
19 -6 1			
1	142	141	0
4	344	344	0
7	604	630	-19
10	308	334	-14
13	-137	115	-32
16	115	170	-20
19	174	131	10
22	-116	72	-14
25	155	138	3
19 -5 1			
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3	174	74	26
6	257	154	39
9	66	46	2
12	-98	145	-31
15	-132	28	-17
18	108	134	-5
21	166	166	0
24	-68	82	-8
19 -4 1			

2	566	559	5
5	826	769	41
8	171	205	-12
11	33	139	-18
14	198	255	-22
17	-126	64	-24
20	115	75	5
23	-82	40	-6
19 -3 1			
1	343	337	3
4	672	631	29
7	141	159	-5
10	-165	90	-37
13	-105	179	-41
16	-202	67	-39
19	173	146	6
22	139	10	13
19 -2 1			
0	51	0	2
3	524	529	-3
6	271	248	10
9	-129	96	-26
12	318	326	-4
15	-81	88	-12
18	224	202	9
21	72	3	3
19 -1 1			
2	-22	7	0
5	255	302	-23
8	291	287	2
11	43	119	-11
14	-194	21	-33
17	126	199	-17
20	80	15	4
19 0 1			
1	152	127	9
4	-83	106	-26
7	-81	74	-17
10	184	185	0
13	239	267	-15
16	148	167	-6
19	190	186	1
19 1 1			
0	230	251	-9
3	159	152	1
6	301	226	33
9	228	105	35
12	197	160	10
15	-3	118	-11
18	136	90	7
21	-131	87	-17
19 2 1			
2	83	109	-4
5	334	323	5
8	325	266	27
11	252	217	12
14	38	44	0
17	167	196	-7
20	140	113	6
19 3 1			
1	251	273	-9
4	191	206	-4
7	107	53	7
10	181	195	-3
13	218	207	3
16	-118	8	-10
19 4 1			
0	142	96	8
3	276	309	-14
6	75	17	4
9	35	22	0
12	186	98	18
15	63	90	-2
19 5 1			
2	207	209	0
5	383	347	16
8	81	33	4
11	159	92	12
14	132	77	8
19 6 1			
1	57	12	2
4	205	115	20
7	272	220	16
10	160	25	17
13	140	46	11
19 7 1			
0	139	81	9
3	199	152	11
6	76	111	-4
9	155	150	0
19 8 1			
2	86	115	-4
5	-17	12	0
8	-83	20	-5
19 9 1			
1	-38	45	-2
20 -27 1			
2	114	111	0
5	-162	52	-20
20 -26 1			
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4	257	193	18
7	258	278	-6
10	410	317	36
20 -25 1			
3	-102	88	-13
6	-94	0	-6
9	135	167	-6
12	295	241	17
20 -24 1			
2	495	506	-5
5	348	335	5
8	206	253	-15
11	311	253	20
14	381	338	24
20 -23 1			
1	53	4	2
4	-215	45	-41
7	29	116	-9
10	62	112	-6
13	166	134	9
16	257	169	23
20 -22 1			
3	402	395	3
6	234	237	0
9	304	255	18
12	220	245	-11
15	315	284	11
18	194	156	8
20 -21 1			
2	-104	17	-10
5	-106	53	-13
8	313	286	11
11	83	116	-7
14	-96	94	-14
17	80	79	0
20 -20 1			
1	405	420	-12
4	510	526	-14
7	648	604	39
10	281	239	27
13	138	141	0
16	146	162	-3
19	352	340	4
20 -19 1			
3	267	197	28
6	205	170	12
9	64	51	1
12	55	161	-19
15	225	228	0
18	229	119	26
21	135	5	12
20 -18 1			
2	472	476	-2
5	445	439	3
8	732	740	-5
11	498	467	26
14	283	281	0
17	382	299	35
20	482	425	27
20 -17 1			
1	-28	112	-14
4	164	154	3
7	277	262	7
10	95	0	8
13	118	162	-11
16	177	147	7
19	265	225	13
22	210	103	21
20 -16 1			
3	307	256	25
6	667	643	17
9	412	397	9
12	384	379	3
15	286	267	7
18	296	273	9
21	251	203	14
20 -15 1			
2	-75	75	-12
5	-68	52	-7
8	97	108	-2
11	-123	61	-19
14	-51	70	-7
17	77	181	-21
20	89	120	-4
23	110	35	7
20 -14 1			
1	271	210	27
4	523	500	16
7	642	632	7
10	543	547	-2
13	481	481	0
16	409	402	3
19	317	298	7
22	326	214	37
20 -13 1			
3	33	73	-4
6	115	160	-13
9	246	258	-5
12	209	270	-26
15	200	165	11
18	219	267	-17
21	84	112	-4
24	167	74	14
20 -12 1			
2	188	140	16
5	582	578	2
8	607	613	-4
11	432	405	16
14	331	317	9
17	397	360	18
20	494	448	24
23	224	207	4
20 -11 1			
1	350	348	1
4	295	271	12
7	235	212	9
10	-118	177	-47
13	389	422	-19
16	276	279	-1
19	109	77	4
22	111	120	-1
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Tetra(pentafluorophenyl)porphinato Copper(II) Page 24

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15	250	243	2
18	259	264	-2

24 -11 1

2	232	219	5
5	202	234	-10
8	157	206	-13
11	-161	5	-20
14	-83	31	-5
17	-150	72	-20

24 -10 1

1	545	548	-1
4	382	372	4
7	447	425	11
10	473	456	8
13	397	405	-3
16	-204	72	-35

24 -9 1

0	-64	61	-6
3	122	169	-10
6	234	245	-3
9	-106	133	-22
12	58	43	1
15	-109	47	-10
18	-146	33	-15

24 -8 1

2	245	266	-8
5	238	205	10
8	452	416	18
11	293	317	-9
14	46	144	-13
17	23	124	-10

24 -7 1

1	18	70	-3
4	-135	67	-18
7	-180	26	-27
10	-22	101	-8
13	247	273	-8
16	-182	18	-24

24 -6 1

0	452	438	7
3	241	256	-5
6	188	209	-6
9	366	383	-7
12	212	208	1
15	184	111	14

24 -5 1

2	201	218	-5
5	106	166	-12
8	83	153	-12
11	155	178	-5
14	-70	1	-3

24 -4 1

1	471	475	-2
4	143	162	-4
7	108	230	-29
10	259	244	4
13	255	227	8

24 -3 1

0	109	138	-5
3	-152	80	-22
6	-180	46	-26
9	135	171	-7
12	-162	77	-23

24 -2 1

2	142	193	-12
5	215	208	2
8	336	333	0
11	198	237	-10

24 -1 1

1	-49	28	-2
4	132	46	10
7	233	210	6
10	-133	43	-13

24 0 1

0	63	108	-7
3	293	302	-4
6	217	227	-3

24 1 1

2	205	165	9

25 -24 1

1	-59	49	-4
4	-90	43	-6

25 -23 1

3	-37	41	-2
6	133	181	-10

25 -22 1

2	189	174	3
5	140	45	12
8	-107	26	-8

25 -21 1

1	132	158	-5
4	114	99	2
7	-93	108	-14
10	106	96	1

25 -20 1

3	317	275	16
6	-85	85	-10
9	100	52	5
12	-39	90	-6

25 -19 1

2	-39	100	-8
5	-216	5	-38
8	64	56	0
11	25	55	-1
14	22	92	-5

25 -18 1

1	208	246	-12
4	-48	161	-21
7	-104	137	-22
10	156	118	7
13	310	299	4

25 -17 1

3	92	143	-9
6	-77	32	-5
9	-22	7	0
12	-70	91	-9
15	-116	78	-13

25 -16 1

2	191	191	0
5	130	211	-20
8	-66	148	-20
11	-143	127	-27
14	-166	34	-20

25 -15 1

1	177	216	-11
4	-89	68	-10
7	-97	15	-7
10	-148	82	-21
13	-88	68	-8
16	-157	71	-20

25 -14 1			
3	-167	28	-24
6	174	245	-22
9	34	118	-9
12	267	239	9
15	78	27	3
25 -13 1			
2	50	99	-5
5	-173	22	-25
8	-111	44	-11
11	61	26	2
14	-207	13	-32
25 -12 1			
1	81	115	-5
4	171	182	-2
7	-87	55	-8
10	231	231	0
13	350	337	5
16	265	175	23
25 -11 1			
0	104	151	-9
3	69	49	4
6	-28	53	-2
9	-164	1	-21
12	-61	76	-6
15	-97	46	-8
25 -10 1			
2	305	276	11
5	121	59	8
8	-126	48	-14
11	365	366	0
14	-144	126	-26
25 -9 1			
1	141	142	0
4	173	189	-4
7	261	157	29
10	124	135	-2
13	-106	57	-10
25 -8 1			
0	-129	54	-15
3	158	102	10
6	113	117	0
9	46	112	-7
12	-28	141	-14
15	-101	49	-8
25 -7 1			
2	-111	42	-11
5	250	247	0
8	179	139	8
11	-133	54	-15
14	-178	21	-22
25 -6 1			
1	317	291	10
4	-40	39	-2
7	52	70	-1
10	-111	9	-8
13	-132	38	-13
25 -5 1			

0	55	57	0
3	147	103	7
6	-69	104	-11
9	-97	135	-19
12	76	126	-6
25 -4 1			
2	176	169	1
5	-186	30	-26
8	-155	87	-22
11	-176	61	-24
25 -3 1			
1	-158	30	-19
4	180	138	8
7	-160	28	-19
10	-86	77	-9
25 -2 1			
0	-119	88	-15
3	15	4	0
6	102	157	-9
25 -1 1			
2	-114	38	-10
5	-128	14	-11
26 -23 1			
1	-53	121	-12
26 -22 1			
3	300	271	9
6	131	186	-11
26 -21 1			
2	99	20	6
5	-148	39	-17
8	-72	36	-4
26 -20 1			
1	317	297	7
4	206	190	4
7	-149	123	-27
10	165	125	7
26 -19 1			
3	-53	14	-2
6	-123	21	-11
9	-169	3	-21
26 -18 1			
2	245	288	-15
5	255	235	6
8	-107	120	-18
11	318	297	7
26 -17 1			
1	182	178	0
4	-130	11	-13
7	-163	22	-20
10	58	14	2
13	193	155	8
26 -16 1			
3	380	351	12
6	206	231	-7

9	89	101	-1
12	304	275	10
26 -15 1			
2	269	261	2
5	176	148	6
8	-182	42	-26
11	172	131	8
14	-126	45	-12
26 -14 1			
1	258	217	13
4	331	333	0
7	185	215	-8
10	310	303	2
13	255	254	0
26 -13 1			
3	438	396	19
6	-42	167	-21
9	-118	44	-11
12	181	209	-7
26 -12 1			
2	576	584	-4
5	328	354	-11
8	105	130	-4
11	318	288	11
14	327	321	2
26 -11 1			
1	236	163	20
4	149	110	7
7	-32	206	-31
10	62	130	-9
13	88	4	5
26 -10 1			
0	500	476	12
3	447	414	15
6	201	242	-12
9	340	329	4
12	308	296	4
26 -9 1			
2	62	144	-12
5	258	256	0
8	50	101	-5
11	-106	40	-9
26 -8 1			
1	350	318	13
4	273	251	7
7	163	211	-12
10	178	212	-8
26 -7 1			
0	200	133	15
3	-87	12	-5
6	-126	94	-18
9	120	155	-6
26 -6 1			
2	415	386	13
5	189	224	-9
8	-84	197	-31
26 -5 1			

1	218	216	0
4	197	166	7
7	-72	104	-11
26 -4 1			
0	318	303	5
3	236	192	11
6	160	212	-12
26 -3 1			
2	-162	41	-19
27 -21 1			
3	-17	139	-13
27 -20 1			
2	189	124	13
5	-62	49	-4
27 -19 1			
1	-24	111	-9
4	-68	54	-5
7	215	175	9
27 -18 1			
3	-53	146	-17
6	214	187	7
9	28	7	0
27 -17 1			
2	-157	86	-24
5	32	4	0
8	-128	120	-21
27 -16 1			
1	-130	64	-15
4	124	64	7
7	-133	17	-12
10	178	82	16
27 -15 1			
3	-142	25	-15
6	-168	22	-21
9	-133	12	-12
27 -14 1			
2	154	105	8
5	113	4	8
8	-167	69	-23
11	71	51	1
27 -13 1			
1	-150	53	-19
4	113	18	8
7	69	144	-11
10	-103	74	-11
27 -12 1			
0	328	313	5
3	401	355	19
6	83	94	-1
9	-47	18	-1
27 -11 1			

```
 2   19   13    0
 5  -76   52   -6
 8 -128   12  -11

   27 -10  1

 1  165  191   -6
 4  190  196   -1
 7  -50   83   -6
10 -121   69  -13

   27  -9  1

 0  246  265   -6
 3 -158   55  -20
 6 -185  112  -34
 9 -195   80  -31

   27  -8  1

 2  -87   20   -5
 5  263  246    5
 8 -149   77  -19

   27  -7  1

 1  181  191   -2
 4 -204   17  -30

   27  -6  1

 0  170   65   16
 3  148   46   12

   28 -18  1

 1  168  140    5
 4  291  217   22

   28 -17  1

 3 -127  131  -23

   28 -16  1

 2 -105   22   -8
 5   51  107   -5

   28 -15  1

 1 -125    4  -11
 4 -126   23  -11

   28 -14  1

 3  185  180    1
 6  190  215   -6

   28 -13  1

 2  -49   28   -2
 5 -108   32   -8

   28 -12  1

 1  204  293  -28
 4  209  246  -10

   28 -11  1

 0  -39  109   -9
 3  -66   80   -7

   28 -10  1

 2  223  237   -4

   28  -9  1

 1   96   47    4
```

Appendix 3. Supplimentary Material for
the X-ray Crystal Structure Determination of $CuTFPPCl_8$.

Figure A3.1. ORTEP diagram for $CuTFPPCl_8$ (50% probability ellipsoids) and numbering scheme for macrocycle.

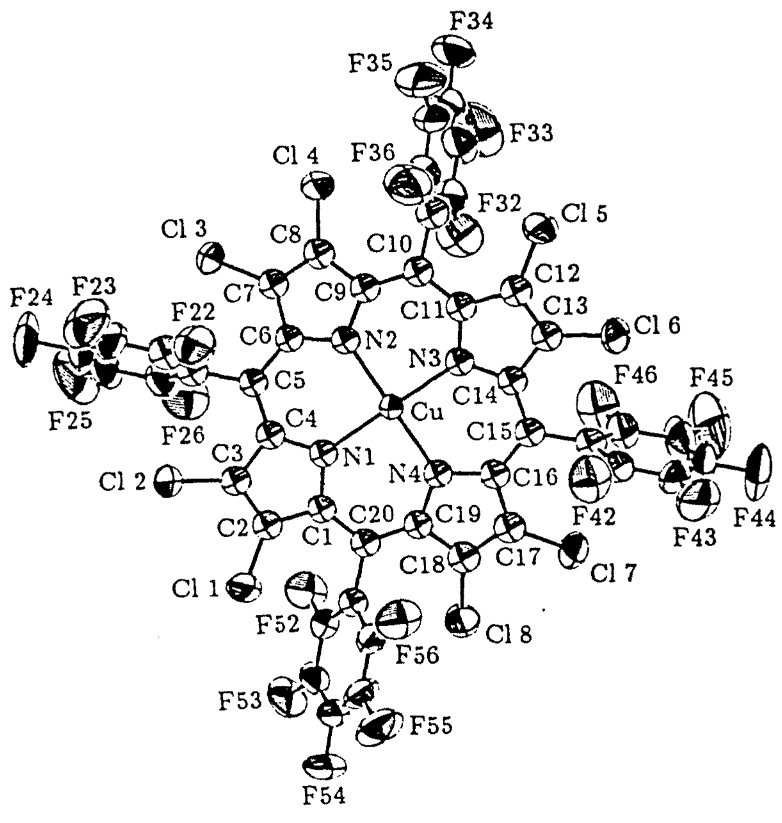

Table A3.1. Crystal and Intensity Collection Data for $CuTFPPCl_8$.

Formula: $CuC_{44}Cl_8N_4F_{20} \cdot CH_2Cl_2$	Formula Weight: 1396.58
Crystal Color: dark red	Habit: prismatic
Crystal Size: 0.33 x 0.52 x 0.63 mm	
Crystal System: triclinic	Space Group: $P\bar{1}$
$a = 11.794(5)$ Å	$\alpha = 87.51(5)$
$b = 14.492(4)$ Å	$\beta = 73.48(5)$
$c = 14.731(2)$ Å	$\gamma = 78.40(3)$
$V = 2364(3)$ Å^3	$Z = 2$
$D = 1.96$ g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 11.5$ cm^{-1}	$T = 294$ K
Enraf-Nonius Cad-4 diffractometer	θ - 2θ scan
Transmission coeff. =	range for data collection: 1-25°
$\pm h = 14, \pm k = 17, \pm l = 17$	
Number of reflections measured: 16705	
Number of independent reflections: 8290	
Goodness of fit for merging data: 1.11	
$R = 0.052$ on F for 7734 reflections with $F_o^2 > 0$	
$R = 0.052$ on F with $F_o^2 > 3\sigma(F_o^2)$	
$wR = 0.014$ on F^2 for 8290 reflections	
Final goodness of fit: 1.78 for 582 parameters and 8290 reflections	

Table A3.2. Final Refined Heavy Atom Parameters x 10^4 for $CuTFPPCl_8$.

x, y, z and $U_{eq}{}^a \times 10^4$

Atom	x	y	z	U_{eq} or B
Cu	2201(.4)	4601(.3)	8305(.3)	284(1)
Cl1	1502(1)	3108(1)	4943(1)	502(3)
Cl2	1485(1)	5302(1)	4548(1)	458(2)
Cl3	3138(1)	8111(1)	6452(1)	504(3)
Cl4	3000(1)	8401(1)	8604(1)	624(3)
Cl5	840(1)	6347(1)	12058(1)	578(3)
Cl6	844(1)	4147(1)	12421(1)	512(3)
Cl7	3341(1)	848(1)	9803(1)	603(4)
Cl8	3747(1)	593(1)	7574(1)	620(4)
N1	2238(3)	4426(2)	6950(2)	2.3(1)*
N2	2238(3)	5969(2)	8080(2)	2.3(1)*
N3	1922(3)	4798(2)	9700(2)	2.4(1)*
N4	2361(3)	3210(2)	8506(2)	2.3(1)*
C1	2172(3)	3605(2)	6552(3)	2.3(1)*
C2	1868(3)	3822(3)	5671(3)	2.5(1)*
C3	1853(3)	4743(3)	5508(3)	2.5(1)*
C4	2118(3)	5126(3)	6307(3)	2.4(1)*
C5	2308(3)	6032(3)	6380(3)	2.3(1)*
C6	2432(3)	6398(3)	7206(3)	2.3(1)*
C7	2727(3)	7301(3)	7300(3)	2.6(1)*

Atom	x	y	z	U_{eq} or B
C8	2674(3)	7421(3)	8211(3)	2.8(1) *
C9	2332(3)	6592(3)	8719(3)	2.5(1) *
C10	2041(3)	6473(3)	9698(3)	2.6(1) *
C11	1740(3)	5650(3)	10150(3)	2.6(1) *
C12	1328(4)	5522(3)	11160(3)	2.9(1) *
C13	1325(3)	4599(3)	11310(3)	2.8(1) *
C14	1753(3)	4130(3)	10393(3)	2.4(1) *
C15	2087(3)	3161(3)	10227(3)	2.5(1) *
C16	2457(3)	2743(3)	9331(3)	2.5(1) *
C17	2932(4)	1751(3)	9100(3)	2.9(1) *
C18	3084(4)	1635(3)	8165(3)	2.9(1) *
C19	2660(3)	2544(3)	7801(3)	2.4(1) *
C20	2467(3)	2710(3)	6907(3)	2.4(1) *
C21	2368(3)	6654(3)	5532(3)	2.7(1) *
C22	1373(4)	7286(3)	5455(3)	458(11)
F22	327(2)	7326(2)	6132(2)	592(7)
C23	1391(6)	7873(3)	4692(4)	651(14)
F23	398(4)	8477(2)	4642(3)	1041(11)
C24	2440(7)	7813(4)	3985(4)	777(18)
F24	2471(5)	8389(3)	3234(3)	1272(14)
C25	3458(6)	7201(4)	4029(3)	682(17)
F25	4501(4)	7160(3)	3338(2)	1140(15)

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Atom	x	y	z	U_{eq} or B
C26	3425(5)	6610(3)	4803(3)	492(12)
F26	4423(3)	6016(2)	4850(2)	731(9)
C31	2205(4)	7224(3)	10290(3)	3.1(1) *
C32	3285(5)	7155(3)	10480(3)	524(12)
F32	4153(3)	6390(2)	10180(2)	709(8)
C33	3553(6)	7860(4)	10938(3)	671(15)
F33	4629(4)	7762(3)	11104(3)	1064(12)
C34	2710(8)	8667(4)	11204(4)	773(19)
F34	2965(4)	9375(2)	11613(2)	1116(13)
C35	1596(7)	8747(3)	11064(3)	709(19)
F35	764(4)	9541(2)	11320(3)	1129(14)
C36	1342(5)	8031(3)	10617(3)	557(13)
F36	257(3)	8127(2)	10478(2)	792(9)
C41	2076(3)	2529(3)	11066(3)	2.7(1) *
C42	1113(4)	2106(3)	11482(3)	420(10)
F42	158(3)	2278(2)	11148(2)	670(8)
C43	1096(5)	1516(3)	12244(3)	559(14)
F43	142(3)	1129(2)	12622(2)	882(10)
C44	2062(6)	1356(4)	12610(3)	689(17)
F44	2039(4)	791(3)	13361(2)	1153(14)
C45	3026(5)	1755(4)	12230(4)	654(14)
F45	3967(4)	1587(3)	12585(3)	1169(13)

Atom	x	y	z	U_{eq} or B
C46	3029(4)	2341(3)	11454(3)	490(11)
F46	4000(3)	2726(2)	11070(2)	759(9)
C51	2593(3)	1880(3)	6289(3)	2.4(1) *
C52	3594(4)	1634(3)	5518(3)	345(9)
F52	4449(2)	2148(2)	5311(2)	538(6)
C53	3734(4)	868(3)	4957(3)	407(10)
F53	4724(3)	641(2)	4216(2)	627(8)
C54	2877(4)	329(3)	5155(3)	451(11)
F54	3029(3)	−439(2)	4622(2)	729(9)
C55	1864(4)	554(3)	5904(3)	455(11)
F55	1018(3)	25(2)	6088(2)	717(8)
C56	1733(4)	1327(3)	6462(3)	393(10)
F56	734(2)	1551(2)	7189(2)	631(7)
CS1	4144(11)	4448(10)	2258(10)	2054(50)
ClS1	4351(2)	3873(3)	3268(3)	2286(15)
ClS2	4720(4)	5382(3)	2089(4)	2479(19)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

Table A3.3. Complete Distances and Angles for $CuTFPPCl_8$.

	Distance(Å)		Distance(Å)
Cu –N1	2.010(3)	C17 –C18	1.350(6)
Cu –N2	2.003(3)	C18 –C19	1.449(5)
Cu –N3	2.011(3)	C19 –C20	1.401(5)
Cu –N4	2.003(3)	C20 –C51	1.498(5)
Cl1 –C2	1.717(4)	C21 –C22	1.365(6)
Cl2 –C3	1.719(4)	C21 –C26	1.386(6)
Cl3 –C7	1.712(4)	C22 –F22	1.340(5)
Cl4 –C8	1.707(4)	C22 –C23	1.378(7)
Cl5 –C12	1.714(4)	C23 –F23	1.332(7)
Cl6 –C13	1.719(4)	C23 –C24	1.362(9)
Cl7 –C17	1.713(4)	C24 –F24	1.354(8)
Cl8 –C18	1.704(4)	C24 –C25	1.358(9)
N1 –C1	1.374(5)	C25 –F25	1.348(7)
N1 –C4	1.371(5)	C25 –C26	1.392(8)
N2 –C6	1.385(5)	C26 –F26	1.329(6)
N2 –C9	1.373(5)	C31 –C32	1.363(6)
N3 –C11	1.375(5)	C31 –C36	1.387(7)
N3 –C14	1.376(5)	C32 –F32	1.342(6)
N4 –C16	1.387(5)	C32 –C33	1.383(8)
N4 –C19	1.371(5)	C33 –F33	1.338(7)
C1 –C2	1.448(5)	C33 –C34	1.364(9)
C1 –C20	1.394(5)	C34 –F34	1.336(8)
C2 –C3	1.342(5)	C34 –C35	1.368(9)
C3 –C4	1.459(5)	C35 –F35	1.342(7)
C4 –C5	1.388(5)	C35 –C36	1.379(8)
C5 –C6	1.405(5)	C36 –F36	1.332(6)
C5 –C21	1.502(5)	C41 –C42	1.376(6)
C6 –C7	1.441(5)	C41 –C46	1.376(6)
C7 –C8	1.343(5)	C42 –F42	1.329(5)
C8 –C9	1.453(5)	C42 –C43	1.380(7)
C9 –C10	1.395(5)	C43 –F43	1.326(6)
C10 –C11	1.400(5)	C43 –C44	1.369(8)
C10 –C31	1.500(6)	C44 –F44	1.345(7)
C11 –C12	1.444(6)	C44 –C45	1.347(8)
C12 –C13	1.347(6)	C45 –F45	1.332(7)
C13 –C14	1.447(5)	C45 –C46	1.393(7)
C14 –C15	1.393(5)	C46 –F46	1.344(6)
C15 –C16	1.392(5)	C51 –C52	1.383(5)
C15 –C41	1.504(5)	C51 –C56	1.377(6)
C16 –C17	1.451(5)	C52 –F52	1.331(5)

	Distance(Å)		Angle(°)
C52 –C53	1.368(6)	N2 –Cu –N1	90.3(1)
C53 –F53	1.346(5)	N3 –Cu –N1	172.3(1)
C53 –C54	1.360(6)	N4 –Cu –N1	90.5(1)
C54 –F54	1.342(5)	N3 –Cu –N2	90.4(1)
C54 –C55	1.370(6)	N4 –Cu –N2	173.7(1)
C55 –F55	1.340(5)	N4 –Cu –N3	89.7(1)
C55 –C56	1.376(6)	C1 –N1 –Cu	125.6(2)
C56 –F56	1.341(5)	C4 –N1 –Cu	126.3(2)
CS1 –ClS1	1.728(15)	C4 –N1 –C1	107.1(3)
CS1 –ClS2	1.613(15)	C6 –N2 –Cu	125.5(2)
		C9 –N2 –Cu	125.7(2)
		C9 –N2 –C6	107.6(3)
		C11 –N3 –Cu	125.9(2)
		C14 –N3 –Cu	126.7(2)
		C14 –N3 –C11	107.1(3)
		C16 –N4 –Cu	126.1(2)
		C19 –N4 –Cu	125.1(2)
		C19 –N4 –C16	107.5(3)
		C2 –C1 –N1	108.9(3)
		C20 –C1 –N1	124.5(3)
		C20 –C1 –C2	126.4(3)
		C1 –C2 –Cl1	129.5(3)
		C3 –C2 –Cl1	122.7(3)
		C3 –C2 –C1	107.7(3)
		C2 –C3 –Cl2	122.9(3)
		C4 –C3 –Cl2	130.0(3)
		C4 –C3 –C2	107.0(3)
		C3 –C4 –N1	108.9(3)
		C5 –C4 –N1	125.1(3)
		C5 –C4 –C3	125.8(3)
		C6 –C5 –C4	123.5(3)
		C21 –C5 –C4	118.1(3)
		C21 –C5 –C6	118.4(3)
		C5 –C6 –N2	125.6(3)
		C7 –C6 –N2	108.4(3)
		C7 –C6 –C5	125.9(3)
		C6 –C7 –Cl3	129.6(3)
		C8 –C7 –Cl3	122.4(3)
		C8 –C7 –C6	107.9(3)
		C7 –C8 –Cl4	122.1(3)

Angle(°)		Angle(°)	
C9 –C8 –Cl4	130.3(3)	C26 –C21 –C22	117.7(4)
C9 –C8 –C7	107.6(3)	F22 –C22 –C21	119.3(4)
C8 –C9 –N2	108.4(3)	C23 –C22 –C21	122.5(4)
C10 –C9 –N2	125.0(3)	C23 –C22 –F22	118.3(4)
C10 –C9 –C8	126.3(3)	F23 –C23 –C22	120.6(5)
C11 –C10 –C9	124.0(4)	C24 –C23 –C22	118.6(5)
C31 –C10 –C9	117.9(3)	C24 –C23 –F23	120.8(5)
C31 –C10 –C11	117.7(3)	F24 –C24 –C23	119.2(6)
C10 –C11 –N3	124.7(3)	C25 –C24 –C23	121.3(6)
C12 –C11 –N3	108.8(3)	C25 –C24 –F24	119.5(6)
C12 –C11 –C10	126.1(4)	F25 –C25 –C24	121.0(5)
C11 –C12 –Cl5	129.4(3)	C26 –C25 –C24	119.4(5)
C13 –C12 –Cl5	122.9(3)	C26 –C25 –F25	119.6(5)
C13 –C12 –C11	107.6(3)	C25 –C26 –C21	120.5(4)
C12 –C13 –Cl6	122.8(3)	F26 –C26 –C21	120.1(4)
C14 –C13 –Cl6	130.0(3)	F26 –C26 –C25	119.4(4)
C14 –C13 –C12	107.2(3)	C32 –C31 –C10	119.2(4)
C13 –C14 –N3	108.8(3)	C36 –C31 –C10	123.8(4)
C15 –C14 –N3	124.6(3)	C36 –C31 –C32	116.8(4)
C15 –C14 –C13	126.1(3)	F32 –C32 –C31	119.4(4)
C16 –C15 –C14	123.9(3)	C33 –C32 –C31	122.9(5)
C41 –C15 –C14	118.1(3)	C33 –C32 –F32	117.7(5)
C41 –C15 –C16	118.0(3)	F33 –C33 –C32	120.7(5)
C15 –C16 –N4	124.8(3)	C34 –C33 –C32	118.9(6)
C17 –C16 –N4	108.3(3)	C34 –C33 –F33	120.4(6)
C17 –C16 –C15	126.8(3)	F34 –C34 –C33	120.1(6)
C16 –C17 –Cl7	129.6(3)	C35 –C34 –C33	120.0(6)
C18 –C17 –Cl7	122.7(3)	C35 –C34 –F34	119.9(6)
C18 –C17 –C16	107.6(3)	F35 –C35 –C34	120.3(5)
C17 –C18 –Cl8	123.2(3)	C36 –C35 –C34	120.1(5)
C19 –C18 –Cl8	129.3(3)	C36 –C35 –F35	119.5(5)
C19 –C18 –C17	107.4(3)	C35 –C36 –C31	121.1(5)
C18 –C19 –N4	108.9(3)	F36 –C36 –C31	119.7(4)
C20 –C19 –N4	124.8(3)	F36 –C36 –C35	119.2(5)
C20 –C19 –C18	126.0(3)	C42 –C41 –C15	121.6(3)
C19 –C20 –C1	123.8(3)	C46 –C41 –C15	121.8(4)
C51 –C20 –C1	117.7(3)	C46 –C41 –C42	116.6(4)
C51 –C20 –C19	118.5(3)	F42 –C42 –C41	119.1(4)
C22 –C21 –C5	120.6(4)	C43 –C42 –C41	122.3(4)
C26 –C21 –C5	121.7(4)	C43 –C42 –F42	118.6(4)

Angle(°)

F43	–C43	–C42	119.9(4)
C44	–C43	–C42	118.9(5)
C44	–C43	–F43	121.1(5)
F44	–C44	–C43	119.0(5)
C45	–C44	–C43	121.1(5)
C45	–C44	–F44	119.9(5)
F45	–C45	–C44	120.6(5)
C46	–C45	–C44	119.0(5)
C46	–C45	–F45	120.4(5)
C45	–C46	–C41	122.1(4)
F46	–C46	–C41	119.1(4)
F46	–C46	–C45	118.8(4)
C52	–C51	–C20	120.8(3)
C56	–C51	–C20	122.0(3)
C56	–C51	–C52	117.2(4)
F52	–C52	–C51	119.8(3)
C53	–C52	–C51	121.6(4)
C53	–C52	–F52	118.6(4)
F53	–C53	–C52	120.3(4)
C54	–C53	–C52	119.8(4)
C54	–C53	–F53	120.0(4)
F54	–C54	–C53	119.9(4)
C55	–C54	–C53	120.5(4)
C55	–C54	–F54	119.5(4)
F55	–C55	–C54	120.1(4)
C56	–C55	–C54	119.1(4)
C56	–C55	–F55	120.8(4)
C55	–C56	–C51	121.8(4)
F56	–C56	–C51	119.3(4)
F56	–C56	–C55	118.9(4)
ClS2	–CS1	–ClS1	111.3(8)

Table A3.4. Observed and Calculated Structure Factors for $CuTFPPCl_8$. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs} - F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

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-12 1 1			
1	56	84	-48
2	26	4	9
3	50	76	-40
-12 2 1			
1	94	121	-61
2	99	91	15
-12 3 1			
1	107	109	-5
-11 1 1			
1	189	184	14
2	170	201	-84
3	127	125	3
4	231	261	-78
5	64	16	46
-11 2 1			
1	100	100	-1
2	38	27	9
3	77	56	33
4	106	129	-53
5	86	72	22
-11 3 1			
1	129	103	57
2	71	64	11
3	96	89	13
4	-29	6	-12
-11 4 1			
1	64	44	27
2	116	110	11
3	89	84	8
-11 5 1			
1	119	109	21
2	39	7	19
-11 6 1			
1	93	86	13
-10 1 1			
1	159	154	13
2	73	44	45
3	336	351	-36
4	197	218	-57
5	212	229	-45
6	189	190	-4
7	118	128	-23
-10 2 1			
1	319	340	-53
2	66	30	47
3	75	19	66
4	184	178	16
5	108	124	-39
6	124	134	-23
7	123	120	5
-10 3 1			
1	183	171	29
2	132	130	5
3	91	101	-20
4	51	30	23
5	22	21	0
6	101	115	-31
-10 4 1			
1	64	79	-28
2	46	36	11
3	136	148	-29
4	85	95	-20
5	44	42	2
6	48	35	14
-10 5 1			
1	70	43	38
2	33	17	12
3	59	41	21
4	142	139	6
5	117	130	-29
-10 6 1			
1	-30	10	-15
2	51	28	24
3	196	197	-1
4	95	102	-14
-10 7 1			
1	68	62	9
2	19	29	-6
3	138	127	24
-10 8 1			
1	77	80	-6
-9 1 1			
1	70	56	24
2	318	319	-2
3	111	103	19
4	179	172	17
5	78	68	18
6	46	25	21
7	46	0	28
8	110	112	-4
9	102	95	13
-9 2 1			
1	127	124	8
2	302	333	-83
3	105	97	18
4	212	222	-27
5	152	158	-16
6	33	9	14
7	125	127	-4
8	12	45	-25
-9 3 1			
1	252	267	-41
2	215	201	36
3	97	56	73
4	80	69	19
5	96	101	-9
6	38	23	13
7	58	41	20
8	95	98	-5
-9 4 1			
1	113	122	-22
2	135	121	34
3	135	118	39
4	121	119	4
5	91	73	34
6	-17	34	-22
7	30	47	-18
-9 5 1			
1	82	70	22
2	67	26	51
3	104	101	6
4	60	76	-28
5	306	301	11
6	58	64	-10
7	55	66	-16
-9 6 1			
1	51	65	-23
2	187	174	32
3	37	30	6
4	143	137	13
5	316	322	-15
6	38	13	16
-9 7 1			
1	31	24	5
2	63	58	9
3	179	200	-54
4	195	192	7
5	208	214	-15
-9 8 1			
1	250	238	28
2	-13	26	-12
3	33	64	-39
4	96	109	-25
-9 9 1			
1	294	299	-12
2	92	81	20
3	155	155	2
-8 1 1			
1	235	254	-57
2	86	58	56
3	137	132	14
4	488	504	-32
5	169	165	11
6	107	114	-19
7	526	525	1
8	96	86	19
9	131	125	14
10	255	256	-2
-8 2 1			
1	290	319	-83
2	208	222	-41
3	105	118	-37
4	378	386	-19
5	151	145	17
6	146	141	14
7	182	171	30
8	134	133	2
9	27	4	10
10	219	212	15
-8 3 1			
1	277	284	-20
2	126	115	29
3	60	28	42
4	127	128	-3
5	106	117	-29
6	94	101	-15
7	280	275	11
8	42	52	-13
9	-22	24	-15
-8 4 1			
1	66	18	61
2	68	73	-9
3	362	379	-40
4	71	60	19
5	39	54	-20
6	102	105	-6
7	53	46	8
8	97	105	-17
9	98	104	-13
-8 5 1			
1	241	245	-12
2	50	11	36
3	174	196	-63
4	27	26	0
5	48	71	-39
6	81	66	26
7	53	54	-2
8	51	71	-29
-8 6 1			
1	190	205	-40
2	189	194	-12
3	239	236	6
4	31	35	-3
5	139	142	-6
6	164	156	18
7	11	31	-12
8	54	63	-12
-8 7 1			
1	94	111	-42
2	174	173	3
3	138	130	18
4	101	109	-18
5	168	196	-77
6	93	84	15
7	49	57	-9
-8 8 1			
1	59	67	-14
2	-7	11	-2
3	33	41	-8
4	61	81	-37
5	166	168	-4
6	182	191	-20
-8 9 1			
1	113	115	-5
2	136	148	-31
3	122	121	2
4	100	95	10
5	39	40	-1
-8 10 1			
1	119	130	-26
2	136	136	1
3	71	59	17
-8 11 1			
1	31	35	-2
-7 1 1			

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1	112	98	40
2	362	330	78
3	242	253	-31
4	54	32	32
5	646	647	-1
6	216	232	-47
7	207	202	14
8	331	348	-42
9	130	116	33
10	148	135	31
11	151	163	-27
	-7	2	1
1	98	105	-22
2	198	187	35
3	263	265	-5
4	152	127	68
5	434	451	-36
6	58	64	-10
7	293	288	10
8	61	27	41
9	34	66	-47
10	95	83	23
11	109	101	16
	-7	3	1
1	44	22	27
2	146	150	-13
3	447	455	-16
4	74	79	-10
5	187	199	-35
6	-22	3	-8
7	84	57	47
8	265	273	-20
9	21	29	-5
10	59	68	-14
11	57	34	25
	-7	4	1
1	63	24	57
2	257	246	29
3	110	118	-23
4	73	76	-7
5	162	164	-5
6	32	13	13
7	227	234	-18
8	240	241	-2
9	-35	7	-20
10	-35	15	-21
	-7	5	1
1	100	93	17
2	30	4	16
3	224	220	10
4	68	31	51
5	144	130	34
6	190	183	18
7	20	11	4
8	197	185	29
9	42	62	-28
10	65	51	19
	-7	6	1
1	51	59	-13
2	146	128	47
3	33	0	17
4	107	123	-41
5	31	2	15
6	153	162	-23
7	119	119	0
8	184	183	3
9	44	72	-42
	-7	7	1
1	318	317	1
2	73	69	8
3	152	144	20
4	277	276	4
5	148	150	-5
6	24	16	4
7	22	56	-39
8	21	19	0
9	33	50	-18
	-7	8	1
1	163	157	16
2	51	23	30
3	233	246	-33
4	101	86	31
5	163	172	-21
6	168	169	-1
7	156	142	32
8	53	61	-10
	-7	9	1
1	265	260	12
2	147	142	11
3	214	217	-9
4	85	78	14
5	18	11	3
6	228	239	-27
7	108	122	-28
	-7	10	1
1	4	14	-2
2	13	5	2
3	114	103	24
4	105	111	-12
5	136	122	30
6	201	198	7
	-7	11	1
1	-8	13	-3
2	189	202	-32
3	78	62	25
4	119	129	-22
	-7	12	1
1	140	141	-1
2	192	191	1
	-6	1	1
1	766	788	-32
2	370	392	-58
3	222	200	68
4	267	253	40
5	214	189	73
6	52	23	37
7	273	284	-29
8	123	121	3
9	136	135	4
10	260	283	-61
11	48	13	29
12	298	293	11
	-6	2	1
1	799	799	0
2	68	75	-19
3	269	258	29
4	384	394	-25
5	158	159	-4
6	146	143	9
7	202	191	29
8	129	122	17
9	48	33	19
10	102	108	-12
11	136	124	27
12	326	320	13
	-6	3	1
1	90	91	-2
2	94	100	-17
3	354	344	24
4	146	161	-46
5	100	111	-29
6	154	150	11
7	138	131	19
8	-7	31	-17
9	207	217	-26
10	39	25	13
11	42	70	-43
12	212	212	0
	-6	4	1
1	127	113	41
2	334	335	-3
3	242	229	36
4	470	469	2
5	84	81	8
6	262	268	-16
7	195	187	19
8	106	107	-2
9	206	213	-18
10	-35	12	-22
11	82	83	-1
	-6	5	1
1	457	449	15
2	168	165	10
3	195	199	-12
4	239	229	28
5	70	33	55
6	220	232	-33
7	58	47	16
8	303	304	-3
9	-18	9	-6
10	12	33	-13
11	157	158	-1
	-6	6	1
1	247	233	40
2	43	42	0
3	30	36	-6
4	212	214	-5
5	315	298	40
6	249	245	10
7	418	426	-16
8	363	369	-12
9	43	39	4
10	142	128	30
	-6	7	1
1	7	6	0
2	218	213	13
3	41	18	21
4	195	195	1
5	613	622	-16
6	194	203	-25
7	41	48	-10
8	128	137	-21
9	9	5	0
10	72	70	4
	-6	8	1
1	275	267	20
2	215	210	13
3	248	250	-3
4	413	415	-5
5	250	259	-22
6	210	206	8
7	68	54	21
8	119	129	-21
9	-27	23	-18
	-6	9	1
1	90	76	28
2	563	549	24
3	60	3	51
4	65	62	6
5	143	126	40
6	39	2	22
7	116	133	-41
8	175	181	-14
	-6	10	1
1	481	488	-12
2	39	0	23
3	103	103	0
4	106	94	26
5	46	49	-4
6	88	75	23
7	25	10	6
	-6	11	1
1	-26	15	-14
2	-30	6	-15
3	57	54	5
4	78	91	-24
5	227	227	0
6	44	33	10
	-6	12	1
1	167	151	36
2	264	258	13
3	45	32	13
4	179	169	22
	-6	13	1
1	111	95	31
2	164	153	25
	-5	1	1
1	273	249	73
2	625	608	29
3	443	453	-21
4	229	220	27
5	618	601	29
6	751	744	10
7	56	28	39
8	400	391	18
9	531	526	9
10	75	73	5
11	438	449	-23
12	54	4	38
13	168	175	-15
	-5	2	1
1	62	59	10
2	497	501	-8
3	198	219	-76
4	38	3	32
5	286	269	45
6	535	535	0
7	390	384	15
8	317	315	5
9	286	291	-12

10	189	179	25
11	334	335	-2
12	229	219	25
13	332	334	-3
-5 3 1			
1	331	318	35
2	59	40	41
3	239	241	-5
4	658	643	24
5	68	69	-2
6	66	74	-19
7	100	92	20
8	122	126	-9
9	-26	10	-13
10	81	77	6
11	157	174	-45
12	64	71	-11
13	214	210	9
-5 4 1			
1	264	266	-6
2	217	221	-11
3	357	325	78
4	70	57	29
5	269	269	0
6	274	261	37
7	488	482	13
8	236	242	-15
9	169	170	0
10	154	162	-20
11	23	37	-12
12	-31	19	-20
-5 5 1			
1	407	415	-19
2	542	542	0
3	500	507	-14
4	201	213	-36
5	-22	37	-37
6	65	43	37
7	314	308	15
8	226	230	-9
9	44	55	-15
10	13	46	-30
11	73	79	-11
12	126	126	0
-5 6 1			
1	462	456	14
2	31	31	0
3	273	271	3
4	422	413	20
5	66	37	46
6	137	149	-34
7	251	241	25
8	80	90	-22
9	-23	6	-9
10	38	42	-4
11	120	102	37
12	53	43	12
-5 7 1			
1	198	205	-21
2	146	154	-25
3	55	59	-8
4	384	384	-1
5	56	31	33
6	338	332	13
7	205	203	7
8	292	277	34
9	52	64	-18
10	45	18	23
11	127	118	18
-5 8 1			
1	30	49	-26
2	103	111	-22
3	423	421	4
4	59	19	46
5	88	57	56
6	248	234	35
7	73	53	32
8	97	56	69
9	206	205	0
10	128	120	16
-5 9 1			
1	131	142	-28
2	144	150	-18
3	268	261	20
4	310	321	-27
5	256	253	7
6	459	449	21
7	200	185	36
8	52	62	-15
9	201	211	-25
-5 10 1			
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2	113	111	4
3	102	99	8
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5	64	72	-15
6	86	74	22
7	28	26	1
8	112	95	32
9	38	31	6
-5 11 1			
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2	72	82	-19
3	41	35	7
4	-19	37	-28
5	-35	12	-22
6	130	112	37
7	313	305	18
-5 12 1			
1	171	163	18
2	119	125	-15
3	138	123	34
4	105	113	-17
5	254	236	40
6	26	30	-2
-5 13 1			
1	171	179	-21
2	287	276	24
3	193	171	49
4	129	112	35
-5 14 1			
1	58	80	-35
-4 1 1			
1	379	357	56
2	316	314	4
3	155	164	-35
4	833	779	71
5	291	268	67
6	689	696	-10
7	225	226	-1
8	137	129	23
9	416	383	69
10	140	121	48
11	114	91	50
12	418	386	64
13	44	20	21
14	39	52	-15
-4 2 1			
1	436	413	53
2	172	177	-17
3	221	201	67
4	55	44	23
5	294	278	45
6	622	587	58
7	49	11	42
8	602	595	12
9	451	427	48
10	171	194	-67
11	290	270	48
12	322	288	76
13	160	143	39
14	43	40	2
-4 3 1			
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2	844	825	24
3	203	190	44
4	373	346	66
5	554	543	20
6	503	493	21
7	100	99	1
8	319	306	34
9	178	156	57
10	161	180	-53
11	-23	12	-12
12	128	120	18
13	64	54	14
14	95	98	-5
-4 4 1			
1	58	50	20
2	107	93	44
3	689	686	4
4	276	263	39
5	125	134	-29
6	64	57	14
7	264	258	17
8	132	119	35
9	107	98	21
10	167	169	-4
11	161	151	27
12	44	35	9
13	36	47	-11
-4 5 1			
1	166	152	48
2	809	782	36
3	243	220	69
4	51	32	33
5	29	48	-30
6	74	82	-18
7	158	141	49
8	393	378	33
9	174	176	-6
10	119	120	0
11	17	22	-3
12	190	171	45
13	56	47	11
-4 6 1			
1	39	32	10
2	372	353	46
3	215	212	8
4	302	303	-5
5	155	167	-36
6	330	299	75
7	218	216	6
8	218	219	-1
9	195	192	5
10	29	60	-41
11	177	164	33
12	341	318	49
-4 7 1			
1	134	130	10
2	115	110	13
3	19	32	-13
4	180	185	-15
5	399	379	43
6	49	22	30
7	37	37	0
8	64	46	26
9	-35	2	-21
10	22	29	-5
11	146	143	6
12	73	46	37
-4 8 1			
1	208	204	9
2	637	648	-18
3	57	56	1
4	605	609	-7
5	285	291	-16
6	130	112	43
7	224	226	-7
8	171	155	40
9	37	39	-2
10	224	222	6
11	212	196	36
-4 9 1			
1	72	78	-14
2	159	164	-15
3	26	39	-14
4	63	36	40
5	412	410	4
6	117	98	44
7	221	235	-36
8	180	162	44
9	64	58	9
10	243	222	48
11	166	166	-1
-4 10 1			
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2	433	442	-18
3	124	139	-40
4	170	167	6
5	445	449	-7
6	279	282	-8
7	336	339	-7
8	41	3	23
9	202	193	21
10	-5	8	-1
-4 11 1			
1	-24	4	-10
2	15	19	-2
3	128	138	-26
4	227	231	-10
5	148	148	0
6	33	39	-5
7	88	97	-18
8	197	182	36
9	253	256	-6

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 4

-4 12 1

1	-33	32	-37
2	-34	32	-37
3	149	142	17
4	128	131	-7
5	121	126	-12
6	102	105	-6
7	106	86	37

-4 13 1

1	149	146	5
2	150	149	2
3	289	290	-2
4	149	150	-4
5	105	119	-30
6	125	131	-12

-4 14 1

1	-32	5	-16
2	157	146	25
3	201	208	-17
4	34	17	11

-3 1 1

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2	90	19	177
3	181	163	67
4	1061	1050	12
5	413	390	54
6	407	377	68
7	332	293	99
8	540	521	36
9	267	254	36
10	265	245	50
11	399	391	19
12	99	71	55
13	74	65	16
14	223	216	16
15	77	80	-5

-3 2 1

1	52	55	-11
2	95	114	-82
3	400	384	39
4	71	49	59
5	79	94	-54
6	254	267	-40
7	439	454	-34
8	357	365	-19
9	57	65	-17
10	131	121	27
11	251	229	54
12	202	182	49
13	308	300	18
14	391	393	-2
15	58	26	31

-3 3 1

1	74	75	-2
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3	47	26	40
4	676	697	-35
5	244	252	-25
6	628	616	20
7	111	131	-66
8	53	68	-31
9	192	191	2
10	129	142	-35
11	174	166	20
12	38	36	1
13	112	115	-8
14	402	399	6

-3 4 1

1	543	549	-12
2	485	482	6
3	165	160	16
4	298	311	-40
5	80	107	-96
6	507	469	73
7	222	236	-46
8	-25	20	-21
9	-30	19	-23
10	24	27	-1
11	119	127	-21
12	160	175	-40
13	81	69	21
14	119	111	16

-3 5 1

1	36	42	-12
2	68	71	-10
3	451	443	17
4	467	477	-23
5	198	199	-3
6	220	197	68
7	856	866	-12
8	166	129	97
9	467	487	-42
10	242	253	-29
11	-13	39	-28
12	26	31	-4
13	221	200	49
14	20	12	3

-3 6 1

1	115	123	-27
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3	124	112	39
4	662	675	-22
5	64	75	-27
6	88	100	-31
7	456	465	-19
8	217	228	-33
9	69	54	24
10	274	296	-58
11	127	130	-6
12	259	249	24
13	134	133	2

-3 7 1

1	660	664	-7
2	253	244	27
3	201	192	29
4	66	47	38
5	130	140	-33
6	620	631	-17
7	278	290	-32
8	268	254	38
9	235	241	-16
10	-31	0	-16
11	290	294	-9
12	503	484	33
13	154	158	-8

-3 8 1

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3	645	630	24
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5	626	624	3
6	207	226	-57
7	450	463	-28
8	388	413	-57
9	260	266	-15
10	55	52	5
11	37	35	1
12	245	234	26

-3 9 1

1	223	216	20
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3	224	224	0
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5	314	305	23
6	347	366	-47
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8	104	89	33
9	17	5	4
10	58	47	15
11	111	94	34
12	209	199	23

-3 10 1

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4	99	111	-30
5	422	404	37
6	69	64	8
7	99	92	17
8	387	391	-7
9	262	235	63
10	106	98	16
11	26	33	-5

-3 11 1

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3	250	253	-8
4	56	51	7
5	283	282	2
6	180	174	15
7	118	116	4
8	235	245	-23
9	172	162	23
10	69	58	16

-3 12 1

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3	58	95	-78
4	37	45	-10
5	227	238	-28
6	99	114	-34
7	234	233	0
8	113	106	15
9	27	8	8

-3 13 1

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3	294	296	-3
4	169	162	17
5	130	134	-9
6	28	42	-13
7	180	181	-2

-3 14 1

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3	80	60	33
4	202	183	45
5	-25	8	-9
6	140	130	20

-3 15 1

1	190	194	-10
2	67	80	-22
3	188	184	8

-2 1 1

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2	620	613	13
3	218	216	4
4	162	156	25
5	246	269	-84
6	349	361	-34
7	962	932	35
8	92	60	78
9	169	184	-48
10	252	245	17
11	64	64	0
12	465	455	21
13	119	114	11
14	110	107	8
15	119	124	-11

-2 2 1

1	193	192	2
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3	292	292	-1
4	379	359	51
5	31	17	20
6	832	803	38
7	376	385	-23
8	90	88	4
9	567	565	4
10	305	302	7
11	360	352	18
12	607	610	-4
13	82	40	63
14	519	515	6
15	142	143	-2

-2 3 1

1	685	678	11
2	198	187	43
3	1242	1190	46
4	486	497	-22
5	380	343	90
6	888	859	36
7	463	422	85
8	254	248	16
9	477	475	4
10	206	213	-20
11	450	458	-18
12	-15	15	-8
13	-22	0	-7
14	212	214	-3
15	96	95	2

-2 4 1

1	777	781	-6
2	781	758	32
3	195	216	-83
4	277	277	-1
5	671	641	47
6	415	407	17
7	158	141	52
8	86	91	-13
9	89	100	-28
10	13	18	-2
11	58	78	-38
12	87	98	-24
13	-24	20	-15
14	195	193	3
15	108	95	24

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 5

-2 5 1

1	224	212	42
2	39	0	41
3	504	524	-42
4	450	446	7
5	258	251	22
6	290	296	-17
7	352	348	8
8	862	852	12
9	147	154	-22
10	79	82	-7
11	204	189	40
12	43	42	2
13	85	97	-27
14	362	352	22

-2 6 1

1	515	507	16
2	910	896	17
3	912	890	27
4	319	329	-29
5	449	432	36
6	80	90	-28
7	712	688	36
8	293	281	33
9	47	30	22
10	144	152	-23
11	230	233	-7
12	69	79	-18
13	135	122	28
14	87	68	30

-2 7 1

1	808	762	61
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3	315	309	16
4	430	392	82
5	360	331	69
6	349	372	-59
7	551	526	45
8	209	187	59
9	73	49	41
10	435	438	-7
11	96	84	25
12	70	6	61
13	149	141	17
14	74	58	23

-2 8 1

1	299	283	43
2	626	636	-17
3	244	248	-11
4	161	135	77
5	325	305	51
6	103	64	83
7	203	182	57
8	338	358	-49
9	354	349	12
10	169	187	-51
11	52	50	2
12	17	39	-17
13	105	112	-14

-2 9 1

1	61	73	-27
2	26	16	8
3	419	418	1
4	181	170	32
5	273	242	80
6	262	253	25
7	194	166	73
8	117	108	21
9	54	86	-64
10	82	103	-47
11	321	302	42
12	28	28	0

-2 10 1

1	-22	23	-20
2	182	182	-1
3	123	110	36
4	354	363	-21
5	-36	5	-24
6	101	83	40
7	443	422	43
8	240	262	-61
9	29	33	-3
10	212	216	-11
11	109	115	-12
12	151	155	-8

-2 11 1

1	234	224	26
2	46	52	-9
3	97	101	-10
4	249	245	11
5	53	66	-23
6	130	139	-24
7	55	46	14
8	38	34	4
9	52	67	-24
10	109	114	-9
11	-13	42	-26

-2 12 1

1	163	191	-84
2	124	136	-34
3	-50	28	-59
4	158	147	28
5	126	115	26
6	-23	21	-16
7	154	151	7
8	85	82	4
9	112	91	39
10	151	159	-18

-2 13 1

1	150	129	51
2	166	152	34
3	384	369	34
4	176	164	30
5	159	141	42
6	358	339	41
7	96	104	-18
8	106	102	8

-2 14 1

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2	18	43	-22
3	604	577	43
4	227	220	17
5	153	139	31
6	119	120	-3
7	59	50	10

-2 15 1

1	127	122	9
2	104	118	-31
3	59	68	-13
4	-54	14	-49
5	78	67	17

-2 16 1

1	82	78	6

-1 1 1

1	424	428	-11
2	510	460	104
3	107	89	80
4	42	42	0
5	1450	1435	11
6	79	52	74
7	483	470	27
8	535	497	71
9	915	885	36
10	202	160	114
11	439	412	56
12	450	409	81
13	132	121	26
14	60	43	24
15	115	99	34
16	161	152	19

-1 2 1

1	263	266	-8
2	540	541	-1
3	730	756	-41
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5	521	483	75
6	830	794	47
7	186	171	50
8	190	187	9
9	769	753	21
10	146	104	109
11	182	177	13
12	398	3[illegible]9	103
13	390	364	56
14	266	256	23
15	188	162	60
16	11	30	-10

-1 3 1

1	62	29	93
2	809	765	60
3	1445	1419	20
4	331	354	-71
5	434	409	58
6	108	96	41
7	508	473	69
8	106	112	-19
9	504	469	67
10	380	329	114
11	144	133	31
12	496	469	50
13	130	144	-37
14	110	90	41
15	-18	13	-7
16	86	59	40

-1 4 1

1	1055	1048	9
2	1883	1862	12
3	1380	1390	-9
4	581	548	59
5	601	582	32
6	133	146	-49
7	579	554	44
8	507	497	19
9	89	72	41
10	416	381	74
11	132	117	39
12	53	61	-14
13	224	230	-16
14	118	103	33
15	134	138	-10

-1 5 1

1	680	685	-7
2	70	88	-65
3	43	2	49
4	274	294	-66
5	646	664	-32
6	63	58	12
7	437	409	60
8	429	424	11
9	91	97	-16
10	25	40	-18
11	507	495	24
12	129	109	46
13	196	188	21
14	151	139	28
15	162	170	-18

-1 6 1

1	647	642	8
2	195	224	-114
3	483	418	130
4	265	278	-42
5	295	259	100
6	106	114	-25
7	95	118	-73
8	86	71	36
9	154	159	-14
10	182	193	-33
11	32	39	-7
12	214	184	73
13	142	137	12
14	128	133	-13
15	189	191	-5

-1 7 1

1	91	109	-70
2	357	364	-19
3	120	157	-150
4	841	853	-15
5	823	838	-20
6	401	348	118
7	146	161	-45
8	281	302	-62
9	45	13	30
10	394	370	52
11	108	98	22
12	664	627	55
13	198	196	5
14	126	124	3

-1 8 1

1	449	439	21
2	166	168	-7
3	224	260	-122
4	509	505	9
5	320	343	-63
6	1098	1074	24
7	594	554	68
8	167	153	39
9	462	437	50
10	121	130	-24
11	83	90	-15
12	92	93	-1
13	31	2	13
14	74	84	-18

-1 9 1

1	483	464	39
2	435	435	-1
3	165	172	-22
4	540	539	0
5	314	328	-38
6	28	3	13
7	178	191	-40
8	411	379	67

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 6

9	17	64	-60
10	74	106	-74
11	181	165	39
12	312	305	14
13	54	55	-2
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1	199	184	43
2	117	139	-69
3	128	134	-17
4	303	285	46
5	188	198	-30
6	159	147	34
7	107	66	83
8	531	523	15
9	123	142	-51
10	299	280	44
11	369	346	49
12	126	130	-9
-1	11	1	
1	242	250	-24
2	28	1	14
3	471	461	20
4	194	199	-14
5	320	319	3
6	361	366	-13
7	18	17	0
8	466	476	-19
9	189	183	16
10	196	199	-6
11	55	60	-7
-1	12	1	
1	29	22	5
2	-47	20	-49
3	183	207	-71
4	104	116	-29
5	228	216	31
6	23	67	-58
7	56	69	-21
8	109	120	-24
9	-41	5	-28
10	131	127	10
-1	13	1	
1	66	80	-26
2	109	110	-2
3	118	100	40
4	323	332	-23
5	31	36	-5
6	30	3	13
7	151	141	22
8	202	196	13
9	122	118	9
-1	14	1	
1	224	206	44
2	274	267	16
3	272	252	47
4	292	294	-5
5	140	134	14
6	402	393	17
7	36	51	-17
8	-18	9	-5
-1	15	1	
1	233	232	2
2	68	78	-18
3	225	224	2
4	54	71	-28
5	92	82	18

6	170	183	-30
-1	16	1	
1	149	140	21
2	335	305	63
3	-32	44	-42
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1	64	65	-1
2	89	89	-3
3	1236	1259	-21
4	281	263	62
5	83	83	0
6	891	848	53
7	114	94	68
8	627	606	34
9	216	184	97
10	556	523	60
11	84	49	67
12	62	67	-9
13	73	75	-2
14	185	181	10
15	232	209	56
16	39	46	-8
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-16	100	75	44
-15	228	203	61
-14	124	119	12
-13	255	249	14
-12	238	206	83
-11	453	449	8
-10	75	49	54
-9	542	535	14
-8	741	732	13
-7	848	804	56
-6	975	924	57
-5	1135	1111	24
-4	466	437	65
-3	331	307	74
-2	229	196	128
-1	320	308	40
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1	380	370	28
2	224	204	81
3	1293	1288	4
4	359	350	25
5	139	133	29
6	470	448	48
7	1072	1052	20
8	379	399	-50
9	299	262	99
10	34	63	-56
11	51	43	13
12	41	24	18
13	95	80	30
14	245	227	43
15	179	157	52
16	36	14	14
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-16	162	153	19
-15	33	12	14
-14	415	409	11
-13	38	5	22
-12	192	195	-7
-11	36	37	-1
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-9	287	277	27
-8	208	201	21
-7	648	652	-7
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-5	461	459	4
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3	54	40	42
4	1269	1270	0
5	1537	1560	-17
6	117	106	40
7	257	251	20
8	259	273	-45
9	154	137	53
10	283	254	77
11	384	372	28
12	342	315	63
13	364	362	4
14	115	114	2
15	438	425	25
16	34	8	14
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-8	73	77	-12
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2	1626	1614	8
3	814	804	17
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5	211	224	-50
6	389	383	14
7	151	153	-9
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9	233	240	-19
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11	248	231	44
12	341	340	3
13	26	28	-2
14	338	326	27
15	156	172	-41
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-15	303	285	41
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-13	422	411	22
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-10	464	479	-30
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-4	1190	1209	-18
-3	166	147	76
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2	986	982	4

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4	786	767	27
5	404	345	138
6	443	450	-17
7	507	515	-17
8	322	344	-63
9	366	366	0
10	438	462	-54
11	41	24	19
12	210	217	-20
13	142	138	10
14	361	340	46
15	46	56	-13
16	-16	20	-9
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-13	127	122	11
-12	-33	47	-58
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-8	397	407	-22
-7	833	792	52
-6	172	150	73
-5	255	226	91
-4	-39	33	-85
-3	279	285	-19
-2	884	916	-40
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1	587	606	-36
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3	119	92	95
4	733	736	-4
5	301	221	210
6	522	529	-13
7	-22	15	-19
8	361	384	-61
9	598	597	1
10	136	169	-108
11	148	174	-77
12	340	329	24
13	248	250	-5
14	419	392	54
15	11	17	-2
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-12	-21	58	-63
-11	134	148	-39
-10	202	215	-39
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-5	896	922	-31
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2	244	233	37
3	328	350	-67
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5	512	556	-93
6	355	343	29
7	553	583	-58
8	505	492	26
9	16	42	-28
10	95	55	78

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 7

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-12	55	74	-36
-11	129	132	-7
-10	458	462	-10
-9	193	189	12
-8	87	105	-52
-7	336	323	33
-6	115	135	-71
-5	406	421	-37
-4	496	479	34
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3	86	99	-45
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5	150	167	-63
6	407	396	26
7	309	340	-88
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9	167	186	-58
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13	279	277	3
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13	41	55	-17
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7	99	102	-6
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5	148	128	47
6	234	231	7
7	91	85	12
8	315	297	41
9	86	77	16
10	186	182	10

Tetra(pentafluorophenyl)octachloroporphinato Cu(II)

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4	195	203	-24
5	155	171	-47
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11	74	70	6
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3	215	217	-7
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5	63	76	-29
6	199	205	-18
7	215	207	21
8	126	139	-34
9	15	70	-72
10	166	178	-31
11	-21	31	-22
12	118	129	-25
13	169	162	15
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2	509	505	7
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5	290	269	56
6	154	162	-24
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10	225	236	-30
11	67	85	-37
12	195	192	6
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14	-26	26	-19
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2	659	674	-25
3	149	171	-83
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6	798	779	25
7	154	155	-3
8	66	85	-46
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9	142	169	-93
10	62	75	-29
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5	70	15	107
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9	387	374	30
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12	64	81	-36
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14	269	262	16
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16	-28	40	-34
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16	78	87	-16
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14	87	79	15
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16	126	134	-18
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3	410	441	-86
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8	652	637	23
9	191	178	41
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-11	155	162	-23
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3	458	493	-87
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5	490	498	-18
6	649	614	58
7	303	307	-12
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9	50	42	15
10	432	432	0
11	339	336	9
12	375	373	4
13	562	558	8
14	98	85	27
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16	83	73	17
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1 2 l			
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-11	85	40	78
-10	335	308	68
-9	49	42	11
-8	737	710	38
-7	360	333	69
-6	35	32	4

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 9

-5	1000	939	66
-4	1731	1737	-3
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6	968	931	42
7	381	369	30
8	548	547	1
9	136	124	36
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11	72	69	6
12	9	23	-8
13	629	607	34
14	96	96	0
15	78	64	24
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-11	237	251	-42
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2	640	641	-2
3	516	500	33
4	782	799	-25
5	13	24	-12
6	757	716	59
7	868	828	51
8	51	64	-36
9	250	268	-54
10	810	812	-2
11	140	143	-7
12	488	518	-62
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14	173	171	4
15	145	138	17
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6	402	415	-33
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11	242	231	31
12	226	185	105
13	388	394	-13
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-11	382	394	-28
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2	65	54	29
3	52	27	50
4	324	320	11
5	718	729	-15
6	1053	1043	9
7	400	385	34
8	84	98	-41

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14	72	84	-23
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	1 7 1		
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-10	66	40	40
-9	666	637	45
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-7	179	160	58
-6	21	3	9
-5	-40	17	-53
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-2	315	313	6
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1	18	37	-29
2	685	708	-37
3	987	988	-1
4	83	100	-59
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6	807	782	34
7	444	395	103
8	635	65C	-25
9	292	316	-70
10	592	610	-30
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	1 8 1		
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-12	107	117	-24
-11	89	100	-26
-10	252	246	16
-9	148	142	15
-8	208	217	-27
-7	215	227	-38
-6	755	783	-41
-5	447	453	-13
-4	803	814	-15
-3	282	306	-74
-2	406	421	-37
-1	312	320	-24
0	653	670	-27
1	64	75	-32
2	326	342	-46
3	-32	24	-46
4	34	44	-19
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6	236	215	63
7	220	267	-156
8	185	184	3
9	20	3	7
10	54	63	-16
11	293	307	-34
12	114	115	-2
13	102	100	3
14	119	132	-29
15	130	117	28
	1 9 1		
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-11	129	146	-46
-10	-36	6	-23
-9	208	237	-88
-8	269	286	-49
-7	253	259	-16
-6	60	85	-59
-5	218	225	-20
-4	616	652	-63
-3	232	229	10
-2	132	123	28
-1	253	267	-45
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1	165	156	28
2	481	479	3
3	337	339	-4
4	66	60	13
5	213	185	79
6	191	182	28
7	613	574	65
8	439	425	29
9	84	121	-101
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11	165	184	-54
12	62	50	17
13	132	132	0
14	67	77	-17
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-12	85	85	-1
-11	233	231	4
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-9	-47	33	-59
-8	112	116	-9
-7	207	217	-29
-6	477	467	19
-5	346	338	20
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-3	242	234	22
-2	412	418	-13
-1	793	764	39
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1	259	237	63
2	427	401	57
3	223	210	37
4	387	369	41
5	64	68	-10
6	76	83	-15
7	151	129	59
8	253	237	42
9	48	43	6
10	89	94	-10
11	189	202	-34
12	436	423	26
13	-24	27	-19
	1 11 1		
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-11	276	261	35
-10	220	187	78
-9	-44	26	-47
-8	291	294	-6
-7	476	465	23
-6	480	480	0
-5	163	175	-37
-4	-22	61	-79
-3	50	78	-59
-2	227	248	-63
-1	662	652	16
0	-34	21	-35
1	248	229	51
2	28	54	-40
3	251	265	-41
4	-32	15	-25

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 10

5	166	161	13
6	280	285	-14
7	-9	15	-5
8	142	149	-19
9	334	354	-50
10	117	116	2
11	15	25	-5
12	55	66	-17
13	273	271	4
	1	12	1
-11	345	331	29
-10	315	311	9
-9	172	181	-24
-8	345	344	2
-7	42	66	-39
-6	180	175	13
-5	23	1	8
-4	249	237	32
-3	85	102	-42
-2	311	300	28
-1	155	160	-14
0	165	152	37
1	50	49	1
2	187	194	-22
3	354	352	4
4	438	408	61
5	232	243	-30
6	116	114	4
7	182	186	-10
8	-29	37	-38
9	58	65	-13
10	74	89	-30
11	162	168	-14
12	120	119	3
	1	13	1
-10	53	51	2
-9	50	53	-4
-8	477	465	21
-7	152	157	-12
-6	191	193	-6
-5	26	68	-62
-4	11	33	-15
-3	97	94	7
-2	572	526	78
-1	497	482	28
0	106	85	45
1	407	397	22
2	221	182	98
3	92	88	8
4	387	358	61
5	130	129	3
6	18	30	-9
7	35	65	-43
8	193	208	-39
9	-19	43	-33
10	153	162	-20
11	80	77	3
	1	14	1
-9	-46	2	-31
-8	111	115	-8
-7	125	146	-52
-6	103	111	-18
-5	242	240	4
-4	164	148	40
-3	316	308	18
-2	133	127	15
-1	188	169	48
0	348	327	47
1	4	23	-9
2	506	487	35
3	-19	22	-14
4	94	90	8
5	369	378	-20
6	413	380	66
7	338	319	40
8	57	80	-41
9	215	208	16
	1	15	1
-7	98	101	-7
-6	72	73	-2
-5	72	99	-55
-4	-22	4	-8
-3	122	133	-28
-2	89	91	-5
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0	210	193	41
1	96	95	3
2	55	31	28
3	397	369	57
4	325	310	34
5	59	67	-12
6	164	159	12
7	222	215	16
8	57	51	8
	1	16	1
-5	210	213	-7
-4	57	64	-9
-3	110	106	9
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2	120	125	-10
3	-25	14	-12
4	101	118	-36
5	-38	30	-34
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1	159	151	17
	2	-16	1
0	105	111	-12
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3	110	102	15
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2	92	105	-28
3	218	204	33
4	58	81	-39
5	107	119	-25
6	138	138	-1
7	21	14	3
	2	-14	1
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1	157	158	-1
2	185	175	25
3	317	303	32
4	29	13	10
5	122	132	-23
6	46	65	-28
7	-20	32	-21
8	77	101	-48
9	111	118	-15
	2	-13	1
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2	36	0	20
3	93	112	-47
4	231	218	33
5	157	161	-10
6	189	170	45
7	400	376	48
8	222	222	-2
9	78	85	-12
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	2	-12	1
0	41	43	-2
1	335	315	46
2	359	345	31
3	22	0	8
4	-8	20	-7
5	49	46	3
6	230	229	1
7	57	66	-14
8	295	300	-12
9	169	141	64
10	421	423	-3
11	421	413	17
	2	-11	1
0	156	156	0
1	102	93	24
2	427	442	-33
3	31	21	9
4	48	54	-10
5	272	266	15
6	405	407	-3
7	113	131	-46
8	375	386	-24
9	117	110	16
10	40	17	18
11	329	307	49
12	209	203	14
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1	45	75	-64
2	83	77	15
3	735	723	17
4	333	343	-24
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6	126	133	-21
7	345	365	-50
8	339	349	-25
9	-47	10	-41
10	20	61	-51
11	54	54	0
12	-44	3	-31
13	71	81	-18
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0	91	101	-30
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2	109	113	-13
3	281	300	-56
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6	149	145	9
7	368	392	-59
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11	278	288	-26
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3	245	212	96
4	883	886	-3
5	409	425	-38
6	543	530	25
7	273	294	-61
8	220	232	-35
9	327	337	-27
10	290	302	-30
11	-27	59	-70
12	104	129	-65
13	126	111	32
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2	201	193	26
3	142	166	-92
4	628	630	-2
5	66	87	-64
6	570	588	-34
7	356	369	-33
8	355	359	-10
9	399	420	-48
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11	59	70	-20
12	148	170	-60
13	151	146	12
14	244	231	30
15	185	170	35
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2	28	26	2
3	24	23	0
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5	688	726	-61
6	17	22	-4
7	436	443	-14
8	281	279	6
9	433	459	-59
10	510	510	0
11	389	396	-17
12	157	173	-47
13	244	257	-35
14	105	100	12
15	76	68	14
16	-20	18	-10
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8	105	100	16
9	85	112	-84
10	16	28	-10
11	190	210	-60
12	136	161	-71
13	147	163	-43
14	-26	11	-13
15	-28	1	-12
16	30	43	-12

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 11

2 -4 1

0	551	564	-27
1	402	373	70
2	1164	1166	-2
3	605	566	68
4	883	852	40
5	167	161	22
6	738	694	64
7	418	449	-75
8	58	60	-5
9	309	339	-86
10	381	386	-12
11	164	161	8
12	289	305	-41
13	378	381	-5
14	-34	8	-21
15	525	528	-4
16	90	90	0

2 -3 1

0	40	25	32
1	438	427	26
2	1054	1053	1
3	1154	1200	-47
4	1461	1463	-1
5	475	427	102
6	555	475	144
7	614	666	-95
8	227	218	28
9	280	264	47
10	325	335	-27
11	208	192	47
12	302	312	-26
13	382	381	3
14	5	37	-21
15	135	126	22
16	14	56	-42

2 -2 1

0	622	599	41
1	25	23	3
2	1621	1583	27
3	778	744	48
4	1550	1543	5
5	66	71	-16
6	259	192	195
7	174	154	71
8	-32	7	-31
9	50	25	39
10	213	205	24
11	279	251	74
12	213	232	-59
13	140	145	-15
14	319	305	32
15	521	496	45
16	106	106	0
17	42	58	-20

2 -1 1

0	515	482	68
1	419	394	63
2	352	325	79
3	335	304	92
4	694	707	-20
5	45	39	16
6	421	437	-39
7	155	135	71
8	20	19	0
9	1231	1245	-16
10	251	243	23
11	104	107	-8
12	-34	24	-33
13	107	104	7
14	118	134	-41
15	523	507	28
16	36	16	14
17	36	49	-14

2 0 1

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-13	126	121	13
-12	74	79	-11
-11	210	219	-24
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1	679	714	-59
2	1060	1110	-54
3	351	359	-22
4	920	950	-37
5	901	886	19
6	1288	1284	3
7	348	367	-51
8	796	824	-39
9	341	331	27
10	27	27	0
11	301	296	12
12	66	75	-18
13	43	40	4
14	40	30	10
15	246	246	0
16	37	35	2
17	152	169	-43

2 1 1

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-14	116	81	70
-13	381	373	17
-12	275	243	78
-11	200	199	2
-10	21	33	-11
-9	262	263	-4
-8	359	328	76
-7	588	563	43
-6	33	5	29
-5	196	160	119
-4	545	519	51
-3	193	170	89
-2	372	357	43
-1	927	870	67
0	156	136	86
1	335	280	162
2	499	508	-20
3	499	515	-34
4	193	210	-78
5	850	842	10
6	831	818	16
7	519	522	-6
8	1033	1058	-27
9	30	37	-10
10	103	103	0
11	679	651	44
12	174	163	32
13	301	287	34
14	581	548	55
15	80	71	16
16	175	175	0
17	19	28	-5

2 2 1

-15	215	193	51
-14	88	73	26
-13	39	40	-1
-12	447	430	35
-11	57	42	23
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-9	49	61	-24
-8	292	288	11
-7	639	626	21
-6	595	568	47
-5	674	694	-33
-4	1324	1355	-27
-3	53	82	-118
-2	778	744	49
-1	76	99	-112
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1	64	7	111
2	226	209	69
3	84	49	122
4	931	953	-27
5	813	842	-40
6	429	447	-43
7	352	356	-11
8	775	804	-43
9	78	77	4
10	469	452	34
11	936	908	33
12	91	86	12
13	114	130	-43
14	114	110	9
15	47	12	29
16	91	27	83
17	87	65	35

2 3 1

-15	19	32	-9
-14	240	221	45
-13	317	298	44
-12	228	219	24
-11	115	125	-25
-10	52	51	2
-9	124	111	37
-8	373	350	54
-7	57	41	33
-6	458	468	-22
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-4	1139	1050	86
-3	899	846	64
-2	-22	14	-25
-1	586	537	89
0	616	634	-32
1	94	109	-75
2	988	990	-2
3	1660	1681	-14
4	736	733	4
5	412	432	-52
6	556	559	-6
7	304	311	-19
8	145	164	-74
9	384	407	-58
10	378	353	58
11	421	406	35
12	111	108	9
13	496	488	14
14	102	104	-4
15	93	88	10
16	310	274	79
17	55	49	7

2 4 1

-15	130	134	-9
-14	158	146	30
-13	398	410	-26
-12	89	80	18
-11	83	67	32
-10	280	269	31
-9	743	725	25
-8	502	511	-18
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-6	472	490	-39
-5	319	340	-64
-4	786	762	33
-3	559	578	-38
-2	1161	1175	-14
-1	342	372	-92
0	91	98	-29
1	1545	1560	-11
2	389	391	-6
3	57	53	14
4	1192	1200	-7
5	344	361	-48
6	156	170	-56
7	188	192	-13
8	727	753	-38
9	81	43	80
10	143	126	49
11	275	252	61
12	116	106	26
13	164	162	4
14	355	347	17
15	298	292	15
16	49	48	1

2 5 1

-15	-14	31	-16
-14	111	90	42
-13	82	90	-16
-12	174	176	-5
-11	239	245	-17
-10	280	265	37
-9	278	286	-20
-8	847	820	35
-7	634	591	69
-6	404	395	22
-5	165	208	-177
-4	21	50	-56
-3	246	230	52
-2	1271	1314	-40
-1	1173	1187	-13
0	868	896	-37
1	792	799	-10
2	554	536	33
3	704	667	57
4	1378	1427	-41
5	620	596	41
6	-27	11	-25
7	290	271	55
8	165	162	8
9	89	77	29
10	32	41	-12
11	-41	15	-38
12	149	173	-71
13	157	173	-47
14	169	170	-1
15	54	70	-26
16	150	168	-46

2 6 1

-15	153	146	15
-14	248	233	36
-13	311	309	4
-12	70	83	-26
-11	190	187	7
-10	301	300	2
-9	657	660	-3
-8	783	736	63
-7	391	363	65
-6	258	267	-27
-5	138	137	2
-4	360	385	-68
-3	454	449	11
-2	1135	1066	67

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 12

-1	286	275	35
0	22	58	-78
1	1136	1143	-6
2	86	40	110
3	393	433	-107
4	1241	1165	67
5	542	568	-51
6	665	681	-27
7	63	88	-75
8	59	72	-33
9	136	131	15
10	351	322	69
11	212	222	-27
12	255	241	36
13	223	200	58
14	254	254	0
15	93	91	3
16	108	125	-39
	2 7 1		
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-13	401	381	40
-12	29	34	-5
-11	13	38	-20
-10	586	580	9
-9	50	37	18
-8	353	337	38
-7	346	336	26
-6	908	901	8
-5	134	146	-42
-4	247	258	-33
-3	487	497	-21
-2	524	512	24
-1	676	704	-47
0	379	364	39
1	446	423	53
2	633	647	-24
3	310	347	-116
4	733	797	-99
5	401	367	79
6	318	333	-42
7	603	547	93
8	144	147	-10
9	449	431	39
10	-32	3	-20
11	291	300	-24
12	94	89	10
13	171	158	33
14	318	332	-32
15	26	67	-51
	2 8 1		
-14	78	93	-28
-13	114	116	-4
-12	7	26	-9
-11	383	380	5
-10	197	207	-27
-9	661	663	-2
-8	381	380	2
-7	140	143	-9
-6	526	508	34
-5	303	291	33
-4	482	467	30
-3	424	432	-19
-2	280	300	-64
-1	373	346	68
0	158	168	-38
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2	43	52	-20
3	58	59	-2
4	519	548	-59
5	239	207	93
6	499	511	-25
7	199	162	106
8	298	299	-3
9	296	334	-107

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11	-12	29	-16
12	289	299	-26
13	244	244	-1
14	84	95	-23
15	84	95	-22
	2 9 1		
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6	153	147	14
7	247	223	57
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9	50	59	-12
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8	112	91	41
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5	217	218	-2
6	195	202	-18
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	4 -9 1		
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3	119	98	55
4	81	82	-2
5	252	238	36
6	78	93	-35
7	238	223	39
8	176	168	23
9	61	71	-19
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12	35	19	12
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9	425	421	7
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11	245	243	4
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5	415	419	-8
6	524	518	11
7	440	411	61
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9	280	262	45
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12	224	221	6
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4	240	258	-57
5	272	264	24
6	84	90	-16
7	133	118	43
8	395	374	47
9	397	389	19
10	368	345	53
11	444	453	-17
12	-15	37	-25
13	143	136	17
14	161	147	33
15	241	238	7
16	167	165	3
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7	768	729	54
8	339	347	-20
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11	262	264	-5
12	184	186	-6

Tetra(pentafluorophenyl)octachloroporphinato Cu(II)

13	152	170	-49
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Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 18

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3	485	485	-1
4	123	118	13
5	191	197	-17
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6	537	541	-7
7	63	64	-1
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7	262	266	-12
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Tetra(pentafluorophenyl-)octachloroporphinato Cu(II)

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10	160	144	44
11	202	193	26
12	190	191	0
13	126	137	-27
14	303	296	16
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16	222	213	22
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6 1 1

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3	198	219	-78
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12	175	185	-30
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14	107	94	28
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6 2 1

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7	1006	1015	-9
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6 3 1

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6 4 1

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6 5 1

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6 6 1

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-7	133	110	57
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8	146	164	-58
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10	337	341	-11
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6 7 1

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6 8 1

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6	528	527	1
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6 9 1

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6	534	554	-38
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8	277	288	-29

Tetra(pentafluorophenyl)octachloroporphinato Cu(II)

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5	381	391	-22
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6	109	99	27
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8	100	114	-37
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4	500	505	-10
5	377	379	-6
6	347	331	37
7	7	64	-72
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6	58	37	29
7	229	244	-44
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	7 11 l		
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3	505	485	38
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9	485	474	20
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11	276	265	26
12	101	107	-12
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6	131	122	20
7	173	169	11
8	14	32	-13
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	7 13 l		
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11	191	182	18
	7 14 l		
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6	245	242	8
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8	162	144	40
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	7 15 l		
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7	113	110	7
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9	100	117	-36
	8 -9 l		
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6	28	38	-9
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8	58	53	7
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	8 -8 l		
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9	59	13	47
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11	143	117	60
12	169	176	-18
13	36	43	-8

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 25

14	211	206	12
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9	201	202	-2
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Tetra(pentafluorophenyl)octachloroporphinato Cu(II)

1	63	83	-46
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	8 10 1		
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3	202	216	-40
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6	260	258	4
7	201	195	14
8	156	165	-24
9	181	173	21

Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 28

10	-23	18	-13
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9 11 1

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6	217	214	8
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8	121	113	17
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10	182	177	12
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12	39	22	14

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11	200	182	41

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8	225	240	-40
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12	172	191	-48

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Tetra(pentafluorophenyl)octachloroporphinato Cu(II) Page 29

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	11	-3	1
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1	38	55	-23
2	139	163	-65
3	198	181	44
4	-18	13	-8
5	97	83	28
6	87	72	27
7	12	50	-36
8	170	190	-53
9	77	86	-16
10	56	39	21
11	94	85	17
12	-29	6	-12

11 -2 1

0	84	71	24
1	45	65	-32
2	154	190	-105
3	175	183	-21
4	25	13	7
5	6	7	0
6	243	229	35
7	102	72	58
8	148	128	46
9	16	2	4
10	71	56	23
11	161	158	7
12	106	125	-44
13	130	138	-16

11 -1 1

0	199	225	-74
1	76	99	-52
2	51	32	23
3	369	381	-27
4	55	79	-46
5	41	73	-55
6	63	51	20
7	29	60	-43
8	42	97	-113
9	131	114	39
10	21	2	6
11	99	104	-10
12	23	27	-2
13	63	64	0

11 0 1

-6	254	262	-20
-5	59	34	28
-4	270	274	-10
-3	105	69	64
-2	58	56	1
-1	136	123	36
0	151	164	-36
1	89	86	6
2	57	32	32
3	131	116	35
4	64	80	-31
5	44	0	28
6	174	179	-12
7	51	45	7
8	59	34	32
9	138	121	40
10	49	33	18
11	145	149	-11
12	33	15	12
13	58	70	-19

11 1 1

-6	168	182	-33
-5	49	3	31
-4	107	100	15
-3	78	75	6
-2	31	15	10
-1	23	3	8
0	188	180	18
1	154	149	11
2	143	135	20
3	61	12	50
4	75	116	-103
5	53	76	-41
6	154	134	48
7	298	330	-84
8	195	206	-29
9	240	264	-65
10	87	61	45
11	40	25	14
12	3	17	-4
13	85	89	-6
14	98	55	65

11 2 1

-6	34	21	9
-5	40	42	-1
-4	52	44	10
-3	112	132	-49
-2	77	103	-56
-1	292	315	-58
0	63	46	25
1	233	218	40
2	281	315	-93
3	240	245	-12
4	53	93	-85
5	65	17	54
6	54	44	14
7	100	115	-34
8	160	156	9
9	208	216	-23
10	121	117	7
11	185	169	37
12	79	100	-43
13	46	26	18
14	255	261	-13

11 3 1

-6	56	37	20
-5	-14	12	-4
-4	166	172	-14
-3	30	3	13
-2	34	36	-2
-1	231	228	6
0	51	69	-32
1	68	21	56
2	308	317	-22
3	144	158	-38
4	78	90	-27
5	235	215	50
6	81	96	-35
7	84	98	-31
8	68	62	9
9	17	9	3
10	4	20	-5
11	143	130	31
12	52	42	11
13	59	27	34
14	314	331	-40

11 4 1

-6	80	81	-2
-5	-19	12	-7
-4	97	109	-26
-3	65	81	-29
-2	-37	25	-34
-1	17	16	0
0	64	22	50
1	147	158	-29
2	39	22	15
3	89	118	-75
4	176	156	52
5	34	40	-7
6	106	94	25
7	101	71	60
8	154	143	28
9	82	90	-18
10	68	82	-27
11	21	25	-2
12	-36	5	-20
13	127	119	16
14	90	91	-1

11 5 1

-6	131	132	-2
-5	76	82	-11
-4	-1	6	0
-3	28	44	-16
-2	130	116	32
-1	143	129	33
0	17	41	-22
1	167	157	26
2	30	51	-24
3	23	5	7
4	305	292	31
5	94	69	48
6	-24	5	-9
7	235	199	87
8	25	47	-25
9	36	19	13
10	321	312	21
11	51	40	13
12	21	53	-33
13	78	103	-50
14	65	60	7

11 6 1

-6	35	24	8
-5	160	175	-38
-4	94	89	10
-3	56	52	5
-2	75	85	-20
-1	190	208	-50
0	137	138	-2
1	291	299	-18
2	201	213	-32
3	147	169	-62
4	227	208	49
5	56	41	21
6	39	56	-25
7	254	230	59
8	210	203	18
9	22	3	7
10	159	166	-16
11	149	157	-19
12	65	63	4
13	165	158	17

11 7 1

-5	122	125	-4
-4	97	111	-29
-3	93	97	-8
-2	-11	33	-18
-1	40	18	17
0	87	92	-10
1	152	157	-11
2	105	104	3
3	230	229	1
4	83	59	44
5	-13	13	-5
6	26	34	-7
7	216	197	49
8	261	279	-45
9	145	126	45
10	52	41	14
11	-22	29	-21
12	68	62	9
13	126	118	17

11 8 1

-5	116	113	5
-4	68	63	7
-3	247	243	11
-2	97	70	48
-1	49	16	30
0	359	357	3
1	67	54	21
2	173	197	-68
3	126	112	33
4	250	245	13
5	160	180	-54
6	246	252	-16
7	221	228	-18
8	-20	7	-7
9	96	71	47
10	151	160	-24
11	-23	46	-38
12	-30	1	-12

11 9 1

-4	90	73	28
-3	246	254	-20
-2	92	88	8
-1	87	77	18
0	226	243	-44
1	38	25	11
2	57	42	20
3	157	154	8
4	-33	25	-28
5	156	200	-127
6	111	87	49
7	155	175	-54
8	90	80	19
9	-24	12	-11
10	125	151	-63
11	33	72	-55
12	209	198	25

11 10 1

-3	177	170	15
-2	46	44	1
-1	59	43	20
0	131	124	15
1	-27	8	-13
2	38	13	17
3	212	220	-20
4	-38	17	-28
5	-33	8	-19
6	-36	15	-24
7	125	125	0
8	126	121	11
9	97	94	5
10	155	149	15
11	115	102	25

11 11 1

-2	72	57	22
-1	206	205	2
0	273	253	45
1	54	62	-12
2	-18	15	-8
3	100	97	5
4	72	55	26
5	136	126	23
6	-32	17	-20
7	111	107	7
8	-40	24	-33
9	-34	9	-18
10	172	165	15

11 12 1

0	106	105	3
1	21	35	-10
2	38	31	6
3	-13	34	-18
4	-10	26	-11
5	62	53	12
6	20	34	-10
7	47	58	-14
8	186	157	63

11 13 1

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2	51	10	30
3	229	224	12
4	119	118	1
5	85	78	12
12	-5	1	
1	51	35	16
2	150	144	14
3	46	20	21
4	37	12	15
5	-16	10	-5
6	57	38	22
7	59	69	-15
12	-4	1	
0	123	131	-17
1	90	93	-5
2	165	162	7
3	54	39	18
4	9	8	0
5	46	35	11
6	36	35	1
7	50	35	16
8	230	237	-16
9	66	77	-19
12	-3	1	
0	102	128	-59
1	142	142	1
2	106	70	62
3	128	160	-86
4	58	44	18
5	124	145	-51
6	34	36	-1
7	-18	10	-6
8	104	79	45
9	99	146	-118
10	87	92	-8
12	-2	1	
0	50	58	-11
1	109	116	-16
2	43	62	-25
3	124	167	-118
4	48	39	11
5	127	114	30
6	1	22	-7
7	32	21	8
8	-15	13	-5
9	30	36	-5
10	138	135	7
11	29	15	8
12	-1	1	
0	-22	43	-36
1	82	83	-1
2	21	32	-8
3	40	8	21
4	238	238	0
5	40	14	19
6	63	51	18
7	65	74	-15
8	-28	21	-18
9	46	37	9
10	220	241	-54
11	38	1	19
12	118	139	-49
12	0	1	
-3	58	46	16
-2	72	61	16
-1	94	96	-4
0	47	68	-32
1	116	149	-86
2	126	124	4
3	210	220	-26
4	79	73	12
5	250	258	-20
6	135	109	56
7	90	97	-15
8	88	84	9
9	95	87	15
10	120	116	8
11	58	63	-7
12	64	47	22
12	1	1	
-4	58	63	-6
-3	46	40	7
-2	71	89	-33
-1	39	49	-12
0	35	5	17
1	194	240	-132
2	46	70	-39
3	23	34	-10
4	117	135	-46
5	154	146	19
6	304	316	-28
7	97	72	47
8	161	150	27
9	268	265	8
10	72	84	-23
11	12	27	-8
12	123	106	35
12	2	1	
-4	39	32	6
-3	50	39	12
-2	126	169	-115
-1	-14	19	-9
0	132	131	1
1	17	37	-16
2	59	28	36
3	182	197	-41
4	128	119	21
5	70	58	19
6	322	347	-60
7	44	6	27
8	72	71	2
9	257	269	-29
10	67	60	10
11	26	2	9
12	145	143	2
12	3	1	
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-2	83	81	4
-1	114	135	-53
0	113	132	-48
1	65	47	27
2	63	12	51
3	170	208	-110
4	69	40	41
5	124	128	-9
6	232	247	-39
7	64	56	13
8	-28	37	-34
9	143	146	-7
10	28	9	10
11	64	46	23
12	139	121	37
12	4	1	
-4	-12	12	-4
-3	34	37	-2
-2	83	48	52
-1	255	277	-57
0	77	69	14
1	33	30	3
2	198	206	-22
3	107	115	-18
4	31	17	10
5	28	4	12
6	50	9	34
7	42	41	1
8	56	50	8
9	154	142	28
10	50	63	-18
11	-36	36	-40
12	59	16	38
12	5	1	
-4	77	59	27
-3	33	31	1
-2	87	52	53
-1	184	179	13
0	112	93	40
1	77	62	26
2	280	284	-9
3	62	87	-48
4	122	119	7
5	174	173	2
6	-37	26	-34
7	-16	5	-4
8	26	4	10
9	234	246	-30
10	59	44	19
11	18	25	-4
12	-16	13	-6
12	6	1	
-3	20	13	3
-2	35	54	-21
-1	63	48	21
0	222	231	-22
1	153	181	-75
2	110	105	11
3	-19	5	-6
4	28	1	12
5	44	57	-19
6	36	25	10
7	103	115	-28
8	45	38	8
9	85	93	-15
10	62	42	25
11	56	66	-14
12	105	99	10
12	7	1	
-3	37	15	14
-2	-5	25	-9
-1	138	139	-1
0	88	90	-4
1	31	25	4
2	135	139	-9
3	46	42	3
4	175	159	39
5	30	39	-8
6	79	102	-51
7	292	305	-32
8	56	37	24
9	64	31	38
10	124	121	6
11	61	91	-54
12	8	1	
-2	64	53	15
-1	184	188	-9
0	83	58	39
1	132	147	-39
2	108	95	27
3	-26	11	-12
4	41	33	7
5	273	276	-6
6	127	140	-31
7	118	144	-65
8	83	75	13
9	-42	1	-26
10	-24	18	-13
11	69	72	-3
12	9	1	
-2	45	14	22
-1	56	32	25
0	-15	14	-6
1	27	16	6
2	192	176	38
3	29	25	3
4	51	39	14
5	184	175	21
6	116	124	-17
7	127	136	-21
8	138	140	-5
9	-26	1	-9
10	22	28	-4
12	10	1	
0	77	80	-6
1	-20	31	-19
2	151	166	-38
3	55	60	-6
4	48	66	-25
5	109	106	6
6	18	8	3
7	117	127	-24
8	190	200	-24
9	18	1	4
12	11	1	
1	5	3	0
2	-28	25	-20
3	-42	21	-33
4	-24	34	-25
5	83	72	19
6	6	41	-22
7	152	153	-2
13	-3	1	
4	50	11	29
5	32	6	13
13	-2	1	
2	126	151	-60
3	57	41	19
4	37	30	5
5	123	110	25
6	24	1	8
7	31	28	2
8	70	63	10
13	-1	1	
1	57	66	-13
2	53	39	16
3	89	103	-29
4	28	2	10
5	107	71	61
6	-18	31	-18
7	58	41	19
8	46	23	20
9	114	103	23

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13 0 1

0	146	140	13
1	69	65	6
2	179	167	28
3	111	101	20
4	59	29	33
5	60	60	0
6	83	68	24
7	86	93	-14
8	43	52	-11
9	41	39	1
10	23	9	6

13 1 1

-1	102	91	19
0	65	82	-28
1	60	70	-16
2	138	147	-19
3	24	0	8
4	52	76	-39
5	131	133	-4
6	126	131	-12
7	96	115	-42
8	188	219	-81
9	65	27	41
10	79	65	22

13 2 1

-1	41	49	-9
0	-13	17	-6
1	129	118	24
2	61	78	-29
3	60	54	7
4	72	19	58
5	157	157	0
6	183	216	-89
7	141	161	-51
8	202	210	-20
9	31	0	13
10	17	28	-6

13 3 1

-1	-27	13	-13
0	-10	22	-8
1	107	96	22
2	39	51	-15
3	44	39	4
4	71	64	10
5	126	141	-37
6	35	1	17
7	61	73	-20
8	98	95	6
9	61	63	-2
10	44	60	-21

13 4 1

-1	53	29	23
0	91	106	-31
1	57	49	10
2	54	88	-62
3	9	13	-1
4	162	182	-51
5	48	11	29
6	93	113	-42
7	102	99	5
8	-8	9	-2
9	109	121	-26
10	83	94	-19

13 5 1

-1	40	15	17
0	21	0	6
1	134	118	35
2	121	155	-87
3	40	17	18
4	128	129	-1
5	20	0	5
6	-16	2	-4
7	19	0	5
8	33	48	-16
9	51	51	0
10	178	181	-8

13 6 1

-1	29	23	4
0	-21	40	-28
1	174	190	-40
2	51	37	16
3	-19	24	-13
4	39	13	18
5	-20	4	-6
6	52	45	9
7	101	95	11
8	29	15	8
9	122	131	-18
10	49	54	-5

13 7 1

0	169	179	-23
1	149	163	-34
2	41	56	-19
3	72	55	25
4	-28	19	-17
5	45	57	-16
6	179	187	-18
7	94	75	32
8	20	82	-85
9	116	121	-12

13 8 1

1	55	41	16
2	19	52	-30
3	67	85	-32
4	69	72	-5
5	61	86	-44
6	153	178	-63
7	32	35	-2
8	69	92	-41

13 9 1

3	102	99	5
4	58	90	-57
5	39	1	19
6	66	56	14

14 3 1

5	36	36	0

14 4 1

5	54	18	31

Appendix 4. Supplimentary Material for
the X-ray Crystal Structure Determination of $H_2TFPPBr_8$.

Figure A4.1. ORTEP diagram for $H_2TFPPBr_8$ unit cell (50% probability ellipsoids) and numbering scheme for macrocycle.

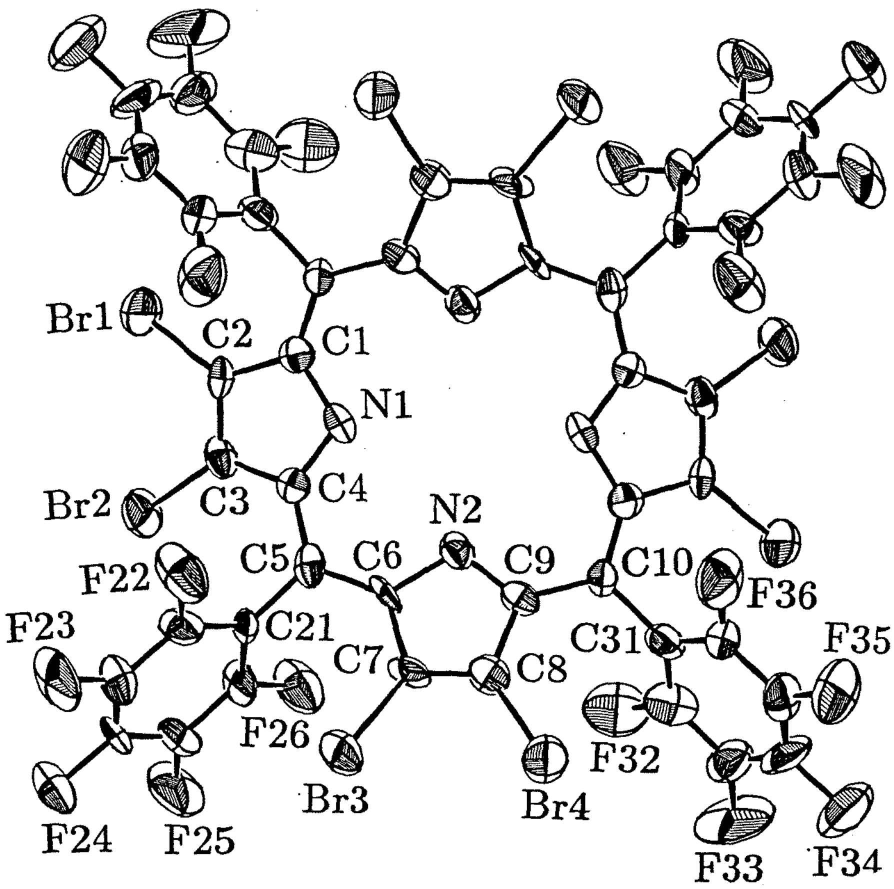

Figure A4.2. ORTEP diagram for $H_2TFPPBr_8$ (50% probability ellipsoids).

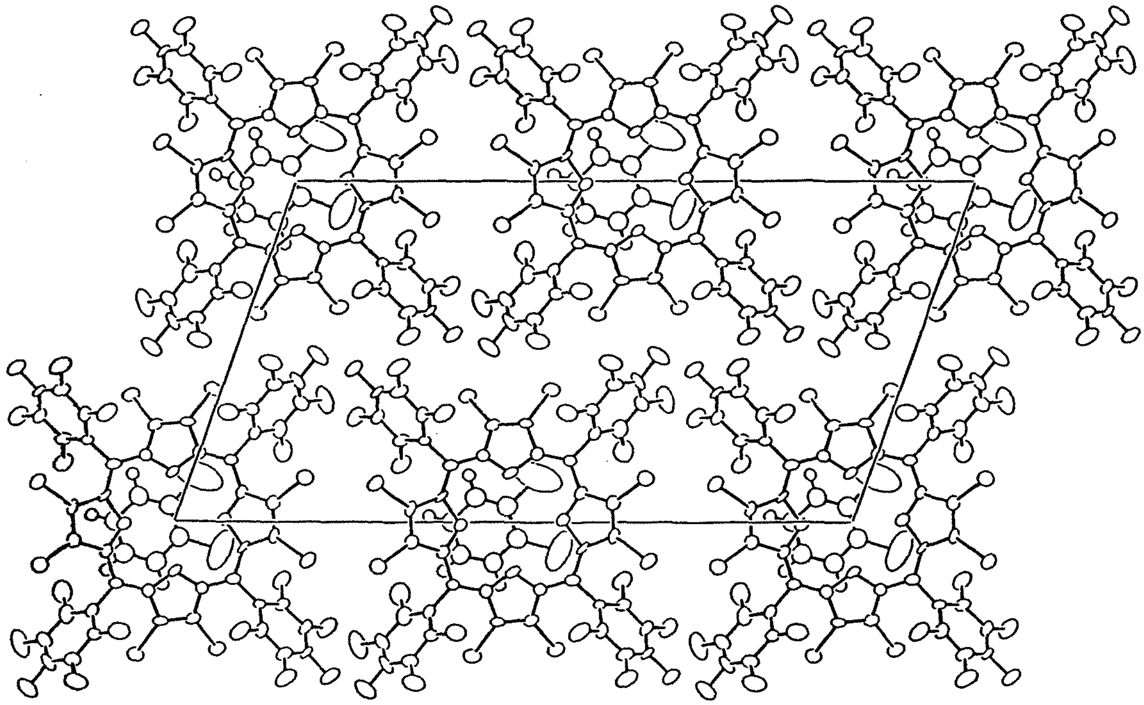

Table A4.1. Crystal and Intensity Collection Data for $H_2TFPPBr_8$.

Formula: $C_{44}H_2Br_8N_4F_{20} \cdot C_6H_4Cl_2$	Formula Weight: 1752.73
Crystal Color: dark brown	Habit: plate
Crystal Size: 0.07 x 0.23 x 0.50 mm	
Crystal System: monoclinic	Space Group: C2
a = 27.634(6) Å	$\alpha = 90$
b = 6.926(2) Å	$\beta = 109.64(2)$
c = 14.844(3) Å	$\gamma = 90$
V = 2675.8(11) $Å^3$	Z = 2
D = 2.18 g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 661.52\ cm^{-1}$	T = 225 K
Enraf-Nonius Cad-4 diffractometer	θ - 2θ scan
Transmission coeff. =	range for data collection: 1.5 - 25°
h = 0 - 32, ±k = 8, ±l = 17	
Number of reflections measured: 4881	
Number of independent reflections: 4710	
Goodness of fit for merging data: 1.61	
R = 0.071 on F for 4409 reflections with $F_o^2 > 0$	
R = 0.043 on F for 3051 reflections with $F_o^2 > 3\sigma(F_o^2)$	
wR = 0.006 on F^2 for 4710 reflections	
Final goodness of fit: 1.41 for 360 parameters and 4710 reflections	

Table A4.2. Final Refined Heavy Atom Parameters x 10^4 for $H_2TFPPBr_8$.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
N1	284(2)	5038(8)	1447(4)	250(17)
N2	730(2)	5258(9)	−78(5)	299(17)
C1	−7(3)	4719(11)	2017(6)	275(20)
C2	323(3)	3789(11)	2910(5)	261(22)
C3	793(3)	3646(11)	2838(5)	302(21)
C4	769(3)	4544(11)	1946(5)	233(19)
C5	1194(3)	4975(11)	1672(5)	274(22)
C6	1166(3)	5546(11)	744(5)	271(23)
C7	1563(3)	6272(11)	397(6)	328(23)
C8	1372(3)	6377(11)	−570(6)	377(22)
C9	847(3)	5672(11)	−869(6)	253(20)
C10	519(3)	5239(11)	−1814(5)	253(20)
Br1	136(.3)	2677	3888(.6)	481(3)
Br2	1315	2186(2)	3700(1)	471(2)
Br3	2209	7260(2)	1132(1)	551(3)
Br4	1725	7554(3)	−1292(1)	651(3)
C21	1712(3)	4858(12)	2391(5)	290(23)
C22	1880(3)	6168(12)	3149(6)	356(22)
C23	2354(3)	6090(15)	3842(6)	472(28)
C24	2678(3)	4601(15)	3811(6)	465(41)

Atom	x	y	z	U_{eq}
C25	2530(3)	3224(14)	3077(6)	458(28)
C26	2061(3)	3425(13)	2403(6)	411(25)
C31	733(3)	5389(13)	−2609(6)	342(22)
C32	1084(3)	4129(14)	−2728(7)	482(26)
C33	1269(4)	4135(16)	−3481(7)	494(27)
C34	1089(4)	5590(20)	−4137(8)	661(33)
C35	760(3)	6899(17)	−4040(6)	566(31)
C36	571(3)	6792(13)	−3299(6)	389(24)
F22	1566(2)	7628(9)	3189(3)	630(14)
F23	2500(2)	7349(10)	4548(3)	773(16)
F24	3145(2)	4448(9)	4492(4)	689(19)
F25	2845(2)	1829(9)	3074(4)	759(18)
F26	1930(2)	2111(9)	1700(3)	621(14)
F32	1255(2)	2688(9)	−2086(4)	688(15)
F33	1603(2)	2915(10)	−3583(4)	972(18)
F34	1264(2)	5765(10)	−4879(4)	901(19)
F35	592(2)	8388(9)	−4676(4)	891(21)
F36	227(2)	8122(7)	−3209(3)	634(15)
Cl1	837(3)	68(9)	832(7)	1480(38)
Cl2	131(5)	16(10)	−1333(7)	1965(60)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table A4.3. Complete Distances and Angles for $H_2TFPPBr_8$.

	Distance(Å)		Distance(Å)
N1 –C1	1.366(10)	C36 –F36	1.363(10)
N1 –C4	1.341(10)	Cl1 –C41	1.763
N2 –C6	1.411(10)	Cl2 –C41'	1.728
N2 –C9	1.349(10)	C41 –C41'	1.377
C1 –C2	1.480(11)	C41 –C46	1.369
C2 –C3	1.342(11)	C41' –C43	1.304
C2 –Br1	1.864(8)	C43 –C44	1.388
C3 –C4	1.444(11)	C43 –H43	0.950
C3 –Br2	1.871(8)	C44 –C45	1.378
C4 –C5	1.399(11)	C44 –H44	0.950
C5 –C6	1.411(11)	C45 –C46	1.373
C5 –C21	1.473(11)	C45 –H45	0.950
C6 –C7	1.449(11)	C46 –H46	0.950
C7 –C8	1.355(11)		
C7 –Br3	1.880(8)		
C8 –C9	1.452(11)		
C8 –Br4	1.863(8)		
C9 –C10	1.422(11)		
C10 –C31	1.489(11)		
C21 –C22	1.397(11)		
C21 –C26	1.380(11)		
C22 –C23	1.367(12)		
C22 –F22	1.347(10)		
C23 –C24	1.379(13)		
C23 –F23	1.317(11)		
C24 –C25	1.402(13)		
C24 –F24	1.349(10)		
C25 –C26	1.351(12)		
C25 –F25	1.303(10)		
C26 –F26	1.339(10)		
C31 –C32	1.360(13)		
C31 –C36	1.374(12)		
C32 –C33	1.376(14)		
C32 –F32	1.350(11)		
C33 –C34	1.372(16)		
C33 –F33	1.296(12)		
C34 –C35	1.326(15)		
C34 –F34	1.348(13)		
C35 –C36	1.368(13)		
C35 –F35	1.370(12)		

Angle(°)				Angle(°)			
C4	–N1	–C1	107.7(6)	C26	–C25	–C24	117.6(8)
C9	–N2	–C6	109.8(6)	F25	–C25	–C24	119.0(8)
C2	–C1	–N1	108.2(6)	F25	–C25	–C26	123.4(8)
C3	–C2	–C1	106.4(7)	C25	–C26	–C21	125.1(8)
Br1	–C2	–C1	129.0	F26	–C26	–C21	118.4(7)
Br1	–C2	–C3	124.1	F26	–C26	–C25	116.6(7)
C4	–C3	–C2	107.1(7)	C32	–C31	–C10	123.3(8)
Br2	–C3	–C2	122.0(6)	C36	–C31	–C10	121.6(7)
Br2	–C3	–C4	130.3(6)	C36	–C31	–C32	115.1(8)
C3	–C4	–N1	110.2(6)	C33	–C32	–C31	125.4(9)
C5	–C4	–N1	124.5(7)	F32	–C32	–C31	118.5(8)
C5	–C4	–C3	125.1(7)	F32	–C32	–C33	116.0(8)
C6	–C5	–C4	124.6(7)	C34	–C33	–C32	115.7(10)
C21	–C5	–C4	119.0(7)	F33	–C33	–C32	124.4(9)
C21	–C5	–C6	116.4(7)	F33	–C33	–C34	119.8(10)
C5	–C6	–N2	123.8(7)	C35	–C34	–C33	121.5(11)
C7	–C6	–N2	105.7(6)	F34	–C34	–C33	120.2(10)
C7	–C6	–C5	130.1(7)	F34	–C34	–C35	118.3(10)
C8	–C7	–C6	108.8(7)	C36	–C35	–C34	120.7(10)
Br3	–C7	–C6	127.2(6)	F35	–C35	–C34	121.8(9)
Br3	–C7	–C8	123.4(6)	F35	–C35	–C36	117.5(8)
C9	–C8	–C7	107.4(7)	C35	–C36	–C31	121.5(8)
Br4	–C8	–C7	122.7(6)	F36	–C36	–C31	117.8(7)
Br4	–C8	–C9	129.4(6)	F36	–C36	–C35	120.7(8)
C8	–C9	–N2	108.2(6)	C41'	–C41	–Cl1	124.3
C10	–C9	–N2	123.7(7)	C46	–C41	–Cl1	116.7
C10	–C9	–C8	127.7(7)	C46	–C41	–C41'	119.0
C31	–C10	–C9	118.4(7)	C41	–C41'	–Cl2	116.7
C22	–C21	–C5	121.8(7)	C43	–C41'	–Cl2	119.6
C26	–C21	–C5	123.6(7)	C43	–C41'	–C41	123.7
C26	–C21	–C22	114.6(7)	C44	–C43	–C41'	117.7
C23	–C22	–C21	123.7(8)	H43	–C43	–C41'	121.5
F22	–C22	–C21	118.6(7)	H43	–C43	–C44	120.8
F22	–C22	–C23	117.7(7)	C45	–C44	–C43	121.2
C24	–C23	–C22	118.3(8)	H44	–C44	–C43	119.4
F23	–C23	–C22	122.2(8)	H44	–C44	–C45	119.4
F23	–C23	–C24	119.6(8)	C46	–C45	–C44	119.1
C25	–C24	–C23	120.8(8)	H45	–C45	–C44	120.5
F24	–C24	–C23	120.2(8)	H45	–C45	–C46	120.5
F24	–C24	–C25	119.1(8)	C45	–C46	–C41	119.3

	Angle(°)
H46 –C46 –C41	119.8
H46 –C46 –C45	120.8

Table A4.4. Observed and Calculated Structure Factors for $H_2TFPPBr_8$. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

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h	-8	0	
0	380	349	6
2	207	266	-7
4	81	113	-1
6	317	261	9
h	-8	1	
-6	269	111	18
-4	-52	207	-13
-2	327	289	6
0	323	122	29
2	116	262	-12
4	320	239	12
6	244	137	11
h	-8	2	
-6	316	248	11
-4	280	54	22
-2	238	152	8
0	-179	114	-12
2	-231	28	-10
4	-202	64	-10
h	-8	3	
-6	-204	78	-13
-4	309	267	6
-2	-182	66	-7
0	-39	93	-2
2	173	99	3
h	-8	4	
-4	177	165	1
-2	97	125	-1
h	-7	0	
1	289	191	16
3	525	453	23
5	200	217	-2
7	270	265	0
9	230	274	-7
11	117	258	-16
13	123	217	-9
15	220	184	4
h	-7	1	
-15	164	219	-6
-13	-46	157	-8
-11	356	220	25
-9	-130	151	-13
-7	39	106	-3
-5	368	303	15
-3	307	352	-10
-1	340	405	-11
1	56	208	-8
3	-156	47	-8
5	378	380	0
7	164	274	-15
9	238	279	-6
11	138	65	4
13	353	279	14
15	110	150	-2
h	-7	2	
-17	205	115	8
-15	278	214	8
-13	405	402	0
-11	-88	118	-7
-9	-19	97	-3
-7	258	308	-9
-5	237	127	14
-3	255	160	13
-1	415	430	-2
1	-187	126	-9
3	132	0	4
5	292	275	2
7	248	243	0
9	-113	47	-4
11	237	288	-7
13	292	347	-9
h	-7	3	
-17	235	175	7
-15	-199	24	-12
-13	198	195	0
-11	186	249	-9
-9	345	187	28
-7	169	152	1
-5	308	253	10
-3	135	227	-9
-1	370	294	9
1	194	233	-3
3	259	242	2
5	196	229	-3
7	245	124	12
9	89	75	0
11	221	122	9
13	223	252	-3
h	-7	4	
-17	65	89	-1
-15	178	234	-7
-13	318	365	-9
-11	-110	111	-8
-9	82	140	-4
-7	380	348	7
-5	377	338	8
-3	344	303	7
-1	221	175	3
1	-301	92	-19
3	329	272	7
5	241	256	-1
7	418	384	7
9	-220	119	-16
11	301	280	3
h	-7	5	
-15	93	190	-8
-13	179	152	2
-11	318	351	-6
-9	84	71	0
-7	156	98	4
-5	253	183	9
-3	422	417	0
-1	191	109	5
1	-41	194	-8
3	-241	94	-13
5	418	301	19
7	281	283	0
9	282	296	-2
h	-7	6	
-15	65	206	-11
-13	149	274	-15
-11	-127	89	-7
-9	133	250	-13
-7	180	231	-5
-5	246	283	-5
-3	-173	61	-7
-1	507	479	5
1	293	106	15
3	-259	256	-24
5	236	292	-6
7	231	267	-3
h	-7	7	
-13	191	167	2
-11	185	243	-7
-9	216	188	3
-7	187	274	-10
-5	-173	26	-7
-3	208	121	5
-1	111	116	0
1	206	140	4
3	403	309	13
5	229	159	5
h	-7	8	
-13	188	201	-1
-11	162	199	-3
-9	-153	201	-17
-7	209	228	-2
-5	217	183	3
-3	319	230	10
-1	276	234	4
1	-177	70	-7
3	-143	158	-8
h	-7	9	
-9	142	186	-3
-7	46	100	-1
-5	225	174	4
-3	460	328	21
h	-6	0	
0	457	442	5
2	368	413	-14
4	334	342	-2
6	675	703	-13
8	285	260	5
10	161	110	5
12	519	543	-9
14	230	166	8
16	112	143	-2
18	141	143	0
20	237	293	-8
h	-6	1	
-20	180	193	-1
-18	320	206	19
-16	169	217	-6
-14	179	146	3
-12	381	317	17
-10	671	717	-21
-8	299	346	-12
-6	276	352	-19
-4	215	285	-15
-2	626	567	26
0	463	399	22
2	455	380	21
4	714	732	-8
6	401	413	-3
8	512	483	10
10	282	274	1
12	357	356	0
14	193	201	0
16	484	459	7
18	351	313	7
20	58	160	-6
h	-6	2	
-22	179	178	0
-20	333	285	9
-18	330	292	7
-16	131	128	0
-14	541	490	18
-12	314	304	2
-10	138	150	-1
-8	399	410	-3
-6	328	310	4
-4	110	247	-20
-2	453	488	-11
0	148	119	2
2	301	346	-8
4	332	289	9
6	473	468	1
8	438	466	-8
10	108	29	3
12	148	156	0
14	468	429	11
16	252	226	3
18	396	359	8
h	-6	3	
-22	164	253	-10
-20	482	390	24
-18	-67	111	-5
-16	341	289	11
-14	63	34	1
-12	402	409	-2
-10	390	427	-11
-8	342	342	0
-6	423	441	-6
-4	703	739	-16
-2	610	679	-24
0	225	200	3
2	276	208	8
4	353	238	21
6	270	275	0
8	330	442	-28
10	458	447	3
12	185	244	-8
14	226	326	-16
16	298	365	-12
18	168	213	-4
h	-6	4	
-22	406	465	-14
-20	149	265	-14
-18	-118	151	-12
-16	126	194	-7
-14	368	370	0
-12	463	460	0
-10	348	332	4
-8	150	146	0
-6	372	324	13
-4	654	685	-13
-2	453	516	-16
0	624	588	13
2	-236	235	-26
4	223	142	8
6	262	322	-10
8	294	239	9
10	282	264	3
12	416	424	-2
14	273	294	-3
16	101	238	-12
h	-6	5	
-22	-118	214	-17
-20	72	76	0
-18	278	210	11
-16	143	215	-8
-14	162	173	-1
-12	-156	106	-13
-10	290	370	-19
-8	490	457	11
-6	244	221	3
-4	263	319	-10
-2	538	521	4
0	315	356	-9

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2	476	429	9
4	652	613	11
6	197	232	-4
8	212	328	-17
10	-209	53	-13
12	341	323	3
14	-39	155	-7
16	392	407	-3
h	-6	6	
-22	-57	100	-3
-20	249	174	9
-18	284	208	12
-16	200	217	-2
-14	557	539	6
-12	245	272	-5
-10	220	179	6
-8	205	201	0
-6	217	248	-4
-4	-47	125	-5
-2	-167	231	-19
0	213	246	-5
2	439	386	10
4	200	250	-5
6	640	656	-4
8	373	436	-12
10	224	128	8
12	171	61	6
14	543	498	11
h	-6	7	
-20	195	66	10
-18	-219	162	-23
-16	333	324	1
-14	379	324	13
-12	544	552	-2
-10	468	434	10
-8	312	309	0
-6	217	36	14
-4	388	434	-10
-2	345	322	3
0	-80	201	-16
2	303	295	1
4	329	91	22
6	355	266	12
8	476	448	5
10	462	445	3
12	189	177	1
h	-6	8	
-20	357	440	-18
-18	362	370	-1
-16	230	236	0
-14	260	215	7
-12	-94	171	-12
-10	312	279	6
-8	260	210	7
-6	-48	161	-8
-4	221	189	3
-2	337	277	8
0	495	496	0
2	261	67	15
4	240	255	-1
6	356	308	6
8	246	260	-1
10	-253	228	-24
h	-6	9	
-18	266	219	6
-16	158	109	4
-14	246	169	9
-12	54	140	-5
-10	257	154	12
-8	407	352	11

-6	261	257	0
-4	178	269	-9
-2	436	416	3
0	189	124	6
2	369	358	1
4	395	346	7
6	28	115	-2
8	79	155	-3
h	-6	10	
-18	234	160	8
-16	372	323	9
-14	-32	219	-13
-12	-224	238	-30
-10	107	161	-3
-8	289	352	-10
-6	135	135	0
-4	179	165	1
-2	418	345	12
0	217	226	-1
2	219	175	4
4	98	88	0
h	-6	11	
-14	195	231	-4
-12	158	212	-5
-10	307	348	-6
-8	208	225	-1
-6	266	138	11
-4	81	243	-11
-2	288	290	0
0	389	445	-14
h	-6	12	
-8	213	126	6
-6	231	16	11
h	-5	0	
1	548	481	33
3	773	739	20
5	562	563	0
7	979	988	-5
9	293	348	-16
11	228	145	14
13	330	252	19
15	602	567	15
17	143	132	1
19	286	227	10
21	421	411	2
23	21	212	-13
h	-5	1	
-25	431	434	0
-23	272	217	8
-21	268	240	4
-19	161	139	2
-17	295	312	-3
-15	386	374	3
-13	341	255	22
-11	440	492	-21
-9	633	598	18
-7	276	265	3
-5	633	638	-2
-3	729	686	25
-1	559	525	14
1	524	500	7
3	261	231	7
5	566	567	0
7	413	405	2
9	324	286	10
11	691	703	-6
13	822	803	9
15	299	215	17

17	711	737	-11
19	484	522	-12
21	311	298	2
23	563	535	8
h	-5	2	
-25	189	99	7
-23	507	491	4
-21	445	456	-3
-19	-77	163	-11
-17	535	560	-9
-15	510	490	7
-13	783	770	7
-11	763	770	-4
-9	837	869	-18
-7	395	370	9
-5	122	172	-7
-3	107	203	-15
-1	589	579	3
1	726	631	33
3	137	120	1
5	401	401	0
7	385	381	1
9	329	404	-23
11	664	698	-16
13	543	550	-2
15	398	432	-10
17	202	218	-2
19	333	395	-14
21	452	468	-4
23	291	269	3
h	-5	3	
-25	197	200	0
-23	453	457	-1
-21	141	8	7
-19	565	560	1
-17	499	557	-22
-15	327	348	-6
-13	611	598	6
-11	605	608	-1
-9	391	412	-7
-7	566	573	-3
-5	575	599	-12
-3	-70	70	-4
-1	532	619	-27
1	-378	350	5
3	795	753	19
5	768	798	-15
7	412	473	-20
9	484	503	-6
11	378	357	6
13	336	338	0
15	338	405	-17
17	35	283	-25
19	288	166	17
21	-226	75	-16
h	-5	4	
-25	311	221	14
-23	466	443	6
-21	303	282	4
-19	175	249	-11
-17	347	342	1
-15	739	733	2
-13	151	250	-17
-11	114	134	-2
-9	416	390	9
-7	649	686	-19
-5	378	380	0
-3	819	864	-23
-1	631	629	0
1	277	152	15
3	488	465	6
5	463	472	-2

7	537	527	3
9	-171	125	-17
11	230	206	3
13	106	98	0
15	650	676	-9
17	-60	170	-9
19	391	434	-9
21	382	253	22
h	-5	5	
-25	454	418	9
-23	207	260	-8
-21	191	261	-11
-19	269	229	7
-17	231	356	-28
-15	488	492	-1
-13	282	308	-6
-11	539	499	17
-9	269	335	-18
-7	328	320	2
-5	495	534	-15
-3	640	600	16
-1	812	845	-13
1	969	1004	-15
3	352	463	-26
5	431	381	13
7	608	574	12
9	619	622	-1
11	303	413	-25
13	491	479	3
15	371	350	4
17	427	370	12
19	196	203	0
h	-5	6	
-25	136	93	3
-23	250	224	4
-21	322	236	16
-19	-197	109	-18
-17	62	112	-3
-15	716	712	2
-13	348	369	-6
-11	184	123	8
-9	891	904	-7
-7	520	526	-2
-5	520	516	1
-3	-69	49	-2
-1	734	723	4
1	449	501	-13
3	310	344	-6
5	664	658	2
7	638	609	10
9	398	325	16
11	174	263	-11
13	293	335	-7
15	539	552	-3
17	203	226	-2
h	-5	7	
-25	-190	122	-15
-23	420	426	-1
-21	300	232	12
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-5	389	408	-5
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-5	304	335	-4
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18	315	322	-1
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-26	270	398	-26
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-16	209	237	-5
-14	613	637	-13
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18	384	405	-6
20	52	163	-8
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8	392	416	-8
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16	479	491	-4
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12	527	514	4
14	738	716	9
16	108	337	-30
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20	356	374	-3

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13	884	904	-13
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-13	306	328	-9
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-9	688	700	-9

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13	706	740	-16
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Tetrakis(Pentafluorophenyl)Octabromo Porphyrin Page 7

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-9	1676	1705	-16
-7	1892	1914	-10
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-3	1051	1065	-9
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13	857	853	2
15	852	836	8
17	586	656	-29
19	413	396	4
21	214	163	6
23	231	254	-3
25	284	201	10

h 1 7

-31	519	495	7
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-15	353	353	0
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-11	374	413	-21
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-7	1502	1479	13
-5	921	931	-7
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5	1521	1507	7
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13	839	815	11
15	215	254	-6
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19	318	287	5
21	503	511	-2
23	470	529	-14

h 1 8

-31	-73	136	-7
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-17	551	522	15
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-13	343	361	-7
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-9	863	873	-7
-7	1818	1844	-13
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7	1215	1184	16
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11	582	547	13
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17	292	321	-5
19	612	565	13
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h 1 9

-31	271	318	-8
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-27	116	155	-3
-25	1156	1126	15
-23	400	336	19
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-11	233	302	-22
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-7	189	205	-3
-5	2695	2740	-15
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17	397	493	-21
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h 1 10

-31	201	93	9
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-27	631	575	21
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-7	1333	1329	2
-5	89	150	-6
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h 1 11

-29	174	234	-7
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-11	195	138	8
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h 1 12

-29	205	61	12
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-23	-53	69	-2
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7	407	464	-13
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h 1 13

-27	383	256	24
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-21	350	385	-8
-19	226	133	12
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-13	400	411	-3
-11	256	322	-13
-9	403	409	-1
-7	244	211	4
-5	1430	1446	-7
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h 1 14

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-23	325	323	0
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-19	198	134	7
-17	-187	215	-27
-15	514	517	-1
-13	475	453	6
-11	163	247	-10
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-7	915	909	2
-5	273	233	6
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1	170	237	-7
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9	293	242	6

h 1 15

-25	369	329	7
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-19	182	271	-11
-17	774	723	19
-15	52	203	-11
-13	309	210	15
-11	-249	145	-23
-9	221	234	-1
-7	505	560	-14
-5	377	414	-8
-3	269	303	-5
-1	-84	199	-13
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h 1 16

-21	291	335	-7
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-17	232	307	-10
-15	950	942	3
-13	424	319	20
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-5	-232	38	-14
-3	-139	77	-6
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1	-142	96	-7

h 1 17

-17	386	285	16
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-9	220	175	4
-7	119	215	-7
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h 2 0

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h 2 1

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26	281	118	22
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h 2 2

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8	2378	2397	-7
10	95	68	3
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14	597	609	-7
16	353	294	19
18	1524	1517	3
20	526	518	3
22	76	185	-11
24	305	341	-7
26	618	576	14
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h 2 3

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-16	1173	1143	19
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-6	1402	1415	-8
-4	1121	1095	19
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20	134	133	0
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h 2 4

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22	431	403	7
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-16	260	274	-4
-14	730	693	26
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-8	1698	1713	-8
-6	1122	1107	10
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-2	1637	1617	10
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h 2 6

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-12	1128	1118	6
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-8	930	908	16
-6	328	337	-4
-4	809	842	-23
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12	423	427	-1
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22	193	207	-1
24	166	196	-2

h 2 7

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h 2 8

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h 2 9

-30	260	291	-5
-28	351	325	5
-26	225	279	-9
-24	177	221	-6
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h 2 10

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-14	495	497	0
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16	262	173	9
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-22	256	293	-7
-20	584	612	-11
-18	262	223	7
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6	417	314	21
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12	471	409	12
14	187	117	4
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-18	419	388	9
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h	2	13	
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-22	320	237	15
-20	654	690	-14
-18	401	472	-21
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17	175	207	-6
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27	103	204	-9
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7	459	408	12
9	633	604	9
11	159	272	-13
13	109	159	-3
15	482	526	-10
h	5	8	
-25	-81	116	-6
-23	324	246	13
-21	530	561	-10
-19	246	269	-4
-17	-81	157	-11
-15	432	430	0
-13	290	221	13
-11	535	512	8
-9	446	416	9
-7	799	795	1
-5	312	268	8
-3	475	450	6
-1	368	488	-27
1	-119	112	-7
3	430	383	9
5	599	580	5
7	572	586	-3
9	193	256	-7
11	94	204	-8
13	149	108	2
15	326	278	6
h	5	9	
-23	214	128	8
-21	233	155	9
-19	180	229	-6
-17	214	214	0
-15	179	134	5
-13	66	142	-5
-11	381	427	-12
-9	86	112	-1
-7	175	94	7
-5	765	744	8
-3	570	576	-1
-1	217	86	11
1	734	608	41
3	157	213	-5
5	290	257	4
7	554	534	4
9	484	501	-3
11	89	161	-4
13	367	220	19
h	5	10	
-23	58	205	-11
-21	314	248	11
-19	-178	112	-14
-17	-41	97	-3
-15	579	511	23
-13	179	262	-12
-11	162	36	8
-9	665	685	-7
-7	350	334	3
-5	-159	37	-7
-3	139	209	-6
-1	606	487	32
1	311	328	-2
3	175	235	-5
5	395	365	5
7	344	273	9
9	345	301	5
h	5	11	
-21	-182	124	-14
-19	484	514	-8
-17	496	432	17
-15	-138	48	-6
-13	335	290	8
-11	-32	77	-2
-9	262	331	-11
-7	289	319	-4
-5	380	330	8
-3	25	159	-6
-1	267	250	2
1	301	261	5
3	509	454	12
5	59	281	-16
7	72	182	-5
h	5	12	
-19	201	190	1
-17	281	218	9
-15	480	458	5
-13	348	311	6
-11	350	247	17
-9	459	509	-11
-7	427	389	7
-5	185	193	0
-3	0	277	-18
-1	402	457	-11
1	303	306	0
3	307	271	5
5	306	210	11
h	5	13	
-17	111	254	-13
-15	96	94	0

Tetrakis(Pentafluorophenyl)Octabromo Porphyrin

-13	-156	111	-9
-11	369	399	-5
-9	265	295	-3
-7	-67	122	-4
-5	443	490	-9
-3	149	310	-16
-1	274	283	-1
h	5	14	
-9	494	424	13
h	6	0	
0	508	517	-3
2	334	329	1
4	238	277	-8
6	613	650	-16
8	183	208	-3
10	81	122	-3
12	491	531	-14
14	105	189	-8
16	195	143	5
18	217	130	9
20	321	317	0
h	6	1	
-20	232	207	3
-18	301	207	15
-16	308	217	16
-14	-128	163	-15
-12	296	276	4
-10	758	753	2
-8	385	359	7
-6	364	374	-3
-4	236	298	-14
-2	606	600	2
0	454	405	17
2	254	363	-24
4	721	732	-5
6	439	438	0
8	507	508	0
10	254	294	-8
12	348	319	6
14	235	223	1
16	476	456	5
18	336	310	5
20	153	156	0
h	6	2	
-22	121	149	-2
-20	136	263	-15
-18	303	268	6
-16	99	99	0
-14	556	557	0
-12	261	272	-2
-10	195	165	4
-8	435	406	10
-6	346	309	10
-4	209	241	-6
-2	443	451	-2
0	230	138	12
2	263	348	-18
4	217	288	-13
6	521	488	12
8	508	510	0
10	-96	28	-3
12	-52	181	-12
14	469	471	0
16	176	235	-7
18	329	350	-4
h	6	3	
-22	211	257	-6
-20	219	382	-29
-18	73	125	-3
-16	244	289	-8
-14	153	82	6
-12	411	403	2
-10	404	443	-12
-8	229	339	-25
-6	424	426	0
-4	672	705	-16
-2	641	702	-25
0	70	184	-9
2	315	255	10
4	196	262	-10
6	85	220	-14
8	398	431	-9
10	491	405	25
12	288	257	5
14	324	336	-2
16	369	342	5
18	253	234	2
h	6	4	
-22	487	469	4
-20	223	251	-4
-18	169	142	2
-16	326	181	26
-14	344	344	0
-12	506	459	16
-10	306	283	5
-8	246	205	7
-6	329	366	-10
-4	659	669	-4
-2	323	464	-34
0	579	581	0
2	143	207	-6
4	133	78	3
6	371	353	4
8	253	243	1
10	284	261	4
12	380	452	-17
14	335	287	8
16	171	253	-9
h	6	5	
-22	351	234	20
-20	220	95	12
-18	216	204	1
-16	234	208	4
-14	242	149	13
-12	164	112	5
-10	351	376	-6
-8	419	425	-2
-6	295	266	6
-4	330	376	-11
-2	520	498	6
0	293	342	-10
2	415	392	4
4	626	627	0
6	226	258	-4
8	279	307	-4
10	119	45	3
12	377	315	12
14	246	169	8
16	295	417	-21
h	6	6	
-22	153	141	1
-20	-167	161	-17
-18	214	204	1
-16	263	233	4
-14	570	559	3
-12	217	252	-6
-10	193	188	0
-8	233	225	1
-6	172	273	-15
-4	160	146	1
-2	349	267	13
0	275	279	0
2	354	408	-9
4	426	239	32
6	625	628	0
8	512	444	16
10	-219	147	-18
12	112	75	1
14	536	471	15
h	6	7	
-20	-130	92	-7
-18	262	165	13
-16	353	314	8
-14	342	293	10
-12	478	563	-27
-10	415	432	-4
-8	321	309	2
-6	268	40	24
-4	442	422	4
-2	300	295	0
0	-89	143	-10
2	307	307	0
4	152	86	3
6	352	242	15
8	451	437	2
10	439	425	2
12	152	195	-3
h	6	8	
-20	391	450	-14
-18	441	361	19
-16	231	243	-1
-14	186	237	-6
-12	227	149	9
-10	244	257	-2
-8	175	209	-4
-6	182	179	0
-4	-87	194	-11
-2	306	287	2
0	504	523	-6
2	119	84	1
4	317	268	6
6	331	300	4
8	146	228	-6
10	160	220	-4
h	6	9	
-18	327	226	16
-16	112	104	0
-14	251	157	12
-12	287	146	19
-10	-141	206	-19
-8	396	353	9
-6	200	253	-6
-4	320	273	7
-2	455	438	3
0	163	119	4
2	307	383	-11
4	305	376	-10
6	224	112	7
8	373	110	26
h	6	10	
-18	270	161	13
-16	297	334	-6
-14	207	215	-1
-12	166	250	-10
-10	94	158	-4
-8	387	353	6
-6	190	137	4
-4	-175	170	-13
-2	354	379	-4
0	88	240	-16
2	209	206	0
4	268	70	14
h	6	11	
-14	254	230	3
-12	124	224	-9
-10	277	337	-9
-8	-68	207	-11
-6	330	129	21
-4	289	274	1
-2	326	272	7
0	337	431	-22
h	6	12	
-8	-47	141	-5
-6	-143	40	-4
h	7	0	
1	200	187	1
3	525	457	22
5	135	162	-2
7	380	289	20
9	197	271	-11
11	161	240	-10
13	158	182	-2
15	308	181	18
h	7	1	
-15	270	231	5
-13	59	151	-6
-11	226	197	4
-9	128	158	-3
-7	142	118	2
-5	411	304	26
-3	243	379	-29
-1	327	400	-17
1	371	260	21
3	-248	58	-21
5	375	375	0
7	314	278	6
9	314	284	5
11	195	129	6
13	328	312	2
15	267	149	14
h	7	2	
-17	-48	92	-3
-15	276	198	11
-13	312	397	-18
-11	-99	77	-5
-9	-127	109	-9
-7	321	309	2
-5	-138	108	-10
-3	69	157	-6
-1	471	437	8
1	187	176	0
3	133	3	5
5	333	275	11
7	223	243	-2
9	175	28	9
11	337	266	12
13	348	359	-2
h	7	3	
-17	259	152	12
-15	248	37	18
-13	380	244	28
-11	271	266	0
-9	291	179	18
-7	116	161	-4
-5	248	237	1
-3	251	241	1

-1	258	276	-2
1	329	244	11
3	305	250	8
5	232	213	2
7	87	144	-3
9	49	70	0
11	243	127	12
13	295	230	9
h	7	4	
-17	189	64	9
-15	-56	205	-13
-13	313	354	-8
-11	208	121	9
-9	260	182	11
-7	269	331	-12
-5	308	338	-5
-3	227	285	-8
-1	210	156	4
1	-227	73	-12
3	396	277	19
5	424	286	26
7	400	395	1
9	178	118	4
11	309	293	2
h	7	5	
-15	205	196	1
-13	230	171	7
-11	378	338	8
-9	95	64	1

-7	165	98	5
-5	-170	179	-18
-3	244	405	-28
-1	-229	91	-13
1	78	229	-8
3	124	82	1
5	337	297	6
7	123	270	-14
9	273	338	-9
h	7	6	
-15	30	189	-10
-13	301	278	4
-11	-143	60	-7
-9	141	267	-15
-7	184	236	-6
-5	244	265	-3
-3	158	63	5
-1	353	477	-20
1	-143	81	-5
3	-169	246	-18
5	297	256	5
7	325	267	8
h	7	7	
-15	-136	24	-5
-13	172	142	2
-11	272	210	9
-9	194	186	0
-7	-40	282	-22
-5	89	83	0

-3	128	133	0
-1	-166	76	-6
1	-201	191	-15
3	-244	279	-25
5	0	179	-6
h	7	8	
-13	305	233	10
-11	-135	237	-20
-9	270	207	8
-7	317	204	15
-5	-69	164	-7
-3	-202	241	-19
-1	222	237	-1
1	-401	50	-32
3	292	138	13
h	7	9	
-9	307	181	16
-7	167	99	4
-5	222	163	5
-3	245	333	-9
h	8	0	
0	328	324	0
2	303	279	4
4	255	148	12
6	205	282	-10
h	8	1	

-6	222	138	8
-4	236	190	5
-2	328	246	14
0	248	116	15
2	213	271	-7
4	338	245	15
6	-44	130	-5
h	8	2	
-6	199	260	-8
-4	-86	55	-3
-2	-145	142	-11
0	176	107	5
2	137	12	4
4	70	67	0
h	8	3	
-6	246	80	15
-4	124	258	-14
-2	-122	31	-3
0	139	99	2
2	-185	66	-8
h	8	4	
-4	132	162	-2
-2	117	115	0

Appendix 5. Supplimentary Material for the X-ray Crystal Structure Determination of NiTFPPBr$_8$.

Figure A5.1. ORTEP diagram for NiTFPPBr$_8$ (50% probability ellipsoids) and numbering scheme for macrocycle.

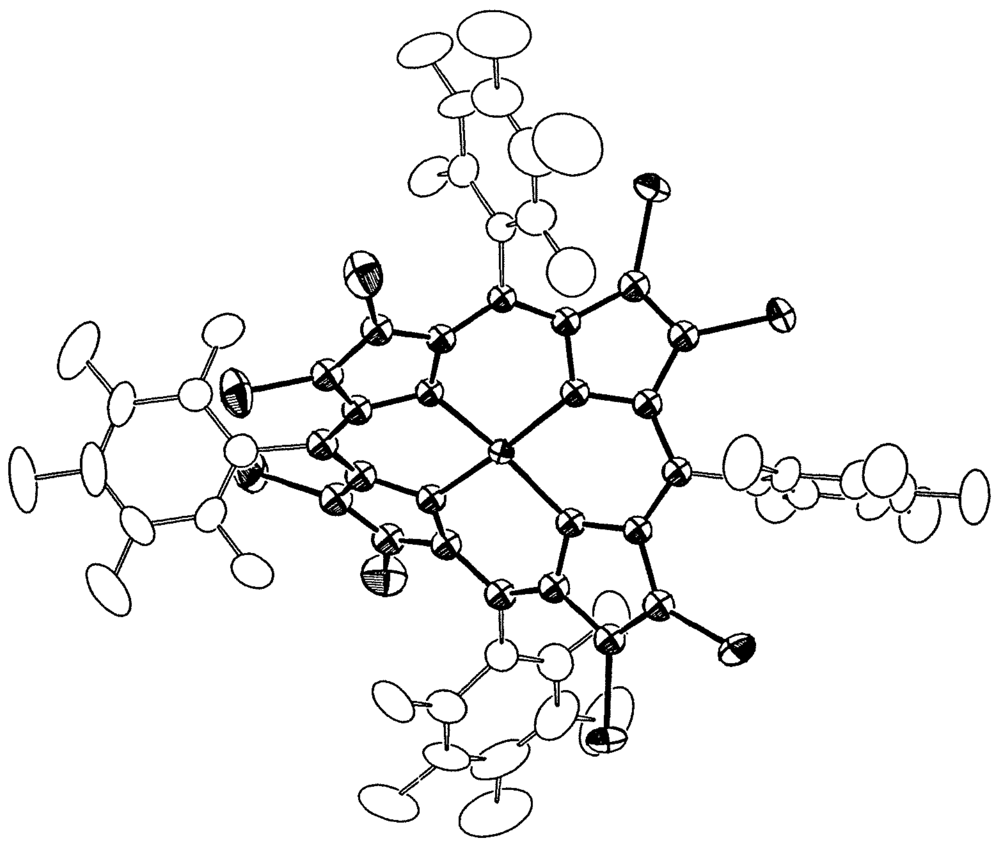

Table A5.1. Crystal and Intensity Collection Data for $NiTFPPBr_8$.

Formula: $NiC_{44}Br_8F_{20}N_4 \cdot \frac{1}{2}CH_2Cl_2$	Formula Weight: 1704.88
Crystal Color: dark purple	Habit: thin parallelepiped
Crystal Size: 0.07 x 0.55 x 0.55 mm	
Crystal System: monoclinic	Space Group: C2/c
$a = 18.178(7)$ Å	$\alpha = 90°$
$b = 22.160(11)$ Å	$\beta = 93.64(4)°$
$c = 24.421(8)$ Å	$\gamma = 90°$
$V = 9818(7)$ Å^3	$Z = 8$
$D = 2.31$ g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 70.2$ cm^{-1}	$T = 295$ K
Enraf-Nonius Cad-4 diffractometer	ω scan
Transmission coeff. =	range for data collection: 1-25°
$h = 0 - 20$, $k = -23 - 26$, $\pm l = 29$	
Number of reflections measured: 16471	
Number of independent reflections: 8602	
Goodness of fit for merging data: 0.95	
$R = 0.042$ on F for 4055 reflections with $F_o^2 > 3\sigma(F_o^2)$	
$wR = 0.005$ on F^2 for 8602 reflections	
Final goodness of fit: 1.22 for 570 parameters and 8602 reflections	

Table A5.2. Final Refined Heavy Atom Parameters x 10^4 for $NiTFPPBr_8$.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq} or B
Ni	3211(.4)	990(.3)	9746(.3)	287(2)
Br1	2973(.4)	3554(.3)	9300(.3)	567(2)
Br2	4338(.4)	3356(.3)	10333(.3)	536(2)
Br3	6243(.4)	918(.3)	10594(.3)	609(2)
Br4	5401(.4)	−372(.3)	11032(.3)	590(2)
Br5	1962(.4)	−611(.4)	11296(.3)	650(2)
Br6	808(.4)	−657(.4)	10119(.3)	640(2)
Br7	1668(.4)	118(.3)	7755(.3)	601(3)
Br8	2181(.4)	1576(.3)	7503(.3)	528(2)
N1	3549(2)	1787(2)	9617(2)	2.4(1)*
N2	3991(2)	873(2)	10293(2)	2.5(1)*
N3	2747(2)	273(2)	9974(2)	2.3(1)*
N4	2559(2)	1028(2)	9104(2)	2.2(1)*
C1	3167(3)	2217(2)	9299(2)	2.3(1)*
C2	3385(3)	2813(3)	9503(3)	2.8(1)*
C3	3935(3)	2737(3)	9887(3)	2.7(1)*
C4	4074(3)	2092(3)	9951(3)	2.7(1)*
C5	4666(3)	1807(3)	10223(2)	2.6(1)*
C6	4653(3)	1191(3)	10316(2)	2.6(1)*

Atom	x	y	z	U_{eq} or B
C7	5226(3)	802(3)	10556(3)	2.9(1) *
C8	4900(3)	301(3)	10733(3)	3.0(1) *
C9	4119(3)	349(3)	10592(2)	2.7(1) *
C10	3544(3)	3(3)	10766(2)	2.6(1) *
C11	2855(3)	15(2)	10493(2)	2.5(1) *
C12	2197(3)	−305(3)	10610(3)	2.9(1) *
C13	1743(3)	−312(3)	10155(3)	2.8(1) *
C14	2093(3)	35(2)	9745(2)	2.3(1) *
C15	1884(3)	93(2)	9196(2)	2.2(1) *
C16	2171(3)	541(3)	8872(2)	2.3(1) *
C17	2022(3)	657(3)	8299(3)	2.8(1) *
C18	2234(3)	1226(3)	8202(3)	2.6(1) *
C19	2547(3)	1472(3)	8710(2)	2.4(1) *
C20	2753(3)	2066(3)	8827(2)	2.4(1) *
C21	5338(4)	2151(3)	10405(3)	3.1(1) *
C22	5765(4)	2426(3)	10036(3)	497(21)
C23	6423(5)	2704(3)	10183(4)	677(30)
C24	6656(5)	2723(4)	10728(5)	838(40)
C25	6248(5)	2467(4)	11116(4)	655(27)

Atom	x	y	z	U_{eq} or B
C26	5584(4)	2192(3)	10962(3)	523(23)
F22	5560(2)	2422(2)	9501(2)	733(14)
F23	6836(3)	2961(2)	9827(2)	1156(19)
F24	7303(3)	2971(2)	10892(2)	1289(22)
F25	6467(3)	2475(2)	11648(2)	1088(17)
F26	5192(2)	1931(2)	11333(2)	695(15)
C31	3695(3)	−375(3)	11268(3)	3.1(1) *
C32	3740(4)	−996(3)	11268(3)	515(23)
C33	3900(4)	−1321(4)	11740(4)	637(27)
C34	3985(4)	−1025(4)	12224(4)	734(29)
C35	3911(5)	−413(4)	12244(3)	797(39)
C36	3771(4)	−102(3)	11763(3)	610(28)
F32	3666(3)	−1281(2)	10790(2)	863(18)
F33	3950(3)	−1909(2)	11730(2)	1245(23)
F34	4126(3)	−1332(2)	12687(2)	1182(19)
F35	3980(4)	−130(2)	12728(2)	1504(31)
F36	3706(3)	498(2)	11794(2)	1066(22)
C41	1325(3)	−336(3)	8942(2)	2.5(1) *
C42	1487(4)	−930(3)	8867(3)	435(20)

Atom	x	y	z	U_{eq} or B
C43	965(6)	−1336(3)	8644(3)	694(30)
C44	277(5)	−1126(5)	8495(4)	835(32)
C45	107(5)	−551(5)	8564(4)	821(33)
C46	621(4)	−155(3)	8791(3)	544(22)
F42	2173(2)	−1130(2)	8996(2)	669(13)
F43	1171(3)	−1908(2)	8566(2)	1108(20)
F44	−206(3)	−1521(3)	8279(3)	1623(23)
F45	−584(3)	−360(3)	8429(2)	1379(24)
F46	422(2)	418(2)	8877(2)	795(14)
C51	2545(4)	2546(3)	8414(3)	2.6(1) *
C52	3047(4)	2812(3)	8107(3)	430(20)
C53	2870(5)	3247(3)	7725(4)	670(28)
C54	2144(6)	3404(3)	7637(3)	686(31)
C55	1624(4)	3146(3)	7931(3)	542(24)
C56	1824(4)	2730(3)	8317(3)	443(21)
F52	3759(2)	2645(2)	8178(2)	676(13)
F53	3375(3)	3512(2)	7442(2)	1040(17)
F54	1945(3)	3816(2)	7248(2)	1050(18)
F55	903(3)	3300(2)	7837(2)	927(15)

Atom	x	y	z	U_{eq} or B
F56	1300(2)	2488(2)	8612(2)	715(13)
CS	0	1890(6)	7500	1339(58)
ClS	38(2)	1464(2)	6925(1)	1750(14)
HS1	−427	2140	7464	12.8 *

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

Table A5.3. Complete Distances and Angles for $NiTFPPBr_8$.

	Distance(Å)		Distance(Å)
Ni –N1	1.902(4)	C17 –C18	1.343(8)
Ni –N2	1.904(4)	C18 –C19	1.439(8)
Ni –N3	1.898(4)	C19 –C20	1.393(8)
Ni –N4	1.906(4)	C20 –C51	1.497(8)
Br1 –C2	1.858(6)	C21 –C22	1.367(10)
Br2 –C3	1.872(6)	C21 –C26	1.407(10)
Br3 –C7	1.863(6)	C22 –C23	1.373(11)
Br4 –C8	1.871(6)	C22 –F22	1.338(8)
Br5 –C12	1.880(6)	C23 –C24	1.373(13)
Br6 –C13	1.861(6)	C23 –F23	1.313(10)
Br7 –C17	1.870(6)	C24 –C25	1.363(13)
Br8 –C18	1.871(6)	C24 –F24	1.336(11)
N1 –C1	1.387(7)	C25 –C26	1.382(11)
N1 –C4	1.392(7)	C25 –F25	1.334(10)
N2 –C6	1.391(7)	C26 –F26	1.322(8)
N2 –C9	1.383(7)	C31 –C32	1.380(9)
N3 –C11	1.395(7)	C31 –C36	1.351(10)
N3 –C14	1.385(7)	C32 –C33	1.374(11)
N4 –C16	1.390(7)	C32 –F32	1.325(8)
N4 –C19	1.376(7)	C33 –C34	1.353(12)
C1 –C2	1.458(8)	C33 –F33	1.305(10)
C1 –C20	1.378(8)	C34 –C35	1.365(12)
C2 –C3	1.337(8)	C34 –F34	1.330(10)
C3 –C4	1.457(8)	C35 –C36	1.372(11)
C4 –C5	1.381(8)	C35 –F35	1.338(10)
C5 –C6	1.384(8)	C36 –F36	1.338(9)
C5 –C21	1.485(9)	C41 –C42	1.364(9)
C6 –C7	1.446(8)	C41 –C46	1.369(9)
C7 –C8	1.344(8)	C42 –C43	1.392(11)
C8 –C9	1.443(8)	C42 –F42	1.342(8)
C9 –C10	1.385(8)	C43 –C44	1.362(13)
C10 –C11	1.380(8)	C43 –F43	1.339(10)
C10 –C31	1.495(9)	C44 –C45	1.325(13)
C11 –C12	1.436(8)	C44 –F44	1.325(11)
C12 –C13	1.342(8)	C45 –C46	1.373(12)
C13 –C14	1.441(8)	C45 –F45	1.347(11)
C14 –C15	1.377(8)	C46 –F46	1.340(8)
C15 –C16	1.392(8)	C51 –C52	1.351(9)
C15 –C41	1.496(8)	C51 –C56	1.378(9)
C16 –C17	1.432(8)	C52 –C53	1.366(11)

		Distance(Å)
C52	–F52	1.348(8)
C53	–C54	1.369(12)
C53	–F53	1.323(10)
C54	–C55	1.350(12)
C54	–F54	1.351(10)
C55	–C56	1.352(10)
C55	–F55	1.360(9)
C56	–F56	1.342(8)
CS	–ClS	1.696(14)
CS	–HS1	0.953

			Angle(°)
N1	–Ni	–N2	90.5(2)
N1	–Ni	–N3	168.4(2)
N1	–Ni	–N4	90.8(2)
N2	–Ni	–N3	90.3(2)
N2	–Ni	–N4	168.5(2)
N3	–Ni	–N4	90.8(2)
C4	–N1	–C1	107.1(4)
C9	–N2	–C6	106.7(4)
C14	–N3	–C11	106.2(4)
C19	–N4	–C16	106.6(4)
C2	–C1	–N1	108.5(5)
C20	–C1	–N1	122.0(5)
C20	–C1	–C2	128.8(5)
C3	–C2	–C1	107.4(5)
C4	–C3	–C2	108.4(5)
C3	–C4	–N1	107.8(5)
C5	–C4	–N1	122.9(5)
C5	–C4	–C3	128.7(5)
C6	–C5	–C4	120.7(5)
C21	–C5	–C4	120.6(5)
C21	–C5	–C6	118.7(5)
C5	–C6	–N2	121.1(5)
C7	–C6	–N2	108.3(5)
C7	–C6	–C5	129.3(5)
C8	–C7	–C6	107.5(5)
C9	–C8	–C7	108.0(5)
C8	–C9	–N2	108.5(5)
C10	–C9	–N2	121.5(5)
C10	–C9	–C8	129.5(5)
C11	–C10	–C9	121.3(5)
C31	–C10	–C9	117.3(5)
C31	–C10	–C11	121.3(5)
C10	–C11	–N3	121.2(5)
C12	–C11	–N3	108.2(5)
C12	–C11	–C10	129.6(5)
C13	–C12	–C11	108.5(5)
C14	–C13	–C12	107.1(5)
C13	–C14	–N3	109.2(5)
C15	–C14	–N3	122.3(5)
C15	–C14	–C13	128.2(5)

Angle(°)		Angle(°)	
C16 –C15 –C14	121.9(5)	F33 –C33 –C34	119.6(7)
C41 –C15 –C14	118.8(5)	C35 –C34 –C33	120.5(8)
C41 –C15 –C16	119.2(5)	F34 –C34 –C33	120.1(8)
C15 –C16 –N4	121.5(5)	F34 –C34 –C35	119.4(8)
C17 –C16 –N4	108.6(5)	C36 –C35 –C34	118.8(8)
C17 –C16 –C15	129.0(5)	F35 –C35 –C34	119.7(8)
C18 –C17 –C16	107.6(5)	F35 –C35 –C36	121.5(8)
C19 –C18 –C17	107.9(5)	C35 –C36 –C31	123.0(7)
C18 –C19 –N4	108.6(5)	F36 –C36 –C31	119.4(6)
C20 –C19 –N4	122.7(5)	F36 –C36 –C35	117.6(7)
C20 –C19 –C18	128.5(5)	C42 –C41 –C15	121.5(5)
C19 –C20 –C1	121.7(5)	C46 –C41 –C15	121.6(6)
C51 –C20 –C1	119.6(5)	C46 –C41 –C42	116.9(6)
C51 –C20 –C19	118.6(5)	C43 –C42 –C41	122.0(6)
C22 –C21 –C5	121.5(6)	F42 –C42 –C41	119.4(6)
C26 –C21 –C5	121.8(6)	F42 –C42 –C43	118.6(6)
C26 –C21 –C22	116.7(6)	C44 –C43 –C42	118.3(8)
C23 –C22 –C21	123.4(7)	F43 –C43 –C42	118.5(7)
F22 –C22 –C21	120.4(6)	F43 –C43 –C44	123.1(8)
F22 –C22 –C23	116.2(7)	C45 –C44 –C43	120.9(9)
C24 –C23 –C22	118.4(8)	F44 –C44 –C43	117.0(8)
F23 –C23 –C22	123.3(8)	F44 –C44 –C45	122.1(9)
F23 –C23 –C24	118.3(8)	C46 –C45 –C44	120.5(9)
C25 –C24 –C23	121.0(9)	F45 –C45 –C44	119.6(8)
F24 –C24 –C23	120.9(8)	F45 –C45 –C46	119.9(8)
F24 –C24 –C25	118.0(8)	C45 –C46 –C41	121.5(7)
C26 –C25 –C24	119.8(8)	F46 –C46 –C41	119.6(6)
F25 –C25 –C24	121.9(8)	F46 –C46 –C45	118.9(7)
F25 –C25 –C26	118.3(7)	C52 –C51 –C20	122.2(6)
C25 –C26 –C21	120.7(7)	C56 –C51 –C20	121.5(6)
F26 –C26 –C21	118.9(6)	C56 –C51 –C52	116.4(6)
F26 –C26 –C25	120.3(7)	C53 –C52 –C51	123.3(7)
C32 –C31 –C10	124.5(6)	F52 –C52 –C51	119.2(6)
C36 –C31 –C10	119.1(6)	F52 –C52 –C53	117.5(6)
C36 –C31 –C32	116.3(6)	C54 –C53 –C52	118.0(8)
C33 –C32 –C31	122.2(7)	F53 –C53 –C52	122.0(7)
F32 –C32 –C31	118.2(6)	F53 –C53 –C54	120.0(8)
F32 –C32 –C33	119.6(6)	C55 –C54 –C53	120.6(8)
C34 –C33 –C32	119.1(8)	F54 –C54 –C53	119.7(8)
F33 –C33 –C32	121.3(7)	F54 –C54 –C55	119.7(7)

Angle(°)

C56 –C55 –C54	119.6(7)
F55 –C55 –C54	120.3(7)
F55 –C55 –C56	120.1(7)
C55 –C56 –C51	122.1(6)
F56 –C56 –C51	119.3(6)
F56 –C56 –C55	118.6(6)
ClS –CS –ClS′	112.4(8)
ClS –CS –HS1	108.8
ClS′ –CS –HS1	108.8
HS1 –CS –HS1′	109.0

Table A5.4. Observed and Calculated Structure Factors for $NiTFPPBr_8$. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

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-21	1	1	
1	162	26	0
2	662	503	6
3	507	36	8
4	-463	30	-7
5	580	395	6
6	448	67	6
7	548	324	6
8	483	579	-3
-21	3	1	
1	451	4	7
2	762	45	20
3	542	194	9
4	-269	20	-2
5	677	521	6
6	744	380	13
7	563	394	5
-21	5	1	
1	-212	4	-1
2	563	469	3
3	294	215	1
4	-332	411	-9
5	-218	627	-16
-20	0	1	
2	1431	1395	3
4	1419	1308	10
6	685	544	6
8	500	307	5
10	397	619	-8
12	894	616	13
-20	2	1	
1	1098	1164	-5
2	961	843	7
3	920	781	8
4	458	697	-10
5	358	38	4
6	-617	82	-13
7	338	38	4
8	564	146	10
9	463	164	6
10	624	501	4
11	217	505	-6
12	-597	403	-16
-20	4	1	
1	647	563	3
2	-240	401	-8
3	575	188	10
4	509	415	3
5	-337	68	-4
6	366	31	4
7	566	338	7
8	-326	30	-3
9	-274	45	-2
10	-103	312	-3
11	482	448	1
-20	6	1	
1	809	477	14
2	1080	922	10
3	551	48	10
4	-629	180	-15
5	358	230	2
6	103	253	-1
7	534	116	9
8	664	510	6
9	637	504	4
10	548	142	9
-20	8	1	
1	-220	325	-5
2	489	688	-7
3	711	583	5
4	816	310	19
5	873	805	3
6	-748	256	-20
7	763	364	15
8	-651	73	-13
-19	1	1	
1	-464	111	-13
2	647	351	17
3	164	294	-3
4	437	547	-6
5	317	282	1
6	1341	1174	22
7	481	218	10
8	1006	951	4
9	508	253	7
10	1220	1060	13
11	44	11	0
12	-276	25	-2
13	-461	20	-8
14	-750	51	-18
15	817	204	20
-19	3	1	
1	383	258	4
2	-91	20	0
3	371	172	6
4	278	405	-5
5	435	241	7
6	501	631	-8
7	336	707	-14
8	-102	120	0
9	938	943	0
10	-642	39	-15
11	-617	388	-18
12	309	273	0
13	552	237	8
14	-292	215	-4
-19	5	1	
1	400	263	5
2	555	29	17
3	-448	18	-11
4	1135	1007	14
5	280	131	2
6	877	906	-2
7	392	75	5
8	931	919	0
9	434	296	3
10	-503	88	-9
11	-241	301	-5
12	134	239	-1
13	-544	17	-9
14	108	84	0
-19	7	1	
1	-404	82	-6
2	441	189	6
3	-441	49	-8
4	951	567	22
5	248	34	2
6	346	40	4
7	462	676	-8
8	833	844	0
9	985	630	19
10	691	694	0
11	807	788	0
12	-615	280	-14
13	565	285	7
-19	9	1	
1	496	228	7
2	880	799	4
3	-339	109	-4
4	404	677	-10
5	419	396	0
6	589	346	7
7	338	440	-2
8	727	414	12
9	632	581	2
10	207	317	-1
11	728	327	13
-19	11	1	
1	731	398	12
2	-611	40	-12
3	-101	87	0
4	235	113	1
5	431	405	0
6	578	254	9
7	314	187	2
8	510	123	7
-18	0	1	
2	953	730	22
4	876	1026	-17
6	-227	299	-8
8	-80	245	-3
10	473	298	7
12	-333	14	-4
14	717	517	10
16	-559	1	-10
-18	2	1	
1	-213	556	-23
2	689	419	18
3	350	331	0
4	947	860	9
5	270	142	3
6	1117	1294	-24
7	811	279	35
8	580	682	-7
9	578	549	1
10	-298	268	-9
11	961	927	3
12	-171	44	-1
13	-106	225	-2
14	490	236	6
15	532	265	7
16	-206	168	-2
17	618	72	11
-18	4	1	
1	735	526	16
2	336	212	4
3	888	781	10
4	457	407	2
5	1061	986	8
6	-240	228	-6
7	550	734	-13
8	-119	138	-1
9	1107	1007	11
10	-290	189	-6
11	-188	429	-9
12	-733	397	-26
13	110	181	0
14	605	281	9
15	-298	369	-7
16	-356	84	-4
-18	6	1	
1	521	243	12
2	988	1029	-4
3	674	371	18
4	654	723	-5
5	429	249	7
6	904	726	16
7	-205	262	-6
8	778	490	20
9	-253	198	-5
10	-617	82	-14
11	873	84	28
12	-147	58	0
13	411	281	3
14	680	27	15
15	277	319	0
16	901	389	20
-18	8	1	
1	470	303	7
2	64	285	-4
3	543	33	17
4	-287	523	-20
5	845	915	-6
6	696	593	7
7	-787	265	-26
8	1160	786	27
9	-451	318	-11
10	597	516	3
11	482	175	6
12	-66	73	0
13	-684	184	-19
14	518	34	8
-18	10	1	
1	336	171	3
2	1340	1158	16
3	309	391	-2
4	808	931	-7
5	234	231	0
6	1250	932	25
7	186	477	-7
8	-420	524	-15
9	752	367	14
10	679	264	13
11	747	603	6
12	-94	345	-4
13	-516	17	-8
-18	12	1	
1	745	426	13
2	-418	269	-8
3	-788	71	-21
4	993	666	18
5	774	518	11
6	-677	219	-17
7	-285	165	-3
8	451	133	6
9	416	277	3
10	571	586	0
-18	14	1	
1	1067	813	15
2	970	458	24
3	425	80	5
4	446	406	1
5	434	259	-4
-17	1	1	
1	-277	325	-13
2	508	508	0

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3	351	123	7
4	909	878	3
5	327	171	5
6	1455	1448	1
7	-335	534	-25
8	601	816	-19
9	1230	1336	-15
10	732	726	0
11	781	579	16
12	531	328	11
13	516	484	1
14	282	83	3
15	700	586	5
16	382	290	2
17	606	807	-8
18	809	646	7
19	729	369	11

-17 3 l

1	1235	1198	5
2	572	434	9
3	583	516	4
4	700	131	31
5	255	506	-12
6	450	689	-17
7	533	530	0
8	-279	223	-8
9	1158	1062	12
10	666	982	-30
11	762	697	5
12	617	620	0
13	769	520	17
14	746	599	7
15	742	862	-6
16	148	409	-4
17	499	810	-12
18	477	282	4

-17 5 l

1	2034	2020	2
2	1655	1739	-16
3	964	1028	-7
4	849	809	4
5	-298	29	-5
6	667	661	0
7	1438	1547	-18
8	-327	27	-6
9	1472	1559	-14
10	-503	110	-15
11	-480	36	-13
12	122	315	-4
13	423	451	-1
14	-113	225	-2
15	209	207	0
16	475	298	4
17	570	506	2
18	-39	142	0

-17 7 l

1	598	575	1
2	504	345	9
3	902	1000	-11
4	554	584	-2
5	802	889	-8
6	857	843	1
7	64	39	0
8	-128	93	-1
9	907	785	11
10	663	625	2
11	670	484	11
12	748	810	-3
13	599	741	-6
14	816	174	23
15	569	621	-2
16	252	126	1
17	-834	54	-21

-17 9 l

1	597	500	6
2	1214	1236	-3
3	336	508	-8
4	681	821	-12
5	-247	183	-5
6	221	173	1
7	473	8	12
8	477	217	10
9	524	498	1
10	-245	177	-3
11	-174	100	-1
12	-754	305	-24
13	478	702	-8
14	613	598	0
15	1277	1198	6
16	-246	133	-2

-17 11 l

1	489	27	13
2	1435	1429	0
3	-608	120	-21
4	814	854	-3
5	-212	454	-14
6	288	419	-5
7	653	157	16
8	-470	378	-13
9	435	77	6
10	651	238	13
11	-581	174	-14
12	697	266	14
13	426	358	1
14	732	345	13

-17 13 l

1	325	322	0
2	988	996	0
3	585	306	9
4	474	609	-5
5	524	216	8
6	-335	3	-4
7	1008	874	8
8	-227	71	-2
9	481	409	2
10	161	136	0
11	330	20	3
12	623	294	9

-17 15 l

1	477	293	4
2	553	150	11
3	-316	37	-3
4	472	686	-8
5	546	40	10
6	246	187	0
7	-441	365	-10
8	416	257	3

-16 0 l

2	1215	881	48
4	1495	1664	-34
6	1007	956	6
8	1127	1010	16
10	490	372	6
12	1774	1426	59
14	282	188	2
16	-77	405	-9
18	611	191	11
20	827	778	2

-16 2 l

1	299	269	1
2	392	529	-9
3	881	748	15
4	562	526	2
5	837	671	17
6	141	242	-2
7	407	14	11
8	-487	320	-23
9	623	345	18
10	-290	275	-10
11	1188	1207	-2
12	338	477	-7
13	204	113	1
14	363	191	5
15	-335	145	-7
16	723	671	3
17	726	487	10
18	-295	41	-3
19	497	543	-1
20	-541	168	-9

-16 4 l

1	865	902	-4
2	2026	2088	-14
3	889	693	21
4	1031	1002	3
5	910	896	1
6	671	683	-1
7	1084	934	19
8	978	902	9
9	-596	34	-22
10	1110	900	26
11	322	166	4
12	854	875	-2
13	-602	129	-21
14	-419	50	-9
15	1198	1033	19
16	-603	188	-14
17	-783	177	-22
18	595	470	4
19	487	7	7
20	631	137	11

-16 6 l

1	1390	1338	8
2	288	458	-8
3	1337	1385	-8
4	460	413	2
5	-461	153	-16
6	1070	1125	-7
7	-292	72	-5
8	361	25	8
9	-458	100	-15
10	647	518	9
11	475	416	3
12	471	580	-6
13	1102	1111	-1
14	435	111	10
15	692	626	3
16	973	747	13
17	631	585	1
18	708	197	14
19	527	372	4

-16 8 l

1	475	61	14
2	484	138	14
3	545	449	6
4	686	486	15
5	412	459	-2
6	339	51	7
7	1031	1013	2
8	656	716	-4
9	360	22	7
10	707	432	18
11	495	74	15
12	-611	178	-22
13	701	542	10
14	594	181	12
15	375	368	0
16	1020	772	14
17	-418	515	-14
18	450	266	4

-16 10 l

1	274	273	0
2	192	235	-1
3	175	280	-3
4	-168	442	-14
5	508	34	16
6	1272	1274	0
7	581	426	9
8	806	711	8
9	601	534	4
10	260	227	0
11	-517	230	-17
12	726	341	15
13	-308	118	-4
14	452	422	0
15	829	425	16
16	340	537	-5
17	278	444	-3

-16 12 l

1	709	747	-3
2	1016	1014	0
3	287	387	-3
4	346	436	-4
5	-278	581	-25
6	378	304	2
7	1418	1345	10
8	1250	1190	7
9	1066	1070	0
10	251	34	2
11	597	539	2
12	909	549	18
13	730	855	-6
14	872	342	21
15	-740	300	-20

-16 14 l

1	789	424	17
2	-714	162	-20
3	826	953	-8
4	160	295	-2
5	606	214	12
6	-150	378	-7
7	949	735	13
8	245	277	0
9	-209	3	-1
10	932	610	16
11	970	723	13
12	585	316	8
13	-458	142	-7

-16 16 l

1	565	109	12
2	-371	140	-5
3	248	195	0
4	420	405	0
5	933	863	4
6	693	66	16
7	-375	466	-11
8	926	821	5
9	753	898	-7

-15 1 l

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 3

1	201	201	0
2	2118	2140	-5
3	293	419	-7
4	1153	1334	-35
5	528	582	-4
6	2014	2002	2
7	896	839	7
8	994	1066	-10
9	515	557	-3
10	729	609	11
11	434	95	12
12	624	62	26
13	337	78	7
14	156	21	1
15	536	256	13
16	355	325	1
17	420	343	3
18	430	271	6
19	-234	313	-5
20	561	206	8
21	-154	199	-1
22	534	246	6
-15	3	1	
1	-294	176	-9
2	320	56	8
3	-332	466	-25
4	1067	868	28
5	388	382	0
6	118	176	-1
7	748	842	-10
8	294	383	-4
9	1171	1225	-8
10	-105	31	0
11	-88	335	-8
12	832	599	22
13	-416	88	-11
14	363	135	6
15	787	443	24
16	439	193	8
17	1130	925	21
18	644	120	14
19	397	127	4
20	733	771	-1
21	-378	182	-5
-15	5	1	
1	383	295	4
2	664	492	15
3	885	733	18
4	835	634	21
5	1149	1108	6
6	1054	818	31
7	1255	1108	23
8	1568	1552	3
9	702	482	17
10	721	648	6
11	1106	1080	3
12	236	386	-6
13	704	534	12
14	559	581	-1
15	469	484	0
16	-223	9	-2
17	701	679	1
18	845	187	27
19	-239	245	-3
20	499	319	4
21	-478	166	-8
-15	7	1	
1	409	161	10
2	1464	1444	3
3	397	540	-9
4	647	587	5
5	941	730	24
6	1732	1675	11
7	592	652	-5
8	2028	1902	26
9	634	497	10
10	727	652	6
11	467	515	-2
12	619	370	15
13	404	602	-12
14	706	521	12
15	258	416	-5
16	404	528	-6
17	614	320	9
18	326	166	2
19	785	792	0
20	379	23	4
-15	9	1	
1	446	231	10
2	-73	233	-4
3	527	422	6
4	891	918	-3
5	169	154	0
6	657	535	10
7	146	392	-8
8	-316	78	-6
9	617	586	2
10	333	323	0
11	742	627	9
12	-80	47	0
13	472	680	-13
14	-170	551	-17
15	354	222	2
16	-552	156	-11
17	-576	430	-17
18	518	522	0
19	1072	824	13
-15	11	1	
1	675	518	12
2	642	324	20
3	60	362	-8
4	488	725	-17
5	1406	1399	1
6	1277	1329	-7
7	550	514	2
8	625	720	-7
9	502	601	-6
10	20	54	0
11	-183	209	-4
12	251	209	1
13	705	606	4
14	447	368	2
15	310	537	-6
16	-538	318	-12
17	255	370	-2
18	-331	296	-6
-15	13	1	
1	320	439	-5
2	813	436	28
3	1130	966	20
4	-373	31	-8
5	1088	1088	0
6	530	470	3
7	438	290	6
8	379	422	-2
9	590	588	0
10	-445	362	-17
11	785	713	4
12	671	613	3
13	-637	540	-23
14	-520	56	-8
15	437	473	-1
16	522	553	-1
-15	15	1	
1	382	222	5
2	489	572	-4
3	-484	172	-14
4	1341	1130	27
5	-339	112	-5
6	361	155	4
7	-313	217	-5
8	-610	98	-14
9	-691	111	-18
10	-752	326	-23
11	281	132	2
12	487	0	7
13	598	190	10
-15	17	1	
1	445	216	5
2	709	689	0
3	399	444	-1
4	-162	199	-2
5	1228	883	24
6	-262	364	-6
7	591	288	8
8	323	203	2
9	460	213	5
10	593	114	11
-14	0	1	
2	1486	1383	22
4	766	689	9
6	719	654	7
8	1591	1604	-2
10	-23	22	0
12	2132	2118	3
14	1232	1100	18
16	1600	1597	0
18	677	441	13
20	455	733	-10
22	218	135	0
-14	2	1	
1	2097	2149	-13
2	890	708	24
3	2359	2327	8
4	662	567	9
5	416	375	2
6	1418	1397	4
7	1598	1735	-31
8	302	446	-8
9	2057	1961	22
10	911	771	16
11	636	553	6
12	1603	1637	-6
13	465	363	5
14	1485	1434	8
15	926	917	0
16	990	974	1
17	-666	17	-24
18	715	469	15
19	788	653	9
20	607	165	11
21	283	359	-1
22	-404	166	-5
23	316	168	1
-14	4	1	
1	1527	1547	-4
2	1644	1776	-31
3	1917	1866	12
4	1575	1430	31
5	1573	1576	0
6	1659	1564	20
7	-498	37	-19
8	685	614	7
9	375	241	6
10	858	528	33
11	1348	1367	-3
12	1223	1189	5
13	1816	1762	10
14	337	354	0
15	-388	55	-9
16	53	131	0
17	205	174	0
18	309	135	4
19	378	254	2
20	571	61	10
21	818	102	20
22	515	0	7
-14	6	1	
1	507	199	17
2	1483	1558	-16
3	336	273	3
4	1826	1791	8
5	800	631	18
6	963	894	9
7	851	798	6
8	366	20	9
9	742	778	-4
10	1513	1448	12
11	581	534	3
12	-181	178	-4
13	404	88	9
14	2273	2175	20
15	938	765	16
16	707	596	8
17	526	467	3
18	934	922	1
19	653	265	12
20	445	564	-3
21	277	15	2
22	1168	993	10
-14	8	1	
1	643	600	3
2	599	76	27
3	994	1003	-1
4	1251	1190	10
5	1059	1010	7
6	1749	1624	26
7	552	584	-2
8	193	482	-13
9	1802	1717	17
10	220	160	1
11	312	351	-1
12	664	486	12
13	703	640	5
14	866	719	13
15	-285	51	-4
16	320	354	-1
17	825	815	0
18	489	127	7
19	-549	162	-10
20	-203	171	-2
21	-869	262	-23
-14	10	1	
1	307	128	5
2	485	789	-27
3	284	22	5
4	2291	2267	5
5	-284	153	-7
6	1497	1467	5
7	-358	215	-11
8	806	699	10
9	259	99	3
10	197	352	-5
11	224	360	-4

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 4

12	-248	268	-8
13	289	428	-6
14	461	158	10
15	576	745	-11
16	-37	638	-14
17	301	193	1
18	1126	999	8
19	-416	462	-11
20	390	113	4
	-14	12	1
1	850	649	20
2	91	402	-10
3	-418	25	-11
4	271	86	4
5	162	234	-1
6	460	473	0
7	540	446	5
8	986	954	3
9	621	493	8
10	431	288	6
11	-319	244	-9
12	490	391	4
13	696	779	-6
14	624	316	10
15	1068	799	17
16	610	372	7
17	84	207	-1
18	613	341	8
	-14	14	1
1	509	658	-11
2	200	625	-22
3	40	690	-31
4	328	7	6
5	-208	392	-11
6	323	370	-1
7	361	203	5
8	485	499	0
9	929	889	3
10	364	507	-7
11	344	274	2
12	1025	765	16
13	-581	253	-14
14	-772	31	-19
15	1146	1106	2
16	482	324	4
	-14	16	1
1	182	289	-2
2	1544	1409	20
3	-414	160	-11
4	436	616	-10
5	295	64	5
6	1342	1220	16
7	637	580	2
8	-398	223	-7
9	-278	32	-2
10	679	111	16
11	366	330	0
12	708	168	15
13	419	293	2
14	436	211	4
	-14	18	1
1	673	436	9
2	686	580	4
3	819	674	7
4	1104	1096	0
5	-387	427	-11
6	992	791	12
7	-461	14	-7
8	434	227	4
9	-409	44	-6
10	421	510	-2
	-14	20	1
1	591	606	0
2	473	99	6
	-13	1	1
1	1026	1021	0
2	1003	989	2
3	-245	51	-5
4	2567	2570	0
5	816	715	13
6	318	133	7
7	578	497	7
8	675	619	6
9	-170	84	-2
10	320	61	8
11	563	315	17
12	1410	1209	35
13	1193	1249	-8
14	1371	1273	16
15	263	513	-12
16	1215	1153	8
17	462	615	-9
18	670	227	22
19	411	331	3
20	966	971	0
21	405	172	4
22	-467	12	-6
23	-407	57	-4
24	844	963	-5
	-13	3	1
1	609	666	-6
2	140	304	-6
3	-286	35	-7
4	-385	15	-13
5	132	70	1
6	1004	1128	-22
7	145	227	-2
8	-156	190	-5
9	394	269	6
10	724	719	0
11	-381	131	-12
12	354	451	-5
13	916	777	15
14	807	571	21
15	865	771	9
16	-218	429	-13
17	764	767	0
18	1475	1468	0
19	841	739	8
20	546	520	1
21	582	250	9
22	661	397	8
23	524	20	7
	-13	5	1
1	599	663	-7
2	1451	1464	-3
3	590	485	10
4	507	536	-2
5	-180	2	-2
6	1170	1201	-5
7	907	938	-4
8	1105	1118	-2
9	1413	1383	5
10	507	532	-1
11	495	343	9
12	1070	1091	-3
13	1385	1296	14
14	278	60	4
15	1008	814	21
16	-241	36	-3
17	-55	377	-8
18	-366	335	-13
19	674	229	20
20	707	348	12
21	598	516	2
22	319	83	2
23	666	746	-2
	-13	7	1
1	1142	1227	-15
2	2628	2723	-26
3	750	703	5
4	725	818	-11
5	994	949	6
6	-465	88	-18
7	852	874	-2
8	2146	2054	23
9	247	53	4
10	311	332	-1
11	370	110	9
12	344	251	3
13	891	752	14
14	1193	1182	1
15	473	676	-13
16	733	164	29
17	400	204	7
18	824	753	5
19	423	285	4
20	753	707	2
21	1125	925	11
22	48	165	0
	-13	9	1
1	546	507	3
2	582	560	1
3	782	761	2
4	1250	1347	-18
5	1234	1251	-2
6	1727	1733	-1
7	264	13	5
8	1129	1246	-19
9	-175	123	-3
10	1979	1928	11
11	586	684	-8
12	1836	1835	0
13	-358	180	-10
14	399	390	0
15	1032	955	8
16	-317	168	-7
17	-359	152	-8
18	-344	285	-7
19	696	731	-1
20	585	449	4
21	-288	387	-6
	-13	11	1
1	1873	1897	-5
2	1019	823	25
3	1065	1069	0
4	885	889	0
5	742	802	-6
6	260	479	-11
7	1372	1310	10
8	-298	4	-6
9	467	428	2
10	1389	1114	41
11	177	248	-1
12	954	823	13
13	518	536	-1
14	-254	72	-4
15	815	515	23
16	630	817	-15
17	726	345	14
18	-672	184	-16
19	-439	2	-5
20	829	428	14
	-13	13	1
1	1169	1064	15
2	480	220	12
3	596	654	-4
4	1301	1167	20
5	-117	470	-15
6	310	343	-1
7	990	988	0
8	1166	1192	-3
9	441	529	-5
10	474	273	9
11	646	402	15
12	731	788	-4
13	505	301	9
14	674	643	2
15	339	443	-3
16	538	556	0
17	92	258	-1
18	-251	128	-2
19	547	476	2
	-13	15	1
1	341	277	2
2	1114	1030	10
3	859	665	18
4	327	148	5
5	180	491	-12
6	756	699	4
7	128	71	0
8	458	512	-3
9	676	485	12
10	714	706	0
11	793	649	11
12	1541	1395	14
13	539	192	9
14	890	827	3
15	-388	32	-4
16	217	431	-4
17	592	398	5
	-13	17	1
1	750	820	-6
2	321	421	-4
3	1037	1048	-1
4	780	662	9
5	-203	266	-6
6	879	850	2
7	-816	374	-30
8	378	475	-3
9	382	397	0
10	400	543	-4
11	1091	931	10
12	901	685	11
13	544	504	1
14	691	386	10
	-13	19	1
1	757	827	-3
2	-381	27	-5
3	1083	1106	-1
4	260	476	-5
5	790	202	20
6	630	185	12
7	205	1	1
8	-280	23	-2
9	324	449	-3
10	624	350	8
	-13	21	1
1	-351	28	-4
2	1139	701	25

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-12 0 1

2	1580	1605	-6
4	5646	5578	13
6	3467	3460	1
8	1965	1910	14
10	2987	2891	25
12	605	784	-19
14	522	318	12
16	1590	1594	0
18	-156	532	-17
20	1284	1005	30
22	606	5	11
24	763	320	12

-12 2 1

1	1487	1458	8
2	-266	31	-7
3	1276	1199	17
4	2530	2551	-6
5	1589	1559	7
6	451	497	-4
7	1375	1345	6
8	221	84	3
9	283	346	-3
10	659	584	7
11	988	1046	-9
12	1114	1059	8
13	885	914	-3
14	440	394	2
15	2037	2082	-9
16	223	499	-12
17	1404	1255	22
18	24	334	-6
19	2083	1945	24
20	426	467	-1
21	994	661	26
22	704	222	14
23	-539	576	-17
24	-465	253	-7

-12 4 1

1	736	706	4
2	1388	1351	9
3	379	0	14
4	-383	200	-18
5	3080	3148	-19
6	2686	2690	-1
7	658	689	-3
8	1740	1797	-14
9	289	392	-6
10	1518	1520	0
11	547	343	14
12	164	171	0
13	1282	1313	-5
14	812	689	12
15	171	204	0
16	777	605	14
17	621	546	5
18	598	458	8
19	1023	1002	2
20	396	355	1
21	1248	1272	-2
22	-785	31	-19
23	159	178	0
24	-433	386	-8

-12 6 1

1	983	1008	-4
2	1812	1811	0
3	1774	1750	6
4	1520	1516	0
5	1112	1120	-1
6	-131	93	-2
7	974	1077	-18
8	858	921	-9
9	648	512	13
10	1231	1153	13
11	325	273	2
12	1937	1885	11
13	424	347	4
14	991	976	1
15	-213	8	-2
16	-479	5	-13
17	291	74	4
18	389	295	3
19	-294	6	-4
20	486	651	-9
21	579	65	10
22	952	743	10
23	-612	4	-10
24	-560	261	-9

-12 8 1

1	948	875	11
2	2017	1971	12
3	511	577	-6
4	614	631	-1
5	763	684	9
6	-408	16	-14
7	786	703	10
8	624	699	-8
9	438	291	8
10	1004	1046	-6
11	791	725	7
12	669	432	18
13	-79	425	-12
14	-465	335	-23
15	911	821	9
16	422	188	8
17	-288	269	-8
18	-283	236	-7
19	492	334	6
20	246	26	1
21	1219	1158	4
22	903	478	16
23	-378	352	-6

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1	1497	1501	-1
2	1967	1887	20
3	795	908	-15
4	903	883	2
5	-10	340	-9
6	833	721	14
7	-346	124	-10
8	1248	1384	-24
9	728	629	9
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11	618	444	12
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13	905	862	4
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15	282	207	2
16	-486	80	-13
17	-102	234	-3
18	346	164	4
19	424	633	-7
20	399	152	4
21	1132	897	13
22	-819	234	-19

-12 12 1

1	472	353	7
2	477	359	7
3	1974	2022	-11
4	139	381	-9
5	1041	1181	-22
6	1148	1211	-10
7	634	524	9
8	1894	1778	24
9	1414	1282	22
10	2066	2045	4
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12	373	133	7
13	487	469	1
14	-305	308	-10
15	-249	0	-3
16	1208	1164	5
17	378	133	4
18	-710	184	-18
19	262	98	1
20	431	112	5
21	-600	31	-10

-12 14 1

1	-425	118	-15
2	-341	149	-9
3	379	41	9
4	225	55	3
5	242	532	-15
6	-267	57	-4
7	773	590	16
8	751	836	-8
9	371	59	8
10	541	18	18
11	616	421	11
12	831	807	2
13	587	661	-4
14	720	643	5
15	958	800	10
16	500	128	8
17	645	298	10
18	1010	912	5
19	867	651	9

-12 16 1

1	1994	1944	10
2	-237	223	-6
3	235	254	0
4	-195	40	-2
5	344	3	7
6	2101	1936	33
7	768	755	1
8	766	589	15
9	576	675	-6
10	-291	311	-10
11	817	726	7
12	-386	73	-5
13	845	839	0
14	-331	388	-9
15	-612	16	-12
16	310	394	-1
17	-330	41	-3

-12 18 1

1	939	849	8
2	1137	1007	15
3	506	186	12
4	-184	84	-2
5	-269	288	-8
6	399	465	-3
7	886	821	5
8	-316	84	-4
9	-437	203	-9
10	430	589	-5
11	417	351	1
12	473	331	3
13	-354	322	-7
14	-335	196	-4

-12 20 1

1	-362	343	-8
2	-394	257	-7
3	-523	202	-11
4	584	531	2
5	-454	35	-7
6	726	540	9
7	218	24	1
8	-629	637	-26
9	-483	163	-8
10	639	435	7

-11 1 1

1	1168	1180	-3
2	2020	2049	-9
3	244	211	1
4	1616	1556	17
5	1654	1633	6
6	357	169	12
7	1002	973	5
8	-401	71	-16
9	745	693	7
10	2377	2433	-16
11	2625	2652	-7
12	856	797	7
13	583	460	10
14	1074	1035	5
15	592	520	5
16	379	671	-22
17	-328	122	-7
18	1273	1282	-1
19	776	470	20
20	952	970	-1
21	-79	358	-6
22	501	306	7
23	782	176	16
24	-312	82	-2
25	657	90	11

-11 3 1

1	470	580	-13
2	1944	1971	-8
3	1911	1963	-16
4	1037	1070	-7
5	889	893	0
6	1916	1842	22
7	1056	1036	4
8	357	403	-3
9	679	556	14
10	596	721	-14
11	2721	2677	11
12	590	662	-7
13	643	626	1
14	1278	1285	-1
15	153	108	0
16	601	473	9
17	476	29	14
18	378	406	-1
19	486	709	-14
20	243	33	3
21	264	104	3
22	286	143	2
23	-743	85	-16
24	1062	941	5
25	845	882	-1

-11 5 1

1	2508	2565	-18
2	245	85	6
3	1791	1838	-14
4	786	762	3
5	2185	2207	-6
6	2154	2215	-18
7	428	532	-10
8	603	662	-6
9	2107	2050	15
10	399	623	-21

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 6

11	1689	1758	-16
12	1362	1391	-5
13	415	345	4
14	1010	1075	-9
15	1676	1593	15
16	2483	2377	23
17	-177	141	-3
18	520	423	5
19	-326	460	-17
20	789	322	26
21	777	703	5
22	358	420	-1
23	504	19	7
24	484	38	6
25	979	669	12

-11 7 1

1	1187	1263	-17
2	1468	1558	-22
3	2494	2484	2
4	1292	1270	5
5	539	491	4
6	2350	2306	12
7	209	160	1
8	950	953	0
9	653	632	2
10	492	34	21
11	2362	2397	-9
12	1264	1179	14
13	559	508	3
14	694	632	5
15	645	666	-1
16	1614	1556	10
17	333	452	-5
18	620	281	16
19	1125	1070	6
20	202	116	1
21	466	282	6
22	-400	453	-10
23	63	294	-2
24	709	274	10

-11 9 1

1	2306	2320	-3
2	2332	2299	9
3	2162	2204	-11
4	1013	1071	-10
5	397	445	-3
6	2617	2636	-5
7	-206	316	-12
8	2017	2013	1
9	1945	1859	20
10	1368	1285	15
11	439	374	4
12	1120	1130	-1
13	-187	21	-2
14	1140	1159	-2
15	1217	1320	-15
16	413	324	3
17	344	316	1
18	295	367	-2
19	449	68	9
20	1566	1433	17
21	-641	52	-13
22	548	702	-5
23	415	153	3

-11 11 1

1	785	649	16
2	1217	1187	5
3	414	214	10
4	538	1	24
5	1051	1123	-12
6	390	551	-13
7	1288	1352	-12
8	938	905	4
9	823	774	5
10	932	999	-9
11	1678	1640	7
12	2006	2015	-1
13	1388	1241	23
14	1786	1717	12
15	740	820	-7
16	-127	15	0
17	1269	1003	31
18	264	253	0
19	1148	1044	7
20	479	287	4
21	-659	142	-13
22	520	180	6

-11 13 1

1	1828	1791	8
2	1673	1681	-1
3	1671	1579	19
4	511	253	14
5	921	934	-1
6	460	337	7
7	375	324	2
8	865	1047	-23
9	912	951	-4
10	789	841	-5
11	447	551	-6
12	608	90	22
13	553	578	-1
14	1138	924	24
15	536	307	10
16	474	130	11
17	724	674	3
18	940	734	11
19	521	383	3
20	539	530	0
21	-257	177	-2

-11 15 1

1	446	462	0
2	609	702	-8
3	739	746	0
4	1417	1344	12
5	1519	1559	-7
6	423	401	1
7	404	345	2
8	496	310	9
9	578	586	0
10	1104	1017	10
11	1074	980	11
12	1036	953	9
13	388	345	1
14	758	828	-5
15	1028	958	5
16	-333	353	-8
17	900	566	15
18	727	445	10
19	-234	217	-3

-11 17 1

1	1036	1035	0
2	490	310	9
3	1128	973	19
4	-248	407	-14
5	1501	1501	0
6	446	65	11
7	809	938	-12
8	787	577	16
9	331	248	2
10	-248	96	-3
11	205	190	0
12	-677	164	-18
13	440	239	4
14	-492	536	-18
15	355	230	2
16	794	559	9
17	-272	46	-2

-11 19 1

1	430	85	10
2	550	324	11
3	259	100	3
4	474	666	-12
5	1054	847	21
6	-157	129	-2
7	1213	1031	15
8	241	513	-7
9	-189	253	-3
10	-275	39	-2
11	-261	273	-4
12	653	650	0
13	719	40	16
14	-702	90	-15

-11 21 1

1	-175	230	-2
2	245	619	-11
3	-494	406	-14
4	502	438	2
5	-732	200	-19
6	1070	945	8
7	-362	135	-5
8	596	787	-8
9	507	773	-10
10	1058	951	6

-10 0 1

2	651	607	7
4	2501	2471	9
6	2624	2645	-6
8	1735	1763	-8
10	2236	2273	-11
12	1682	1617	15
14	170	395	-10
16	280	364	-4
18	2049	1974	14
20	944	1189	-26
22	112	462	-8
24	716	295	12
26	935	847	3

-10 2 1

1	2490	2580	-30
2	910	926	-3
3	988	975	3
4	419	454	-4
5	-387	107	-20
6	1181	1168	3
7	-219	170	-9
8	2844	2943	-30
9	1101	1107	-1
10	3019	3067	-13
11	509	373	11
12	3586	3682	-25
13	1279	1253	5
14	490	134	17
15	882	778	13
16	-279	550	-25
17	1684	1697	-2
18	1391	1267	18
19	175	213	0
20	436	379	2
21	356	379	0
22	466	614	-7
23	728	430	13
24	1005	701	14
25	214	236	0
26	443	658	-5

-10 4 1

1	3744	3766	-5
2	618	685	-11
3	4560	4543	3
4	1138	1060	19
5	560	598	-5
6	1572	1546	7
7	2631	2638	-2
8	862	709	25
9	1233	1231	0
10	1363	1340	5
11	-300	162	-10
12	797	781	2
13	2023	1989	8
14	1396	1306	17
15	591	711	-10
16	-382	245	-13
17	1236	1099	19
18	278	429	-6
19	610	176	19
20	-164	19	-1
21	1669	1610	8
22	710	4	22
23	556	496	1
24	651	251	10
25	-656	50	-10
26	-265	351	-4

-10 6 1

1	467	421	5
2	455	247	17
3	1320	1274	12
4	457	507	-5
5	264	417	-11
6	550	607	-7
7	1693	1704	-3
8	912	899	2
9	436	398	2
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11	700	818	-16
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13	1209	1075	22
14	2038	2026	2
15	903	943	-4
16	1378	1353	4
17	1037	1008	3
18	735	386	23
19	-290	19	-4
20	747	646	7
21	778	630	10
22	970	1077	-9
23	-563	87	-9
24	-195	214	-2
25	785	708	2

-10 8 1

1	4400	4443	-10
2	296	365	-4
3	4361	4392	-7
4	314	339	-1
5	1962	1986	-6
6	944	928	2
7	535	568	-3
8	1909	1906	0
9	1087	1074	2
10	1092	1036	9
11	262	167	3
12	317	222	4
13	705	775	-7
14	224	18	3
15	-203	308	-9
16	384	317	3
17	705	696	0
18	964	772	18

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II)

19	762	655	8
20	845	886	-3
21	410	485	-3
22	-613	169	-12
23	-687	345	-15
24	259	30	1
	-10	10	1
1	2220	2236	-4
2	956	876	13
3	977	937	7
4	-352	31	-11
5	471	313	11
6	895	907	-1
7	2037	2081	-11
8	671	657	1
9	1119	1133	-2
10	560	498	5
11	538	373	11
12	1848	1886	-8
13	1184	1092	13
14	1758	1658	19
15	544	616	-5
16	1095	986	13
17	1576	1531	7
18	927	920	0
19	1559	1592	-4
20	998	978	1
21	1113	637	26
22	95	282	-1
23	474	135	5
24	-593	394	-12
	-10	12	1
1	1076	1014	10
2	953	861	14
3	1126	1180	-9
4	349	204	6
5	784	657	15
6	958	910	7
7	960	1024	-9
8	756	624	14
9	1861	1782	17
10	466	563	-7
11	1312	1270	6
12	479	524	-2
13	1253	1175	11
14	991	1008	-2
15	-214	165	-4
16	167	186	0
17	-282	257	-8
18	-232	238	-5
19	-622	111	-18
20	-209	283	-3
21	702	164	13
22	622	581	1
	-10	14	1
1	482	233	13
2	1395	1498	-20
3	407	619	-16
4	908	936	-3
5	1050	1029	2
6	285	70	5
7	1305	1379	-13
8	536	379	9
9	1428	1445	-3
10	1178	1189	-1
11	303	361	-2
12	-308	118	-6
13	-170	370	-9
14	435	306	5
15	73	88	0
16	875	551	23
17	359	240	3
18	661	317	11
19	714	146	15
20	406	307	2
21	-167	391	-4
	-10	16	1
1	190	276	-2
2	756	853	-10
3	988	814	20
4	2377	2288	20
5	770	673	9
6	-184	403	-12
7	299	398	-4
8	499	267	12
9	237	161	1
10	1035	1009	3
11	1453	1253	29
12	735	643	7
13	401	451	-2
14	183	118	1
15	-450	262	-9
16	-742	2	-19
17	947	459	21
18	-521	26	-8
19	428	194	4
	-10	18	1
1	237	187	1
2	1656	1574	14
3	452	415	2
4	740	953	-21
5	1043	947	11
6	506	307	9
7	319	382	-2
8	1170	1110	7
9	387	134	7
10	363	573	-10
11	1151	1120	3
12	270	126	2
13	456	176	6
14	-380	41	-4
15	286	78	2
16	371	41	4
17	988	701	14
	-10	20	1
1	-310	3	-5
2	631	628	0
3	894	1018	-12
4	381	414	-1
5	238	80	2
6	662	577	4
7	221	288	-1
8	1361	1085	23
9	749	545	9
10	1444	1097	29
11	374	584	-6
12	-379	662	-18
13	527	52	8
14	886	266	22
	-10	22	1
1	1031	983	3
2	-273	124	-3
3	1126	816	20
4	371	218	3
5	755	208	18
6	35	184	-1
7	936	594	17
8	862	825	2
9	409	372	0
	-9	1	1
1	834	825	2
2	3253	3249	1
3	1811	1877	-24
4	3639	3708	-19
5	2163	2174	-3
6	1202	1267	-18
7	1222	1296	-21
8	1489	1523	-10
9	2986	3033	-14
10	-237	4	-6
11	421	562	-14
12	1485	1506	-4
13	-198	8	-3
14	486	489	0
15	1181	1257	-13
16	-160	159	-3
17	768	724	4
18	2519	2401	25
19	281	317	-1
20	-301	226	-7
21	1483	1431	6
22	2317	2271	7
23	413	450	-1
24	1108	1067	3
25	549	449	2
26	1414	1105	19
27	995	812	8
	-9	3	1
1	1565	1583	-6
2	2342	2411	-24
3	439	240	19
4	2508	2516	-2
5	796	750	9
6	1445	1442	1
7	3632	3687	-15
8	1692	1723	-9
9	3605	3687	-22
10	1847	1859	-3
11	1032	1118	-17
12	3480	3558	-20
13	1123	1018	18
14	1606	1616	-2
15	-394	92	-14
16	784	642	14
17	557	627	-5
18	447	430	0
19	113	89	0
20	-212	107	-2
21	895	1064	-15
22	315	459	-5
23	550	663	-5
24	540	466	2
25	-491	53	-6
26	-918	326	-24
	-9	5	1
1	2808	2772	11
2	927	912	3
3	5093	5170	-16
4	-109	99	-2
5	452	449	0
6	970	1058	-20
7	2465	2460	1
8	1256	1323	-17
9	911	853	10
10	1386	1373	3
11	977	908	11
12	-443	97	-18
13	869	817	7
14	318	199	4
15	958	985	-3
16	1944	1862	17
17	1012	934	9
18	1077	1066	1
19	581	423	8
20	1869	1804	10
21	816	588	15
22	484	345	5
23	233	46	2
24	683	427	7
25	818	859	-1
26	-238	99	-1
	-9	7	1
1	2522	2517	1
2	2219	2215	1
3	-123	120	-3
4	274	84	8
5	2229	2221	2
6	1379	1309	18
7	2681	2775	-29
8	521	554	-3
9	909	1121	-39
10	1388	1390	0
11	1113	1136	-4
12	1548	1532	3
13	325	234	4
14	290	299	0
15	957	989	-4
16	2065	2087	-4
17	351	272	3
18	376	45	8
19	983	962	2
20	594	665	-4
21	631	267	16
22	1059	857	18
23	428	624	-5
24	1367	863	27
25	293	53	2
	-9	9	1
1	406	282	9
2	4890	4851	11
3	2022	2005	5
4	1086	1093	-1
5	1768	1739	8
6	2059	2093	-10
7	1540	1541	0
8	731	621	13
9	321	286	1
10	2636	2676	-11
11	1060	1100	-6
12	172	63	2
13	234	252	0
14	375	36	9
15	1879	1860	3
16	415	189	8
17	705	421	19
18	-304	419	-14
19	534	707	-11
20	559	441	5
21	843	965	-9
22	-366	181	-4
23	-276	421	-6
24	-457	6	-5
25	591	38	8
	-9	11	1
1	2291	2278	3
2	1265	1219	9
3	2786	2753	10
4	1411	1384	6
5	803	715	12
6	1174	1103	13
7	-83	63	0
8	1075	1063	2
9	1401	1356	9
10	1300	1145	28
11	985	984	0
12	1108	1088	3

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 8

13	269	190	2
14	311	523	-11
15	898	740	15
16	590	418	10
17	637	479	10
18	613	613	0
19	-321	559	-19
20	-197	330	-6
21	552	251	7
22	899	593	12
23	579	403	4
24	530	10	6
	-9	13	1
1	1672	1658	3
2	259	362	-5
3	1010	942	10
4	127	96	0
5	340	17	9
6	-266	257	-12
7	1237	1115	21
8	-82	95	-1
9	101	309	-6
10	632	424	15
11	746	799	-5
12	1871	1921	-10
13	1212	1269	-8
14	725	816	-8
15	492	250	10
16	621	723	-7
17	1112	891	22
18	1657	1522	19
19	410	620	-9
20	264	164	1
21	1184	1056	7
22	129	379	-3
	-9	15	1
1	1998	2072	-18
2	942	991	-6
3	535	557	-1
4	825	786	4
5	976	921	7
6	-228	79	-4
7	640	600	3
8	2687	2607	19
9	1272	1356	-13
10	1635	1594	7
11	435	174	10
12	1118	1058	7
13	206	436	-8
14	661	674	0
15	934	733	17
16	1168	977	20
17	811	802	0
18	1045	957	5
19	201	167	0
20	831	89	19
21	477	844	-13
	-9	17	1
1	-500	1	-17
2	958	932	3
3	2242	2282	-9
4	743	767	-2
5	639	576	5
6	1325	1228	15
7	1745	1635	20
8	936	931	0
9	-272	26	-4
10	1220	1057	21
11	-364	32	-7
12	487	625	-8
13	728	718	0
14	445	173	8
15	475	103	7
16	-375	102	-5
17	584	127	10
18	490	249	5
19	624	300	8
	-9	19	1
1	-478	280	-20
2	269	7	4
3	276	588	-16
4	1160	1023	17
5	1275	1302	-3
6	449	455	0
7	473	429	2
8	537	630	-6
9	712	708	0
10	82	15	0
11	983	1081	-7
12	963	1075	-8
13	-619	321	-17
14	837	164	22
15	582	427	4
16	295	175	1
	-9	21	1
1	549	290	12
2	165	288	-3
3	978	887	9
4	-535	351	-15
5	197	199	0
6	875	474	20
7	359	22	4
8	286	228	1
9	380	739	-13
10	850	700	7
11	150	294	-2
12	-253	325	-5
13	1007	822	10
	-9	23	1
1	1507	1338	15
2	736	65	18
3	-228	394	-7
4	612	143	11
5	620	211	11
6	383	238	2
7	1281	1214	5
	-8	0	1
2	3290	3280	3
4	3533	3484	14
6	1004	1022	-4
8	1412	1370	12
10	1654	1721	-20
12	3322	3400	-21
14	289	147	5
16	357	367	0
18	1158	1171	-1
20	849	846	0
22	649	532	6
24	476	276	6
26	-702	368	-16
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Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 9

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8	1091	1080	1
9	1206	1192	1
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12	456	46	11

13	1319	1283	3
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15	503	776	-12
16	320	335	0
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1	-232	507	-17
2	1112	1171	-7
3	-270	176	-5
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5	739	573	12
6	524	56	15
7	237	204	0
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9	415	418	0
10	242	139	1
11	1030	1125	-6
12	751	539	8
13	420	684	-9
14	828	269	19
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2	890	816	4
3	778	355	16
4	1061	1211	-11
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6	921	955	-2
7	611	91	12
8	-899	259	-28
9	1006	1080	-4
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2	7961	7871	12
3	5562	5596	-7
4	2538	2610	-28
5	3813	3902	-25
6	940	982	-13
7	2884	2918	-11
8	327	304	2
9	1376	1410	-10
10	1672	1809	-46
11	1490	1525	-9
12	3097	3136	-11
13	451	321	9
14	2255	2360	-28
15	2610	2684	-18
16	3040	3044	0
17	598	509	5
18	1594	1412	27
19	1277	1199	9
20	307	338	-1
21	534	758	-14
22	732	725	0
23	295	445	-5
24	927	742	13
25	1731	1688	5
26	371	735	-11
27	243	112	1
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2	526	605	-20
3	5009	5003	1
4	2330	2394	-26
5	8020	8287	-38
6	5581	5729	-30
7	6656	6786	-22
8	2193	2200	-2
9	318	374	-5
10	887	984	-22

11	369	511	-14
12	5396	5518	-24
13	3572	3694	-31
14	945	1099	-25
15	984	1098	-16
16	2370	2384	-3
17	866	781	8
18	-151	12	-1
19	593	466	6
20	2617	2608	1
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22	741	541	12
23	683	38	21
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25	-386	518	-17
26	261	182	1
27	309	383	-1
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1	1194	1201	-2
2	2125	2162	-15
3	982	1066	-30
4	2323	2300	8
5	5302	5329	-5
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7	922	932	-2
8	1017	1036	-5
9	477	121	29
10	887	811	15
11	1733	1761	-8
12	1275	1185	20
13	3689	3701	-3
14	605	612	0
15	157	469	-14
16	1778	1751	5
17	487	12	13
18	780	594	13
19	2871	2832	7
20	998	795	16
21	2150	2000	24
22	542	345	7
23	660	877	-14
24	-322	38	-4
25	671	619	2
26	426	35	5
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28	269	478	-3
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3	2568	2532	12
4	1250	1268	-6
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6	2119	2136	-6
7	1076	1130	-15
8	2729	2692	12
9	3836	3875	-10
10	730	683	7
11	360	284	5
12	2179	2189	-2
13	1991	1979	3
14	482	410	4
15	1767	1642	25
16	1129	1189	-8
17	613	593	1
18	187	708	-24
19	-283	323	-9
20	436	312	4
21	396	329	2
22	1280	1326	-5
23	1059	1012	4
24	-614	41	-17
25	-346	82	-3
26	281	168	1

27	-478	579	-16
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2	3288	3342	-16
3	1992	2047	-20
4	2029	2035	-2
5	1656	1672	-5
6	1738	1775	-12
7	2694	2686	2
8	1058	1049	1
9	2377	2444	-21
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13	506	620	-10
14	622	387	17
15	807	718	9
16	2759	2723	8
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21	-608	92	-16
22	417	203	6
23	-110	23	0
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25	350	55	3
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3	1193	1266	-19
4	1573	1611	-11
5	210	108	3
6	158	107	1
7	3176	3189	-3
8	913	929	-2
9	721	716	0
10	1806	1842	-9
11	2447	2472	-6
12	336	507	-11
13	418	586	-12
14	308	233	3
15	3490	3480	2
16	1541	1604	-10
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18	1491	1456	4
19	2302	2215	15
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21	-154	231	-3
22	770	426	17
23	1200	878	18
24	521	167	6
25	1190	864	16
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2	433	143	18
3	194	204	0
4	553	509	4
5	700	592	14
6	3793	3797	-1
7	749	818	-9
8	2032	2091	-16
9	2810	2803	1
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12	-431	23	-14
13	-208	312	-10
14	-477	10	-16
15	-331	342	-14
16	379	83	8
17	-472	519	-27

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II)

18	640	667	-1
19	915	1019	-9
20	563	296	10
21	1335	1103	22
22	339	303	0
23	560	4	8
24	588	748	-5

-5 15 1

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3	1507	1457	11
4	243	461	-13
5	176	87	2
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7	934	867	9
8	881	813	9
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10	1557	1553	0
11	294	449	-8
12	644	854	-20
13	1011	1003	0
14	-324	295	-11
15	659	597	4
16	1319	1224	12
17	960	746	18
18	1249	1096	17
19	909	607	21
20	1953	1859	10
21	658	369	8
22	-135	32	0
23	-516	126	-7

-5 17 1

1	593	425	13
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3	1419	1421	0
4	1570	1635	-14
5	-77	363	-10
6	376	245	6
7	2264	2350	-21
8	1088	1116	-4
9	1439	1361	13
10	1784	1808	-4
11	2245	2254	-2
12	552	615	-4
13	407	252	6
14	-363	49	-7
15	631	675	-3
16	828	784	3
17	1271	1034	25
18	-444	252	-8
19	345	157	3
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-5 19 1

1	266	345	-3
2	1680	1663	3
3	2407	2445	-9
4	416	500	-5
5	2048	2004	9
6	-290	248	-9
7	509	627	-8
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-5 21 1

1	-252	63	-4
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6	494	347	7
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14	1082	891	12
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-5 23 1

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9	-419	428	-14
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12	490	176	6

-5 25 1

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5	442	196	5
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-4 0 1

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28	1897	1723	15

-4 2 1

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5	763	791	-9
6	6301	6507	-37
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8	1697	1737	-15
9	650	656	-1
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14	1603	1719	-25
15	4241	4388	-32
16	1764	1649	20
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18	1121	953	19
19	2562	2497	12
20	1809	1735	12
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22	552	644	-5
23	385	231	4
24	-150	214	-3
25	983	942	3
26	933	832	5
27	891	1181	-15
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-4 4 1

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13	617	678	-7
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26	919	1181	-15
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-4 6 1

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19	726	673	3
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26	832	974	-7
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-4 8 1

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25	1494	1321	13
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-4 10 1

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-4 12 1

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3	440	321	5
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16	527	392	4
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8	1618	1742	-46
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12	2511	2503	2
13	1540	1568	-5
14	2011	2051	-9
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16	1263	1140	17
17	990	905	9
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19	-330	353	-12

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21	775	681	7
22	926	798	10
23	668	46	21
24	-283	451	-13
25	1023	1057	-3
26	384	568	-7
27	-487	280	-9
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4	2562	2578	-6
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6	2872	2870	0
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8	3582	3575	2
9	276	181	6
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11	855	727	21
12	1651	1658	-1
13	-336	25	-9
14	719	669	4
15	-292	79	-5
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17	518	529	0
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19	-373	231	-10
20	1019	979	4
21	549	532	0
22	1693	1474	21
23	914	773	11
24	182	281	-2
25	647	497	7
26	972	657	15
27	0	266	-2
28	482	581	-3
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1	5947	5920	5
2	3130	3049	27
3	12026	11335	79
4	4735	4682	12
5	4580	4545	8
6	1011	1043	-10
7	1928	1870	22
8	556	505	8
9	1183	1019	42
10	1747	1768	-6
11	-147	338	-14
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13	1790	1757	7
14	2574	2564	2
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16	1773	1816	-7
17	819	696	10
18	777	970	-18
19	1771	1780	-1
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21	1447	1295	19
22	-386	65	-8
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25	-202	106	-2
26	709	597	4
27	-468	145	-6
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11	2636	2669	-10
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17	729	727	0
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20	517	137	12
21	553	116	15
22	641	751	-7
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24	1245	1262	-1
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26	511	137	7
27	707	595	4
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7	267	219	3
8	2124	2076	16
9	2616	2554	19
10	223	324	-5
11	2447	2413	9
12	1468	1387	18
13	2035	2033	0
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17	1676	1640	6
18	1803	1699	17
19	1179	1091	9
20	1281	1398	-14
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5	1889	1896	-2
6	2669	2665	1
7	1032	1101	-15
8	2907	2888	5
9	3455	3482	-7
10	902	844	9
11	1875	1893	-4
12	363	388	-1
13	2953	2934	5
14	-385	145	-12
15	550	578	-2
16	1067	1108	-5
17	2895	2888	1
18	1196	1207	-1
19	430	632	-10
20	-542	14	-12
21	444	371	2
22	1044	858	15

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 14

23	1828	1713	15
24	244	605	-8
25	531	683	-4
26	485	797	-10
-3 13 l			
1	479	407	7
2	986	895	19
3	1534	1573	-11
4	2972	3001	-8
5	1572	1544	7
6	436	617	-19
7	987	907	14
8	843	787	8
9	1804	1810	-1
10	1641	1612	6
11	2735	2724	2
12	603	636	-3
13	715	579	12
14	137	129	0
15	492	567	-5
16	635	546	6
17	481	422	3
18	432	165	8
19	889	903	-1
20	846	928	-6
21	1222	1233	-1
22	1194	957	16
23	616	826	-8
24	387	85	3
25	858	141	18
-3 15 l			
1	1185	1201	-3
2	837	825	1
3	2023	2096	-21
4	107	203	-2
5	472	254	14
6	531	20	25
7	1716	1752	-8
8	973	899	11
9	804	475	34
10	1395	1406	-2
11	-336	57	-9
12	3036	3095	-14
13	635	538	7
14	-479	145	-17
15	1295	1225	10
16	-304	284	-10
17	361	141	5
18	109	1	0
19	-623	143	-19
20	2333	2232	16
21	743	113	16
22	-66	196	-1
23	-587	115	-8
-3 17 l			
1	2141	2105	9
2	1492	1501	-1
3	481	425	4
4	1278	1230	9
5	1287	1288	0
6	549	358	13
7	1899	1831	16
8	1702	1778	-16
9	656	624	2
10	1129	1066	9
11	2593	2603	-2
12	1383	1366	2
13	453	518	-3
14	176	399	-7
15	782	702	6
16	31	480	-12
17	466	736	-16

18	921	817	8
19	1241	1039	14
20	1660	1457	17
21	867	933	-3
-3 19 l			
1	309	245	2
2	1585	1632	-9
3	720	711	1
4	100	95	0
5	660	644	1
6	395	104	10
7	-428	87	-12
8	1209	1124	12
9	1487	1360	21
10	284	332	-1
11	1312	1223	12
12	-203	254	-6
13	256	251	0
14	-289	65	-4
15	449	418	1
16	890	583	16
17	678	695	0
18	380	65	4
19	1334	1304	2
-3 21 l			
1	1539	1631	-16
2	-261	70	-5
3	836	688	14
4	295	418	-5
5	-188	155	-3
6	929	915	1
7	863	899	-3
8	893	836	5
9	759	665	7
10	653	906	-21
11	-354	305	-11
12	-190	430	-8
13	821	620	10
14	1007	750	15
15	-476	458	-14
16	646	430	7
17	-694	80	-14
-3 23 l			
1	1426	1506	-12
2	-541	104	-17
3	-573	29	-18
4	602	237	18
5	805	764	3
6	659	572	4
7	1032	729	20
8	594	327	9
9	755	586	8
10	340	762	-15
11	311	139	2
12	-219	172	-2
13	1124	1195	-5
-3 25 l			
1	-662	108	-15
2	594	290	9
3	307	406	-2
4	890	726	8
5	-282	102	-3
6	329	485	-4
7	565	424	4
8	791	870	-4
-2 0 l			
2	3639	3780	-44
4	5020	5033	-2

6	6393	6422	-5
8	456	354	11
10	1670	1784	-31
12	1155	1183	-4
14	1873	1904	-6
16	719	497	18
18	3387	3372	3
20	3518	3494	4
22	2980	2987	-1
24	619	586	1
26	1506	1387	13
28	545	644	-3
-2 2 l			
1	2175	2180	-2
2	2736	2641	37
3	1236	1047	97
4	1169	1037	61
5	339	324	2
6	3832	3796	10
7	4757	4726	7
8	3641	3658	-4
9	9305	9689	-41
10	2720	2781	-17
11	187	58	2
12	3598	3595	0
13	513	472	2
14	1579	1588	-1
15	1995	1957	7
16	2018	2078	-12
17	583	704	-9
18	-256	5	-3
19	1760	1709	8
20	1746	1759	-2
21	-193	215	-4
22	438	806	-22
23	1331	1193	15
24	740	314	21
25	1307	1200	11
26	678	457	10
27	1513	1243	20
28	1141	502	28
-2 4 l			
1	5624	5501	24
2	-102	126	-8
3	3911	3766	40
4	2901	2862	14
5	1337	1218	49
6	8220	8260	-5
7	8351	8354	0
8	3078	3036	13
9	1771	1853	-28
10	495	520	-2
11	1840	1805	9
12	5306	5316	-2
13	4756	4810	-11
14	1259	1322	-10
15	430	28	12
16	1434	1455	-3
17	467	482	0
18	1962	2048	-16
19	212	384	-5
20	497	41	14
21	2464	2479	-2
22	1026	1012	1
23	498	461	1
24	-660	25	-22
25	783	905	-8
26	444	225	4
27	228	20	1
28	-417	404	-9
-2 6 l			
1	6169	6041	23

2	3370	3325	14
3	3211	3147	21
4	6661	6585	13
5	1445	1520	-31
6	767	762	1
7	448	494	-6
8	2356	2365	-3
9	840	773	13
10	1326	1320	1
11	341	324	1
12	3358	3394	-9
13	3171	3102	18
14	2811	2777	8
15	2481	2539	-13
16	2353	2472	-25
17	1684	1663	3
18	1918	1922	0
19	1454	1438	2
20	1763	1860	-16
21	1438	1459	-2
22	-352	415	-14
23	414	295	4
24	773	715	3
25	547	352	7
26	292	475	-4
27	800	127	17
28	-227	615	-11
-2 8 l			
1	1087	1040	16
2	3097	3130	-10
3	7996	7987	1
4	3389	3300	26
5	3387	3405	-5
6	1817	1849	-12
7	3035	3011	7
8	1396	1375	6
9	568	441	16
10	2261	2294	-10
11	2504	2526	-6
12	694	675	2
13	761	721	5
14	565	349	14
15	527	381	9
16	771	627	12
17	3043	2991	11
18	1264	1134	16
19	1378	1340	4
20	548	178	13
21	2385	2391	0
22	-356	280	-10
23	-387	88	-7
24	-449	288	-13
25	1046	1074	-1
26	310	502	-4
27	701	421	8
-2 10 l			
1	2011	1989	8
2	4271	4252	4
3	941	933	2
4	1001	1067	-18
5	860	877	-4
6	-233	347	-23
7	2159	2194	-12
8	2926	2893	10
9	1382	1360	5
10	3241	3278	-10
11	-222	308	-14
12	1879	1878	0
13	1361	1330	6
14	522	511	0
15	634	767	-12
16	2585	2641	-13
17	316	610	-15
18	1492	1507	-2

19	1046	957	8
20	-367	116	-7
21	263	459	-6
22	-91	342	-5
23	208	447	-6
24	754	733	0
25	725	510	7
26	872	679	8
	-2	12	1
1	819	851	-6
2	1994	2048	-18
3	2981	2960	6
4	252	326	-5
5	1816	1835	-6
6	1299	1337	-10
7	2973	2995	-6
8	987	1060	-15
9	1911	1919	-2
10	1867	1850	4
11	1463	1406	12
12	1066	1086	-3
13	934	1022	-12
14	-218	24	-3
15	1521	1570	-9
16	607	394	13
17	1261	1100	20
18	681	728	-3
19	1264	1280	-1
20	543	242	10
21	757	711	2
22	1031	1074	-3
23	284	689	-11
24	510	81	6
25	662	985	-13
	-2	14	1
1	1277	1296	-4
2	857	770	15
3	2046	2015	9
4	2169	2213	-13
5	1362	1389	-6
6	2264	2208	16
7	884	863	3
8	572	308	21
9	521	385	10
10	562	390	13
11	1027	980	7
12	-266	189	-7
13	1241	1251	-1
14	1001	1100	-13
15	313	7	6
16	387	97	8
17	-103	123	-1
18	402	616	-10
19	-282	85	-4
20	833	592	16
21	298	576	-10
22	386	532	-3
23	393	526	-3
24	-511	106	-7
	-2	16	1
1	-129	50	-1
2	1424	1393	7
3	722	623	11
4	1272	1336	-13
5	359	49	11
6	1534	1504	6
7	1090	1089	0
8	718	800	-9
9	898	816	10
10	714	539	16
11	1222	1192	4
12	2109	2075	7
13	998	898	11
14	208	22	2
15	-418	281	-14
16	1144	1056	10
17	1281	1304	-2
18	1014	846	14
19	-336	319	-10
20	-490	94	-8
21	552	139	7
22	866	1075	-10
	-2	18	1
1	752	542	21
2	971	1066	-14
3	1802	1839	-8
4	535	425	8
5	1329	1329	0
6	290	450	-8
7	-253	131	-6
8	524	509	1
9	2034	1979	11
10	753	587	14
11	-226	57	-3
12	364	264	3
13	912	901	1
14	625	463	10
15	1707	1598	17
16	-164	48	-1
17	128	333	-4
18	557	128	9
19	1276	1076	13
20	483	449	0
21	863	489	13
	-2	20	1
1	1628	1586	8
2	653	572	6
3	-515	17	-18
4	-419	322	-18
5	656	728	-6
6	1441	1399	7
7	1619	1566	9
8	116	307	-5
9	1071	1095	-3
10	542	566	-1
11	-508	112	-16
12	470	60	12
13	351	582	-11
14	253	269	0
15	903	978	-4
16	-669	193	-18
17	851	772	3
18	98	667	-12
	-2	22	1
1	636	643	0
2	1202	1013	24
3	460	391	3
4	703	744	-3
5	-264	125	-5
6	-147	282	-5
7	580	494	5
8	1291	1335	-6
9	598	768	-12
10	-530	101	-10
11	1128	1013	8
12	-565	307	-14
13	479	337	3
14	702	356	12
15	-788	144	-19
	-2	24	1
1	715	220	17
2	677	473	9
3	479	855	-19
4	1405	1326	8
5	-248	188	-3
6	1430	1332	9
7	1067	1106	-2
8	1293	1065	17
9	596	218	10
10	-277	482	-10
11	1281	877	27
	-2	26	1
1	387	276	2
2	-280	143	-3
3	943	531	19
	-1	1	1
1	2397	2376	9
2	1319	1277	27
3	1303	1302	0
4	610	378	53
5	5460	5415	9
6	2094	2056	13
7	222	188	1
8	6007	5962	7
9	684	722	-4
10	2993	2921	18
11	1881	1730	34
12	735	572	16
13	605	408	15
14	1783	1607	35
15	1113	1034	11
16	2911	2863	11
17	849	355	36
18	782	891	-10
19	1582	1623	-6
20	830	617	16
21	956	1041	-8
22	30	14	0
23	1167	1136	3
24	1049	1185	-13
25	339	392	24
26	1913	1766	20
27	263	257	0
28	368	366	0
	-1	3	1
1	2528	2525	1
2	1036	1001	20
3	3026	3059	-11
4	1809	1800	4
5	5550	5433	23
6	845	941	-29
7	3641	3542	27
8	7675	7535	20
9	571	410	17
10	2403	2373	8
11	1560	1519	9
12	1373	1364	1
13	1112	1197	-14
14	818	884	-8
15	3886	3910	-5
16	154	381	-7
17	412	279	5
18	744	642	8
19	740	758	-1
20	2131	2117	2
21	607	119	21
22	819	607	15
23	-175	211	-3
24	-372	150	-7
25	459	474	0
26	821	647	11
27	1072	1146	-4
28	1464	1464	0
	-1	5	1
1	4541	4562	-5
2	2693	2561	50
3	2043	1996	21
4	4802	4756	10
5	671	635	9
6	1009	912	31
7	293	194	8
8	-299	177	-18
9	-332	196	-19
10	5468	5371	19
11	287	303	-1
12	311	129	7
13	979	979	0
14	811	765	5
15	1055	1148	-13
16	1111	1051	7
17	1830	1851	-4
18	808	653	13
19	3678	3599	16
20	666	690	-1
21	873	784	7
22	694	638	3
23	435	465	-1
24	685	726	-2
25	518	535	0
26	703	59	15
27	1088	1201	-7
28	1317	1036	17
	-1	7	1
1	1063	1080	-6
2	521	638	-29
3	1772	1763	3
4	4782	4789	-1
5	2326	2280	17
6	1155	1174	-6
7	1504	1577	-27
8	2381	2400	-6
9	3088	3127	-11
10	6930	6893	6
11	511	453	5
12	1683	1739	-14
13	589	685	-10
14	1811	1745	14
15	354	301	2
16	267	170	2
17	3188	3189	0
18	601	597	0
19	1576	1604	-4
20	562	795	-16
21	519	689	-10
22	-386	325	-13
23	782	445	19
24	1603	1589	1
25	482	464	0
26	591	468	4
27	920	822	4
	-1	9	1
1	1617	1614	0
2	6483	6394	15
3	4135	4100	9
4	2221	2216	1
5	2424	2418	2
6	2566	2605	-13
7	561	642	-13
8	864	786	16
9	529	469	7
10	1390	1357	8
11	332	181	7
12	1679	1739	-15
13	2309	2221	23
14	322	295	1
15	2520	2536	-3

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 16

16	1542	1457	14
17	1991	2038	-9
18	764	628	9
19	524	285	10
20	310	266	1
21	937	859	6
22	1064	963	9
23	522	425	4
24	1244	1204	4
25	-191	396	-5
26	691	600	3
27	389	511	-2
	-1	11	1
1	2042	1981	21
2	4567	4544	5
3	1393	1460	-22
4	3544	3507	10
5	1649	1551	31
6	4559	4618	-14
7	487	538	-6
8	402	262	10
9	391	288	7
10	1042	1062	-3
11	2667	2729	-17
12	1674	1690	-3
13	1852	1851	0
14	1456	1436	3
15	433	7	12
16	2325	2218	23
17	355	100	6
18	437	310	5
19	592	374	10
20	519	531	0
21	457	404	2
22	890	1160	-23
23	948	841	7
24	392	204	3
25	-671	382	-16
26	1164	1156	0
	-1	13	1
1	2066	2153	-29
2	2200	2133	21
3	946	920	5
4	2348	2370	-7
5	4577	4556	4
6	700	742	-6
7	1930	1912	5
8	849	873	-3
9	2450	2413	10
10	534	500	3
11	3379	3459	-21
12	630	761	-13
13	1185	1118	10
14	1038	967	9
15	1329	1402	-11
16	544	375	9
17	2257	2229	5
18	-306	180	-6
19	1722	1637	12
20	313	61	4
21	791	340	21
22	600	257	12
23	455	431	0
24	726	375	10
25	797	643	5
	-1	15	1
1	2202	2209	-2
2	2554	2611	-17
3	112	111	0
4	2664	2683	-5
5	1202	1197	1
6	327	248	4

7	926	937	-1
8	1727	1721	1
9	320	437	-7
10	1367	1326	8
11	1001	1074	-10
12	1031	1072	-5
13	1370	1349	3
14	904	994	-10
15	529	566	-2
16	1211	1077	16
17	599	768	-12
18	1036	1083	-4
19	1082	1110	-2
20	520	327	7
21	432	516	-2
22	791	327	13
23	564	382	4
	-1	17	1
1	1334	1305	6
2	1480	1495	-3
3	1277	1263	2
4	439	526	-7
5	1080	984	15
6	647	693	-4
7	2691	2754	-16
8	1518	1593	-15
9	308	12	6
10	1209	1210	0
11	418	19	11
12	414	417	0
13	1384	1298	13
14	804	582	17
15	1142	1096	5
16	408	1	8
17	254	344	-2
18	577	446	6
19	1139	1197	-4
20	515	9	7
21	613	644	-1
22	-634	262	-12
	-1	19	1
1	564	211	20
2	-450	49	-15
3	-396	7	-11
4	398	509	-7
5	1897	1996	-22
6	1335	1259	12
7	916	813	12
8	257	352	-3
9	1062	926	17
10	970	992	-2
11	627	415	14
12	1432	1299	19
13	1052	1105	-6
14	1388	1367	2
15	-377	435	-16
16	561	398	5
17	637	24	13
18	668	303	11
19	797	592	8
20	137	380	-3
	-1	21	1
1	1445	1292	24
2	516	448	4
3	-359	259	-12
4	799	699	9
5	345	166	6
6	-353	328	-14
7	1601	1637	-6
8	754	640	9
9	798	346	30
10	1170	937	26

11	-255	200	-5
12	428	379	2
13	1077	1026	3
14	681	709	-1
15	222	203	0
16	826	137	21
17	367	263	1
	-1	23	1
1	1014	939	8
2	701	632	5
3	458	25	11
4	625	565	4
5	768	505	18
6	581	258	15
7	1948	2043	-12
8	-381	84	-5
9	-506	476	-17
10	612	36	15
11	419	32	5
12	566	39	10
13	571	309	7
14	-385	316	-7
	-1	25	1
1	602	333	8
2	451	74	6
3	-529	235	-11
4	715	632	3
5	1010	991	1
6	867	731	7
7	512	334	4
8	532	391	4
9	824	891	-3
	0	0	1
2	6234	6292	-11
4	3699	3698	0
6	2844	2864	-6
8	4394	4439	-12
10	2582	2564	6
12	160	99	1
14	1542	1526	4
16	1355	1358	0
18	-493	57	-21
20	2781	2847	-18
22	665	552	9
24	726	749	-2
26	1023	1056	-4
28	955	654	18
	0	2	1
0	4063	3979	23
1	2914	2913	0
2	1145	1151	-5
3	1958	1929	16
4	2227	2206	10
5	688	534	49
6	3409	3254	52
7	1290	1253	14
8	3214	3191	7
9	5865	5750	23
10	3515	3545	-9
11	5361	5486	-28
12	1664	1669	-1
13	5493	5624	-28
14	1689	1724	-10
15	-178	244	-9
16	883	920	-6
17	1510	1561	-12
18	2642	2661	-5
19	1348	1359	-2
20	2002	2061	-15
21	902	807	13

22	1100	1112	-1
23	1204	1169	5
24	1730	1807	-16
25	1047	1086	-5
26	441	265	7
27	228	467	-7
28	752	704	2
	0	4	1
0	476	481	-1
1	3752	3643	36
2	397	290	33
3	1727	1751	-14
4	4247	4161	24
5	3807	3864	-18
6	2776	2751	10
7	3037	2987	18
8	1481	1480	0
9	1355	1331	9
10	3463	3424	12
11	5416	5399	3
12	570	657	-12
13	433	267	11
14	1579	1488	25
15	3478	3558	-23
16	1479	1513	-8
17	1037	939	16
18	3777	3851	-19
19	2835	2854	-5
20	527	205	18
21	974	839	17
22	2445	2486	-10
23	1807	1787	4
24	665	747	-7
25	411	311	4
26	830	959	-9
27	364	615	-9
28	-683	565	-30
	0	6	1
0	2744	2710	12
1	2345	2335	4
2	7925	7822	18
3	5147	5080	16
4	5382	5417	-8
5	1541	1543	0
6	6213	6206	1
7	4676	4606	18
8	198	249	-4
9	179	250	-5
10	2141	2087	21
11	969	880	22
12	982	941	9
13	1482	1422	17
14	1229	1160	15
15	687	635	6
16	1062	1171	-20
17	854	652	26
18	1172	1203	-5
19	2021	2126	-27
20	283	66	5
21	-116	415	-13
22	328	120	6
23	1167	1015	21
24	161	540	-17
25	-173	319	-8
26	725	702	1
27	642	343	11
28	1412	1466	-5
	0	8	1
0	964	878	28
1	4626	4682	-15
2	2830	2875	-18
3	44	195	-9

4	1329	1357	-14
5	2774	2799	-10
6	3419	3456	-12
7	1381	1432	-23
8	4088	3950	39
9	2794	2745	18
10	533	453	12
11	736	766	-6
12	1635	1587	16
13	1263	1288	-7
14	1303	1248	13
15	2989	2941	14
16	1579	1636	-13
17	1611	1573	8
18	808	931	-15
19	1688	1645	9
20	1134	1075	9
21	667	513	12
22	443	114	12
23	268	490	-10
24	755	878	-12
25	515	692	-8
26	744	839	-5
27	855	466	19

0 10 1

0	3352	3408	-17
1	759	694	20
2	1986	1942	20
3	1175	1164	4
4	2092	2038	24
5	459	430	5
6	525	596	-15
7	2363	2356	3
8	1977	2016	-16
9	2909	2936	-10
10	826	844	-4
11	660	536	20
12	2298	2292	2
13	1623	1642	-5
14	1328	1335	-1
15	1249	1213	7
16	2895	2875	5
17	1871	1865	1
18	1425	1373	9
19	1290	1296	-1
20	1313	1428	-19
21	-167	58	-2
22	694	937	-24
23	1483	1509	-4
24	959	1078	-9
25	914	955	-2
26	584	680	-4

0 12 1

0	2395	2446	-17
1	326	263	7
2	206	7	8
3	100	208	-6
4	5781	5764	3
5	1694	1683	4
6	223	10	8
7	1576	1580	-1
8	-148	136	-6
9	2627	2629	0
10	3581	3623	-13
11	55	267	-8
12	581	661	-11
13	580	560	2
14	710	743	-4
15	1463	1394	16
16	428	204	12
17	1751	1730	4
18	918	811	13
19	1108	966	20
20	689	477	15

21	1131	1188	-7
22	693	751	-5
23	-249	359	-8
24	613	703	-4
25	1675	1578	10

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0	360	46	14
1	891	882	2
2	709	687	4
3	2764	2802	-14
4	1145	1198	-17
5	2733	2715	6
6	874	940	-15
7	-209	99	-7
8	652	634	2
9	2931	2965	-11
10	737	701	5
11	633	654	-2
12	1439	1428	2
13	1706	1657	13
14	2317	2285	9
15	772	758	1
16	2347	2353	-1
17	-71	245	-5
18	251	52	4
19	1155	1330	-28
20	988	948	4
21	675	656	1
22	468	45	8
23	935	917	1
24	790	848	-3

0 16 1

0	2717	2718	0
1	598	524	11
2	2146	2174	-10
3	3814	3934	-35
4	1946	1990	-15
5	1878	1833	15
6	2784	2822	-13
7	721	823	-18
8	352	247	7
9	761	726	5
10	1148	1140	1
11	-47	29	0
12	479	569	-8
13	435	190	15
14	2246	2213	9
15	333	315	0
16	443	483	-2
17	849	850	0
18	993	784	24
19	1159	1164	0
20	1104	952	12
21	-546	306	-14
22	1565	1690	-13

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0	651	775	-14
1	-360	99	-15
2	497	447	5
3	354	317	2
4	1909	1960	-16
5	670	621	6
6	564	751	-25
7	959	953	1
8	1068	1046	4
9	1678	1788	-31
10	579	446	12
11	1424	1489	-15
12	898	904	0
13	2272	2198	20
14	1546	1497	10
15	-343	117	-9

16	1151	1105	7
17	427	386	2
18	1213	1195	1
19	1436	1516	-9
20	618	390	8
21	812	712	5

0 20 1

0	1941	1907	7
1	1882	1871	3
2	186	221	-1
3	-78	129	-2
4	425	113	16
5	1931	1985	-16
6	875	760	16
7	-162	571	-32
8	197	380	-9
9	1374	1255	25
10	767	830	-8
11	667	603	6
12	-337	190	-11
13	360	366	0
14	146	42	1
15	338	240	3
16	-358	150	-6
17	1051	1098	-4
18	693	925	-14

0 22 1

0	238	108	2
1	352	505	-11
2	897	822	10
3	1309	1327	-3
4	854	928	-10
5	138	156	0
6	574	317	19
7	107	44	0
8	1898	1803	23
9	1131	1132	0
10	-412	261	-17
11	694	818	-9
12	567	328	10
13	161	232	-1
14	207	650	-18
15	257	715	-18

0 24 1

0	259	360	-2
1	-498	102	-13
2	-549	129	-18
3	142	165	0
4	-581	97	-18
5	-191	194	-3
6	-469	143	-12
7	463	282	6
8	388	1	7
9	28	150	-1
10	380	52	6
11	394	447	-1

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0	-632	165	-13
1	987	763	17
2	542	571	-1
3	271	26	3
4	511	167	11

1 1 1

0	211	41	31
1	831	731	72
2	1147	1140	4
3	298	269	5
4	1669	1590	35

5	146	63	2
6	7318	7097	33
7	3649	3552	25
8	1460	1339	25
9	3446	3502	-14
10	3165	3050	28
11	2028	1999	6
12	1095	941	22
13	385	156	9
14	3856	3923	-15
15	789	876	-9
16	1874	1905	-6
17	1154	1143	1
18	2561	2528	6
19	513	625	-7
20	515	405	5
21	804	622	13
22	661	352	15
23	567	319	10
24	378	361	0
25	-324	145	-5
26	1055	946	9
27	1018	738	13
28	-339	75	-3

1 3 1

0	1906	1879	14
1	759	625	68
2	341	269	16
3	2658	2538	46
4	495	422	17
5	2323	2244	31
6	3424	3378	14
7	5807	5686	23
8	3695	3605	24
9	911	795	20
10	1480	1532	-12
11	2767	2588	45
12	2797	2789	1
13	1223	1274	-9
14	4125	4146	-4
15	2306	2362	-13
16	750	541	17
17	3440	3495	-12
18	1294	1282	1
19	1818	1753	11
20	-444	53	-11
21	1216	1257	-5
22	620	611	0
23	1554	1456	13
24	467	182	9
25	1168	1069	9
26	913	970	-3
27	-42	51	0
28	-476	72	-6

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0	1815	1768	23
1	4581	4472	26
2	719	682	13
3	3879	3701	49
4	1466	1427	18
5	2225	2243	-7
6	3343	3371	-8
7	26	254	-10
8	3311	3304	2
9	288	79	10
10	565	295	25
11	4688	4557	28
12	2755	2702	14
13	1180	1088	15
14	327	111	7
15	3512	3524	-2
16	1010	1146	-17
17	2156	2240	-17
18	-522	128	-16

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II)

19	775	786	-1
20	1087	1333	-30
21	894	761	11
22	1005	1061	-5
23	488	573	-4
24	-242	414	-10
25	664	809	-10
26	319	47	3
27	672	104	12
28	961	729	10
	1 7 l		
0	2991	2968	7
1	708	713	-1
2	484	387	18
3	1307	1338	-13
4	4381	4343	9
5	3335	3282	16
6	2449	2523	-27
7	6630	6584	7
8	2596	2612	-5
9	1148	1194	-12
10	3338	3268	19
11	2309	2265	13
12	525	525	0
13	686	752	-7
14	501	171	17
15	1688	1643	8
16	1131	1077	6
17	625	318	17
18	504	35	14
19	1458	1567	-16
20	1269	1306	-4
21	1806	1929	-20
22	1131	858	18
23	897	891	0
24	944	1049	-9
25	-691	483	-21
26	299	390	-1
27	966	774	9
	1 9 l		
0	4554	4418	32
1	4435	4415	4
2	1055	1040	4
3	1924	1962	-15
4	2211	2264	-20
5	340	151	14
6	408	398	1
7	2941	2951	-3
8	2078	2023	18
9	921	924	0
10	4565	4681	-27
11	838	1023	-32
12	858	757	14
13	1746	1740	1
14	1693	1585	22
15	926	787	15
16	945	886	6
17	1613	1660	-7
18	3129	3036	18
19	131	413	-8
20	822	962	-11
21	915	754	12
22	198	138	1
23	572	677	-5
24	525	205	10
25	381	300	1
26	797	458	11
27	844	353	15
	1 11 l		
0	1541	1496	15
1	1984	1934	17
2	2250	2291	-14
3	2465	2372	32
4	1838	1808	10
5	1075	1080	-1
6	1633	1676	-14
7	2271	2320	-16
8	2152	2200	-15
9	4590	4619	-6
10	1639	1522	30
11	1991	2034	-11
12	990	984	0
13	2007	1955	12
14	-271	316	-12
15	224	340	-4
16	476	260	9
17	880	862	1
18	2247	2260	-2
19	631	315	14
20	500	551	-2
21	810	434	20
22	202	357	-3
23	238	249	0
24	413	281	2
25	-343	18	-3
26	-535	65	-7
	1 13 l		
0	4151	4178	-6
1	444	440	0
2	574	665	-13
3	109	258	-6
4	257	225	1
5	286	115	7
6	788	815	-4
7	1153	1250	-21
8	1070	931	25
9	3021	3042	-5
10	1911	1936	-6
11	433	208	11
12	778	828	-6
13	1095	1022	10
14	592	733	-12
15	1623	1660	-6
16	716	678	3
17	1214	1225	-1
18	649	581	4
19	1267	1292	-2
20	847	784	4
21	-313	205	-6
22	727	482	8
23	658	572	2
24	-656	54	-11
25	114	103	0
	1 15 l		
0	1806	1840	-9
1	1116	1084	6
2	1045	1019	5
3	-13	334	-10
4	3527	3545	-4
5	1059	1054	0
6	1033	1042	-1
7	943	942	0
8	388	242	7
9	930	1000	-10
10	950	988	-5
11	765	739	2
12	1094	1041	7
13	1543	1501	7
14	746	890	-14
15	-431	265	-15
16	-114	132	-1
17	985	943	4
18	364	362	0
19	-433	540	-21
20	-472	187	-10
21	448	383	1
22	-114	13	0
23	417	98	4
	1 17 l		
0	1546	1582	-8
1	1668	1648	4
2	1002	1005	0
3	696	822	-15
4	-464	275	-24
5	-351	74	-10
6	1031	1049	-2
7	477	228	13
8	126	419	-11
9	489	643	-12
10	1178	1271	-15
11	1750	1713	7
12	1443	1373	11
13	1135	1242	-14
14	523	324	9
15	551	438	6
16	-473	311	-16
17	660	663	0
18	412	124	7
19	-269	336	-5
20	-659	280	-13
21	722	105	13
	1 19 l		
0	1128	1055	11
1	1988	1953	8
2	744	784	-4
3	1187	1254	-11
4	1093	1052	6
5	316	324	0
6	600	739	-13
7	652	501	11
8	408	215	7
9	722	720	0
10	429	228	8
11	2035	1995	8
12	-285	601	-27
13	657	719	-4
14	576	424	8
15	1462	1461	0
16	458	95	6
17	1103	1002	6
18	-408	182	-5
19	959	509	18
	1 21 l		
0	1349	1269	12
1	523	269	13
2	1365	1390	-4
3	412	310	4
4	1036	910	15
5	-203	387	-11
6	768	749	1
7	332	8	6
8	-329	368	-14
9	493	115	13
10	1492	1462	4
11	905	973	-6
12	1085	1124	-4
13	221	10	1
14	961	806	9
15	-277	501	-10
16	970	495	20
17	-574	103	-9
	1 23 l		
0	1133	1099	4
1	920	1006	-9
2	-376	24	-8
3	886	905	-1
4	509	446	3
5	1095	851	25
6	201	406	-7
7	61	30	0
8	168	18	1
9	1060	1046	0
10	296	326	0
11	-412	89	-5
12	799	675	5
13	746	901	-7
	1 25 l		
0	-133	74	0
1	861	424	19
2	711	533	7
3	754	381	14
4	871	636	12
5	-287	135	-3
6	781	283	18
7	781	37	19
8	690	301	12
	2 0 l		
0	4488	4551	-17
2	3424	3422	0
4	8236	8161	12
6	4907	4938	-6
8	3161	3116	13
10	4091	4167	-18
12	3330	3278	12
14	837	797	4
16	4672	4685	-2
18	528	655	-8
20	316	102	4
22	910	1037	-11
24	1466	1315	18
26	-473	27	-7
28	773	722	2
	2 2 l		
0	613	583	14
1	1005	1056	-32
2	285	118	24
3	953	935	8
4	4252	4122	33
5	4949	4773	39
6	1380	1301	29
7	6887	6699	30
8	3448	3356	25
9	868	769	16
10	943	745	28
11	1869	1946	-18
12	2242	2140	23
13	1244	1247	0
14	833	738	9
15	533	467	4
16	934	927	0
17	2892	2984	-20
18	909	895	1
19	415	528	-5
20	1636	1730	-14
21	355	256	3
22	2386	2361	4
23	1001	667	25
24	278	217	1
25	1573	1580	0
26	995	745	12
27	352	110	3
28	1523	1531	0
	2 4 l		
0	2039	2028	5
1	3444	3427	5
2	888	860	12

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 19

3	1340	1259	39
4	339	180	19
5	782	839	-18
6	2185	2147	14
7	1072	971	30
8	709	826	-24
9	422	359	6
10	127	329	-9
11	2457	2307	41
12	1648	1572	16
13	923	738	21
14	1550	1459	16
15	1452	1453	0
16	1512	1536	-4
17	1366	1310	8
18	-186	271	-6
19	2098	2120	-4
20	1379	1380	0
21	1865	1806	9
22	1649	1614	5
23	465	249	7
24	647	461	9
25	326	512	-6
26	1524	1520	0
27	421	553	-3
28	734	738	0
	2 6 1		
0	663	655	2
1	2906	2870	12
2	5751	5691	11
3	261	231	3
4	3280	3257	7
5	1885	1884	0
6	9607	9563	5
7	317	232	7
8	865	914	-11
9	597	539	8
10	4332	4383	-12
11	3145	3076	19
12	2462	2564	-21
13	4268	4249	4
14	533	425	7
15	1302	1304	0
16	1574	1617	-6
17	502	518	0
18	420	471	-2
19	667	885	-18
20	1089	1067	2
21	1124	1106	2
22	-372	94	-7
23	673	76	21
24	-360	127	-6
25	392	8	6
26	644	20	12
27	608	637	-1
	2 8 1		
0	3942	3833	29
1	1224	1264	-15
2	997	953	14
3	3535	3550	-4
4	539	469	11
5	670	627	9
6	456	509	-7
7	282	241	3
8	621	270	41
9	2516	2513	1
10	1351	1402	-13
11	3373	3406	-9
12	1935	1977	-11
13	520	316	14
14	203	461	-12
15	2391	2430	-9
16	2393	2390	0
17	654	701	-3
18	-323	403	-13
19	2213	2209	0
20	341	318	0
21	908	1079	-16
22	215	28	2
23	-267	40	-3
24	1914	1974	-8
25	1883	1925	-4
26	535	216	6
27	493	896	-14
	2 10 1		
0	1527	1532	-1
1	1019	1100	-24
2	1727	1693	12
3	1384	1407	-8
4	2887	2911	-8
5	3522	3444	22
6	3481	3530	-14
7	2875	2907	-10
8	1341	1342	0
9	2070	2100	-9
10	3685	3697	-3
11	235	451	-14
12	798	741	7
13	1276	1268	1
14	2150	2101	11
15	2100	2033	14
16	3885	3949	-14
17	483	115	13
18	343	124	5
19	-337	371	-11
20	989	952	3
21	1116	1062	5
22	930	716	15
23	1113	1115	0
24	1757	1900	-13
25	-679	499	-19
26	412	312	1
	2 12 1		
0	1579	1534	14
1	1247	1202	12
2	2403	2440	-12
3	137	116	0
4	-153	32	-3
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Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 22

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12	412	115	8
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15	-390	345	-9
16	-541	417	-15
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7 21 1

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4	-341	169	-8
5	1558	1410	22
6	578	837	-19
7	700	501	12

8	1032	874	11
9	1319	1006	25
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11	575	440	4
12	788	644	6
13	1158	1221	-4
14	-752	438	-22

7 23 1

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5	464	494	-1
6	553	447	3
7	1140	814	20
8	769	41	19
9	331	511	-4

8 0 1

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2	4158	4114	11
4	4054	4065	-3
6	476	26	31
8	4784	4898	-25
10	56	226	-4
12	1505	1580	-16
14	1199	1246	-7
16	4083	3936	31
18	3414	3518	-21
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24	482	645	-5
26	-474	231	-7

8 2 1

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3	2711	2761	-17
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6	746	662	15
7	3986	4011	-6
8	3090	3030	17
9	5217	5362	-30
10	-91	55	-1
11	1667	1655	3
12	1834	1878	-11
13	1371	1313	10
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18	710	824	-8
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20	390	209	4
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22	1062	843	17
23	636	756	-6
24	507	735	-7
25	-913	23	-21
26	764	419	10

8 4 1

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4	1125	1072	14
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6	2645	2709	-21
7	257	292	-2

8	583	644	-8
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14	395	133	9
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16	833	902	-6
17	1594	1612	-2
18	1074	1066	0
19	580	714	-7
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22	1598	1599	0
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25	729	374	9

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6	4145	4135	2
7	1523	1512	3
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9	1472	1492	-5
10	980	1068	-15
11	1636	1646	-2
12	910	869	3
13	-408	351	-21
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20	-333	57	-4
21	917	713	13
22	615	446	7
23	451	776	-10
24	124	112	0
25	813	332	13

8 8 1

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2	809	827	-3
3	1759	1715	14
4	951	986	-7
5	1041	1057	-3
6	2625	2624	0
7	1170	1141	6
8	554	392	15
9	544	488	5
10	365	434	-4
11	561	303	17
12	2164	2174	-2
13	2610	2647	-9
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18	1089	918	15
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4	2453	2420	10
5	245	210	1
6	2028	2036	-2
7	2843	2931	-25
8	2768	2687	22
9	1604	1636	-7
10	901	869	4
11	1386	1404	-3
12	288	376	-4
13	642	583	5
14	1507	1444	10
15	310	423	-4
16	138	99	0
17	551	304	10
18	770	732	2
19	287	124	2
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7	1283	1365	-16
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9	1153	1051	16
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12	996	1047	-6
13	1331	1278	8
14	818	802	1
15	600	676	-5
16	358	593	-11
17	496	161	11
18	617	588	1
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21	-572	294	-9
22	-355	185	-3

8 14 1

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3	462	124	16
4	1626	1640	-3
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7	562	498	4
8	867	806	7
9	590	525	5
10	618	620	0
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12	545	238	14
13	986	814	17
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15	569	508	3
16	947	743	17
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18	628	127	11
19	890	567	12
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15	943	751	15
16	1035	909	7
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18	1316	1218	6
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8 18 1

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9	618	487	8
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17	336	110	2

8 20 1

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5	576	440	7
6	-215	431	-12
7	135	52	0
8	284	531	-10
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11	404	377	0
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7	551	227	8
8	-446	23	-6
9	1357	1288	5
10	575	593	0
11	526	365	4

8 24 1

0	139	441	-5

Tetra(pentafluorophenyl)octabromoporphinato Nickel(II) Page 26

1	342	162	2
2	466	222	5
3	881	417	22
4	702	631	3

9 1 l

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17	1006	931	7
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19	1027	1121	-8
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23	873	814	2
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25	686	455	6

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12	494	512	-1
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17	-182	73	-2
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19	-178	64	-1
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23	1195	1225	-1
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17	1085	1123	-4
18	661	572	5
19	782	891	-7
20	775	1089	-22
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22	670	716	-1
23	722	67	13
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9 7 l

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6	1102	1148	-10
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9	2014	2048	-9
10	2880	2932	-14
11	1916	1921	-1
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13	1619	1617	0
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15	760	706	4
16	2227	2245	-3
17	557	27	15
18	1103	953	14
19	1073	976	8
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21	1575	1487	9
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16	2554	2557	0
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18	2196	2073	20
19	1846	1833	1
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9 11 l

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7	4495	4557	-13
8	1263	1250	2
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16	909	868	3
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9 13 l

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19	-713	271	-15
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21	454	770	-9

9 15 l

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9 17 l

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15	-67	85	0
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9 19 l

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7	572	283	13
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8	2237	2299	-18

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21	902	1022	-9
22	-457	407	-12
23	999	369	22
24	388	145	3

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6	1463	1454	2
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8	1205	1193	2
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11	1432	1487	-11
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14	1777	1801	-4
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13	987	1021	-3
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19	543	790	-8
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21	573	587	0

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9	638	776	-12
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13	470	623	-9
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15	886	752	10
16	573	205	9
17	318	136	2
18	-431	273	-8
19	1004	740	11

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2	1191	959	32
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7	382	102	8
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12	717	662	3
13	1308	1269	4
14	696	921	-12
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3	-196	254	-11
4	269	389	-8
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6	751	709	5
7	197	14	4
8	793	670	16
9	1495	1545	-11
10	481	236	14
11	1227	1274	-8
12	500	709	-18
13	2176	2228	-11
14	1277	1294	-2
15	454	300	6
16	637	712	-5
17	1346	1355	-1
18	616	601	0
19	-462	179	-10
20	1409	1343	7
21	818	239	16
22	2568	2489	8
23	1127	909	11

11 3 1

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2	196	80	3
3	-476	52	-25
4	3272	3239	9
5	2081	2134	-16
6	496	508	-1
7	2243	2286	-12
8	3298	3284	3
9	931	973	-6
10	-227	83	-4
11	355	403	-2
12	2603	2598	1
13	702	810	-10
14	192	292	-3
15	1084	1114	-3
16	190	140	0
17	-445	270	-13
18	-375	166	-8
19	522	326	7
20	-274	118	-3
21	-349	439	-8
22	-221	201	-2
23	-107	811	-16

11 5 1

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1	335	439	-8
2	480	157	22
3	1121	1145	-5
4	622	467	19
5	673	751	-10
6	1279	1343	-14
7	2637	2642	-1
8	933	843	13
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10	928	954	-3
11	1140	1166	-4
12	-472	235	-19
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14	1195	1357	-23
15	864	923	-6

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17	1536	1489	6
18	-188	354	-7
19	41	421	-7
20	1153	1204	-4
21	531	349	4
22	-435	435	-9
23	-422	84	-4
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1	816	905	-14
2	1821	1818	0
3	1607	1580	7
4	2278	2320	-12
5	1692	1678	3
6	2466	2524	-16
7	1224	1221	0
8	1245	1196	9
9	156	247	-2
10	851	823	2
11	-117	201	-3
12	755	764	0
13	238	330	-3
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15	396	369	1
16	1143	960	19
17	871	975	-9
18	-115	210	-2
19	-423	38	-8
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22	-609	112	-8
	11	9	1
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2	749	728	2
3	1445	1414	7
4	1975	1922	13
5	2083	2112	-7
6	1744	1749	-1
7	1627	1647	-4
8	691	565	12
9	539	598	-5
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11	759	604	14
12	623	773	-13
13	466	222	10
14	885	811	6
15	838	824	1
16	661	687	-1
17	1021	1027	0
18	-443	314	-13
19	88	111	0
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	11	11	1
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3	857	801	7
4	491	473	1
5	528	411	8
6	402	546	-9
7	3094	3143	-12
8	1263	1213	8
9	391	10	11
10	2563	2572	-2
11	518	509	0
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13	2185	2100	16
14	328	64	5
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17	588	335	10
18	1955	1999	-4
19	625	52	10
20	125	382	-3
	11	13	1
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1	1823	1862	-9
2	421	493	-4
3	439	574	-10
4	337	210	5
5	217	61	3
6	678	428	19
7	2546	2544	0
8	428	672	-17
9	1708	1633	13
10	381	569	-11
11	268	327	-2
12	825	754	6
13	500	49	13
14	885	883	0
15	723	807	-6
16	611	44	12
17	920	633	13
18	567	522	1
19	534	143	7
	11	15	1
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3	-442	467	-27
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5	71	80	0
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7	613	456	10
8	1646	1457	32
9	591	411	10
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15	327	500	-4
16	860	42	21
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4	880	799	8
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7	366	307	2
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9	2084	1966	21
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	11	21	1
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6	2448	2514	-18
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12	804	811	0
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3	3114	3100	3
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6	1792	1811	-4
7	4084	4091	-1
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14	1110	1007	12
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22	652	198	9
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6	871	746	17
7	2246	2289	-11
8	716	615	10
9	1155	1263	-18
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12	1752	1676	15
13	278	357	-3
14	2579	2642	-13
15	1068	1081	-1

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18	936	837	7
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3	3952	3957	-1
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6	1199	1182	3
7	184	227	-1
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18	1663	1602	8
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2	1274	1187	16
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4	1090	1186	-16
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6	1949	1916	8
7	444	334	6
8	679	645	3
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10	381	247	5
11	777	773	0
12	857	755	10
13	1335	1349	-1
14	734	651	6
15	516	597	-4
16	902	807	7
17	184	236	-1
18	404	4	5
19	621	618	0
20	540	579	-1
21	1013	782	9
	12	10	1
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1	364	285	4
2	469	347	8
3	2037	2067	-7
4	-539	255	-27
5	-96	243	-5
6	1863	1838	5
7	853	953	-12
8	-287	391	-16
9	598	589	0
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11	487	84	14
12	332	216	3
13	-306	255	-8
14	779	735	3
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17	468	367	2
18	-493	352	-10
19	249	175	0
20	986	656	13

12 12 1

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3	-271	297	-11
4	1540	1637	-19
5	1583	1571	2
6	-198	254	-7
7	118	292	-4
8	138	369	-7
9	687	541	11
10	1206	1070	17
11	515	75	15
12	702	624	5
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14	-634	360	-28
15	-320	415	-9
16	1485	1307	16
17	1036	874	8
18	684	473	6
19	883	621	10

12 14 1

0	749	623	12
1	1176	1176	0
2	254	68	4
3	2259	2224	7
4	-337	148	-8
5	1793	1803	-1
6	212	49	2
7	512	246	12
8	1386	1457	-11
9	652	581	5
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11	259	68	3
12	554	489	4
13	1153	1102	3
14	-580	9	-11
15	226	559	-8
16	508	477	0
17	1221	1044	10

12 16 1

0	812	638	15
1	617	381	16
2	312	403	-4
3	256	200	1
4	463	501	-2
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6	294	115	4
7	197	394	-6
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9	469	226	9
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12	1396	1238	13
13	510	76	8
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12 18 1

0	633	557	5
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2	335	266	2
3	1727	1672	9
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5	664	653	0
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12 20 1

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7	575	313	7
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13 1 1

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2	1483	1499	-4
3	440	440	0
4	1031	1029	0
5	792	956	-23
6	128	265	-4
7	761	658	11
8	231	235	0
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11	372	126	8
12	1109	1006	13
13	1263	1225	5
14	656	686	-2
15	657	721	-4
16	-682	230	-26
17	-68	515	-12
18	1017	917	8
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20	-628	130	-10
21	649	425	5
22	449	752	-8

13 3 1

0	423	292	8
1	1403	1343	13
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4	1490	1535	-10
5	857	991	-20
6	772	892	-15
7	618	630	-1
8	601	484	9
9	628	496	10
10	1835	1837	0
11	2227	2175	11
12	313	180	4
13	2455	2432	5
14	820	886	-6
15	809	763	3
16	944	1027	-8
17	-152	181	-2
18	746	462	15
19	1159	947	13
20	422	245	3
21	912	715	7

13 5 1

0	1154	1170	-3
1	1803	1821	-4
2	1481	1560	-18
3	1047	973	12
4	1693	1644	11
5	270	413	-8
6	-145	326	-11
7	428	563	-10
8	403	687	-22
9	333	4	8
10	744	820	-8
11	1911	1898	2
12	1685	1593	16
13	1181	1192	-1
14	758	887	-11
15	857	903	-4
16	1060	1030	3
17	818	885	-5
18	619	494	4
19	1094	859	13
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13 7 1

0	547	670	-12
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2	1685	1731	-10
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6	960	1046	-12
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12	2253	2276	-4
13	676	715	-3
14	895	959	-6
15	1486	1460	3
16	473	401	3
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19	-794	395	-21
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13 9 1

0	-78	225	-4
1	2202	2153	12
2	397	377	1
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6	1275	1229	7
7	728	524	17
8	531	47	19
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11	306	408	-4
12	458	372	4
13	656	343	17
14	1580	1466	16
15	421	496	-3
16	450	270	4
17	-152	799	-20
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13 11 1

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3	940	956	-2
4	669	465	16
5	1489	1455	6
6	-330	7	-7
7	570	237	17
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9	525	623	-6
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16	418	526	-3
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13 13 1

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10	985	1083	-10
11	870	824	4
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13	760	481	12
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13 15 1

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6	1298	1304	0
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9	733	412	19
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12	-360	138	-4
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13 17 1

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5	356	381	0
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7	718	481	11
8	898	643	13
9	787	668	5
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11	388	137	4
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13 19 1

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6	806	429	15
7	705	886	-8
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14 0 1

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Tetra(pentafluorophenyl)octabromoporphinato Nickel(II)

2	1345	1313	6
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14	2	1	
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2	1824	1828	0
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6	1163	1071	15
7	293	389	-4
8	366	316	2
9	527	422	6
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11	338	397	-2
12	900	938	-4
13	1018	901	12
14	873	783	8
15	-390	158	-9
16	-207	369	-8
17	654	569	3
18	472	91	6
19	647	463	5
20	788	222	14
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1	707	613	10
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3	405	480	-5
4	1267	1254	2
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7	674	703	-2
8	603	645	-3
9	2040	2038	0
10	891	755	14
11	550	575	-1
12	536	222	15
13	400	529	-6
14	952	991	-3
15	565	794	-15
16	807	691	8
17	608	885	-13
18	481	679	-6
19	1551	1360	14
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3	306	677	-28
4	753	646	11
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7	1910	1948	-8
8	1188	1244	-8
9	575	602	-2
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11	1239	1236	0
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14	-233	254	-6
15	-262	389	-10
16	-357	35	-4
17	-348	401	-8
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19	561	637	-2
14	8	1	
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2	452	57	15
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4	272	456	-9
5	1743	1659	17
6	451	321	6
7	1292	1305	-2
8	704	572	11
9	1015	1017	0
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11	361	127	6
12	492	535	-2
13	897	869	2
14	810	643	12
15	683	325	12
16	-649	153	-14
17	93	310	-2
18	774	215	15
19	1276	1141	8
14	10	1	
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1	1365	1317	8
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3	1714	1661	10
4	2417	2406	2
5	1648	1646	0
6	535	536	0
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8	106	86	0
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12	607	338	13
13	701	398	16
14	661	413	9
15	875	910	-1
16	470	207	5
17	-419	175	-6
14	12	1	
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4	328	279	1
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6	527	259	13
7	270	71	4
8	474	315	7
9	1731	1711	3
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11	1558	1478	11
12	893	341	24
13	1788	1763	2
14	1491	1407	7
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16	-786	292	-19
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3	215	39	2
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9	619	551	2
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7	226	281	-1
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1	553	718	-16
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3	652	679	-2
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5	163	412	-10
6	556	672	-9
7	1490	1432	10
8	933	868	7
9	1406	1416	-1
10	560	548	0
11	1274	1268	0
12	826	634	16
13	157	375	-6
14	1298	1228	8
15	-161	371	-8
16	315	838	-19
17	1147	935	13
18	994	918	3
19	-195	368	-4
15	3	1	
0	781	718	7
1	1523	1467	11
2	243	491	-13
3	2013	1980	7
4	1684	1647	7
5	893	850	5
6	116	314	-6
7	1208	1208	0
8	1078	1168	-12
9	1415	1339	12
10	527	628	-7
11	713	790	-6
12	-158	341	-7
13	581	423	8
14	-86	165	-1
15	955	888	5
16	882	833	2
17	1194	815	22
18	687	386	9
19	476	182	5
15	5	1	
0	373	186	8
1	1385	1365	3
2	452	306	8
3	1297	1130	27
4	-604	243	-30
5	626	605	1
6	1343	1296	7
7	541	418	8
8	851	910	-6
9	241	442	-8
10	251	332	-2
11	-465	495	-26
12	-153	386	-9
13	-290	476	-16
14	-137	143	-1
15	-530	342	-13
16	1171	1040	8
17	302	402	-2
18	852	602	10
15	7	1	
0	95	237	-3
1	752	768	-1
2	934	887	6
3	-227	49	-3
4	604	688	-7
5	1209	1231	-3
6	215	351	-5
7	798	674	11
8	476	516	-2
9	-508	268	-19
10	373	0	8
11	849	632	17
12	675	660	1
13	273	424	-5
14	707	662	2
15	411	22	5
16	871	568	13
17	571	369	5
18	702	36	13
15	9	1	
0	2078	1988	20
1	714	606	9
2	747	753	0
3	1260	1222	5
4	304	557	-14
5	1813	1751	12
6	272	78	4
7	580	623	-3
8	269	181	2
9	369	216	5
10	337	4	6
11	574	680	-7
12	663	772	-8
13	620	553	2
14	756	5	19
15	-632	219	-13
16	440	108	5
17	-462	7	-5
15	11	1	
0	1081	885	23
1	819	612	18
2	718	534	14

Appendix 6. Supplimentary Material for the X-ray Crystal Structure Determination of $CuTFPPBr_8$.

Figure A6.1. ORTEP diagram for $CuTFPPBr_8$ (50% probability ellipsoids) and numbering scheme for macrocycle.

Table A6.1. Crystal and Intensity Collection Data for $CuTFPPBr_8$.

Formula: $CuC_{44}Br_8F_{20}N_4 \bullet \frac{1}{2}CH_2Cl_2$	Formula Weight: 1709.72
Crystal Color: dark purple	Habit: irregular plate
Crystal Size: 0.11 x 0.41 x 0.40 mm	
Crystal System: monoclinic	Space Group: C2/c
a = 18.099(4) Å	$\alpha = 90$
b = 22.326(4) Å	$\beta = 92.31$
c = 24.303(5) Å	$\gamma = 120$
V = 9814(3) $Å^3$	Z = 8
D = 2.32 g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 7.07$ mm^{-1}	T = 294 K
Enraf-Nonius Cad-4 diffractometer	ω scan
	range for data collection: 1-25
$\pm h = 21$, $\pm k = 26$, l = 0 - 28	
Number of reflections measured: 18304	
Number of independent reflections: 8610	
R = 0.047 on F for 3625 reflections with $F_o^2 > 3\sigma(F_o^2)$	
wR = 0.007 on F^2 for 8610 reflections	
Final goodness of fit: 1.18 for 570 parameters and 8610 reflections	

Table A6.2. Final Refined Heavy Atom Parameters x 10^4 for $CuTFPPBr_8$.

x, y, z and $U_{eq}{}^a \times 10^4$

Atom	x	y	z	U_{eq} or B
Cu	3220(.5)	995(.4)	9755(.4)	306(3)
Br1	2998(.5)	3559(.4)	9321(.4)	512(3)
Br2	4340(.5)	3356(.4)	10352(.4)	492(3)
Br3	6255(.5)	938(.4)	10623(.5)	563(3)
Br4	5418(.5)	−362(.4)	11029(.5)	572(3)
Br5	1968(.6)	−673(.5)	11292(.4)	584(3)
Br6	812(.5)	−681(.5)	10131(.5)	597(3)
Br7	1632(.6)	175(.4)	7758(.4)	554(3)
Br8	2168(.5)	1617(.4)	7511(.4)	484(3)
N1	3590(3)	1809(3)	9617(3)	2.6(1)*
N2	4008(3)	879(3)	10332(3)	2.3(1)*
N3	2752(3)	241(3)	9979(3)	2.3(1)*
N4	2532(3)	1045(3)	9109(3)	2.2(1)*
C1	3202(4)	2227(3)	9308(4)	2.7(2)*
C2	3422(4)	2813(3)	9514(3)	2.4(2)*
C3	3952(4)	2742(3)	9892(4)	2.5(2)*
C4	4093(4)	2106(3)	9959(4)	2.7(2)*
C5	4672(4)	1815(3)	10240(4)	3.0(2)*
C6	4662(4)	1201(3)	10350(3)	2.5(2)*

Atom	x	y	z	U_{eq} or B
C7	5230(4)	811(3)	10593(4)	3.1(2) *
C8	4911(4)	301(3)	10751(4)	2.9(2) *
C9	4128(4)	349(3)	10608(4)	2.7(2) *
C10	3550(4)	−18(3)	10767(4)	2.5(2) *
C11	2858(4)	−26(3)	10492(3)	2.5(2) *
C12	2211(4)	−350(3)	10619(4)	2.8(2) *
C13	1761(4)	−335(3)	10158(4)	2.7(2) *
C14	2097(4)	15(3)	9754(3)	2.2(2) *
C15	1877(4)	108(3)	9205(4)	2.4(2) *
C16	2147(4)	570(3)	8881(4)	2.5(2) *
C17	2000(4)	703(3)	8309(4)	2.4(2) *
C18	2220(4)	1255(3)	8206(4)	2.8(2) *
C19	2540(4)	1495(3)	8712(3)	2.3(2) *
C20	2775(4)	2084(3)	8840(4)	2.4(2) *
C21	5346(5)	2163(4)	10436(4)	3.0(2) *
C22	5779(5)	2435(4)	10039(5)	504(30)
C23	6443(6)	2705(4)	10198(6)	662(44)
C24	6668(6)	2694(5)	10760(7)	810(52)
C25	6231(6)	2456(5)	11140(6)	667(39)

Atom	x	y	z	U_{eq} or B
C26	5570(5)	2181(4)	10985(5)	500(30)
F22	5579(3)	2440(3)	9517(3)	726(19)
F23	6862(3)	2958(3)	9836(3)	1179(27)
F24	7321(3)	2943(3)	10912(3)	1283(29)
F25	6464(3)	2448(3)	11664(3)	1015(22)
F26	5179(3)	1928(3)	11364(2)	679(21)
C31	3694(4)	−403(4)	11261(4)	2.6(2) *
C32	3758(5)	−1012(4)	11246(5)	481(29)
C33	3914(6)	−1349(5)	11716(6)	709(42)
C34	3983(7)	−1076(6)	12206(6)	769(42)
C35	3900(7)	−473(6)	12242(5)	823(50)
C36	3753(6)	−149(4)	11776(5)	638(37)
F32	3714(4)	−1289(2)	10758(3)	902(25)
F33	3985(4)	−1934(3)	11692(3)	1248(30)
F34	4117(4)	−1390(3)	12668(3)	1223(25)
F35	3936(5)	−193(3)	12729(3)	1558(44)
F36	3673(4)	447(3)	11812(3)	1071(29)
C41	1314(4)	−307(4)	8957(4)	2.5(2) *
C42	1473(5)	−908(4)	8865(4)	419(26)

Atom	x	y	z	U_{eq} or B
C43	952(7)	−1295(4)	8659(4)	624(39)
C44	251(6)	−1088(5)	8525(5)	786(39)
C45	86(6)	−508(5)	8589(5)	719(37)
C46	608(5)	−134(4)	8812(4)	526(29)
F42	2155(3)	−1113(2)	8993(2)	633(17)
F43	1134(3)	−1871(2)	8587(3)	974(25)
F44	−241(4)	−1477(3)	8318(3)	1414(27)
F45	−602(3)	−316(3)	8466(3)	1287(30)
F46	423(3)	446(2)	8893(2)	690(17)
C51	2588(5)	2566(3)	8425(4)	2.3(2) *
C52	3097(5)	2820(4)	8120(4)	410(27)
C53	2946(6)	3255(4)	7739(4)	575(33)
C54	2215(7)	3428(4)	7650(5)	614(38)
C55	1679(5)	3177(4)	7952(5)	508(32)
C56	1872(5)	2751(4)	8344(4)	421(28)
F52	3808(3)	2635(2)	8177(2)	649(17)
F53	3458(4)	3525(3)	7457(3)	1012(23)
F54	2042(4)	3844(3)	7271(3)	1082(25)
F55	971(3)	3345(2)	7862(3)	911(20)

Atom	x	y	z	U_{eq} or B
F56	1330(3)	2526(2)	8635(3)	705(18)
CS	0	1918(7)	7500	1069(63)
ClS	36(2)	1500(2)	6912(2)	1397(15)
HS	429	2164	7528	10.2 *

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

Table A6.3. Complete Distances and Angles for $CuTFPPBr_8$.

	Distance(Å)		Distance(Å)
Cu –N1	1.969(6)	C17 –C18	1.323(11)
Cu –N2	1.977(6)	C18 –C19	1.442(11)
Cu –N3	1.971(6)	C19 –C20	1.413(11)
Cu –N4	1.968(6)	C20 –C51	1.503(11)
Br1 –C2	1.884(7)	C21 –C22	1.405(13)
Br2 –C3	1.887(8)	C21 –C26	1.379(13)
Br3 –C7	1.874(8)	C22 –C23	1.386(15)
Br4 –C8	1.857(8)	C22 –F22	1.305(12)
Br5 –C12	1.856(8)	C23 –C24	1.411(18)
Br6 –C13	1.882(8)	C23 –F23	1.313(13)
Br7 –C17	1.885(8)	C24 –C25	1.349(18)
Br8 –C18	1.870(8)	C24 –F24	1.344(15)
N1 –C1	1.373(10)	C25 –C26	1.382(15)
N1 –C4	1.378(10)	C25 –F25	1.325(13)
N2 –C6	1.384(10)	C26 –F26	1.311(11)
N2 –C9	1.372(10)	C31 –C32	1.366(13)
N3 –C11	1.390(10)	C31 –C36	1.375(13)
N3 –C14	1.381(9)	C32 –C33	1.386(15)
N4 –C16	1.373(10)	C32 –F32	1.338(11)
N4 –C19	1.392(10)	C33 –C34	1.340(17)
C1 –C2	1.452(11)	C33 –F33	1.313(14)
C1 –C20	1.387(11)	C34 –C35	1.357(18)
C2 –C3	1.310(11)	C34 –F34	1.339(14)
C3 –C4	1.450(11)	C35 –C36	1.362(16)
C4 –C5	1.390(11)	C35 –F35	1.339(15)
C5 –C6	1.398(11)	C36 –F36	1.341(12)
C5 –C21	1.507(12)	C41 –C42	1.392(12)
C6 –C7	1.453(11)	C41 –C46	1.367(12)
C7 –C8	1.340(11)	C42 –C43	1.359(14)
C8 –C9	1.449(11)	C42 –F42	1.342(10)
C9 –C10	1.395(11)	C43 –C44	1.377(16)
C10 –C11	1.395(11)	C43 –F43	1.340(12)
C10 –C31	1.490(11)	C44 –C45	1.339(16)
C11 –C12	1.423(11)	C44 –F44	1.328(14)
C12 –C13	1.359(11)	C45 –C46	1.357(15)
C13 –C14	1.413(11)	C45 –F45	1.339(13)
C14 –C15	1.393(11)	C46 –F46	1.355(11)
C15 –C16	1.397(11)	C51 –C52	1.332(12)
C15 –C41	1.486(11)	C51 –C56	1.366(12)
C16 –C17	1.436(11)	C52 –C53	1.362(14)

Distance(Å)		Angle(°)	
C52 –F52	1.354(10)	N1 –Cu –N2	90.1(2)
C53 –C54	1.386(15)	N1 –Cu –N3	171.0(2)
C53 –F53	1.319(12)	N1 –Cu –N4	91.2(2)
C54 –C55	1.360(15)	N2 –Cu –N3	89.9(2)
C54 –F54	1.336(13)	N2 –Cu –N4	171.5(2)
C55 –C56	1.380(14)	N3 –Cu –N4	90.2(2)
C55 –F55	1.345(12)	C4 –N1 –C1	108.2(6)
C56 –F56	1.332(11)	C9 –N2 –C6	108.3(6)
CS –ClS	1.710(17)	C14 –N3 –C11	106.6(6)
CS –HS	0.950	C19 –N4 –C16	107.3(6)
		C2 –C1 –N1	107.3(6)
		C20 –C1 –N1	123.2(7)
		C20 –C1 –C2	128.8(7)
		C3 –C2 –C1	108.3(7)
		C4 –C3 –C2	108.6(7)
		C3 –C4 –N1	107.2(6)
		C5 –C4 –N1	122.6(7)
		C5 –C4 –C3	129.7(7)
		C6 –C5 –C4	122.5(7)
		C21 –C5 –C4	119.9(7)
		C21 –C5 –C6	117.6(7)
		C5 –C6 –N2	121.4(7)
		C7 –C6 –N2	107.0(6)
		C7 –C6 –C5	130.5(7)
		C8 –C7 –C6	108.5(7)
		C9 –C8 –C7	107.4(7)
		C8 –C9 –N2	108.3(6)
		C10 –C9 –N2	122.4(7)
		C10 –C9 –C8	128.8(7)
		C11 –C10 –C9	122.8(7)
		C31 –C10 –C9	117.0(7)
		C31 –C10 –C11	120.2(7)
		C10 –C11 –N3	121.0(7)
		C12 –C11 –N3	109.1(6)
		C12 –C11 –C10	129.3(7)
		C13 –C12 –C11	106.3(7)
		C14 –C13 –C12	109.1(7)
		C13 –C14 –N3	108.3(6)
		C15 –C14 –N3	122.2(7)
		C15 –C14 –C13	129.4(7)

Angle(°)		Angle(°)	
C16 –C15 –C14	123.8(7)	F33 –C33 –C34	119.0(11)
C41 –C15 –C14	117.3(7)	C35 –C34 –C33	120.2(12)
C41 –C15 –C16	118.8(7)	F34 –C34 –C33	121.0(11)
C15 –C16 –N4	121.8(7)	F34 –C34 –C35	118.8(11)
C17 –C16 –N4	107.6(6)	C36 –C35 –C34	119.5(11)
C17 –C16 –C15	130.0(7)	F35 –C35 –C34	121.3(11)
C18 –C17 –C16	109.3(7)	F35 –C35 –C36	119.2(11)
C19 –C18 –C17	107.3(7)	C35 –C36 –C31	122.9(10)
C18 –C19 –N4	107.9(6)	F36 –C36 –C31	117.7(9)
C20 –C19 –N4	122.1(7)	F36 –C36 –C35	119.4(10)
C20 –C19 –C18	129.7(7)	C42 –C41 –C15	121.6(7)
C19 –C20 –C1	123.1(7)	C46 –C41 –C15	123.2(8)
C51 –C20 –C1	119.3(7)	C46 –C41 –C42	115.2(8)
C51 –C20 –C19	117.4(7)	C43 –C42 –C41	121.8(8)
C22 –C21 –C5	118.2(8)	F42 –C42 –C41	119.0(7)
C26 –C21 –C5	121.5(8)	F42 –C42 –C43	119.1(8)
C26 –C21 –C22	120.1(9)	C44 –C43 –C42	119.5(10)
C23 –C22 –C21	119.9(9)	F43 –C43 –C42	119.2(9)
F22 –C22 –C21	122.0(9)	F43 –C43 –C44	121.3(9)
F22 –C22 –C23	118.1(9)	C45 –C44 –C43	120.3(11)
C24 –C23 –C22	118.5(11)	F44 –C44 –C43	117.9(10)
F23 –C23 –C22	121.2(10)	F44 –C44 –C45	121.8(11)
F23 –C23 –C24	120.3(10)	C46 –C45 –C44	119.0(11)
C25 –C24 –C23	120.9(12)	F45 –C45 –C44	119.7(10)
F24 –C24 –C23	118.4(11)	F45 –C45 –C46	121.2(10)
F24 –C24 –C25	120.7(11)	C45 –C46 –C41	124.0(9)
C26 –C25 –C24	120.9(11)	F46 –C46 –C41	117.7(8)
F25 –C25 –C24	119.3(11)	F46 –C46 –C45	118.3(9)
F25 –C25 –C26	119.6(10)	C52 –C51 –C20	122.4(8)
C25 –C26 –C21	119.6(9)	C56 –C51 –C20	120.1(7)
F26 –C26 –C21	121.4(9)	C56 –C51 –C52	117.6(8)
F26 –C26 –C25	119.0(9)	C53 –C52 –C51	123.9(9)
C32 –C31 –C10	124.5(8)	F52 –C52 –C51	119.3(8)
C36 –C31 –C10	119.9(8)	F52 –C52 –C53	116.8(8)
C36 –C31 –C32	115.5(8)	C54 –C53 –C52	117.9(10)
C33 –C32 –C31	122.3(9)	F53 –C53 –C52	123.6(9)
F32 –C32 –C31	118.7(8)	F53 –C53 –C54	118.6(9)
F32 –C32 –C33	118.8(9)	C55 –C54 –C53	119.9(10)
C34 –C33 –C32	119.6(11)	F54 –C54 –C53	119.8(10)
F33 –C33 –C32	121.4(10)	F54 –C54 –C55	120.3(10)

Angle(°)

C56	–C55	–C54	119.3(9)
F55	–C55	–C54	119.6(9)
F55	–C55	–C56	121.1(9)
C55	–C56	–C51	121.4(9)
F56	–C56	–C51	121.6(8)
F56	–C56	–C55	117.0(8)
ClS	–CS	–ClS′	113.8(9)
ClS	–CS	–HS	108.4
ClS	–CS	–HS′	108.4
HS	–CS	–HS′	109.5

Table A6.4. Observed and Calculated Structure Factors for $CuTFPPBr_8$. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

Tetra(pentafluorophenyl)octabromoporphinato Copper(II) Page 1

-21 1 1			
1	-475	25	-7
2	774	540	10
3	368	120	4
4	711	104	17
5	98	486	-7
6	-395	24	-5
7	570	416	4
-21 3 1			
1	-464	117	-7
2	328	68	3
3	290	154	2
4	225	48	1
5	448	480	0
6	722	358	12
-21 5 1			
1	551	57	9
2	622	493	4
3	844	217	22
4	568	361	6
-20 0 1			
2	1563	1503	6
4	1528	1499	2
6	294	794	-18
8	-91	163	-1
10	573	617	-1
-20 2 1			
1	1190	1139	4
2	946	896	3
3	744	770	-1
4	622	730	-5
5	427	7	6
6	-394	120	-6
7	509	20	9
8	741	268	16
9	407	229	3
10	-447	485	-14
11	344	583	-6
-20 4 1			
1	903	586	16
2	-527	565	-20
3	372	261	2
4	705	564	6
5	359	3	4
6	-117	32	0
7	-442	414	-12
8	379	7	4
9	669	5	14
10	-175	320	-4
-20 6 1			
1	815	567	11
2	948	825	7
3	289	52	2
4	437	207	5
5	-688	253	-18
6	467	438	0
7	510	32	8
8	718	482	9
9	1090	433	32
-20 8 1			
1	491	236	6
2	713	633	3
3	486	565	-2
4	312	432	-2
5	682	722	-1
6	-331	195	-4
7	476	505	0
-19 1 1			
1	353	11	5
2	546	452	3
3	468	371	3
4	760	550	10
5	140	428	-6
6	1333	1254	7
7	529	249	8
8	1069	969	7
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12	463	22	7
13	541	79	9
14	388	149	4
-19 3 1			
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6	889	717	10
7	694	794	-5
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11	-63	258	-2
12	396	108	4
13	602	20	11
14	633	310	9
-19 5 1			
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3	-510	156	-10
4	1245	1101	12
5	-351	213	-6
6	662	923	-14
7	236	12	2
8	894	982	-5
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11	-589	280	-14
12	-288	192	-3
13	-420	54	-5
-19 7 1			
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3	-228	70	-2
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6	507	57	9
7	597	763	-7
8	680	853	-8
9	928	690	12
10	761	786	-1
11	1163	794	22
12	315	234	1
-19 9 1			
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3	514	115	8
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5	596	544	1
6	-479	389	-12
7	500	408	2
8	759	296	16
9	750	670	3
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-19 11 1			
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3	-690	62	-15
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5	-301	383	-7
6	540	360	5
7	401	239	3
-18 0 1			
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4	651	902	-16
6	471	308	5
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12	639	87	14
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16	401	45	4
-18 2 1			
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3	-45	216	-2
4	759	835	-5
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7	707	254	17
8	712	711	0
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10	-526	339	-14
11	909	1001	-6
12	-236	118	-2
13	597	258	9
14	311	270	0
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16	-374	241	-5
-18 4 1			
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3	1051	787	20
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5	982	1013	-2
6	623	329	11
7	427	711	-12
8	549	154	10
9	1037	1045	0
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11	-828	279	-26
12	613	418	6
13	-364	158	-5
14	407	344	1
15	858	404	17
16	350	141	3
-18 6 1			
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2	1165	1019	12
3	212	550	-10
4	915	800	7
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6	427	616	-7
7	-197	207	-3
8	674	628	2
9	-501	184	-10
10	469	191	6
11	210	160	0
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13	552	265	7
14	-193	6	-1
15	-578	263	-11
-18 8 1			
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2	113	374	-4
3	787	136	23
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6	650	728	-3
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8	893	808	4
9	726	243	16
10	590	510	2
11	525	98	8
12	897	50	25
13	372	224	2
14	263	2	2
-18 10 1			
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3	142	241	-1
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6	1087	995	6
7	518	524	0
8	585	509	2
9	605	424	6
10	386	159	4
11	837	732	5
12	-592	388	-14
-18 12 1			
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3	647	7	14
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5	199	648	-12
6	689	287	13
7	611	231	10
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-18 14 1			
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-17 1 1			
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2	417	229	5
3	614	240	14
4	703	907	-14
5	523	233	9
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7	-256	528	-14
8	1052	1079	-2
9	1349	1407	-6
10	1008	785	15
11	927	554	21
12	530	365	5
13	807	561	12
14	696	5	17
15	320	573	-7
16	-449	300	-9
17	733	827	-4
18	204	631	-10

-17 3 1

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3	390	368	0
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5	503	480	0
6	641	551	4
7	-351	447	-13
8	436	126	7
9	1412	1333	8
10	870	979	-7
11	953	776	11
12	1015	717	18
13	811	482	15
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15	1198	768	27
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-17 5 1

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5	-680	94	-20
6	759	786	-1
7	1160	1372	-20
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11	514	6	9
12	752	460	12
13	165	513	-8
14	879	293	22
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17	-591	376	-13

-17 7 1

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5	933	838	6
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7	-251	400	-8
8	525	55	10
9	832	852	-1
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11	491	442	1
12	1025	963	4
13	736	554	7
14	-396	155	-5
15	992	732	13
16	219	146	0

-17 9 1

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3	592	654	-3
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5	532	84	11
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8	-179	281	-4
9	30	356	-4
10	527	70	9
11	789	61	21
12	-109	294	-3
13	905	630	13
14	439	378	1
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-17 11 1

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3	606	22	14
4	1048	1006	3
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8	400	393	0
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-17 13 1

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3	745	395	14
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5	282	187	1
6	815	40	23
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11	-404	27	-4

-17 15 1

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-16 0 1

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10	62	253	-2
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16	681	567	4
18	227	168	0
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-16 2 1

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3	786	817	-2
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13	-740	55	-21
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15	585	36	12
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-16 4 1

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-16 6 1

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13	418	1020	-29
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16	1036	825	11
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-16 8 1

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-16 10 1

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3	578	202	12
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12	545	420	3
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-16 12 1

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3	91	459	-8
4	692	506	8
5	413	560	-5
6	409	421	0
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12	670	657	0
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-16 14 1

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-16 16 1

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-15 1 1

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3	386	456	-3
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-15 3 1

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-15 5 1

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17	958	723	11
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19	441	360	1
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-15 7 1

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14	983	709	15
15	700	534	6
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19	1123	935	9
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-15 9 1

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5	635	395	11
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-15 11 1

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3	445	490	-1
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6	1494	1580	-10
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-15 13 1

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5	915	1004	-6
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9	635	508	4
10	180	335	-2
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12	895	753	6
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-15 15 1

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5	357	91	4
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-15 17 1

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6	115	326	-2
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-14 0 1

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6	655	692	-2
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16	1438	1492	-5
18	255	455	-4
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-14 2 1

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6	1285	1265	2
7	1870	1947	-13
8	542	409	6
9	2079	2033	7
10	510	515	0
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12	1394	1528	-15
13	560	488	3
14	1366	1355	1
15	1191	1072	10
16	815	842	-1
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19	828	672	6
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-14 4 1

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3	1978	1881	17
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7	-138	228	-3
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12	1380	1334	4
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15	713	136	18
16	-813	170	-23
17	340	237	1
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19	483	444	1
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21	291	135	1
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-14 6 1

1	583	309	13
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6	1222	1291	-8
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13	-380	286	-8
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17	526	572	-1
18	1290	895	24
19	500	347	3
20	-676	580	-19
21	-585	93	-8

-14 8 1

1	1079	777	28
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3	370	703	-18
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7	702	436	14
8	632	541	4
9	1865	1770	12
10	463	344	4
11	523	469	2
12	510	414	3
13	1010	704	18
14	406	519	-3
15	351	309	0
16	343	210	2
17	1029	623	18
18	-545	30	-7
19	581	125	8
20	730	338	10

-14 10 1

1	-249	338	-8
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3	399	133	6
4	2166	2140	4
5	263	183	1
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8	747	681	3
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12	-564	106	-11
13	-556	429	-15
14	-635	83	-12
15	573	1062	-21
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17	-418	357	-7
18	798	981	-7
19	574	615	-1

-14 12 1

1	-183	550	-14
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3	491	311	6
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5	-148	198	-2
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8	1269	1137	11
9	603	140	12
10	567	399	5
11	489	461	0
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13	856	847	0
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16	-519	299	-8
17	401	250	2
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-14 14 1

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3	869	1067	-15

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9	1049	987	3
10	784	722	2
11	591	500	2
12	764	681	2
13	379	144	2
14	182	328	-1
15	1207	1063	6
16	708	428	6
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2	1568	1483	9
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4	609	577	1
5	574	358	6
6	1400	1305	7
7	-657	379	-15
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9	422	63	4
10	740	180	11
11	743	498	6
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1	786	768	0
2	891	629	11
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4	1415	1218	12
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6	-332	477	-6
7	932	19	16
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6	610	129	22
7	541	475	3
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11	505	556	-2
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14	1087	968	9
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16	1338	1391	-5
17	659	570	3
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19	-743	243	-19
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1	790	915	-13
2	816	664	14
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6	1413	1532	-18
7	-422	123	-11
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9	245	178	1
10	540	720	-11
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Tetra(pentafluorophenyl)octabromoporphinato Copper(II) Page 8

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-8 2 1

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-8 18 1

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22	1411	1569	-12
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24	-645	414	-15
25	1759	1606	12
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16	826	363	18
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Tetra(pentafluorophenyl)octabromoporphinato Copper(II) Page 15

18	727	660	2
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9	410	180	4
10	789	501	12
11	361	492	-3
12	-243	233	-3
13	-504	343	-10
	3	25	1
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1	597	476	4
2	-204	522	-10
3	589	576	0
4	354	162	3
5	770	973	-11
6	869	447	18
7	438	42	6
8	-85	95	0
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0	3939	3915	7
2	1388	1420	-12
4	1734	1712	7
6	-127	254	-9
8	7572	7493	11
10	1165	1164	0
12	339	86	5
14	6062	6084	-3
16	2853	2812	6
18	1143	1304	-13
20	982	1159	-12
22	3165	3194	-4
24	-164	575	-10
26	967	1053	-4
28	729	714	0
	4	2	1
0	760	768	-3
1	506	493	2
2	757	683	18
3	190	251	-4
4	4919	4838	17
5	392	313	7
6	1545	1532	3
7	5893	5779	20
8	2080	2077	0
9	1014	919	14
10	1075	1030	6
11	704	667	3
12	355	109	6
13	3779	3733	8
14	2717	2779	-11
15	1665	1523	17
16	1375	1461	-8
17	3100	3083	2
18	710	732	-1
19	664	234	12
20	-292	443	-8
21	1779	1848	-6
22	-348	289	-6
23	1140	1102	2
24	-638	319	-14
25	502	334	3
26	900	1018	-5

27	-593	147	-9
28	649	779	-4

4 4 1

0	2742	2730	5
1	1401	1368	11
2	931	924	1
3	7913	7915	0
4	3159	3120	11
5	1375	1300	21
6	4456	4396	13
7	914	834	13
8	631	668	-4
9	1255	1222	6
10	3761	3616	32
11	789	857	-7
12	857	812	4
13	1214	1191	2
14	1394	1480	-10
15	3635	3761	-23
16	610	641	-1
17	1712	1771	-6
18	260	95	2
19	1856	1772	8
20	197	399	-3
21	88	639	-10
22	429	320	2
23	738	264	12
24	607	234	8
25	865	485	13
26	1473	1416	3
27	414	500	-1

4 6 1

0	5041	4944	22
1	459	413	5
2	1736	1705	10
3	4063	4063	0
4	4022	3987	8
5	539	516	2
6	1525	1427	25
7	1077	1022	10
8	1974	1862	27
9	1547	1541	1
10	3322	3323	0
11	2250	2239	2
12	2681	2687	-1
13	533	141	15
14	956	963	0
15	3687	3706	-3
16	3340	3269	12
17	1320	1400	-7
18	1382	1321	5
19	624	468	5
20	1513	1469	3
21	818	592	8
22	1059	1061	0
23	1011	787	9
24	-177	307	-3
25	1233	997	12
26	441	669	-5
27	-140	236	-1

4 8 1

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2	710	670	6
3	2787	2828	-12
4	3155	3132	6
5	4329	4284	10
6	2751	2810	-16
7	4410	4458	-10
8	335	210	5
9	3652	3632	4
10	1554	1399	28
11	1283	1333	-7
12	1344	1313	4
13	3689	3682	1
14	996	1040	-4
15	1314	1143	18
16	538	922	-22
17	1543	1553	-1
18	606	298	9
19	2215	2177	4
20	1919	1891	2
21	-240	9	-1
22	1330	1209	7
23	1827	1621	16
24	930	374	16
25	618	439	4
26	865	292	14

4 10 1

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1	449	570	-12
2	1665	1697	-8
3	651	503	16
4	1963	1939	6
5	3258	3301	-11
6	693	758	-7
7	931	1003	-10
8	1495	1533	-7
9	112	369	-8
10	2377	2340	8
11	1389	1304	12
12	2880	2794	17
13	358	310	1
14	1542	1528	2
15	1020	1148	-11
16	1418	1332	9
17	616	68	14
18	691	292	13
19	1221	1100	8
20	-592	141	-10
21	-135	509	-7
22	1573	1712	-10
23	1433	1257	10
24	-515	40	-5
25	-837	92	-13

4 12 1

0	1782	1801	-6
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2	903	828	10
3	622	634	-1
4	2712	2715	0
5	168	396	-9
6	472	293	10
7	288	355	-3
8	2131	2111	4
9	658	605	4
10	319	258	2
11	3419	3401	3
12	2901	2902	0
13	611	473	7
14	367	398	-1
15	344	532	-6
16	-601	153	-14
17	441	590	-5
18	2061	2072	-1
19	-636	136	-12
20	-649	500	-19
21	1833	1886	-4
22	552	689	-4
23	1319	1393	-4
24	-582	221	-8

4. 14 1

0	883	944	-10
1	1232	1298	-11
2	888	949	-7
3	2368	2404	-8
4	490	440	3
5	623	70	25
6	3074	3101	-6
7	1237	1271	-4
8	3811	3771	8
9	1278	1270	1
10	2753	2765	-2
11	1447	1524	-10
12	2522	2485	6
13	1487	1531	-5
14	2023	1894	17
15	-165	257	-3
16	612	503	4
17	2318	2248	9
18	321	531	-5
19	-493	6	-7
20	792	630	6
21	1510	1347	11
22	770	2	13
23	766	136	12

4 16 1

0	141	172	0
1	1430	1457	-4
2	1351	1403	-8
3	2309	2250	11
4	1344	1316	4
5	624	466	9
6	2825	2898	-15
7	1354	1309	5
8	2647	2676	-5
9	512	252	9
10	630	607	1
11	203	39	1
12	2223	2298	-12
13	480	228	7
14	173	306	-2
15	557	176	10
16	1633	1528	10
17	338	59	3
18	-560	37	-9
19	880	879	0
20	1335	1074	15
21	-256	903	-20
22	75	497	-5

4 18 1

0	1141	1186	-7
1	217	378	-5
2	490	781	-19
3	908	768	12
4	607	238	16
5	987	945	3
6	244	229	0
7	1100	1074	2
8	1334	1326	0
9	1721	1598	16
10	1103	1142	-3
11	369	328	1
12	971	899	5
13	759	9	22
14	788	595	9
15	1605	1357	23
16	-386	559	-14
17	-158	361	-4
18	-306	979	-28
19	852	776	3
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4 20 1

0	320	399	-3
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2	-393	120	-7
3	1105	1038	6
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5	1589	1579	1
6	734	389	17
7	694	226	18
8	305	360	-1
9	1174	1191	-1
10	412	301	3
11	-339	475	-12
12	528	364	5
13	1392	1335	5
14	1291	1269	1
15	-228	170	-2
16	705	26	14
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4 22 1

0	920	1004	-9
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2	278	157	2
3	194	237	0
4	-629	129	-16
5	510	446	2
6	900	915	0
7	1000	1048	-3
8	-19	453	-7
9	972	877	6
10	-334	394	-9
11	639	686	-2
12	725	777	-2
13	-493	42	-7
14	873	778	4

4 24 1

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3	-349	260	-6
4	454	140	6
5	-729	38	-17
6	566	147	10
7	510	79	8
8	705	538	6
9	515	5	8
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4 26 1

0	730	778	-3
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5 1 1

0	7209	7134	12
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2	2640	2576	21
3	4778	4672	23
4	1918	1928	-3
5	1864	1916	-16
6	9296	9227	8
7	3161	3073	23
8	3192	3203	-2
9	1820	1843	-5
10	3599	3601	0
11	794	909	-11
12	2816	2806	1
13	888	967	-7
14	503	47	12
15	725	858	-8
16	1654	1655	0
17	-920	394	-34
18	799	798	0
19	1288	1363	-5
20	2061	2165	-11
21	-317	8	-2
22	497	239	5

23	609	13	10
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25	748	936	-8
26	209	222	0
27	697	88	12

5 3 1

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2	1388	1416	-9
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4	683	643	6
5	1094	1063	7
6	375	278	7
7	2020	2000	5
8	1162	1075	16
9	945	891	7
10	1898	1892	1
11	-84	286	-5
12	1726	1624	17
13	1212	1265	-6
14	197	33	1
15	2317	2415	-15
16	2774	2860	-14
17	1552	1614	-6
18	484	304	4
19	1155	1291	-9
20	1271	1224	3
21	2718	2774	-6
22	2471	2617	-16
23	555	696	-4
24	956	853	4
25	793	340	13
26	1028	583	17
27	-763	536	-20

5 5 1

0	234	84	9
1	1165	1149	4
2	854	845	1
3	6749	6689	14
4	9303	9119	22
5	4114	4038	18
6	2173	2211	-11
7	420	95	16
8	4640	4650	-2
9	2535	2479	13
10	1760	1735	5
11	2450	2424	5
12	4295	4310	-3
13	2956	2941	3
14	1617	1650	-4
15	680	466	11
16	1079	1177	-9
17	1088	1009	6
18	364	508	-4
19	128	12	0
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23	829	519	10
24	1541	1351	12
25	547	557	0
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27	592	429	3

5 7 1

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2	523	441	9
3	382	411	-2
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5	2461	2371	25
6	1004	901	17
7	3707	3646	14
8	750	863	-14
9	647	701	-5
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11	1532	1591	-10
12	4702	4608	17
13	3284	3266	3
14	737	688	3
15	1649	1724	-10
16	1594	1572	2
17	3003	3006	0
18	382	428	-1
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20	484	353	3
21	-310	205	-3
22	1440	1403	2
23	724	281	10
24	1709	1558	10
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26	712	278	9

5 9 1

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2	1449	1472	-5
3	2309	2373	-17
4	783	953	-26
5	3564	3548	4
6	984	1057	-11
7	1071	1029	6
8	1818	1835	-3
9	605	29	27
10	-302	197	-8
11	1187	1152	4
12	340	478	-6
13	2897	2910	-2
14	798	837	-3
15	2135	2098	5
16	831	955	-8
17	579	770	-9
18	2046	1922	14
19	-573	211	-11
20	-983	255	-28
21	376	39	3
22	1422	1521	-6
23	1245	1175	3
24	413	368	0
25	293	187	1
26	1738	1716	1

5 11 1

0	1166	1175	-2
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2	3801	3826	-6
3	478	399	5
4	1350	1408	-11
5	2323	2406	-20
6	1175	1211	-5
7	723	794	-7
8	1355	1391	-6
9	1315	1201	17
10	513	514	0
11	2304	2235	13
12	682	595	5
13	490	646	-8
14	1095	1087	0
15	828	915	-6
16	-296	240	-5
17	1961	1958	0
18	687	547	5
19	-391	382	-9
20	-404	260	-6
21	1131	1095	2
22	631	98	9
23	791	1086	-12
24	-1004	78	-21
25	1026	779	8

5 13 1

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2	2421	2441	-4
3	2705	2666	9
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5	2041	2053	-2
6	797	625	16
7	1646	1679	-5
8	2555	2658	-22
9	447	433	0
10	721	588	9
11	2518	2459	11
12	356	298	1
13	1275	1369	-10
14	307	196	2
15	581	448	5
16	1490	1518	-2
17	-431	370	-11
18	1088	878	13
19	325	463	-3
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21	-131	240	-1
22	1550	1575	-1
23	-489	322	-7

5 15 1

0	1291	1330	-8
1	221	190	0
2	774	854	-8
3	2557	2640	-18
4	1529	1510	3
5	998	812	19
6	1557	1484	11
7	2645	2685	-8
8	516	527	0
9	1467	1505	-5
10	263	259	0
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12	2386	2388	0
13	1627	1718	-11
14	779	490	14
15	1296	1239	5
16	818	667	7
17	846	628	10
18	725	738	0
19	522	27	7
20	845	1094	-12
21	506	84	6
22	450	11	4

5 17 1

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3	1929	1904	4
4	513	519	0
5	602	718	-7
6	1514	1555	-5
7	185	362	-4
8	1786	1751	5
9	1286	1269	1
10	336	518	-6
11	-551	412	-19
12	1505	1645	-16
13	757	634	6
14	532	659	-5
15	-647	25	-14
16	595	641	-1
17	590	639	-1
18	-285	4	-2
19	855	577	10
20	339	403	-1

5 19 1

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2	726	675	3
3	208	33	2
4	428	177	7
5	392	135	6
6	732	108	24
7	886	918	-2
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10	347	439	-2
11	298	663	-13
12	799	433	16
13	146	286	-2
14	-163	611	-13
15	338	12	3
16	-172	531	-9
17	1091	1351	-16
18	553	354	4

5 21 1

0	274	546	-13
1	876	1208	-28
2	1071	1106	-3
3	905	1003	-7
4	1032	1214	-16
5	751	8	23
6	1002	1110	-8
7	1391	1423	-3
8	3048	2990	9
9	793	858	-3
10	134	399	-5
11	-298	521	-12
12	562	308	7
13	182	176	0
14	1335	1413	-6
15	834	821	0
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5 23 1

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2	902	854	3
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4	511	841	-16
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6	980	1131	-10
7	553	161	9
8	-410	254	-7
9	-275	452	-9
10	812	710	4
11	662	703	-1
12	-614	8	-11

5 25 1

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2	622	317	9
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4	790	1128	-19
5	702	166	14
6	1327	1272	4

6 0 1

0	757	782	-7
2	7970	8025	-7
4	190	222	-1
6	3356	3358	0
8	695	796	-12
10	1663	1573	16
12	975	1047	-7
14	1460	1373	10

16	1828	1901	-8
18	1542	1496	4
20	2692	2584	13
22	-613	17	-10
24	1858	1892	-3
26	-382	595	-12

6 2 1

0	1648	1646	0
1	97	188	-3
2	3595	3576	5
3	813	713	19
4	759	724	6
5	3788	3727	15
6	1709	1672	10
7	1370	1299	15
8	192	420	-11
9	980	867	16
10	2110	2169	-13
11	1706	1851	-26
12	3485	3519	-7
13	1282	1240	5
14	668	604	3
15	1296	1225	7
16	-632	250	-18
17	-468	94	-8
18	-280	304	-5
19	-771	179	-19
20	-327	731	-18
21	857	742	4
22	84	574	-8
23	-197	188	-1
24	-466	395	-9
25	1331	1152	10
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27	602	947	-12

6 4 1

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4	439	451	-1
5	945	958	-2
6	176	380	-11
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11	2547	2527	4
12	895	946	-5
13	-206	550	-18
14	510	590	-4
15	-388	59	-7
16	60	80	0
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18	1840	1874	-3
19	1451	1394	4
20	373	186	3
21	1305	1242	4
22	361	494	-2
23	792	952	-6
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25	694	724	0
26	418	534	-2
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6 6 1

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3	1924	1945	-6
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5	-231	318	-15
6	799	844	-6
7	2363	2430	-18
8	1301	1325	-4
9	1241	1095	23
10	7404	7347	8
11	1169	1089	10
12	3151	3165	-2
13	744	674	5
14	3133	3015	22
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20	1957	1968	-1
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22	606	24	9
23	399	16	4
24	1005	918	3
25	415	536	-2
26	545	1151	-20

6 8 1

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5	2262	2299	-9
6	2103	2059	11
7	229	57	3
8	-290	112	-7
9	281	508	-12
10	1814	1824	-2
11	1269	1272	0
12	1301	1293	1
13	2137	2176	-6
14	539	257	10
15	783	876	-6
16	1043	1130	-7
17	1566	1577	-1
18	419	300	3
19	2142	2167	-3
20	1162	1119	2
21	1220	1285	-4
22	716	371	9
23	2287	2220	6
24	423	410	0
25	379	129	2

6 10 1

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2	3928	3949	-4
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4	5927	5928	0
5	2406	2426	-5
6	1200	1104	15
7	382	499	-7
8	268	184	2
9	2087	2101	-2
10	2704	2729	-5
11	1489	1382	16
12	2972	2990	-3
13	-501	101	-13
14	1597	1669	-9
15	1071	904	14
16	1005	573	27
17	519	395	4
18	-533	42	-9
19	1348	1290	4
20	-289	60	-2
21	1044	458	24
22	-473	77	-5
23	-524	352	-9
24	166	195	0
25	-1050	71	-22

6 12 1

0	998	1019	-4
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3	1052	1078	-3
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5	2098	2140	-9
6	1313	1267	7
7	894	1035	-16
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13	2442	2384	9
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15	-346	376	-8
16	111	484	-6
17	752	976	-10
	12	16	1
0	543	481	2
1	-152	387	-7
2	242	315	-1
3	442	427	0
4	490	214	8
5	1027	1018	0
6	562	13	12
7	587	469	4
8	642	880	-13
9	707	603	4
10	1005	946	3
11	780	233	19
12	1344	1352	0
13	-320	58	-3
14	855	1023	-9
15	834	575	10
	12	18	1
0	312	222	2
1	377	235	3
2	804	659	8
3	1934	1864	9
4	1225	1271	-4
5	1078	918	11
6	548	293	8
7	1550	1523	2
8	1682	1609	7
9	-154	248	-2
10	-459	19	-6
11	402	209	3
12	897	839	3
13	668	634	1
	12	20	1
0	-302	295	-8
1	981	653	18

2	616	302	9
3	278	367	-2
4	530	437	3
5	-258	65	-2
6	454	673	-7
7	688	322	11
8	-374	181	-5
9	867	509	15
	12	22	1
0	721	584	5
	13	1	1
0	2637	2612	7
1	363	429	-3
2	765	879	-11
3	658	225	24
4	956	864	9
5	1031	1027	0
6	600	559	2
7	968	923	4
8	503	590	-4
9	683	441	13
10	1308	1236	8
11	522	260	9
12	758	1031	-19
13	1183	1116	6
14	771	726	2
15	-373	442	-11
16	848	365	20
17	635	532	3
18	1129	1109	1
19	864	266	18
20	767	218	13
21	725	513	6
22	-376	644	-12
	13	3	1
0	255	14	6
1	1504	1511	-1
2	537	307	12
3	678	749	-6
4	1313	1373	-8
5	1430	1522	-14
6	951	963	-1
7	931	868	5
8	518	665	-8
9	434	513	-3
10	1559	1533	3
11	2150	2168	-2
12	-496	203	-12
13	2178	2059	17
14	947	982	-2
15	627	840	-10
16	956	1022	-4
17	292	107	2
18	601	617	0
19	1156	1158	0
20	-207	695	-10
21	1102	993	5
22	-61	318	-2
	13	5	1
0	731	770	-5
1	1518	1639	-20
2	1794	1772	3
3	1395	1365	4
4	1539	1524	2
5	404	166	7
6	126	365	-6
7	422	410	0
8	296	629	-15
9	-282	191	-5
10	1436	1391	5

11	2217	2294	-12
12	2198	2194	0
13	1357	1457	-10
14	807	1002	-12
15	1116	1049	5
16	1120	1098	1
17	1137	1071	4
18	724	601	4
19	1098	922	9
20	791	450	11
21	1059	634	17
	13	7	1
0	631	552	7
1	3764	3782	-3
2	1845	1868	-4
3	2576	2576	0
4	-277	66	-4
5	1747	1661	13
6	961	1104	-14
7	664	810	-10
8	376	31	6
9	1018	983	3
10	817	875	-4
11	-176	396	-7
12	2304	2340	-5
13	1252	924	27
14	1141	1073	5
15	1502	1558	-5
16	281	400	-2
17	1563	1530	3
18	544	127	8
19	-485	262	-8
20	505	441	1
	13	9	1
0	262	150	3
1	2624	2616	1
2	612	354	13
3	1900	1905	0
4	981	842	12
5	522	443	3
6	1238	1074	17
7	760	542	13
8	724	294	20
9	1204	1151	5
10	515	467	2
11	-258	405	-9
12	-75	95	0
13	977	857	8
14	1783	1664	13
15	211	322	-2
16	254	310	-1
17	-114	710	-15
18	548	59	8
19	620	279	8
20	973	1092	-6
	13	11	1
0	688	496	16
1	734	768	-2
2	-251	358	-9
3	1386	1328	7
4	626	368	12
5	1923	1863	9
6	289	405	-3
7	605	454	7
8	837	1017	-14
9	-562	510	-23
10	602	254	12
11	607	775	-9
12	842	851	0
13	902	857	2
14	1842	1676	18
15	480	518	-1

16	778	880	-5
17	697	466	7
18	580	180	8
	13	13	1
0	612	301	18
1	721	487	13
2	632	477	7
3	871	1004	-10
4	1462	1580	-14
5	542	424	4
6	455	590	-6
7	-419	451	-15
8	1193	1040	13
9	1133	1238	-9
10	787	1017	-15
11	965	925	2
12	651	583	2
13	376	382	0
14	574	487	2
15	965	306	26
16	412	312	2
17	1050	857	10
	13	15	1
0	2054	1976	15
1	243	217	0
2	361	410	-1
3	-253	104	-3
4	1398	1490	-10
5	269	239	0
6	1470	1372	10
7	239	89	1
8	647	529	5
9	582	122	11
10	-109	399	-6
11	-601	573	-22
12	-231	140	-2
13	105	44	0
14	234	62	1
15	250	377	-2
	13	17	1
0	649	435	10
1	718	618	5
2	704	648	2
3	179	77	1
4	257	310	-1
5	861	146	26
6	44	9	0
7	1009	690	18
8	858	655	10
9	434	758	-12
10	581	267	8
11	-670	35	-13
12	-441	255	-7
	13	19	1
0	574	494	3
1	349	300	1
2	589	744	-7
3	557	113	10
4	759	632	5
5	-322	477	-10
6	417	323	2
7	1082	785	17
8	609	134	11
9	379	161	3
	13	21	1
0	197	489	-8
1	694	321	12

14 0 1

0	860	815	6
2	1392	1384	1
4	1467	1382	12
6	-534	46	-14
8	1470	1594	-16
10	2115	2100	2
12	1544	1605	-6
14	1176	1227	-4
16	1113	1274	-11
18	-434	310	-7
20	1071	1044	1

14 2 1

0	425	511	-6
1	2778	2791	-2
2	1823	1780	7
3	-87	476	-13
4	-247	288	-7
5	1006	943	6
6	1029	966	6
7	824	544	19
8	733	674	3
9	247	85	2
10	665	616	2
11	497	454	1
12	1038	1062	-1
13	588	864	-15
14	1263	1202	5
15	-97	165	-1
16	551	279	7
17	782	702	3
18	-651	181	-12
19	1211	873	18
20	472	370	2
21	664	383	6

14 4 1

0	-275	302	-13
1	1037	977	6
2	-485	119	-13
3	276	580	-14
4	1566	1423	20
5	115	255	-2
6	1205	1098	12
7	949	824	10
8	724	581	8
9	2048	2132	-13
10	1060	1094	-3
11	164	341	-3
12	-45	530	-11
13	453	576	-4
14	1349	1370	-1
15	1058	946	7
16	948	961	0
17	695	637	2
18	668	861	-8
19	1317	1375	-3
20	1193	1070	6

14 6 1

0	1828	1829	0
1	1079	980	10
2	-343	200	-8
3	352	382	-1
4	834	928	-8
5	1785	1633	23
6	-272	62	-3
7	2127	2016	18
8	930	943	-1
9	859	726	9
10	1355	1218	14
11	1354	1407	-5
12	709	19	20
13	-482	266	-11
14	-359	109	-5
15	-63	400	-5
16	-604	126	-12
17	-599	378	-14
18	1574	1431	11
19	-47	594	-9
20	525	514	0

14 8 1

0	795	788	0
1	697	468	14
2	552	128	14
3	-544	348	-21
4	306	331	0
5	1911	1809	15
6	515	599	-4
7	1587	1509	10
8	664	618	2
9	808	686	7
10	-554	327	-17
11	-275	209	-4
12	403	244	3
13	648	607	1
14	786	729	2
15	644	416	8
16	103	5	0
17	907	402	20
18	726	446	9
19	992	1120	-6

14 10 1

0	1890	1821	14
1	1576	1449	17
2	998	933	5
3	1685	1551	18
4	2307	2357	-8
5	2107	2134	-4
6	370	227	3
7	623	809	-11
8	179	10	1
9	1166	1125	3
10	834	1033	-14
11	473	239	6
12	679	313	13
13	783	736	2
14	876	449	18
15	1333	1375	-3
16	108	132	0
17	-357	189	-4
18	902	856	2

14 12 1

0	1474	1523	-8
1	607	670	-3
2	318	386	-2
3	459	333	4
4	512	382	5
5	702	832	-8
6	588	622	-1
7	571	82	13
8	118	255	-2
9	1776	1798	-2
10	668	502	7
11	1467	1530	-6
12	253	362	-2
13	1658	1731	-7
14	1909	1756	16
15	620	19	11
16	517	136	7

14 14 1

0	673	847	-14
1	1000	996	0
2	1213	1081	12
3	567	140	12
4	449	249	5
5	653	345	12
6	578	171	12
7	-596	99	-13
8	762	566	9
9	-181	700	-18
10	864	782	4
11	-396	394	-10
12	63	401	-4
13	636	44	12
14	824	1089	-14
15	128	2	0

14 16 1

0	-262	385	-10
1	718	99	20
2	730	680	2
3	1276	1084	16
4	661	866	-11
5	-315	401	-9
6	654	124	14
7	-380	129	-5
8	219	525	-7
9	842	839	0
10	1408	1476	-5
11	1592	1537	4
12	398	278	2

14 18 1

0	-234	642	-18
1	351	234	2
2	-399	319	-8
3	1373	1357	1
4	135	460	-6
5	464	647	-6
6	976	563	20
7	276	862	-20
8	512	641	-4
9	-487	235	-8

14 20 1

0	484	239	6
1	611	42	11

15 1 1

0	1758	1733	5
1	1155	952	22
2	645	265	18
3	595	693	-6
4	2532	2597	-12
5	122	382	-6
6	662	299	17
7	1454	1401	6
8	456	754	-15
9	1362	1444	-9
10	60	486	-9
11	1279	1277	0
12	1362	1226	12
13	722	410	12
14	1528	1458	6
15	298	378	-1
16	868	948	-4
17	679	848	-7
18	1221	906	17
19	49	379	-3

15 3 1

0	876	1020	-19
1	1675	1628	7
2	593	629	-2
3	2364	2234	23
4	2053	1965	14
5	935	743	15
6	948	687	20
7	1052	1220	-16
8	1433	1489	-6
9	1474	1454	2
10	1103	1024	6
11	1032	854	13
12	539	375	5
13	514	508	0
14	50	50	0
15	1001	776	12
16	600	732	-5
17	727	530	7
18	513	316	4
19	-51	29	0

15 5 1

0	-282	52	-6
1	1273	1275	0
2	429	259	5
3	1187	1102	9
4	721	109	25
5	156	360	-5
6	1294	1287	0
7	745	239	23
8	796	606	11
9	650	559	4
10	-436	232	-9
11	589	556	1
12	-256	491	-11
13	684	227	15
14	864	602	13
15	-512	410	-13
16	1421	1308	9
17	494	542	-1
18	524	783	-8
19	650	848	-7

15 7 1

0	291	23	5
1	835	1015	-15
2	874	866	0
3	613	69	18
4	935	900	2
5	1523	1489	4
6	362	418	-1
7	762	746	1
8	670	720	-2
9	572	383	7
10	19	14	0
11	772	630	7
12	900	649	14
13	558	320	7
14	1112	822	18
15	694	144	14
16	864	699	7
17	-810	124	-18
18	-61	163	0

15 9 1

0	2220	2187	7
1	909	692	16
2	1013	481	37
3	1567	1330	29
4	781	647	8
5	2192	2159	5
6	689	115	20
7	500	605	-4
8	-257	11	-2
9	-489	394	-15
10	-448	163	-8
11	936	876	3
12	761	795	-1
13	577	686	-4

Appendix 7. Supplimentary Material for
the X-ray Crystal Structure Determination of $ZnTFPPBr_8$.

Figure A7.1. ORTEP diagram for $ZnTFPPBr_8$ (50% probability ellipsoids) and numbering scheme for macrocycle. Unlabelled C atoms have the same number as the attached F atom.

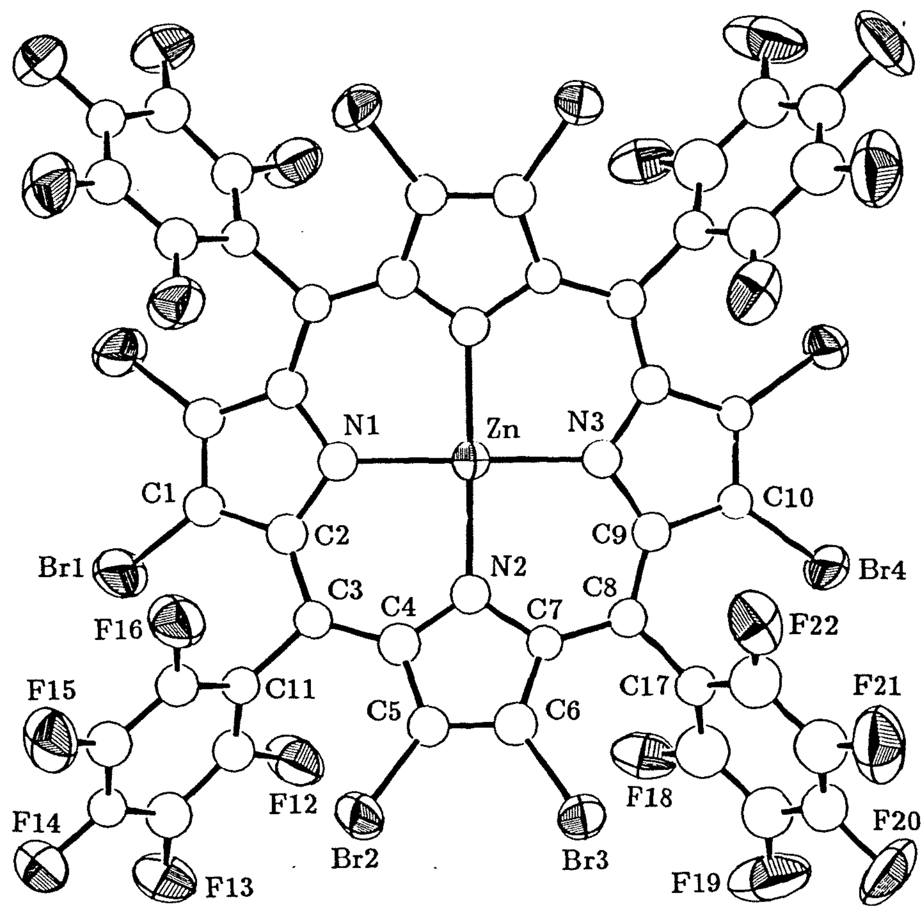

Figure A7.2. ORTEP diagram for ZnTFPPBr$_8$ unit cell (50% probability ellipsoids). The representation is a projection down the b axis (c is horizontal) with water molecules shown with shaded quadrants.

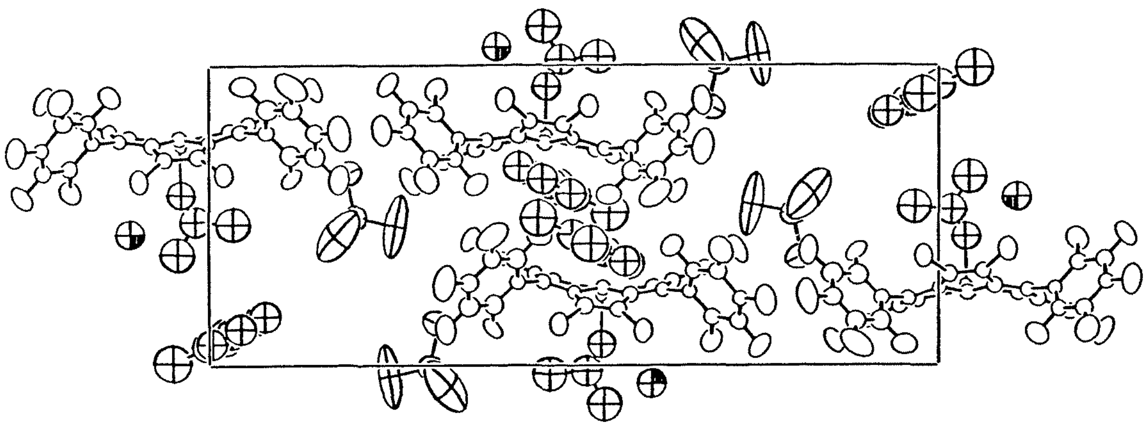

Table A7.1. Crystal and Intensity Collection Data for $ZnTFPPBr_8$.

Formula: $ZnC_{44}Br_8N_4F_{20}$•CCl_4•$C_6H_4Cl_2$•-(C_3H_6O,CH_4O)$_{1/2}$•[C_3H_6O,2(H_2O)]$_{1/2}$	Formula Weight: 2062.03
Crystal Color: purple	Habit: hexagonal prism
Crystal Size: 0.30 x 0.12 x 0.11 mm	
Crystal System: orthorhombic	Space Group: Pnma
a = 12.053 (4) Å	$\alpha = 90$
b = 18.453 (6) Å	$\beta = 90$
c = 29.259 (10) Å	$\gamma = 90$
V = 6508 (4) Å^3	Z = 4
D = 2.10 g cm^{-3}	
MoKα Radiation	$\lambda = 0.71073$ Å
$\mu = 5.60$ mm^{-1}	T = 295 K
Enraf-Nonius Cad-4 diffractometer	ω scan
Transmission coeff. =	range for data collection: 1-20
$\pm h = 11$, $k = 0$-17, $l = 0$-28	
Number of reflections measured: 6539	
Number of independent reflections: 3151	
R = 0.066 on F for 1398 reflections with $F_o^2 > 3\sigma(F_o^2)$	
wR = 0.020 on F^2 for 3151 reflections	
Final goodness of fit: 1.74 for 294 parameters and 3151 reflections	

Table A7.2. Final Refined Heavy Atom Parameters x 10^4 for $ZnTFPPBr_8$.

x, y, z and $U_{eq}{}^a \times 10^4$

Atom	x	y	z	U_{eq} or B	
Zn	2496(3)	2500	5394(1)	535(11)	
Br1	3871(2)	3419(1)	7258(1)	859(9)	
Br2	1145(2)	5433(1)	5949(1)	694(8)	
Br3	1366(2)	5459(1)	4795(1)	647(8)	
Br4	4192(2)	3416(1)	3570(1)	666(8)	
N1	2609(17)	2500	6087(7)	3.0(5)	*
N2	2583(11)	3611(7)	5400(6)	3.0(3)	*
N3	2829(16)	2500	4714(7)	2.9(5)	*
C1	3234(14)	2866(9)	6799(6)	3.2(5)	*
C2	2805(15)	3104(10)	6361(6)	3.2(5)	*
C3	2502(15)	3813(10)	6216(6)	2.8(4)	*
C4	2347(15)	4021(11)	5770(7)	3.4(5)	*
C5	1866(15)	4701(11)	5607(7)	3.3(5)	*
C6	1975(15)	4691(11)	5147(7)	3.6(5)	*
C7	2428(14)	4021(10)	5009(6)	2.3(4)	*
C8	2780(14)	3823(9)	4578(7)	2.9(4)	*
C9	3041(14)	3112(10)	4462(6)	2.9(5)	*
C10	3547(13)	2866(8)	4029(5)	2.4(4)	*
C11	2450(15)	4355(10)	6592(6)	2.7(5)	*
C12	3133(17)	4891(12)	6647(7)	3.3(5)	*

Atom	x	y	z	U_{eq} or B
C13	3121(18)	5422(12)	6987(7)	4.1(5) *
C14	2221(16)	5353(11)	7292(7)	2.9(4) *
C15	1475(18)	4830(12)	7269(7)	4.0(5) *
C16	1598(16)	4350(12)	6907(7)	3.5(5) *
C17	2761(16)	4389(11)	4222(6)	3.0(5) *
C18	3532(20)	4929(14)	4207(8)	5.3(6) *
C19	3532(19)	5443(13)	3868(8)	4.9(6) *
C20	2736(18)	5398(13)	3554(8)	4.3(5) *
C21	1958(20)	4894(14)	3552(9)	5.4(6) *
C22	2001(20)	4359(14)	3895(9)	5.3(6) *
F12	3972(10)	4977(6)	6349(4)	757(38)
F13	3822(11)	5941(7)	7030(4)	938(47)
F14	2156(11)	5844(7)	7642(4)	989(51)
F15	637(11)	4799(7)	7559(4)	904(45)
F16	811(10)	3822(7)	6893(4)	801(41)
F18	4313(9)	4962(6)	4530(5)	747(40)
F19	4281(12)	5974(7)	3880(5)	1230(62)
F20	2727(14)	5938(8)	3219(5)	1362(63)
F21	1181(13)	4888(8)	3230(4)	1200(57)
F22	1219(10)	3869(7)	3876(4)	786(41)

Atom	x	y	z	U_{eq} or B	
Cl1a	1358(20)	2500	3140(9)	1546(100)‡	
Cl2a	−361(50)	2500	2455(9)	2865(255)‡	
Cl3a	−688(35)	1737(18)	3230(11)	3416(198)‡	
Cl1b	−2042(27)	2500	2899(16)	2321(187)‡	
Cl2b	−488(26)	2500	3610(11)	1774(128)‡	
Cl3b	−92(26)	1774(15)	2828(10)	2243(137)‡	
C2b	−606(18)	1829(12)	6066(7)	10.8(7)	*
Cl1o	958(16)	1295(11)	229(7)	17.6(8)	*‡
Cl2o	90(14)	2300	−488(6)	18.0(7)	*‡

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

‡ Population Parameter, 0.5

Table A7.3. Complete Distances and Angles for $ZnTFPPBr_8$.

	Distance(Å)		Distance(Å)
Zn –N1	2.03(2)	C18 –F18	1.34(3)
Zn –N2	2.053(14)	C19 –C20	1.33(3)
Zn –N3	2.03(2)	C19 –F19	1.33(3)
Zn –O a	2.158	C20 –C21	1.32(3)
Zn –Cl2o	3.167	C20 –F20	1.40(3)
Br1 –C1	1.853(17)	C21 –C22	1.41(4)
Br2 –C5	1.891(19)	C21 –F21	1.33(3)
Br3 –C6	1.90(2)	C22 –F22	1.31(3)
Br4 –C10	1.854(15)	C a –Cl1a	1.775
N1 –C2	1.39(3)	C a –Cl2a	1.663
N2 –C4	1.35(2)	C a –Cl3a	1.710
N2 –C7	1.38(2)	C b –Cl1b	1.715
N3 –C9	1.37(3)	C b –Cl2b	1.613
C1 –C1	1.35(2)	C b –Cl3b	1.664
C1 –C2	1.45(3)	O a –C1a	1.227
C2 –C3	1.42(3)	C1a –C2a	1.504
C3 –C4	1.37(3)	C1a –C3a	1.500
C3 –C11	1.49(3)	O b –C1b	1.205
C4 –C5	1.46(3)	C1b –C2b	1.431
C5 –C6	1.35(3)	C1o –C2o	1.380
C6 –C7	1.41(3)	C1o –C6o	1.380
C7 –C8	1.38(3)	C1o –Cl1o	1.680
C8 –C9	1.39(3)	C2o –C3o	1.380
C8 –C17	1.48(3)	C2o –Cl2o	1.669
C9 –C10	1.48(2)	C3o –C4o	1.380
C10 –C10	1.35(2)	C4o –C5o	1.380
C11 –C12	1.30(3)	C5o –C6o	1.380
C11 –C16	1.38(3)		
C12 –C13	1.40(3)		
C12 –F12	1.34(2)		
C13 –C14	1.41(3)		
C13 –F13	1.28(3)		
C14 –C15	1.32(3)		
C14 –F14	1.37(2)		
C15 –C16	1.39(3)		
C15 –F15	1.32(3)		
C16 –F16	1.36(2)		
C17 –C18	1.36(3)		
C17 –C22	1.33(3)		
C18 –C19	1.37(3)		

Angle(°)				Angle(°)			
N1	–Zn	–N2	89.4(7)	C10	–C10	–C9	107.9(14)
N1	–Zn	–N3	164.8(8)	C12	–C11	–C3	125.2(18)
N2	–Zn	–N3	89.8(7)	C16	–C11	–C3	121.4(17)
N2	–Zn	–N2'	174.1(6)	C16	–C11	–C12	113.3(18)
C2	–N1	–C2	106.3(17)	C13	–C12	–C11	128.0(20)
C7	–N2	–C4	109.1(15)	F12	–C12	–C11	119.2(18)
C9	–N3	–C9	110.8(17)	F12	–C12	–C13	112.7(18)
C1	–C1	–Br1	123.4(13)	C14	–C13	–C12	113.3(19)
C2	–C1	–Br1	128.4(13)	F13	–C13	–C12	125.9(20)
C2	–C1	–C1	107.6(15)	F13	–C13	–C14	120.8(19)
C1	–C2	–N1	109.1(16)	C15	–C14	–C13	123.9(19)
C3	–C2	–N1	121.4(17)	F14	–C14	–C13	117.3(17)
C1	–C2	–N1	109.1(16)	F14	–C14	–C15	118.8(18)
C3	–C2	–N1	121.4(17)	C16	–C15	–C14	115.7(19)
C3	–C2	–C1	129.3(16)	F15	–C15	–C14	121.3(19)
C4	–C3	–C2	125.2(17)	F15	–C15	–C16	123.0(19)
C11	–C3	–C2	114.0(16)	C15	–C16	–C11	125.7(19)
C11	–C3	–C4	120.6(17)	F16	–C16	–C11	120.3(17)
C3	–C4	–N2	125.2(17)	F16	–C16	–C15	113.9(17)
C5	–C4	–N2	107.7(16)	C18	–C17	–C8	121.9(18)
C5	–C4	–C3	127.1(18)	C22	–C17	–C8	119.4(19)
C4	–C5	–Br2	128.6(14)	C22	–C17	–C18	118.6(20)
C6	–C5	–Br2	125.5(15)	C19	–C18	–C17	121.8(22)
C6	–C5	–C4	105.8(17)	F18	–C18	–C17	119.4(20)
C5	–C6	–Br3	119.4(15)	F18	–C18	–C19	118.7(21)
C7	–C6	–Br3	130.4(15)	C20	–C19	–C18	117.2(22)
C7	–C6	–C5	109.6(17)	F19	–C19	–C18	119.3(21)
C6	–C7	–N2	107.1(15)	F19	–C19	–C20	123.4(21)
C8	–C7	–N2	124.6(16)	C21	–C20	–C19	123.9(22)
C8	–C7	–C6	127.9(17)	F20	–C20	–C19	116.4(20)
C9	–C8	–C7	122.9(17)	F20	–C20	–C21	119.6(20)
C17	–C8	–C7	116.9(16)	C22	–C21	–C20	117.7(23)
C17	–C8	–C9	119.9(16)	F21	–C21	–C20	120.6(22)
C8	–C9	–N3	127.1(17)	F21	–C21	–C22	121.7(22)
C10	–C9	–N3	106.5(15)	C21	–C22	–C17	120.7(22)
C8	–C9	–N3	127.1(17)	F22	–C22	–C17	123.8(21)
C10	–C9	–N3	106.5(15)	F22	–C22	–C21	115.4(21)
C10	–C9	–C8	126.3(16)	Cl2a	–C a	–Cl1a	113.9
C9	–C10	–Br4	128.8(12)	Cl3a	–C a	–Cl1a	109.8
C10	–C10	–Br4	123.2(12)	Cl3a	–C a	–Cl2a	106.2

Cl2b	–C b	–Cl1b	114.4
Cl3b	–C b	–Cl1b	106.8
Cl3b	–C b	–Cl2b	110.6
C2a	–C1a	–O a	123.5
C3a	–C1a	–O a	122.9
C3a	–C1a	–C2a	113.6
C2b	–C1b	–O b	119.9
C2b	–C1b	–C2b	119.9
C6o	–C1o	–C2o	120.0
Cl1o	–C1o	–C2o	119.3
Cl1o	–C1o	–C6o	120.7
C3o	–C2o	–C1o	120.0
Cl2o	–C2o	–C1o	118.2
Cl2o	–C2o	–C3o	121.8
C4o	–C3o	–C2o	120.0
C5o	–C4o	–C3o	120.0
C6o	–C5o	–C4o	120.0
C5o	–C6o	–C1o	120.0

Table A7.4. Observved and Calculated Structure Factors for $ZnTFPPBr_8$. The colmuns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs} - F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceeding F_{obs} indicates that F^2_{obs} is negative.

Tetra(pentafluorophenyl)octabromoporphinato Zinc(II) Page 1

0 0 1			
2	1577	1318	105
4	274	372	-15
6	237	204	2
8	2550	2498	13
10	266	60	11
12	1143	1204	-14
14	1439	1416	5
16	2681	2717	-7
18	1302	1325	-4
20	-156	37	-2
22	1987	1972	2
24	1979	1878	16
26	-153	221	-5
28	186	17	2
1 0 1			
1	491	95	92
2	988	1070	-45
3	1511	1375	64
4	1419	1370	23
5	269	15	19
6	3447	3358	25
7	412	557	-36
8	3455	3305	41
9	615	637	-5
10	150	27	5
11	5769	5740	5
12	847	846	0
13	2288	2352	-19
14	409	154	26
15	1555	1514	11
16	1563	1485	21
17	663	404	39
18	1167	1225	-14
19	241	35	8
20	936	929	1
21	864	826	6
22	914	834	14
23	485	543	-6
24	260	325	-4
25	-106	231	-7
26	855	599	32
27	1127	1080	7
28	45	267	-6
2 0 1			
0	3785	3574	57
1	713	852	-58
2	2046	2080	-14
3	3579	3821	-71
4	281	469	-39
5	1710	1662	19
6	151	386	-34
7	3028	3052	-7
8	1281	1178	36
9	1950	2013	-22
10	732	619	28
11	3023	3184	-47
12	249	170	7
13	-32	262	-14
14	1209	1206	0
15	407	665	-46
16	-187	171	-11
17	347	540	-26
18	641	512	19
19	3766	3724	9
20	685	628	8
21	567	471	11
22	-284	117	-12
23	836	861	-4
24	563	593	-3
25	705	513	22
26	1223	1027	33
27	446	356	6
3 0 1			
1	1668	1815	-61
2	1601	1483	45
3	2685	2682	0
4	1900	1855	16
5	414	523	-24
6	2168	2116	18
7	1897	1834	21
8	5019	4984	7
9	866	832	9
10	1527	1448	25
11	1636	1652	-5
12	-58	110	-3
13	732	872	-34
14	1053	1071	-4
15	-268	233	-22
16	737	724	2
17	845	899	-11
18	247	99	7
19	-110	203	-7
20	205	210	0
21	247	341	-6
22	56	253	-7
23	404	530	-12
24	1014	865	24
25	984	1001	-2
26	338	124	9
27	765	673	11
4 0 1			
0	4803	4849	-10
1	1912	1879	11
2	1062	981	26
3	1329	1277	18
4	633	632	0
5	2408	2590	-61
6	667	632	8
7	397	296	14
8	1420	1549	-44
9	1537	1531	1
10	2774	2851	-22
11	321	339	-2
12	1021	1028	-1
13	-108	187	-8
14	312	264	4
15	439	177	24
16	1886	1828	15
17	990	1059	-15
18	493	333	17
19	1695	1658	9
20	696	509	24
21	10	275	-9
22	-16	207	-4
23	639	442	21
24	2211	2162	10
25	414	88	15
26	1240	1109	22
5 0 1			
1	721	753	-8
2	348	237	13
3	1063	1133	-22
4	1212	1350	-46
5	1494	1418	23
6	1149	1199	-15
7	791	761	7
8	2138	2131	1
9	1113	1181	-19
10	877	799	17
11	3513	3548	-8
12	2355	2290	17
13	1992	1946	12
14	-92	78	-2
15	1354	1363	-2
16	463	371	10
17	-148	8	-3
18	-134	91	-3
19	173	91	2
20	943	1117	-33
21	-199	10	-4
22	941	885	8
23	252	203	2
24	558	577	-1
25	-283	223	-12
6 0 1			
0	3872	3959	-20
1	1878	1842	10
2	330	45	19
3	1144	1288	-43
4	1419	1369	14
5	2483	2395	24
6	498	235	31
7	1914	1819	26
8	1096	995	24
9	2685	2554	34
10	1219	1333	-30
11	636	668	-5
12	811	953	-30
13	400	321	8
14	374	554	-22
15	-302	226	-20
16	922	943	-4
17	1128	1108	4
18	498	388	10
19	1509	1535	-5
20	623	708	-11
21	630	572	6
22	1300	1231	12
23	-208	146	-6
24	-329	273	-17
7 0 1			
1	2158	2244	-24
2	1107	1142	-9
3	-80	36	-1
4	1220	1289	-18
5	640	617	4
6	556	362	25
7	1546	1459	22
8	1408	1604	-54
9	512	16	35
10	1219	1145	17
11	844	1021	-37
12	-331	155	-19
13	-258	204	-14
14	-82	345	-16
15	265	247	1
16	833	826	1
17	1155	1073	15
18	731	779	-6
19	476	353	10
20	484	642	-17
21	316	168	6
22	585	572	1
8 0 1			
0	1857	1825	8
1	469	438	3
2	998	943	11
3	909	789	23
4	855	707	26
5	169	104	2
6	611	662	-8
7	565	698	-20
8	166	509	-31
9	595	733	-21
10	911	984	-14
11	489	454	3
12	394	182	14
13	859	683	26
14	850	755	14
15	493	625	-15
16	1401	1290	21
17	425	527	-9
18	-165	272	-10
19	633	537	10
20	419	468	-4
9 0 1			
1	540	443	11
2	423	584	-19
3	171	88	2
4	-292	76	-12
5	929	904	4
6	796	630	24
7	407	76	18
8	162	159	0
9	198	335	-8
10	499	264	19
11	1323	1178	28
12	1404	1368	7
13	168	188	0
14	522	309	17
15	55	244	-5
16	674	628	5
17	450	113	17
10 0 1			
0	-180	115	-5
1	626	356	27
2	715	673	5
3	257	76	6
4	489	495	0
5	288	61	8
6	305	92	9
7	220	271	-2
8	-66	223	-5
9	936	1075	-23
10	165	26	2
11	287	309	-1
12	-341	90	-12
13	415	462	-3
14	668	609	6
11 0 1			
1	367	286	5
2	509	205	20
3	422	163	14
4	-258	29	-6
5	517	605	-9
6	364	340	1
7	100	419	-16
8	658	577	8
0 1 1			
1	249	616	-96
3	628	693	-20
5	2651	2917	-80
7	1250	1246	1
9	506	503	0
11	1538	1654	-30
13	634	725	-15
15	1007	1063	-10
17	1147	1257	-21
19	1925	1916	1
21	1479	1367	18
23	253	427	-9
25	489	371	7
27	808	748	5
1 1 1			

2	642	416	78
3	954	1087	-67
4	1679	1581	42
5	543	403	34
6	1514	1305	81
7	161	284	-14
8	3138	3339	-62
9	171	335	-21
10	21	7	0
11	3260	3220	11
12	199	284	-8
13	-250	47	-13
14	592	463	23
15	780	836	-13
16	2098	2059	11
17	213	278	-5
18	386	332	5
19	403	224	15
20	575	557	2
21	940	982	-8
22	777	791	-2
23	445	521	-8
24	187	185	0
25	311	365	-3
26	-132	176	-5
27	1114	1056	9

2 1 1

0	4290	4056	57
1	1955	1923	13
2	1921	1956	-14
3	920	900	7
4	425	485	-14
5	1907	1955	-19
6	768	835	-22
7	1231	1091	49
8	1930	1962	-11
9	1826	1758	23
10	1669	1540	42
11	-351	61	-30
12	356	320	5
13	321	258	7
14	1398	1382	4
15	-174	27	-5
16	1962	1941	6
17	-100	329	-19
18	-48	167	-4
19	1006	1020	-2
20	-188	147	-8
21	565	589	-3
22	1243	1257	-3
23	-306	29	-11
24	1283	1172	21
25	399	20	16
26	389	359	2
27	216	147	2

3 1 1

1	3267	3256	3
2	452	75	49
3	4154	4078	18
4	1958	1761	69
5	685	689	-1
6	1874	1744	45
7	-243	2	-15
8	1093	996	30
9	504	490	2
10	-81	338	-27
11	1048	1191	-44
12	584	478	19
13	2248	2281	-9
14	362	267	10
15	875	936	-14
16	887	974	-20
17	154	92	2

18	541	543	0
19	-13	252	-8
20	552	500	6
21	456	366	8
22	85	112	0
23	437	319	9
24	401	265	9
25	1297	1281	3
26	301	119	7
27	668	454	20

4 1 1

0	576	468	24
1	368	288	12
2	1411	1398	4
3	4167	4093	17
4	2112	1874	76
5	1368	1409	-14
6	225	450	-34
7	929	876	15
8	774	735	9
9	125	166	-2
10	478	465	2
11	191	113	4
12	261	315	-5
13	162	178	0
14	1685	1700	-4
15	606	563	7
16	491	446	5
17	556	452	13
18	522	394	14
19	1809	1769	9
20	220	138	3
21	285	366	-6
22	-337	276	-22
23	535	412	11
24	220	309	-4
25	359	277	5
26	18	114	-1

5 1 1

1	1997	1981	5
2	664	751	-22
3	1130	1131	0
4	801	812	-3
5	-114	108	-5
6	746	902	-42
7	788	955	-45
8	2275	2173	29
9	853	765	20
10	-30	314	-17
11	1282	1232	13
12	-159	30	-4
13	747	655	17
14	737	740	0
15	320	354	-3
16	1185	1189	-1
17	1265	1285	-4
18	480	378	10
19	204	120	3
20	316	392	-6
21	424	71	18
22	432	583	-15
23	621	500	12
24	417	133	15
25	303	104	7

6 1 1

0	232	65	9
1	445	288	20
2	78	211	-7
3	-279	36	-15
4	813	789	5
5	1387	1464	-23
6	507	517	-1
7	369	61	22
8	641	420	34
9	840	765	15
10	510	341	21
11	885	941	-12
12	991	997	-1
13	312	170	9
14	248	157	5
15	707	683	3
16	1031	973	11
17	1128	1077	10
18	456	355	9
19	565	368	19
20	288	219	3
21	252	418	-11
22	-115	98	-2
23	586	606	-2
24	709	506	21

7 1 1

1	873	977	-25
2	826	782	9
3	324	280	4
4	317	112	13
5	521	468	7
6	-179	171	-10
7	111	83	0
8	342	350	0
9	321	298	2
10	417	242	15
11	1190	1259	-16
12	861	817	8
13	371	287	7
14	-346	65	-16
15	509	497	1
16	358	36	14
17	-356	157	-17
18	-184	55	-4
19	-144	213	-7
20	521	711	-22
21	-379	72	-15
22	369	327	2

8 1 1

0	820	772	9
1	497	503	0
2	645	419	30
3	414	184	18
4	369	328	3
5	484	549	-8
6	281	81	9
7	323	350	-2
8	-173	116	-5
9	1255	1361	-25
10	765	701	10
11	344	20	14
12	400	441	-3
13	542	665	-16
14	867	724	21
15	137	166	0
16	428	443	-1
17	347	23	12
18	-367	22	-14
19	-415	54	-18
20	-312	155	-11

9 1 1

1	154	60	2
2	439	474	-3
3	355	462	-10
4	315	106	10
5	277	166	6
6	443	208	17
7	415	410	0
8	592	589	0
9	200	205	0
10	362	520	-15
11	470	144	21
12	-299	280	-18
13	477	402	6
14	-261	33	-7
15	337	534	-17
16	275	152	5
17	551	474	7

10 1 1

0	201	192	0
1	209	226	0
2	216	158	2
3	570	537	3
4	531	545	-1
5	225	184	1
6	372	441	-5
7	340	411	-5
8	341	15	11
9	413	446	-2
10	-126	168	-4
11	306	3	9
12	-221	38	-5
13	-196	191	-7
14	444	337	7

11 1 1

1	439	351	6
2	507	159	21
3	356	70	11
4	280	181	4
5	337	84	10
6	501	307	14
7	-254	202	-10
8	286	161	5

0 2 1

2	466	605	-36
4	1007	1116	-36
6	568	487	14
8	988	1029	-10
10	2684	2719	-8
12	2879	2857	4
14	447	481	-3
16	68	151	-2
18	733	671	8
20	527	356	13
22	1002	953	6
24	477	642	-13
26	1336	1178	20

1 2 1

1	2347	2694	-150
2	252	466	-52
3	972	1097	-58
4	714	731	-5
5	-174	184	-18
6	2107	2157	-19
7	205	135	6
8	2523	2603	-27
9	1137	1144	-2
10	2131	2108	7
11	1107	1030	23
12	456	380	12
13	1078	1125	-13
14	-378	72	-30
15	1269	1261	2
16	556	472	13
17	778	874	-21
18	1102	1195	-23
19	391	372	2
20	-105	270	-11
21	574	451	15

Tetra(pentafluorophenyl)octabromoporphinato Zinc(II)

22	753	842	-15
23	173	184	0
24	549	588	-4
25	1479	1373	21
26	179	339	-8
27	143	331	-8
2 2 1			
0	2829	2878	-16
1	1564	1402	65
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Tetra(pentafluorophenyl)octabromoporphinato Zinc(II) Page 4

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16	849	889	-8
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18	1707	1702	1
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20	150	213	-2
21	671	726	-7
22	298	55	9
23	-325	118	-13
24	169	234	-2
25	997	1006	-1

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3	346	306	5
4	-154	64	-6
5	942	994	-14
6	562	647	-18
7	1825	1770	16
8	956	1082	-35
9	2453	2460	-1
10	1037	1116	-21
11	386	517	-19
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13	-155	45	-4
14	1012	1113	-24
15	720	539	28
16	796	654	23
17	2269	2259	2

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18	369	381	-1
19	741	771	-4
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25	629	422	19
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6	1672	1703	-9
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12	296	398	-10
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14	388	60	19
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16	1082	1080	0
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22	910	833	11
23	476	578	-10
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18	627	594	3
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11	1741	1687	14
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14	251	442	-18
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14	458	485	-2
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9 7 1			
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9 8 1			
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3	199	49	3
4	457	438	1
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6	437	526	-8
7	134	51	1
8	693	467	23
9	-178	72	-3
10	743	765	-2
11	-473	4	-23
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10 8 1			
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4	275	37	7
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6	425	474	-4
0 9 1			
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9	1792	1858	-13
11	665	718	-7
13	-223	153	-7
15	-249	26	-6
17	680	700	-2
19	1039	1104	-8
21	-317	38	-7
23	621	629	0
1 9 1			
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8	2270	2285	-4
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13	884	843	8
14	-223	245	-15
15	-195	162	-8
16	913	872	7
17	-153	2	-3
18	556	663	-14
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22	-269	34	-7
23	516	597	-8
24	232	240	0
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5	636	618	3
6	281	207	6
7	-343	47	-21
8	844	851	-1
9	994	1022	-6
10	786	775	2
11	-33	340	-18
12	-73	265	-11
13	-325	33	-16
14	142	344	-13
15	300	436	-12
16	1339	1362	-5
17	581	563	2
18	392	508	-11
19	587	618	-3
20	-222	66	-5
21	233	56	5
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3 9 1

1	1213	1109	27
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3	2563	2531	8
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5	384	459	-10
6	360	365	0
7	61	15	0
8	1289	1309	-5
9	392	366	2
10	-78	109	-2
11	1091	1014	17
12	505	660	-23
13	1559	1557	0
14	351	153	12
15	1367	1389	-4
16	690	798	-17
17	413	505	-9
18	458	406	4
19	289	0	8
20	306	304	0
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22	343	123	9
23	-264	9	-6

4 9 1

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5	-184	137	-8
6	-86	112	-3
7	144	359	-16
8	284	327	-3
9	-224	115	-9
10	-278	80	-12
11	408	336	7
12	443	429	1
13	-313	165	-17
14	759	856	-16
15	779	837	-9
16	-37	146	-2
17	652	668	-2
18	-278	304	-19
19	1165	1254	-17
20	340	330	0
21	194	13	3
22	266	399	-8

5 9 1

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3	702	681	3
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8	1495	1539	-10
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14	425	216	14
15	464	493	-2
16	-119	408	-20
17	555	594	-4
18	355	314	2
19	273	47	7
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6 9 1

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2	-124	310	-15
3	781	725	9
4	619	499	16
5	700	690	1
6	-134	229	-9
7	604	823	-36
8	358	421	-6
9	-31	63	0
10	97	191	-3
11	209	384	-12
12	-128	202	-6
13	-176	275	-12
14	-414	174	-23
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16	656	452	21
17	481	179	19
18	-302	248	-15
19	307	122	7

7 9 1

1	448	170	20
2	127	205	-3
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6	559	526	3
7	58	301	-10
8	176	162	0
9	532	440	9
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14	492	476	1
15	-118	53	-1
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8 9 1

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2	214	47	4
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9	747	774	-3
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13	-312	182	-13
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9 9 1

1	259	230	1
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7	640	654	-1
8	847	723	16
9	383	91	13
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0 10 1

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14	394	246	8
16	2793	2616	30
18	1047	1232	-26
20	164	45	1
22	426	480	-3

1 10 1

1	1657	1616	11
2	576	693	-23
3	1689	1729	-11
4	628	683	-10
5	420	531	-16
6	1370	1369	0
7	213	379	-15
8	2020	2016	0
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10	240	273	-2
11	2174	2121	13
12	117	197	-3
13	1349	1315	8
14	-273	36	-10
15	845	627	33
16	2307	2340	-7
17	712	552	20
18	1208	1126	15
19	-349	27	-13
20	811	774	5
21	-367	181	-17
22	308	182	6
23	-316	186	-13

2 10 1

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4	817	857	-8
5	3102	3084	4
6	281	415	-14
7	1215	1291	-19
8	340	500	-20
9	912	945	-7
10	-95	51	-1
11	946	987	-8
12	827	759	12
13	553	519	4
14	1363	1340	5
15	278	256	1
16	381	548	-17
17	-104	26	-1
18	-279	66	-9
19	2119	2060	12
20	335	16	11
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22	336	445	-8

3 10 1

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3	636	741	-20
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6	353	241	9
7	519	454	8
8	3270	3394	-30
9	390	288	9
10	913	869	8
11	1010	1084	-16
12	118	273	-8
13	297	377	-6
14	653	732	-12
15	363	282	6
16	802	819	-2
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19	163	348	-9
20	585	386	18
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4 10 1

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7	-314	100	-16
8	1240	1266	-6
9	685	750	-11
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11	311	105	10
12	1305	1215	19
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15	650	457	21
16	904	904	0
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19	457	723	-30
20	77	273	-6
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5 10 1

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7	429	245	15
8	1596	1607	-2
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10	1008	957	9
11	1519	1395	26
12	1231	1090	27
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16	-113	314	-11
17	335	559	-20
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6 10 1

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2	578	407	20
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7	783	760	3
8	265	110	6
9	1567	1481	18
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11	191	256	-3
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7 10 1

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6	425	429	0
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8	886	766	18
9	198	241	-2
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12	317	297	1
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14	398	533	-11
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8 10 1

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5	292	252	2
6	299	331	-2
7	-303	60	-10
8	217	149	2
9	640	665	-2
10	368	30	13
11	279	122	6
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9 10 1

1	450	80	18
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3	346	146	9
4	333	190	7
5	404	429	-1
6	606	621	-1
7	95	175	-2

0 11 1

1	302	431	-10
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5	2751	2628	23
7	241	92	5
9	497	532	-3
11	1275	1186	14
13	441	481	-3
15	584	455	10
17	2029	2049	-3
19	524	534	0
21	614	527	6

1 11 1

1	518	533	-2
2	907	980	-17
3	635	622	2
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6	2259	2133	32
7	138	212	-3
8	1398	1438	-10
9	-91	227	-8
10	220	206	0
11	1516	1574	-14
12	85	220	-5
13	383	432	-5
14	-89	119	-2
15	1027	1016	2
16	751	752	0
17	385	501	-10
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21	457	389	5

2 11 1

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2	1594	1735	-39
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4	260	398	-13
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7	607	758	-27
8	1065	1137	-16
9	1069	1138	-15
10	821	878	-10
11	-365	31	-18
12	321	341	-1
13	342	333	0
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15	457	293	13
16	181	321	-7
17	-195	30	-4
18	-327	9	-11
19	1139	1138	0
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3 11 1

1	412	499	-11
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3	1128	1243	-28
4	497	405	11
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6	200	397	-16
7	504	551	-6
8	916	944	-5
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10	641	628	1
11	1259	1135	26
12	652	617	4
13	1398	1391	1
14	367	248	8
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16	190	304	-6
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18	279	106	6
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4 11 1

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2	1231	1232	0
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4	947	890	11
5	326	380	-5
6	624	588	5
7	1317	1336	-4
8	-157	212	-9
9	655	766	-18
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11	660	421	27
12	518	463	5
13	326	178	8
14	607	477	14
15	294	122	7
16	238	97	4
17	438	136	17
18	417	277	9
19	908	1001	-14

5 11 1

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3	263	65	8
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5	705	674	4
6	1368	1330	8
7	473	442	3
8	555	662	-14
9	331	243	5
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11	538	384	15
12	309	26	10
13	-459	49	-24
14	585	536	5
15	174	287	-5
16	414	330	6
17	761	720	5
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6 11 1

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4	467	391	7
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6	380	289	6
7	328	197	7
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15	333	385	-3
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7 11 1

1	1005	962	7
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3	195	76	3
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8 11 1

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9 11 1

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0 12 1

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1 12 1

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2 12 1

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11	98	251	-6
12	489	424	6
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14	811	848	-5
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5	237	406	-14
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8	690	642	7
9	922	879	7
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13	578	596	-2
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10	1393	1398	-1
11	518	695	-22
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3	1148	1108	8
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6	505	404	11
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9	99	266	-7
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11	264	585	-31
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7	385	266	9
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10	957	973	-2
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16	-453	179	-25
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18	186	270	-3
3 13 1			
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11	282	88	7
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7	1213	1187	5
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7	431	25	19
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9	271	459	-14
10	241	351	-6
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5	761	653	14
6	-371	36	-15
7	62	356	-12
8	-166	142	-4
9	-150	170	-5
10	477	429	4
11	463	476	-1
12	-421	66	-18
7 13 1			
1	502	260	17
2	-216	85	-5
3	415	28	16
4	319	151	7
5	-344	41	-12
6	294	288	0
7	-136	127	-3
8	741	734	0
0 14 1			
0	1930	1983	-9
2	1427	1378	7
4	392	505	-8
6	233	263	-1
8	510	344	10
10	628	743	-11
12	-504	14	-20
14	1115	973	16
16	563	516	3
1 14 1			
1	1400	1434	-7
2	476	613	-17
3	-446	3	-26
4	736	646	13
5	-240	115	-8
6	-398	81	-20
7	-357	14	-15
8	962	886	13
9	560	493	7
10	-229	223	-11
11	-333	97	-13
12	78	43	0
13	-283	67	-9
14	-292	139	-11
15	465	429	3
16	266	171	4
17	519	443	6
2 14 1			
0	581	612	-4
1	541	554	-1
2	698	621	10
3	320	161	8
4	498	453	4
5	361	247	7
6	-181	178	-7
7	801	782	2
8	-310	58	-11
9	604	686	-10
10	519	522	0
11	363	272	6
12	709	800	-12
13	-223	114	-6
14	358	116	11
15	-410	206	-21
16	165	84	1
3 14 1			
1	791	658	19
2	-205	220	-10
3	391	393	0
4	-244	81	-7
5	303	62	9
6	687	664	3
7	-355	50	-14
8	530	269	21
9	393	465	-6
10	1065	1030	6

11	-246	299	-16
12	214	12	4
13	-239	286	-14
14	-404	93	-17
15	603	534	6

4 14 1

0	-356	3	-14
1	-302	130	-12
2	274	414	-10
3	-207	53	-5
4	168	162	0
5	-376	74	-16
6	270	101	6
7	422	517	-9
8	-131	154	-4
9	557	633	-8
10	606	757	-19
11	-333	215	-16
12	640	526	12
13	-444	252	-27
14	-153	406	-18

5 14 1

1	1090	1027	10
2	410	331	5
3	-307	148	-12
4	92	195	-3
5	360	368	0
6	415	513	-9
7	-273	145	-10
8	625	506	12
9	416	386	2
10	749	582	19
11	161	76	1
12	-342	149	-13

6 14 1

0	480	596	-11
1	344	60	11
2	38	232	-5
3	-55	23	0
4	261	161	4
5	-244	321	-16
6	386	246	8
7	736	786	-6
8	136	20	1
9	509	533	-2

7 14 1

1	197	183	0
2	385	332	3
3	-320	233	-15

0 15 1

1	171	316	-5
3	855	890	-4
5	507	636	-10
7	1100	1203	-14
9	1914	1800	17
11	697	648	4
13	-259	118	-5
15	-302	230	-9

1 15 1

1	831	763	10
2	716	689	3
3	510	435	7
4	241	246	0
5	188	310	-6
6	1370	1285	16
7	291	75	8
8	416	315	7
9	1023	920	16
10	608	472	14
11	437	376	4
12	284	344	-3
13	1081	1155	-12
14	172	181	0

2 15 1

0	-155	250	-9
1	60	12	0
2	1534	1507	5
3	375	39	15
4	557	545	1
5	260	402	-10
6	-425	119	-22
7	280	241	2
8	-343	66	-13
9	242	452	-15
10	843	741	14
11	260	251	0
12	681	497	19
13	195	179	0
14	766	644	14

3 15 1

1	1609	1647	-8
2	481	153	21
3	75	63	0
4	-240	161	-9
5	88	225	-4
6	987	933	8
7	483	217	18
8	1005	1054	-8
9	426	293	9
10	317	637	-29
11	650	665	-1
12	-320	70	-10
13	196	125	2

4 15 1

0	834	758	10
1	653	529	13
2	244	374	-8
3	53	23	0
4	-430	0	-20
5	467	218	16
6	186	369	-10
7	1037	991	7
8	-179	278	-11
9	640	518	12
10	528	340	14
11	409	174	12

5 15 1

1	1177	1213	-6
2	629	634	0
3	532	547	-1
4	238	334	-5
5	366	284	5
6	780	527	28
7	-250	263	-13
8	153	207	-1

6 15 1

0	450	387	4
1	292	402	-7
2	574	518	5
3	194	129	1

0 16 1

0	806	953	-16
2	1335	1125	27
4	-293	71	-7
6	451	181	11
8	1036	937	11
10	-204	316	-10
12	565	411	9

1 16 1

1	276	219	2
2	447	427	1
3	1106	1189	-15
4	-331	194	-15
5	476	442	3
6	813	742	9
7	-285	185	-12
8	1176	1141	6
9	557	392	14
10	257	112	5
11	675	737	-7

2 16 1

0	1051	1062	-1
1	-226	8	-5
2	517	357	13
3	1255	1207	8
4	477	542	-6
5	1209	1261	-9
6	93	129	0
7	-238	512	-32
8	304	115	7
9	310	495	-14
10	534	379	12
11	326	241	4

3 16 1

1	-222	163	-7
2	309	183	6
3	224	440	-14
4	-183	81	-4
5	381	426	-3
6	947	819	18
7	501	278	16
8	891	837	7
9	289	284	0

4 16 1

0	1532	1356	32
1	292	312	-1
2	-308	75	-10
3	507	469	3
4	429	48	17
5	633	620	1
6	172	211	-1
7	256	297	-2

0 17 1

1	250	355	-4
3	958	1013	-6
5	1125	1072	6
7	323	376	-2

1 17 1

1	1307	1218	15
2	321	76	9
3	602	638	-4
4	-253	265	-13
5	439	10	18
6	-161	304	-11
7	390	25	14

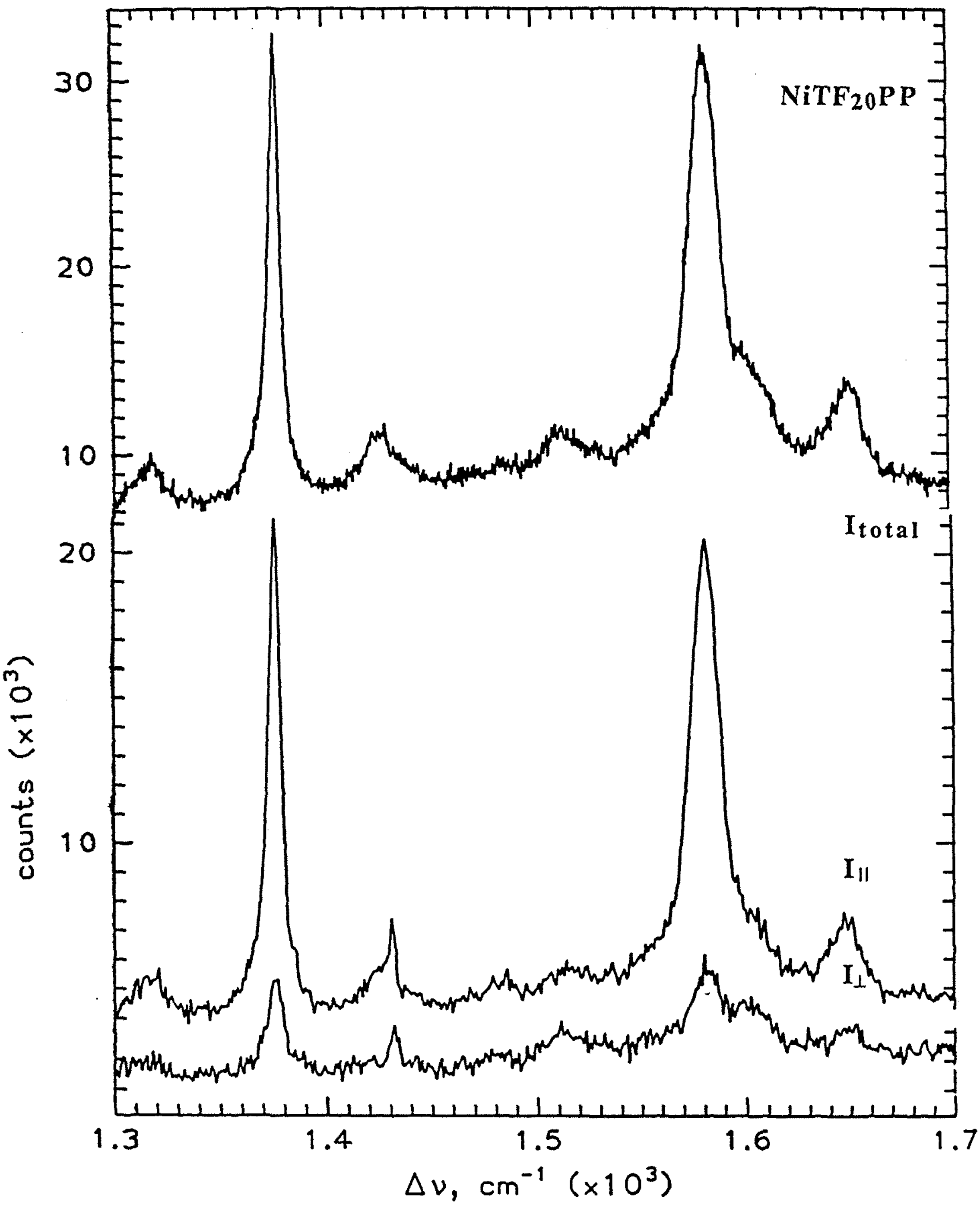
2 17 1

0	2014	1913	20
1	309	35	9
2	-216	104	-5
3	223	129	3
4	-403	210	-21
5	567	461	9
6	230	74	4

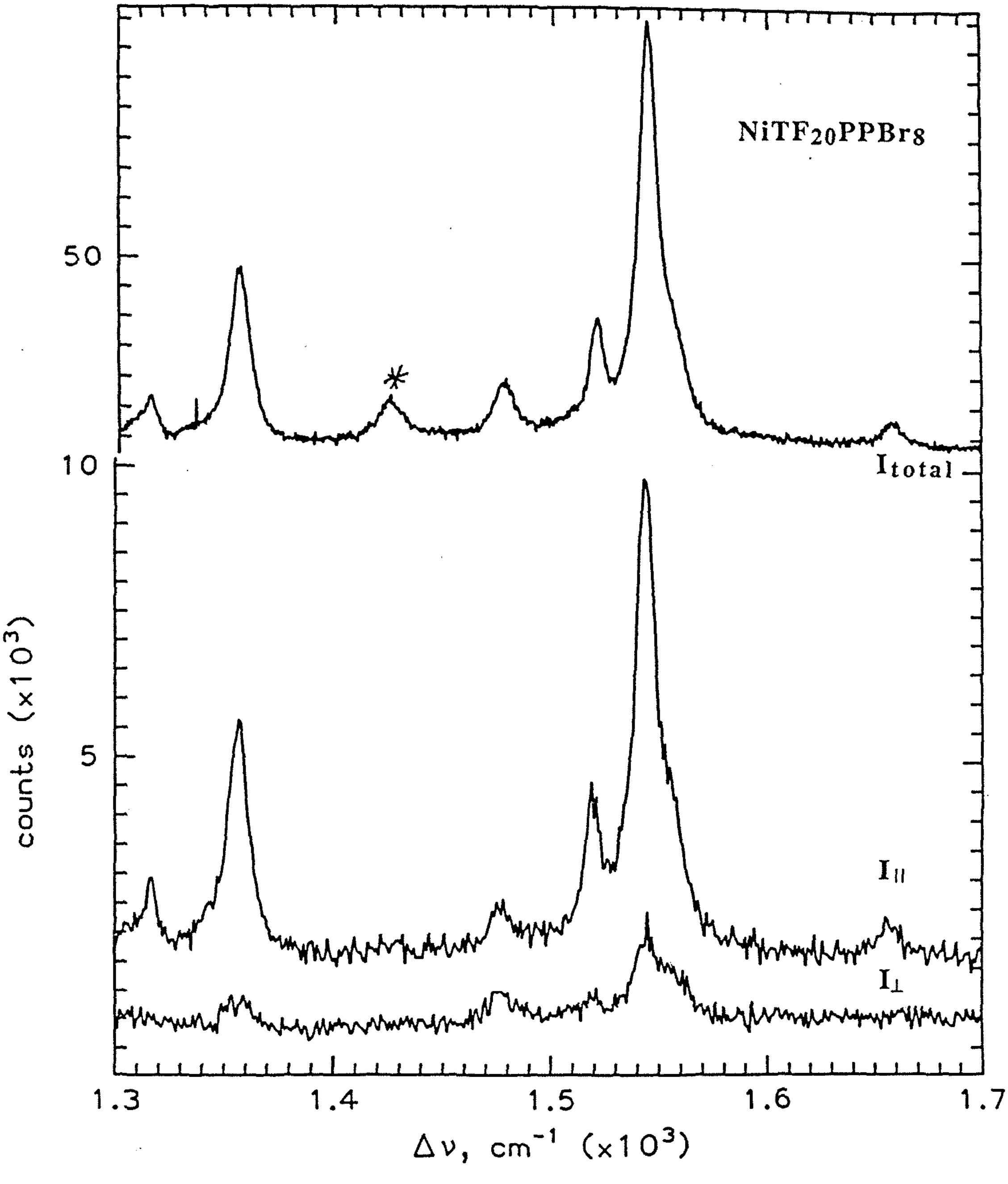
3 17 1

1	110	71	0
2	24	206	-4
3	657	826	-21

Appendix 8. Resonance Raman Spectra of NiTFPP and NiTFPPBr8.



(solvent: I_{total} = CH_2Cl_2, $I_{polarized}$ = CCl_4; 442 nm excitation)



* = **Solvent**

(solvent: I_{total} = CH_2Cl_2, $I_{polarized}$ = CCl_4; 442 nm excitation)