X-RAY STRUCTURAL STUDIES OF SOME GROUP VIII
COMPOUNDS WITH CATALYTIC IMPLICATIONS

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To Jeanie

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KEY TO ABBREVIATIONS

LIPS	ligand-induced proton shift
H ₂ dmg	dimethylglyoxime
dmg	dimethylglyoxime dianion
Hdmg	dimethylglyoxime monoanion
H ₂ dmg ₂	bis(dimethylglyoximate) with relative proton positions unspecified
sulfa	sulfanilamide
dhph	1,4-dihydrazinophthalazine
dhphpy	1,4-dihydrazinophthalazinebis (2- pyridinecarboxaldehyde)
pyca	2-pyridinecarboxaldehyde
clan	4-chloroaniline
H ₂ dph	diphenylglyoxime
H ₂ mpg	methylphenylglyoxime
fph	pentafluorophenyl
cp	cyclopentadienyl anion
tpp	triphenylphosphine
an	aniline
4-FPYTSC	4-formylpyridinethiosemicarbazone

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X-RAY STRUCTURAL STUDIES OF SOME GROUP VIII
COMPOUNDS WITH CATALYTIC IMPLICATIONS

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X-ray structural investigations of compounds containing Group VIII metal atoms are presented. The compounds studied illustrate interatomic interactions which may be of importance in catalytic processes. The structures of metal-containing compounds were solved by locating the heavy atoms in Patterson functions and locating the remaining atoms in Fourier syntheses. The direct method of symbolic addition was used in the one, all light-atom case presented. Trial structures were refined by the method of least-squares.

The crystal structure of trans-chloro(dimethylglyoximate)(dimethylglyoxime)(4-chloroaniline)cobalt(III) illustrates an unusual ligand-induced proton shift. Both neutral and dianionic dimethylglyoxime groups are found in the complex and the 4-chloroaniline ligand is oriented over the dianionic dimethylglyoxime. The structure of trans-bis(dimethyl-

glyoximato)bis(4-chloroaniline)cobalt(III) chloride shows that complex to contain two monoatomic dimethylglyoxime ligands and the 4-chloroaniline ligands to be skewed relative to the diglyoxime ligands. The crystal structure of trans-chlorobis(diphenylglyoximato)(4-chloroaniline)cobalt(III) is described. Trends in the structures of these compounds and in the previously reported structures of similar compounds are discussed. Ultraviolet and infrared spectra of these compounds are given.

The synthesis of a novel chelating ligand capable of binding two metal ions is described. The characterizations, including crystal structures, of its protonated form, 1,4-dihydrazinophthalazinebis(2-pyridiniumcarboxaldehyde) nitrate dihydrate, and of a nickel complex, μ -chlorotetraaqua[1,4-dihydrazinophthalazinebis(2-pyridinecarboxaldehyde)]dinickel(II) chloride dihydrate, are presented. The planar ligand is shown to bind two nickel ions with a separation of 3.603 (1) Å. A chloride ion occupies a bridging site in the plane of the nickel atoms and the ligand. The magnetic moment per nickel atom of the chloride bridged complex was determined to be 2.74 B.M. at 40°C. The plausibility of structurally similar complexes mimicking the nitrogen-fixing enzyme nitrogenase is also discussed.

The X-ray crystal structures of 1-(π -cyclopentadienyl)-1-triphenylphosphine-2,3,4,5-tetrakis(pentafluorophenyl)cobaltole and 1-(π -cyclopentadienyl)-1-triphenylphosphine-2,3,4,5-tetrakis(pentafluorophenyl)rhodole are reported.

These compounds are viewed as stabilized intermediates in the catalyzed cyclization of acetylenes. In each case the metal atom forms a metallocycle by σ -bonding to the terminal carbons of a butadiene-like fragment. The π -bonding in the metallocycle appears to be delocalized.

CHAPTER 1 INTRODUCTION

Western civilization has demonstrated the efficiency-oriented phenomenon of expending large amounts of energy to find ways of requiring less human energy. This is evident in the evolution from animal trails to freeways and from muscle to sophisticated, high-energy machinery. On the molecular scale the more efficient path is provided by catalysts. As alchemists searched for the "philosopher's stone" many chemists have been seeking catalysts. The application of catalysis is now advancing through the development of an understanding of the mechanisms of catalytic processes.

Life processes are dependent upon chemical reactions controlled by enzymes. "It is not generally appreciated how little is understood about the mechanisms by which enzymes bring about their extraordinary and specific rate acceleration."¹ Investigation of enzymes should not only be fundamental in the understanding and maintenance of life processes but also should contribute to developing more efficient industrial processes.

Much of the investigation of enzymes has concerned the use of model compounds. "Model building and the application of material analogues are becoming increasingly important for the elucidation of fundamental problems of biochemical

structure and reactivity."² X-ray structural studies of enzyme models are important for the exploration of structure-activity relationships. Solid state studies of enzyme model compounds are of particular relevance because of the high degree of order the macromolecular enzymes themselves possess.

While electrostatic and hydrogen-bonding forces are usually considered the major binding forces in enzyme-substrate interactions, the strong charge-solvating and hydrogen-bonding ability of water tends to reduce the possibility of obtaining large binding energies from these forces. To explain the large binding energies found, "hydrophobic forces" are presumed to exist in these intermolecular interactions in aqueous solution.³ The enthalpies of mixing of aromatic liquids with aliphatic liquids indicate that aromatic molecules prefer an aromatic environment.^{4,5} "Stacking interactions" involving the π -systems of aromatic groups within the enzyme's protein structure may account for part of the "hydrophobic forces" and contribute to the orientation of the enzyme-substrate interaction.³ The ligand-induced proton shift (LIPS) observed in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$ [the key to abbreviations is given on page x] is an indication of the importance of this π -type interaction. A further examination of LIPS was undertaken and is presented in this work.

The design of enzyme models is often based on sparse structural information about the prosthetic group of the enzyme. Efforts to mimic the nitrogen-fixing enzyme nitrogenase

have been concerned with the metal to nitrogen bond. The probable binuclear nature of the enzyme's active site^{6,7} has largely been ignored. The structures of a novel binucleating ligand and its nickel(II) complex are presented here as a first step in the construction of a new generation of models for nitrogenase.

When the mechanism of a chemical process is believed to be understood, stable compounds similar to the intermediates of the reaction may be prepared and examined to support the proposed mechanism. One proposed mechanism for the catalyzed cyclization of acetylenes would have a five-membered ring containing a metal atom and a cyclobutadiene fragment as one of the intermediates.⁸⁻¹³ The first structure of such a stabilized intermediate containing a cobalt atom and the structure of the rhodium analog are presented in this study.

CHAPTER 2 SYNTHESIS AND CHARACTERIZATION

Synthesis

Crystals of all cobaloxime compounds were generously provided by R. C. Palenik* and were used without recrystallization.

M. D. Rausch and R. H. Gastinger synthesized the metallocycles containing cobalt¹⁴ and rhodium.¹⁵ They supplied well-formed crystals of those metallocycles for X-ray structural studies.

Unless otherwise indicated all solvents were reagent grade and were used without further purification. All preparations were carried out in air. All melting points were taken on a Mel-temp apparatus in open capillaries and are uncorrected.

The published method¹⁶ was used to prepare dhph for succeeding experiments. To 6.40g (49.0 mmoles) 1,2-dicyanobenzene (98%; Aldrich Chemical Company, Milwaukee, Wisc.) in 12.5 ml 1,4-dioxane was added a mixture of 15.0 ml (ca. 250 mmoles) hydrazine hydrate (85%; Fisher Scientific Company, Fair Lawn, N. Y.) and 4.0 ml glacial acetic acid (reagent; Baker and Adamson, Morristown, N. J.). After being heated

*These complexes were prepared using standard procedures¹⁷ with synthetic details to be published at a later date.

for three hours the mixture was cooled and the red product was collected (yield, ca. 40%). The decomposition temperature of 193°C was in agreement with the reported value.

A solution of 0.0955g (0.50 mmoles) of the previously prepared dhph in 40 ml absolute ethanol was added to a solution of 0.237g (1.0 mmoles) $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (reagent; Matheson, Coleman and Bell, Norwood, Ohio) and 0.095 ml (0.99 mmoles) pyca (99%; Aldrich) in 40 ml absolute ethanol. Upon slow, almost complete, evaporation in air of that solution olive green crystals of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ formed.

Analogous procedures were carried out replacing $\text{NiCl}_2 \cdot \text{H}_2\text{O}$ with $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (reagent; Fisher), ZnCl_2 (reagent; Mallinckrodt Chemical Works, St. Louis, Mo.) and $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ (reagent; Matheson, Coleman and Bell) without success in obtaining a crystalline product. Similar procedures were followed with the addition of ca. 0.2 ml of 12 M hydrochloric acid (reagent, 38%; Baker and Adamson) to solutions of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ and $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$. Again, no suitable products were formed. Attempts to separate and recrystallize reaction products from water, water-ethanol, methanol and pyridine failed to give a crystalline product. When CuCl_2 was present, gas evolved from the reaction mixture.

Additional attempts were made to isolate complexes similar to $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3$ using dhph obtained by recrystallization from hot water of $\text{H}_2\text{dhphSO}_4$ (ICN·K and K Laboratories, Inc., Plainview, N. Y.) to which an equivalent

amount of KOH (certified A.C.S.; Fisher) had been added. Those attempts were unsuccessful.

The red-orange plates of $\text{H}_2\text{dhphpy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ used in crystallographic studies had been recrystallized from water. The crude product formed upon cooling a solution made by adding 0.190g (1.0 mmole) dhph in 20 ml warm water to a solution containing 0.583g (2.0 mmoles) $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (reagent; Mallinckrodt) and 0.89 ml (9.4 mmoles) pyca in 10 ml warm water followed by drop-wise addition of nitric acid (reagent, 71%; Baker and Adamson) to a pH less than 1.

Also, $\text{H}_2\text{dhphpy}(\text{NO}_3)_2$ was prepared by first adding 1.90 ml (20.0 mmoles) pyca to a suspension of 2.878g (10.0 mmoles) $\text{H}_2\text{dhphSO}_4$ in 100 ml water. A brick-red solid formed upon addition of 1.11g (ca. 17 mmoles) KOH. After washing with water and drying in air, the brick-red solid was suspended in 100 ml of 95% ethanol and 1.30 ml (21 mmoles) of nitric acid were added. Small red-orange needles of $\text{H}_2\text{dhphpy}(\text{NO}_3)_2$ which decompose at 126°C were filtered, washed with ethanol, and then ether and air dried (yield 4.0g, 75%).

Freshly prepared hydrated metal hydroxides were reacted with $\text{H}_2\text{dhphpy}(\text{NO}_3)_2$ in methanol. Each of the metal hydroxides was filtered after adding 1 M KOH to aqueous solutions of $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (reagent; J. T. Baker Chemical Company, Phillipsburg, N. J.), $\text{Fe}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (reagent; G. Frederick Smith Chemical Company, Columbus, Ohio) and $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (reagent; Matheson, Coleman and Bell). After

the reaction mixtures were stirred until there was no further change in color, they were filtered and the filtrates were allowed to evaporate. Only the reaction with nickel(II) hydroxide produced a crystalline product. Attempts to recrystallize that maroon product from methanol, ethanol, ethanol-water, and 2-propanol did not yield crystals suitable for crystallographic studies.

Discussion of Characterization

The microanalyses recorded in Table 1 were performed by Galbraith Laboratories, Inc., Knoxville, Tennessee, for the dhphpy compounds and by Atlantic Microlab, Inc., Atlanta, Georgia, for the cobaloxime complexes. The calculated percentages of carbon, hydrogen, and nitrogen for the dhphpy compounds correlate well with the measured percentage. Two water molecules per molecule of dhphpy in each are indicated by the elemental analysis. This is confirmed in the structural determination. Similarly, the elemental analysis of $\text{ClCo}(\text{H}_2\text{dmg})(4\text{-nitroaniline})$ is in agreement with the expected formula with two water molecules present. Based on the measured density and crystallographic data the molecular weight of $[\text{Co}(\text{H}_2\text{dmg}_2)(4\text{-methylaniline})]\text{Cl}$ should be 596. This is greater than its formula weight of 538.9 and the presence of molecules of solvation is expected. Three water molecules or one molecule of the ethanol solvent per formula could account for the difference. Neither of these possi-

Table 1
Elemental Analyses of Selected Compounds

	%C		%H		%N	
	found	calc.	found	calc.	found	calc.
$\text{ClCo}(\text{H}_2\text{dmg}_2)(4\text{-nitroaniline}) \cdot 2\text{H}_2\text{O}$	33.87	33.71	4.87	4.85	16.90	16.85
$[\text{Co}(\text{H}_2\text{dmg}_2)(4\text{-methylaniline})_2]\text{Cl}$	48.03	49.03	6.23	5.99	14.27	15.59
$\cdot 3\text{H}_2\text{O}$		44.56		6.46		14.17
$\cdot \text{C}_2\text{H}_5\text{OH}$		49.28		6.55		14.37
$\text{H}_2\text{dhphpy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$	45.36	45.29	4.12	4.18	26.10	26.40
$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$	32.39	32.65	3.84	3.84	15.22	15.23

bilities is confirmed by the CHN analysis (see Table 1).

IR spectra of samples as mineral oil mulls between polished plates of fused sodium chloride were recorded on a Beckman Model IR10 grating spectrophotometer from 4000 to 500 cm^{-1} . The spectra were calibrated using the 1601.0 cm^{-1} absorption of a polystyrene film. IR spectra of selected compounds are reported in Table 2. The IR spectra of the bis(diglyoxime)cobalt(III) complexes with aniline derivatives exhibit many features of similar cobalt complexes with nitriles and isonitriles described by Batyr *et al.*¹⁸ The spectra of the cobaloximes show the absorption assigned¹⁸ to the C=N stretch between 1550 cm^{-1} and 1580 cm^{-1} . The absorptions associated¹⁸ with the N-O band at ca. 1245 cm^{-1} and ca. 1095 cm^{-1} are present also. A weak absorption in the 1700-1800 cm^{-1} range appears in some of the spectra but with low resolution. Peaks in this region have been assigned¹⁹ to the O...H-O bridge between the dioximate ligands. The presence of a symmetrical bridge has been suggested²⁰ to rationalize this low frequency.

Absorption spectra in the ultraviolet region were recorded on a Cary Model 15 spectrophotometer. Spectra of solutions were measured from 26.7 kK (375 m μ) to 47.6 kK (210 m μ) using the double beam method with the pure solvent as the reference. Solutions of the cobaloxime complexes in methanol (spectroquality; Matheson, Coleman and Bell) and solutions of the dhphpy compounds in 0.1 M hydrochloric

Table 2
Infrared Spectra^a of Selected Compounds

$\text{ClCo}(\text{H}_2\text{dmg}_2) -$ (dmg) (clan)	$\text{ClCo}(\text{H}_2\text{dmg}) -$ (dmg) (sulfa)	$\text{ClCo}(\text{H}_2\text{dmg}_2) -$ (4-nitroaniline)	$\text{ClCo}(\text{H}_2\text{dpg}_2) -$ (clan)	$\text{ClCo}(\text{H}_2\text{mpg}_2) -$ (clan)
3525 (s)	3565 (s)	3535 (s)		
3425 (s)		3410 (s)	3400 (m, b)	3480 (m, b)
	3195 (s)			3360 (m)
	3105 (s)			3165 (m)
2395 (b, w)		2405 (w, b)		3065 (m)
1907 (w)	2305 (b, w)			
1778 (b, w)	1930 (w)			1897 (w)
1643 (m)	1780 (b, w)		1610 (w)	
		1598 (s)	1580 (w)	1595 (m)
1563 (s)	1564 (s)	1563 (s)	1530 (m)	1543 (s)
1483 (m)	1494 (w)	1530 (s)	1490 (s)	1490 (s)
			1445 (s)	1445 (s)
	1323 (s)	1343 (s)		
1242 (s)	1244 (s)	1244 (s)	1292 (m)	1263 (s)
1203 (s)		1200 (m)		
1156 (w)	1186 (w)	1168 (w)		

Table 2 - continued

$\text{ClCo}(\text{H}_2\text{dmg}) -$ (dmg) (clan)	$\text{ClCo}(\text{H}_2\text{dmg}) -$ (dmg) (sulfa)	$\text{ClCo}(\text{H}_2\text{dmg}_2) -$ (4-nitroaniline)	$\text{ClCo}(\text{H}_2\text{dpg}_2) -$ (clan)	$\text{ClCo}(\text{H}_2\text{mpg}_2) -$ (clan)
1085 (s)	1152 (s) 1084 (s)	1088 (s)	1130 (s)	1138 (m) 1085 (w) 1007 (s) 958 (m)
973 (b)	972 (m) 922 (m) 837 (m) 824 (m)	971 (m) 858 (s) 818 (w) 798 (w)	1013 (m) 920 (w) 885 (s) 823 (w)	825 (m)
825 (m)				
742 (m)		743 (m)	757 (w)	780 (m)
705 (m)		686 (m)	730 (s)	733 (s)
645 (w)	670 (m)		685 (s)	685 (s)

^aEach column contains the respective absorption peaks (cm^{-1}) and the relative intensity (s, strong; m, moderate; w, weak; b, broad).

Table 2 - extended

$[\text{Co}(\text{Hdmg})_2]^{2-}$ (clan) $_2\text{Cl}_3$	$[\text{Co}(\text{H}_2\text{dmg})_2]^{2-}$ (4-methylalaniline) $_2\text{Cl}_3$	$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4]^{4-}$ (dhppy) Cl_3	$\text{H}_2\text{dhppy} \cdot$ $(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$
	3420 (m, b)	3280 (s, b)	3460 (s, b)
3125 (s)			2050 (w, b)
			1750 (w, b)
2415 (w)	2400 (w, b)	1620 (m)	1609 (s)
2380 (w)		1517 (s)	1552 (s)
1892 (w)		1465 (s)	
1785 (b, w)		1380 (s)	1290 (s)
		1296 (w)	
	1638 (w)	1285 (w)	
1612 (m)	1600 (s)	1260 (w)	1168 (w)
1582 (s)	1570 (s)	1224 (m)	
1493 (s)	1506 (s)	1137 (s)	1141 (m)
			1115 (s)
		1096 (w)	
1234 (s)	1228 (s)		1057 (m)
1205 (s)	1197 (m)	1010 (w)	950 (w)
	1168 (w)	912 (w)	914 (w)

Table 2 - extended - continued

$[\text{Co}(\text{Hdmg})_2]_2^{2-}$ (clan) ₂ Cl ₂	$[\text{Co}(\text{H}_2\text{dmg}_2) -$ (4-methylalaniline) ₂]Cl ₂	$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4 -$ (dhphpy)]Cl ₃	$\text{H}_2\text{dhphpy} -$ (NO ₃) ₂ · 2H ₂ O
1083 (s)	1076 (s)	865 (w)	870 (w)
1008 (m)	1013 (m)	824 (w)	
967 (m)	968 (m)	768 (m)	775 (m)
			758 (s)
819 (m)			
805 (m)	808 (m)		
735 (m)	743 (m)		
700 (m)	701 (w)		
647 (m)			

acid were used. The UV spectra are reported in Table 3.

The UV spectra of all these compounds are dominated by intense charge transfer bands. Yamano et al.²¹ report three bands in this region for compounds of the formula $[\text{Co}(\text{H}_2\text{dmg})_2\text{A}_2]$ where A is an aniline derivative. These three bands are present in $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ and $[\text{Co}(\text{H}_2\text{dmg})_2(4\text{-methyl-aniline})_2]\text{Cl}$. The band between 25.0 and 27.5 kK (400 to 360 m μ) was assigned²¹ to the charge transfer from the aniline ligand to the cobalt ion. In agreement with this assignment the band for the complex of the more basic 4-methylaniline at 27.6 kK is lower in frequency than that for the analogous complex of clan at 28.9 kK. The band near 33.0 kK (300 m μ) was assigned²¹ to the charge transfer from the cobalt ion to the dioximate ligand. The band near 40.0 kK (250 m μ) was assigned²¹ to the intra-Hdmg $\pi \rightarrow \pi^*$ transition.

The UV spectra of cobaloxime complexes with a chloride ligand trans to a substituted aniline show three bands, also. One band is between 27.0 and 33.0 kK (370 to 300 m μ). The other bands lie near 39.0 kK (255 m μ) and 43.0 kK (230 m μ). No assignments have been made for these three bands.

The charge transfer spectrum of a solution of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ in 0.1 M HCl exhibits the same absorptions as that of a solution of $\text{H}_2\text{dhphpy}(\text{NO}_3)_2$ in 0.1 M HCl. The intense bands at 25.4, 32.7, and 37.3 kK (395, 305, and 268 m μ) are presumably due to the aromatic system of the ligand.

Table 3
Ultraviolet Spectra^{a,b} of Selected Compounds

[Co(Hdmg) ₂ (clan) ₂]Cl	28.9(16000)	[32.7]	39.7(21000)
[Co(H ₂ dmg) ₂ (4-methylaniline) ₂]Cl	27.6(11000)	32.8(7400)	39.7(16000)
ClCo(H ₂ dmg)(dmg)(clan)	32.7(9200)	39.5(24000)	44.8(24000)
ClCo(H ₂ mpg ₂)(clan)	31.1(7300)	39.8(27000)	[44.1]
ClCo(H ₂ dpg ₂)(clan)	29.7(12000)	37.6(43000)	42.4(42000)
ClCo(H ₂ dmg ₂)(4-nitroaniline)	27.2(20000)	[39.6]	42.9(33000)
H ₂ dhpmpy(NO ₃) ₂ ·2H ₂ O	25.4(5600)	32.8(4600)	37.3(4600)
[Ni ₂ Cl(H ₂ O) ₄ (dhpmpy)]Cl ₃ ·2H ₂ O	25.4(25000)	32.7(20000)	37.3(20000)

^aThe compound name is followed by the absorption frequencies (kK) with the extinction coefficients in parentheses.

^bFrequencies listed in square brackets are for poorly resolved peaks.

The magnetic moment per nickel atom of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})-(\text{dhphpy})]\text{Cl}_3$ was determined to be 2.74 B.M. at 40°C. Data for this calculation^{22,23} were obtained using a Varian A-60A Analytical NMR Spectrometer and aqueous solutions containing 2% by volume t-butanol as the indicator. This magnetic moment is in agreement with those of binuclear complexes of nickel reported by Ball and Blake.²⁴ Their complexes of the general formula $[\text{Ni}(\text{dhph})]_2\text{X}_4 \cdot n\text{H}_2\text{O}$ (X = Cl, Br, or I) had room temperature effective magnetic moments ranging from 2.79 to 2.89 B.M. As in the case of $[\text{Ni}(\text{dhph})]_2\text{X}_4 \cdot n\text{H}_2\text{O}$, where two Ni^{2+} ions are bridged by a conjugated system, spin-spin interaction is indicated in $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$.

CHAPTER 3 X-RAY DIFFRACTION EXPERIMENTAL

Except where noted in the text, the experimental methods described in this section were used in preliminary crystallographic examination, collection and processing of data, and refinement of trial structures.

Data obtained using precession and Weissenberg X-ray photographic techniques²⁵⁻²⁷ were used in determining the preliminary space groups and cell constants. After centering fifteen intense reflections on a computer-controlled Syntex P1 diffractometer and selecting an indexing consistent with preliminary photographs, accurate cell constants with estimated standard deviations were obtained from least-squares fittings of 2θ , ω , χ , and ϕ for those reflections. In each case the orientation matrix for data collection and the unit cell volume with its standard deviation were derived from these data. The calculated density was in agreement with the density measured by the flotation method²⁸ except in the cases of the metal-containing heterocycles. The specific gravity of the flotation liquid was measured to ± 0.01 with a precision hydrometer. Relevant crystallographic data for each of the compounds studied are given in Table 4.

The suitability of a crystal for data collection was determined by its physical shape and size, the ease with

Table 4

Crystallographic Data for A, $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})\cdot 2\text{H}_2\text{O}$; B, $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})\cdot \text{C}_2\text{H}_5\text{OH}$; C, $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$; D, $\text{H}_2\text{dhphpy}(\text{NO}_3)_2\cdot 2\text{H}_2\text{O}$; E, $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3\cdot 2\text{H}_2\text{O}$; F, $\text{C}_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$; G, $\text{C}_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$; H, $\text{ClCo}(\text{H}_2\text{mpg}_2)(\text{clan})$; I, $\text{ClCo}(\text{H}_2\text{dmg}_2)(4\text{-nitroaniline})\cdot 2\text{H}_2\text{O}$; J, $[\text{Co}(\text{H}_2\text{dmg}_2)(4\text{-methylaniline})_2]\text{Cl}$

Compound ^a	Formula	Crystal System	Systematic Absences	Space Group
A	$\text{C}_{14}\text{Cl}_2\text{CoH}_{20}\text{N}_5\text{O}_4\cdot 2\text{H}_2\text{O}$	triclinic	none	$\text{P}\bar{1}$
B	$\text{C}_{34}\text{Cl}_2\text{CoH}_{28}\text{N}_5\text{O}_4\cdot \text{C}_2\text{H}_5\text{OH}$	monoclinic	$h0\ell:h+\ell=2n+1$	$\text{P}2_1/n$
C	$\text{C}_{20}\text{Cl}_3\text{CoH}_{25}\text{N}_6\text{O}_4$	triclinic	none	$\text{P}\bar{1}$
D	$\text{C}_{20}\text{H}_{18}\text{N}_{10}\text{O}_6\cdot 2\text{H}_2\text{O}$	monoclinic	$hk\ell:h+k=2n+1$ $h0\ell:\ell=2n+1$	$\text{C}2/c$
E	$\text{C}_{20}\text{Cl}_4\text{H}_{24}\text{N}_8\text{Ni}_2\text{O}_4\cdot 2\text{H}_2\text{O}$	monoclinic	$hk\ell:h+k=2n+1$ $h0\ell:\ell=2n+1$	$\text{C}2/c$
F	$\text{C}_{51}\text{CoF}_{20}\text{H}_{20}\text{P}\cdot ?$	triclinic	none	$\text{P}\bar{1}$
G	$\text{C}_{51}\text{F}_{20}\text{H}_{20}\text{PRh}\cdot ?$	triclinic	none	$\text{P}\bar{1}$
H*	$\text{C}_{24}\text{Cl}_2\text{CoH}_{24}\text{N}_5\text{O}_4$	triclinic	none	$\text{P}1$ or $\text{P}\bar{1}$
I*	$\text{C}_{14}\text{ClCoH}_{20}\text{N}_6\text{O}_6\cdot 2\text{H}_2\text{O}$	orthorhombic	$hk0:h+\ell=2n+1$	Pmmn or $\text{Pm}2_1n(\text{Pm}2_1)$
J*	$\text{C}_{22}\text{ClCoH}_{32}\text{N}_6\text{O}_4\cdot ?$	monoclinic	$h0\ell:\ell=2n+1$	$\text{P}2/c$ or Pc

^aData for compounds marked with an asterisk were obtained from photographic techniques.

Table 4 - extended

Compound	a ° (Å)	b ° (Å)	c ° (Å)	α (°)	β (°)	γ (°)	Volume ° (Å ³)
A	7.494(3)	11.838(4)	13.758(6)	106.31(3)	91.25(3)	112.79(3)	1068.3(7)
B	15.363(13)	12.385(3)	18.535(13)	90	96.55(7)	90	3503(4)
C	6.386(4)	8.710(5)	12.719(5)	90.55(4)	105.16(4)	98.83(4)	673.9(6)
D	20.480(3)	11.166(2)	10.704(2)	90	102.99(2)	90	2385.0(8)
E	15.016(6)	15.527(7)	28.704(17)	90	115.78(3)	90	6027(5)
F	11.680(3)	14.008(4)	20.455(9)	114.08(3)	107.41(3)	106.72(2)	2572.9(1.7)
G	11.715(4)	14.015(6)	20.420(6)	114.07(3)	106.97(3)	107.28(3)	2574.3(1.5)
H*	7.95	13.26	13.75	98.1	102.7	105.9	1330
I*	21.66	13.68	14.97	90	90	90	4436
J*	13.2	11.2	19.9	90	110.6	90	2750

Table 4 - extended

Compound	Molecular Weight	Z	ρ calc. (g/cm ³)	ρ meas. (g/cm ³)	Crystal Dimensions (mm ³)	Radiation Used	μ (cm ⁻¹)
A	488.22	2	1.518	1.52	0.24x0.18x0.07	MoK α	11.2
B	746.54	4	1.415	1.43	0.18x0.20x0.05	MoK α	7.1
C	578.75	1	1.426	1.44	0.19x0.31x0.35	MoK α	10.0
D	530.46	4	1.477	1.47	0.34x0.31x0.18	MoK α	1.3
E	735.73	8	1.622	1.63	0.29x0.30x0.14	MoK α	18.1
F	1102.79	2	1.423	1.59	0.27x0.31x0.50	MoK α	4.9
G	1146.57	2	1.479	1.60	0.14x0.24x0.43	MoK α	4.6
H*	576.3	2	1.439	1.47			
I*	498.8	8	1.494	1.50			
J*	538.9	4	1.300	1.44			

Table 4 - extended

Compound	μ r	2 θ Range	K	No. of Unique Reflections	No. of Observed Reflections
A	~0.2	0-45	2.0	2807	2000
B	~0.1	0-45	1.5	4364	2017
C	~0.2	0-45	2.0	1771	1662
D	~0.04	0-45	2.0	1573	1093
E	~0.5	0-45	2.0	3981	2959
F	~0.1	0-45	2.0	6772	5479
G	~0.1	0-45	2.0	6766	5235

which the reflections were centered on the diffractometer, and the values of the refined cell constants with their estimated standard deviations compared to the cell constants obtained by photographic methods. All intensity measurements were made with a Syntex P1 diffractometer at ambient temperature. All unique reflections up to a limiting 2θ value were measured using a variable speed θ - 2θ scan technique. The scan rate was determined from a fast three-second counting scan of the reflection peak and varied linearly from $1^\circ/\text{minute}$ for counting rates of 150.0 c/sec. or less to $24^\circ/\text{minute}$ for 1500.0 c/sec. or more. The intensity, I , was defined:

$$I = (\text{scan rate}) \left[(\text{total scan counts}) - \frac{(\text{background counts})}{(\text{background to scan rate})} \right].$$

Peaks were scanned from 1° below $K\alpha_1$ to 1° above $K\alpha_2$. Measurements of the background count were made at the limits of each scan. The estimated standard deviation, $\sigma(I)$, of each reflection was taken to be:

$$\sigma(I) = \left[(\text{total scan counts}) + \frac{(\text{background counts})}{(\text{background to scan ratio})^2} \right]^{1/2}.$$

For molybdenum radiation, the incident beam was monochromatized by a low order reflection of graphite. Any changes in the system were detected by measuring four standard reflections after each 96 intensity measurements.

A standardized data set was obtained by scaling the data to the initial value of the sum of the measured intensities of the standard reflections. The scaled in-

tensities of duplicate or equivalent reflections were averaged. Reflections with an intensity greater than $K\sigma(I)$, where K is given in Table 4, were considered reliable. The unreliable reflections with $I < K\sigma(I)$ were identified by a minus sign and not included in further steps of the structure solution. Corrections for Lorentz-polarization were of the form:

$$\frac{1}{L_p} = \frac{\sin 2\theta}{(1 + \cos^2 2\theta)}.$$

To obtain a set of observed structure factors, F_{obs} 's, the monochromator was also assumed to be 50% perfect crystal and 50% mosaic crystal.

Scattering factors were obtained from Hanson, Herman, Lea, and Skillman;²⁹ Stewart, Davidson, and Simpson;³⁰ Doyle and Turner;³¹ and are uncorrected for anomalous dispersion. The natural log of the scale factor and the overall temperature factor were initially estimated from a Wilson pilot.³² The initial choice of a centric or acentric space group was made on the basis of calculated intensity statistics.³³

In the case where molecules contained at least one heavy atom (Atomic Number ≥ 16) the approximate positional coordinates were determined using a Patterson function³⁴ of the form:

$$P(UVW) = \frac{2}{V} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)|^2 \cos 2\pi(hU + kV + lW).$$

Using the location of the heavy atom(s) in a structure

factor calculation allowed a sufficient number of reflection phases, $\alpha(hkl)$'s, to be assigned. The magnitude of the structure factor, $|F_{hkl}|$, and the phase may be defined by the following equations:²⁷

$$A_{hkl} = \sum_j f_j \cos 2\pi(hx_j + hy_j + lz_j)$$

$$B_{hkl} = \sum_j f_j \sin 2\pi(hx_j + hy_j + lz_j)$$

$$|F_{hkl}| = (A_{hkl}^2 + B_{hkl}^2)^{1/2}$$

$$\alpha_{hkl} = \tan^{-1}(B_{hkl}/A_{hkl}),$$

where f_j is the scattering factor for atom j .

Additional atomic positions could then be determined through the use of Fourier syntheses³⁴ of the form:

$$(XYZ) = \frac{2}{v} \sum_{h=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F_{hkl}| \cos 2\pi[(hX+kY+lZ)-\alpha_{hkl}].$$

The positional coordinates of atoms in the trial structure were estimated from the Fourier generated electron density map using a FORTRAN computer program, BOOTHIT1, written in the course of this work. A description and listing of BOOTHIT1 is contained in Appendix A. Alternate structure factor calculations and Fourier syntheses were repeated until all nonhydrogen atoms were located.

In the case of a compound not containing a heavy atom but having a centrosymmetric space group, the direct method of symbolic addition was used. The FORTRAN computer programs, FAME-MAGIC-LINK-SYMP1, developed by E. B. Fleischer, R. B.

K. Dewar, and A.L. Stone^{35,36} were used to generate possible solutions to the phase problem. The programs first converted $|F_{\text{obs}}|$'s to normalized structure factors, E 's, through the definitions:

$$(F_{\text{absolute}})^2 = \left(\frac{1}{K^2}\right) |F_{\text{obs}}|^2 e^{(T \sin \theta)/\lambda}$$

and

$$E^2 = (F_{\text{absolute}})^2 / \epsilon \sum_i^N f_i^2$$

where the scale factor, K , and the overall temperature factor, T , were generated by a Wilson plot; where ϵ was a symmetry factor applied to reflections in special zones; and where f_i 's were the scattering factors for N atoms. The programs then assigned symbols representing the phases to six of the largest E 's having the greatest number of interactions, i.e., for E_h and E_m there exists E_{h-m} . For such reflections the probability, p , that the phase of E_h is the same as $\sum_{m=0}^N (E_m E_{h-m})$ is given by:

$$p = 0.5 + 0.5 \tanh \left(\frac{\sigma_3}{\sigma_2^{1.5}} |E_h| \left| \sum_{m=0}^N E_m E_{h-m} \right| \right)$$

where

$$\sigma_n = \sum_{j=1}^N z_j^n$$

with N being the number of atoms in the unit cell and z_j being the atomic number of the j^{th} atom. The programs, when given minimum acceptable probability criteria, iteratively assigned relative signs to the phase symbols. Combinations of these

signed phase symbols were finally used in conjunction with their structure factors to generate E-maps. The positional coordinates of most nonhydrogen atoms were determined from one of these E-maps. Structure factor calculations and Fourier syntheses were used to refine the atomic positions and, as in the heavy atom case, to locate any previously un-found nonhydrogen atoms of the trial structure.

The trial structure was refined by least-squares minimization³⁴ of the function:

$$\text{Residual} = \sum w (|F_{\text{obs}}| - |F_{\text{calc}}|)^2$$

where

$$\sqrt{w} = |F_{\text{obs}}| / |F_{\text{low}}| \quad \text{for } |F_{\text{obs}}| < |F_{\text{low}}|$$

$$\sqrt{w} = 1.0 \quad \text{for } |F_{\text{low}}| \leq |F_{\text{obs}}| \leq |F_{\text{high}}|$$

and

$$\sqrt{w} = |F_{\text{high}}| / |F_{\text{obs}}| \quad \text{for } |F_{\text{obs}}| > |F_{\text{high}}|$$

F_{low} and F_{high} are constants given in Table 4. Prior to refinement, an overall scale factor was chosen such that the sum of F_{obs} equaled the sum of F_{calc} . Isotropic temperature factors were used in the first three cycles of refinement and then anisotropic temperature factors of the form:

$$\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$$

were used. The reliability index, R , was defined by:

$$R = \frac{\sum ||F_{\text{obs}}| - |F_{\text{calc}}||}{\sum |F_{\text{obs}}|}$$

Calculations were performed on an IBM 370/165 computer with programs written or modified by Dr. Gus J. Palenik, except where previously noted. The refinement of each structure is outlined in Table 5.

Table 5

Schemes of Refinement

Compound	R-index with all nonhydrogen atoms from Fourier synthesis	Refinement with isotropic thermal parameters	No. of cycles	R-index	No. of cycles	Refinement ^a with anisotropic thermal parameters
$\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan}) \cdot 2\text{H}_2\text{O}$	0.27		3	0.095	3	0.066
$\text{C}^t\text{Co}(\text{H}_2\text{dpg}_2)(\text{clan}) \cdot \text{C}_2\text{H}_5\text{OH}$	0.229		3	0.132	3	0.093
$[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$	0.255		3	0.141	6	0.056
$\text{H}_2\text{dhpppy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$	0.32		3	0.134	3*	0.076
$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpppy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$	0.21		3	0.090	3	0.052
$\text{C}_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$	0.26		3	0.137	9	0.077
$\text{C}_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$	0.168		3	0.105	9	0.065

^aThe block-diagonal approximation to the full matrix was used, except where marked with an asterisk.

Table 5 - extended

Compound	Refinement ^a with hydrogen atoms in- cluded isotropically but not refined		Refinement ^a with hydrogen atoms refined isotropically		F _{low}	F _{high}
	No. of cycles	R-index	No. of cycles	R-index		
$\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan}) \cdot 2\text{H}_2\text{O}$	3	0.052	6	0.047	18.0	49.0
$\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan}) \cdot \text{C}_2\text{H}_5\text{OH}$	3	0.087	9	0.075	55.0	145.0
$[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$	3	0.038	9	0.033	4.5	12.0
$\text{H}_2\text{dhphpy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$	-	-	6	0.050	8.0	22.0
$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$	6	0.048	-	-	32.0	86.0
$\text{C}_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$	-	-	-	-	17.5	35.0
$\text{C}_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$	-	-	-	-	17.5	35.0

CHAPTER 4

AN INVESTIGATION OF LIGAND-INDUCED PROTON SHIFT: THE CRYSTAL AND MOLECULAR STRUCTURES OF TRANS-CHLORO(DIMETHYLGLYOXIMATO)-(DIMETHYLGLYOXIME) (4-CHLOROANILINE) COBALT(III) DIHYDRATE, TRANS-CHLOROBIS(DIPHENYLGLYOXIMATO) (4-CHLOROANILINE) COBALT(III) ETHANOLATE, AND TRANS-BIS(DIMETHYLGLYOXIMATO) BIS(4-CHLOROANILINE) COBALT(III) CHLORIDE.

The stability of bis(dimethylglyoxime)metal complexes has long been known and their importance in both qualitative and quantitative analysis has been widely recognized.^{37,38} Metal complexes of Hdmg have been used to study the trans-effect³⁹ and the trans-influence^{40,41} of various ligands in octahedral complexes. Since the structural determination of the B₁₂ coenzyme the trans-bis(dimethylglyoxime)cobalt complexes have become of considerable interest.⁴²⁻⁴⁴ Schrauzer⁴² has stated that to be capable of mimicking B₁₂ a complex is required only to have a cobalt ion in the presence of a strong-binding planar ligand. Because Co(H₂dmg₂) complexes successfully mimic the reactions of a cobalt ion in the corrin ring and because they are synthetically expedient, complexes of Co(H₂dmg₂) have been investigated extensively in solution as models for B₁₂.⁴⁵

Until very recently there have been few structural data on Co(H₂dmg₂) complexes.^{40,41,46-52} Except for the work of Palenik et al.⁴⁶ no structural investigation has been made of the interaction between the axial ligand and the equatorial Hdmg ligands. This interaction may be of considerable consequence.

Although sulfonamides are potent inhibitors of carbonic anhydrase they do not form strong coordination bonds with transition metal ions. Therefore, an interaction of the aromatic ring of the sulfonamide with the carbonic anhydrase protein has been proposed⁵³ to make a large contribution to the observed stability of the carbonic anhydrase-sulfonamide complex. Since a cobalt atom can replace the zinc atom in carbonic anhydrase with only a 50% decrease in activity, complexes of $\text{Co}(\text{H}_2\text{dmg}_2)$ may prove to be useful models for investigating the interaction of sulfonamides with carbonic anhydrase.

An apparent ligand-induced proton shift (LIPS) was observed⁴⁶ in $\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{sulfa})$ which should be formulated $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$. To investigate further the LIPS phenomena and to examine interligand interactions within this type of complex the determination of the structures of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$, $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$, and $\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{clan})$ was undertaken.

Structure Solution and Refinement for $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan}) \cdot 2\text{H}_2\text{O}$

The heavy atom method was used with the positions of the cobalt atom and of the ionic chloride ligand estimated from a sharpened Patterson function. The magnitude of the Patterson function for the Co to Cl vectors was of the same order as that for the Co to Co vector. The positions of the heavy atoms, therefore, appeared ambiguous and several combinations were used in Fourier syntheses to determine their actual lo-

cations. Successive Fourier syntheses then revealed the locations of all nonhydrogen atoms in the compound. Three cycles of full-matrix least-squares refinement with individual isotropic thermal parameters and then three cycles of least-squares refinement using the block approximation with individual anisotropic thermal parameters reduced R to 0.066. A difference Fourier synthesis then indicated the absence of additional nonhydrogen atoms and revealed the positions of all hydrogen atoms. An outline of the refinement is given in Table 5. The refinement was terminated after the parameter shifts for the nonhydrogen atoms were less than one-tenth of their corresponding estimated standard deviations.

The scattering factors for cobalt, chlorine, oxygen, nitrogen, and carbon were from Hanson *et al.*²⁹ while those for hydrogen were from Stewart *et al.*³⁰ A list of the observed and calculated structure factors has been published and is available.⁴⁶ The final positional and thermal parameters are given in Tables 6 and 7.

Structure Solution and Refinement for $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan}) \cdot \text{C}_2\text{H}_5\text{OH}$

The nonstandard space group $\text{P2}_1/\text{n}$ was chosen since the standard $\text{P2}_1/\text{c}$ space group would require a very large value for β . The position of the cobalt atom was estimated from a sharpened Patterson function. The location of atoms and the refinement proceeded as in the case of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan}) \cdot 2\text{H}_2\text{O}$. Two atoms, O(S1) and C(S1), of an apparent solvent mole-

Table 6
Final Atomic Parameters of Nonhydrogen Atoms for ClCo(H₂dmg)-(dmg)(clan)^a

Atom	x	y	z	β_{11}	β_{22}
Co	19148(12)	36142(8)	21611(6)	1287(16)	454(7)
Cl(1)	-1353(2)	2445(1)	1882(1)	148(3)	65(2)
Cl(2)	8142(4)	10300(2)	3785(2)	512(9)	67(2)
O(11)	1633(7)	4573(4)	534(3)	305(13)	95(5)
O(12)	1742(6)	4621(4)	4260(3)	304(13)	89(5)
O(21)	2285(7)	2611(4)	3796(3)	314(13)	104(5)
O(22)	1944(7)	2468(4)	17(3)	298(13)	114(6)
N(1)	4821(7)	4589(5)	2375(3)	157(12)	93(6)
N(11)	1600(7)	4753(5)	1536(3)	179(12)	75(6)
N(12)	1693(7)	4792(4)	3347(3)	156(12)	58(5)
N(21)	2289(7)	2459(5)	2788(3)	191(13)	72(5)
N(22)	2144(7)	2398(5)	980(3)	168(12)	74(5)
C(11)	1403(8)	5758(6)	2145(5)	170(15)	67(7)
C(12)	1443(8)	5772(6)	3208(5)	168(15)	59(6)
C(13)	1247(10)	6794(6)	1785(5)	268(19)	85(8)
C(14)	1310(10)	6815(7)	4067(5)	281(20)	100(8)
C(21)	2584(9)	1516(6)	2201(17)	214(17)	66(7)
C(22)	2509(9)	1475(6)	1124(5)	164(15)	65(7)
C(23)	3010(14)	584(8)	2593(7)	530(32)	112(10)
C(24)	2779(12)	465(7)	277(6)	410(27)	121(10)
C(1)	5676(7)	5999(5)	2722(4)	96(13)	70(6)
C(2)	6105(9)	6655(6)	3753(5)	198(16)	71(7)
C(3)	6866(9)	7971(6)	4082(5)	221(17)	91(8)
C(4)	7201(10)	8629(6)	3382(6)	195(17)	73(7)
C(5)	6809(10)	7972(7)	2340(5)	237(19)	99(8)
C(6)	6047(9)	6644(6)	2005(5)	191(16)	82(7)
O(w1)	6682(7)	3785(5)	646(4)	264(13)	148(7)
O(w2)	6802(7)	3830(5)	3690(3)	276(13)	166(7)

^aAll values are $\times 10^4$ except for Co which are $\times 10^5$. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.

Table 6 - extended

β_{33}	β_{12}	β_{13}	β_{23}
276(4)	822(17)	219(13)	157(9)
53(1)	78(4)	25(3)	14(2)
138(2)	65(7)	46(7)	46(4)
36(3)	168(14)	7(9)	44(6)
32(3)	167(13)	70(9)	33(6)
41(3)	199(14)	74(10)	70(6)
30(3)	199(14)	31(9)	25(6)
37(3)	123(14)	29(10)	50(7)
35(3)	108(14)	24(10)	26(7)
35(3)	71(13)	30(9)	19(6)
41(3)	123(14)	41(10)	39(7)
35(3)	99(13)	21(10)	12(7)
53(4)	101(17)	25(13)	41(9)
51(4)	73(16)	30(13)	14(8)
76(5)	190(21)	-5(16)	55(10)
62(5)	214(22)	50(16)	-6(10)
56(4)	134(18)	47(14)	44(9)
60(5)	110(17)	52(13)	24(9)
102(7)	347(31)	148(24)	106(14)
73(6)	301(28)	87(20)	11(12)
44(4)	72(15)	23(11)	44(8)
47(4)	89(17)	4(13)	28(9)
42(4)	95(19)	4(14)	8(9)
82(6)	61(18)	23(16)	39(10)
69(5)	99(20)	83(16)	95(11)
52(4)	104(18)	56(13)	52(9)
80(4)	241(16)	102(11)	100(8)
53(3)	295(16)	20(10)	22(7)

Table 7
Final Parameters for the Hydrogen Atoms for ClCo(H₂dmg)(dmg)-(clan)^a

Atom [Bonded to]	Distance	x	y	z	B
H(B1) [O(22)]	1.16(8)	153(10)	335(7)	17(5)	6.3(1.8)
H(B2) [O(21)]	1.13(8)	184(10)	345(7)	402(5)	6.7(1.8)
H(2) [C(2)]	0.89(5)	591(7)	621(5)	420(4)	2.0(1.1)
H(3) [C(3)]	0.99(7)	726(10)	858(7)	478(5)	6.7(1.9)
H(5) [C(5)]	0.90(7)	709(10)	838(7)	187(5)	5.8(1.7)
H(6) [C(6)]	1.01(5)	568(7)	609(5)	127(4)	2.0(1.1)
H(7) [N(1)]	1.03(7)	522(10)	434(6)	166(5)	6.1(1.7)
H(8) [N(1)]	0.83(6)	518(9)	428(6)	278(5)	4.5(1.5)
H(11) [C(13)]	0.96(8)	243(11)	753(7)	212(6)	8.2(2.1)
H(12) [C(13)]	0.79(9)	37(11)	692(7)	203(6)	8.5(2.2)
H(13) [C(13)]	1.00(1)	102(10)	663(7)	103(5)	7.1(1.9)
H(14) [C(14)]	1.02(7)	46(9)	639(6)	453(5)	5.8(1.7)
H(15) [C(14)]	0.78(7)	62(9)	708(6)	388(5)	4.9(1.5)
H(16) [C(14)]	0.87(8)	228(11)	734(8)	456(6)	8.6(2.2)
H(21) [C(23)]	0.86(10)	414(12)	59(8)	248(6)	9.6(2.4)
H(22) [C(23)]	0.92(9)	239(12)	-21(8)	211(6)	9.3(2.4)
H(23) [C(23)]	0.97(9)	266(12)	52(8)	326(7)	9.8(2.5)
H(24) [C(24)]	1.03(9)	242(12)	44(8)	-46(7)	9.4(2.4)
H(25) [C(24)]	0.84(10)	396(12)	58(8)	29(6)	9.1(2.3)
H(26) [C(24)]	1.00(7)	210(10)	-38(7)	40(5)	5.9(1.7)
H(w1) [O(w1)]	0.70(8)	659(11)	319(7)	69(6)	7.2(2.0)
H(w1') [O(w1)]	0.80(13)	771(16)	438(11)	72(9)	15.2(3.7)
H(w2) [O(w2)]	0.79(7)	736(10)	420(7)	425(5)	6.6(1.8)
H(w2') [O(w2)]	0.71(7)	747(10)	371(6)	337(5)	6.0(1.8)

^aThe hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (in Å), the positional parameters with estimated standard deviations ($\times 10^3$), and the isotropic thermal parameter (in Å²).

cule were located before refinement. The scheme of the refinement is outlined in Table 5.

Although the compound was crystallized from ethanol, difference Fourier syntheses at various stages of refinement failed to indicate the position of an additional atom in the solvent molecule. Because a large region of relative high electron density existing near C(S1) could be indicative of an atom with high disorder and because ethanol was the solvent, a molecule of ethanol was assumed to be present for the purposes of determining the formula, molecular weight, and density.

The cobalt, chlorine, oxygen, nitrogen, and carbon scattering factors were taken from Hanson *et al.*²⁹ and those for hydrogen from Stewart *et al.*³⁰ Table B-1 is a list of observed and calculated structure factors for $\text{ClCo}(\text{H}_2\text{dpg})_2(\text{clan})$. The final positional and thermal parameters are shown in Tables 8 and 9.

Structure Solution and Refinement
for $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$

With one molecule per unit cell in the centric $\text{P}\bar{1}$ space group the cobalt atom and the chloride anion were required to lie on centers of symmetry. The sharpened Patterson function was in agreement with the chloride ion at $0\frac{1}{2}0$ when the cobalt atom is placed at 000. The remaining atoms were located in a similar manner as in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$. An outline of the refinement is given in Table 5.

Table 8

The Final Atomic Parameters for the Nonhydrogen Atoms of $\text{ClCo}(\text{H}_2\text{dpg})_2(\text{clan})^a$

Atom	x	y	z	β_{11}	β_{22}
Co	3339(1)	3017(2)	2961(1)	33(1)	58(1)
Cl(1)	3101(2)	4797(3)	3049(2)	45(2)	68(3)
Cl(2)	6313(4)	60(5)	1153(3)	96(4)	151(6)
O(11)	3953(5)	3496(7)	1583(4)	47(5)	82(9)
O(12)	4349(5)	2916(10)	4348(4)	41(5)	210(13)
O(21)	2763(6)	2628(8)	4340(4)	54(5)	130(11)
O(22)	2334(5)	3078(8)	1587(4)	42(5)	102(9)
N(1)	3495(6)	1461(9)	2903(6)	29(6)	97(12)
N(11)	4172(6)	3351(7)	2306(4)	41(6)	41(8)
N(12)	4368(7)	3168(9)	3660(5)	56(7)	78(11)
N(21)	2534(7)	2738(9)	3635(5)	50(6)	85(11)
N(22)	2312(6)	2882(9)	2294(4)	39(6)	62(9)
C(11)	4970(8)	3533(10)	2591(6)	24(7)	88(14)
C(12)	5080(8)	3361(11)	3373(6)	44(8)	101(15)
C(13)	5698(8)	3915(12)	2191(6)	38(8)	70(12)
C(14)	5956(9)	3431(11)	3862(7)	42(8)	82(14)
C(21)	1706(8)	2557(10)	3364(6)	46(8)	58(12)
C(22)	1575(7)	2672(10)	2562(5)	28(6)	66(12)
C(23)	1055(8)	2220(10)	3832(6)	54(8)	50(12)
C(24)	709(8)	2583(10)	2146(6)	52(8)	46(12)
C(1)	4167(8)	1048(11)	2486(6)	54(9)	46(11)
C(2)	5012(9)	858(11)	2798(7)	65(10)	65(14)
C(3)	5687(9)	544(11)	2387(8)	53(9)	62(13)
C(4)	5487(9)	448(11)	1654(8)	69(10)	53(13)
C(5)	4661(10)	592(13)	1341(7)	74(10)	123(18)
C(6)	3990(8)	883(11)	1733(7)	45(8)	67(13)
C(1A)	5975(8)	3387(11)	1614(7)	35(8)	92(15)
C(2A)	6642(9)	3760(13)	1251(7)	54(9)	111(16)
C(3A)	7077(8)	4683(12)	1485(7)	36(8)	97(15)
C(4A)	6831(9)	5248(13)	2052(8)	46(9)	108(15)
C(5A)	6157(9)	4877(12)	2413(7)	69(10)	93(15)

Table 8 - extended

β_{33}	β_{12}	β_{13}	β_{23}
19(0)	-7(3)	2(1)	-4(2)
40(1)	8(5)	11(3)	-13(4)
100(3)	71(9)	96(5)	-15(7)
21(3)	12(11)	6(6)	26(8)
16(3)	-17(16)	-8(6)	7(13)
20(3)	-35(13)	3(6)	8(9)
21(3)	-18(13)	-4(5)	12(10)
34(4)	-9(13)	7(8)	-15(12)
13(3)	23(11)	-6(6)	14(8)
26(4)	7(15)	-1(8)	7(12)
20(3)	-15(14)	6(7)	-21(11)
16(3)	-12(14)	13(6)	6(11)
23(4)	5(16)	16(9)	28(13)
18(4)	-5(18)	7(9)	0(13)
23(4)	20(17)	20(9)	23(14)
28(5)	-11(17)	-8(10)	5(13)
23(4)	4(15)	12(9)	-2(12)
15(4)	24(15)	-4(8)	7(11)
17(4)	-43(17)	3(8)	-9(12)
28(5)	26(16)	-1(10)	30(12)
30(5)	-5(18)	-18(10)	20(14)
36(6)	-17(19)	-7(11)	15(15)
45(6)	45(18)	4(12)	2(15)
46(6)	58(19)	40(12)	20(15)
37(6)	19(23)	44(12)	70(17)
33(5)	-69(17)	9(10)	-29(14)
39(5)	5(17)	31(10)	4(15)
29(5)	10(21)	22(11)	2(16)
45(6)	-12(19)	9(11)	46(16)
43(6)	-28(21)	30(11)	18(19)
32(5)	7(22)	11(11)	2(17)

Table 8 - continued

Atom	x	y	z	β_{11}	β_{22}
C(1B)	6675(9)	2815(14)	3687(7)	61(9)	113(16)
C(2B)	7444(9)	2801(13)	4142(7)	59(9)	89(15)
C(3B)	7498(9)	3363(15)	4781(7)	56(10)	189(23)
C(4B)	6828(9)	4051(16)	4937(7)	59(10)	207(22)
C(5B)	6047(10)	4094(14)	4476(7)	73(11)	148(19)
C(1C)	664(9)	1226(12)	3750(7)	66(10)	73(14)
C(2C)	20(9)	872(12)	4199(7)	66(10)	96(16)
C(3C)	-212(9)	1576(14)	4700(8)	32(8)	183(23)
C(4C)	184(9)	2563(12)	4813(7)	61(10)	112(17)
C(5C)	826(8)	2872(11)	4368(6)	60(8)	41(11)
C(1D)	593(9)	2121(12)	1437(6)	54(8)	83(14)
C(2D)	-224(9)	1992(14)	1046(7)	56(9)	116(16)
C(3D)	-951(9)	2410(12)	1345(7)	50(9)	105(17)
C(4D)	-888(8)	2847(12)	2044(7)	42(8)	77(14)
C(5D)	-69(8)	2975(12)	2447(6)	30(7)	63(12)
O(S1)	1418(9)	4904(10)	944(5)	190(13)	136(13)
C(S1)	1450(26)	4854(22)	182(12)	512(49)	196(30)

^aAll values are $\times 10^4$. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.

Table 8 - continued - extended

β_{33}	β_{12}	β_{13}	β_{23}
39(6)	-11(22)	-24(11)	13(18)
39(5)	-24(21)	-4(11)	24(17)
32(5)	-59(24)	13(11)	-5(18)
18(5)	-47(26)	0(10)	-39(19)
28(5)	-90(25)	7(11)	0(18)
28(5)	-27(19)	-3(11)	-20(15)
28(5)	-24(21)	7(11)	13(16)
44(6)	-21(21)	-26(11)	-5(19)
26(5)	16(19)	26(10)	-10(14)
28(4)	-31(19)	-7(9)	8(14)
28(5)	-4(20)	7(10)	-16(16)
34(5)	13(23)	-34(10)	-39(19)
42(6)	11(19)	-31(11)	50(16)
51(6)	-13(20)	-8(11)	6(18)
40(5)	-30(18)	17(9)	7(16)
39(5)	67(23)	45(12)	-23(14)
59(11)	224(71)	194(38)	45(34)

Table 9
Final Parameters for Hydrogen Atoms for $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})^a$

Atom [Bonded to]	Distance	x	y	z	B
H(B1)		303(9)	344(12)	153(8)	11.6(5.1)
H(B2)		352(7)	277(9)	439(5)	4.3(2.7)
H(2) [C(2)]	0.84(10)	514(7)	87(9)	325(5)	4.3(2.8)
H(3) [C(3)]	0.95(14)	627(9)	47(12)	260(7)	9.8(4.5)
H(5) [C(5)]	0.80(10)	445(6)	54(8)	93(5)	4.1(2.8)
H(6) [C(6)]	1.00(10)	336(7)	84(9)	152(5)	4.7(3.0)
H(7) [N(1)]	0.93(11)	305(7)	107(10)	264(6)	5.9(3.3)
H(8) [N(1)]	1.02(15)	382(9)	103(13)	332(8)	11.7(4.6)
H(1A) [C(1A)]	1.05(12)	558(7)	278(10)	135(6)	6.0(3.2)
H(2A) [C(2A)]	0.94(10)	680(6)	329(8)	89(5)	4.0(2.7)
H(3A) [C(3A)]	1.18(15)	759(9)	514(13)	117(7)	10.5(4.8)
H(4A) [C(4A)]	1.12(12)	711(7)	604(10)	227(6)	5.7(3.3)
H(5A) [C(5A)]	0.86(9)	601(6)	525(8)	227(5)	2.4(2.4)
H(1B) [C(1B)]	1.07(9)	654(6)	236(8)	320(5)	3.0(2.6)
H(2B) [C(2B)]	1.12(19)	796(11)	224(16)	398(9)	14.6(6.6)
H(3B) [C(3B)]	0.68(13)	792(9)	351(11)	487(7)	9.1(4.4)
H(4B) [C(4B)]	0.74(10)	690(7)	403(9)	533(6)	5.3(3.0)
H(5B) [C(5B)]	0.55(14)	586(9)	406(12)	471(7)	11.2(4.6)
H(1C) [C(1C)]	0.81(13)	76(8)	69(10)	352(7)	8.3(4.1)
H(2C) [C(2C)]	1.04(19)	3(12)	7(15)	403(9)	15.8(6.3)
H(3C) [C(3C)]	0.96(12)	-63(8)	140(10)	504(7)	8.2(4.0)
H(4C) [C(4C)]	0.92(12)	4(8)	305(10)	515(6)	6.0(3.0)
H(5C) [C(5C)]	1.00(8)	106(5)	362(6)	447(4)	0.5(1.9)
H(1D) [C(1D)]	1.05(9)	116(6)	175(7)	128(5)	3.0(2.4)
H(2D) [C(2D)]	1.10(9)	-41(6)	160(8)	52(5)	2.8(2.6)
H(3D) [C(3D)]	0.97(14)	-145(9)	219(12)	101(7)	10.1(4.4)
H(4D) [C(4D)]	1.04(10)	-136(6)	343(8)	212(5)	3.8(2.7)
H(5D) [C(5D)]	0.70(8)	25(5)	316(7)	224(4)	1.5(2.0)

^aThe hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (Å), the positional parameters with estimated standard deviations ($\times 10^3$), and the isotropic thermal parameters ($\text{\AA}^2$).

The scattering factors for cobalt, oxygen, nitrogen, and carbon were from Hanson *et al.*,²⁹ those for hydrogen were from Stewart *et al.*,³⁰ and those for chlorine were from Doyle and Turner.³¹ The observed and calculated structure factors are given in Table B-2. Lists of final positional and thermal parameters may be found in Tables 10 and 11.

Results and Discussion

The atomic numbering and thermal ellipsoids of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$, $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$, and $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ are shown in ORTEP⁵⁴ drawings in Figures 1, 2, and 3, respectively. The individual bond distances for these three compounds together with those of two related compounds, $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$ ⁴⁶ and $[\text{Co}(\text{Hdmg})_2(\text{an})_2]\text{Cl}$,⁵² are tabulated in Table 12. The corresponding bond angles are given in Table 13.

In each case the two dmg or dpg groups are approximately planar as demonstrated by the deviations from least-squares planes in Tables 14-16. The dmg groups of each complex are linked by two intramolecular hydrogen bonds (see Table 17).

As in the case of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$ ⁴⁶ the hydrogen bridges between the dmg groups in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ were found to be asymmetrical with both hydrogen atoms bonded to the same dmg ligand. The $\text{O}(21)\cdots\text{H}(\text{B}2)$ and $\text{O}(22)\cdots\text{H}(\text{B}1)$ distances of 1.13(8) and 1.16(8) Å, respectively, compared to the $\text{O}(12)\cdots\text{H}(\text{B}2)$ and $\text{O}(11)\cdots\text{H}(\text{B}1)$ distances of 1.36(8) and 1.37(8) Å indicate the formulation H_2dmg and dmg for the two

Table 10
The Final Atomic Parameters for Nonhydrogen Atoms of $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$.^a

Atom	x	y	z	β_{11}	β_{22}
Co	0(0)	0(0)	0(0)	817(11)	628(5)
Cl(1)	0(0)	50000(0)	0(0)	2653(30)	664(12)
Cl(2)	32052(23)	26440(24)	55881(8)	5254(48)	6743(52)
O(11)	4450(2)	1508(2)	573(1)	97(4)	126(3)
O(12)	-3514(3)	531(2)	-1814(1)	125(5)	144(3)
N(1)	-846(3)	1678(2)	816(2)	116(5)	77(3)
N(11)	2490(3)	1399(2)	-160(2)	105(5)	83(3)
N(12)	-1339(3)	923(2)	-1288(1)	118(5)	91(3)
C(1)	97(4)	1928(3)	1978(2)	148(7)	90(3)
C(2)	2160(4)	2812(3)	2368(2)	195(8)	136(4)
C(3)	3103(5)	3034(4)	3474(3)	224(9)	231(6)
C(4)	1982(6)	2386(5)	4181(3)	317(11)	311(8)
C(5)	-77(6)	1504(5)	3818(3)	320(11)	300(8)
C(6)	-1012(4)	1282(4)	2704(2)	193(8)	185(5)
C(11)	2176(4)	2274(3)	-990(2)	159(7)	76(3)
C(12)	-124(4)	1982(3)	-1665(2)	185(7)	87(3)
C(13)	3887(4)	3459(3)	-1239(2)	216(8)	116(4)
C(14)	-937(5)	2830(4)	-2658(3)	289(10)	169(5)

^aAll values are $\times 10^4$ except those for Co, Cl(1) and Cl(2) which are $\times 10^5$. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.

Table 10 - extended

β_{33}	β_{12}	β_{13}	β_{23}
332(3)	226(12)	169(9)	-43(6)
873(8)	451(29)	1194(26)	131(15)
482(7)	-1987(79)	-431(28)	-982(29)
57(1)	9(5)	11(4)	-12(3)
57(1)	40(6)	-20(4)	15(3)
45(1)	28(6)	30(4)	-9(3)
47(1)	26(6)	30(4)	-21(3)
41(1)	53(6)	7(4)	-7(3)
47(2)	47(8)	27(5)	-24(4)
63(2)	-25(9)	59(6)	-42(5)
72(2)	-85(12)	-3(8)	-93(6)
49(2)	2(15)	-11(8)	-59(7)
51(2)	-22(15)	64(8)	1(7)
52(2)	-11(10)	36(6)	-12(5)
52(2)	42(7)	73(6)	-4(4)
46(2)	68(8)	56(6)	6(4)
77(2)	12(9)	109(7)	16(5)
68(2)	68(11)	47(8)	75(6)

Table 11
Final Parameters for Hydrogen Atoms for $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}^a$

Atom [Bonded to]	Distance	x	y	z	B
H(B1) [O(12)]	1.07(3)	-408(8)	-35(4)	-133(3)	5.5(0.8)
H(2) [C(2)]	0.85(3)	280(4)	321(3)	190(2)	3.5(0.6)
H(3) [C(3)]	0.91(4)	447(6)	361(4)	366(3)	6.0(0.8)
H(5) [C(5)]	0.98(4)	-92(6)	105(4)	431(3)	6.6(0.9)
H(6) [C(6)]	0.96(3)	-248(5)	73(3)	244(2)	3.9(0.6)
H(7) [N(1)]	0.88(2)	-299(4)	146(3)	64(2)	2.1(0.5)
H(8) [N(1)]	0.94(2)	-52(4)	262(3)	49(2)	2.7(0.5)
H(11) [C(13)]	0.90(4)	349(6)	440(4)	-131(3)	5.7(0.8)
H(12) [C(13)]	0.89(4)	417(7)	315(5)	-185(4)	9.0(1.2)
H(13) [C(13)]	0.91(4)	513(6)	353(5)	-67(3)	7.3(1.0)
H(14) [C(14)]	0.86(4)	-181(7)	217(5)	-314(3)	9.0(1.2)
H(15) [C(14)]	0.80(5)	-14(8)	360(6)	-274(4)	10.0(1.3)
H(16) [C(14)]	1.01(5)	-213(8)	337(6)	-252(4)	11.0(1.4)

^aThe hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (Å), the positional parameters with estimated standard deviations ($\times 10^3$), and the isotropic thermal parameters (Å²).

Figure 1

An ORTEP drawing of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})\cdot 2\text{H}_2\text{O}$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms and water molecules have been omitted for clarity.

Figure 2

An ORTEP drawing of $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})\cdot\text{C}_2\text{H}_5\text{OH}$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms and $\text{C}_2\text{H}_5\text{OH}$ molecule have been omitted.

Figure 3

An ORTEP drawing of $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms have been omitted.

Table 12
Selected Interatomic Distances (Å) in Some Cobaloxime
Complexes with Their Estimated Standard Deviations.^a

	ClCo(H ₂ dmg) (clan)	ClCo(H ₂ dpg) ₂ (clan)
Co-N(1)	1.999(6)	1.946(11)
Co-N(11)	1.872(5)	1.908(9)
Co-N(12)	1.884(5)	1.935(11)
N(11)-O(11)	1.337(6)	1.356(11)
N(12)-O(12)	1.329(6)	1.316(12)
N(11)-C(11)	1.311(8)	1.298(15)
N(12)-C(12)	1.308(8)	1.292(16)
C(11)-C(12)	1.457(9)	1.455(16)
C(11)-C(13)	1.488(10)	1.487(17)
C(12)-C(14)	1.487(10)	1.536(18)
O(11)...O(22)	2.497(7)	2.540(11)
O(11)-H(B)	1.37(8)	1.41(14)
O(12)-H(B)	1.36(8)	1.30(10)
Co-Cl(1)	2.257(2)	2.244(4)
Co-N(21)	1.908(5)	1.887(10)
Co-N(22)	1.906(5)	1.897(9)
N(21)-O(21)	1.348(6)	1.321(12)
N(22)-O(22)	1.359(6)	1.337(11)
N(21)-C(21)	1.280(8)	1.331(16)
N(22)-C(22)	1.288(8)	1.313(14)
C(21)-C(22)	1.468(9)	1.483(15)
C(21)-C(23)	1.486(11)	1.457(17)
C(22)-C(24)	1.498(11)	1.464(17)
O(12)...O(21)	2.479(7)	2.460(12)
O(21)-H(8)	1.13(8)	1.16(10)
O(22)-H(B)	1.16(8)	1.17(15)

*Distance given is for O(11)...O(12')≡O(12)...O(11')

^aValues for [Co(H₂dmg)₂](an)₂Cl are listed with atomic numbering corresponding to the compounds of this work.

Table 12 - extended

$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{sulfa})^{46}$	$[\text{Co}(\text{H}_2\text{dmg}_2)(\text{clan})_2]\text{Cl}$	$[\text{Co}(\text{H}_2\text{dmg}_2)(\text{an})_2]\text{Cl}^{52}$
2.023(8)	2.003(2)	2.001(5)
1.870(8)	1.906(2)	1.885(6)
1.884(8)	1.889(2)	1.889(5)
1.323(11)	1.340(3)	1.353(6)
1.344(11)	1.362(3)	1.333(6)
1.289(14)	1.299(3)	1.286(10)
1.293(13)	1.290(3)	1.303(10)
1.494(16)	1.477(4)	1.463(7)
1.532(17)	1.483(4)	1.482(12)
1.488(16)	1.485(4)	1.476(11)
2.507(11)	2.495(3)*	2.491(8)*
1.50	1.44(3)	1.29
1.60	1.07(3)	1.21
2.235(3)		
1.905(8)		
1.896(8)		
1.326(10)		
1.338(11)		
1.292(12)		
1.290(14)		
1.447(17)		
1.494(17)		
1.488(16)		
2.479(11)		
0.90		
1.04		

Table 13
Selected Intramolecular Angles ($^{\circ}$) in Some Cobaloxime Complexes
with Their Estimated Standard Deviations.^a

	$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{clan})$	$\text{ClCo}(\text{h}_2\text{dpg}_2)(\text{clan})$
N(1)-Co-N(11)	90.5(2)	94.8(4)
N(1)-Co-N(12)	91.5(2)	92.1(4)
N(1)-Co-N(21)	88.4(2)	87.1(4)
N(1)-Co-N(22)	88.6(2)	88.6(4)
N(11)-Co-N(12)	82.6(2)	81.3(4)
N(11)-Co-N(22)	98.8(2)	100.0(4)
N(11)-Co-N(21)	178.8(2)	177.5(4)
N(12)-Co-N(21)	98.1(2)	97.0(4)
N(12)-Co-N(22)	178.6(2)	178.5(4)
N(21)-Co-N(22)	80.6(2)	81.7(4)
Cl(1)-Co-N(11)	90.6(2)	87.7(3)
Cl(1)-Co-N(12)	90.6(2)	89.1(3)
Cl(1)-Co-N(21)	90.5(2)	90.4(3)
Cl(1)-Co-N(22)	89.4(2)	90.2(3)
Cl(1)-Co-N(1)	177.8(2)	177.4(3)
Co-N(1)-C(1)	119.7(4)	118.6(8)
Co-N(11)-O(11)	121.9(4)	123.3(7)
Co-N(12)-O(12)	122.2(4)	121.2(8)
Co-N(21)-O(21)	123.2(4)	123.5(8)
Co-N(22)-O(22)	123.3(4)	120.7(7)
Co-N(11)-C(11)	116.0(4)	116.7(8)
Co-N(12)-C(12)	115.6(4)	114.1(9)
Co-N(21)-C(21)	116.6(4)	116.8(8)
Co-N(22)-C(22)	117.0(4)	117.4(8)
O(11)-N(11)-C(11)	122.1(5)	119.7(9)
O(12)-N(12)-C(12)	122.3(5)	123.8(11)
O(21)-N(21)-C(21)	120.3(5)	119.4(10)
O(22)-N(22)-C(22)	119.8(5)	121.7(10)
N(11)-O(11) $\cdots$ O(22)	99.7(3)	95.9(6)
N(12)-O(12) $\cdots$ O(21)	99.7(3)	99.2(7)
N(21)-O(21) $\cdots$ O(12)	96.9(3)	98.2(7)
N(22)-O(22) $\cdots$ O(11)	96.0(3)	100.1(6)

Table 13 - extended

$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{sulfa})^{46}$	$[\text{Co}(\text{H}_2\text{dmg}_2)(\text{clan})_2]\text{Cl}$	$[\text{Co}(\text{H}_2\text{dmg}_2)(\text{an})_2]\text{Cl}^{52}$
90.5(3)	89.8(1)	91.5(4)
91.7(3)	93.2(1)	93.0(5)
89.3(3)		
87.8(3)		
82.0(4)	80.8(1)	80.8(3)
98.7(4)		
179.3(4)		
98.7(3)		
179.2(4)		
80.6(3)		
89.6(3)		
88.5(3)		
90.5(3)		
91.9(3)		
179.7(2)		
119.1(6)	119.7(1)	119.5(7)
123.0(6)	121.3(1)	121.4(6)
122.6(6)	122.7(1)	122.9(7)
121.6(6)		
123.6(6)		
116.4(7)	116.9(2)	116.8(9)
117.4(7)	117.7(2)	117.8(9)
116.3(7)		
116.8(7)		
120.5(9)	121.8(2)	121.8(12)
120.0(8)	119.6(2)	119.2(10)
122.2(8)		
120.1(9)		
98.3(6)		
97.8(6)		
99.2(5)		
96.8(6)		

Table 13 - continued

	$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{clan})$	$\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$
N(11)-C(11)-C(12)	112.8(6)	112.1(10)
N(11)-C(11)-C(13)	122.9(6)	125.6(11)
N(12)-C(12)-C(11)	113.1(6)	115.5(11)
N(12)-C(12)-C(14)	122.5(6)	119.5(11)
N(21)-C(21)-C(22)	113.5(6)	112.2(10)
N(21)-C(21)-C(23)	112.4(7)	120.9(11)
N(22)-C(22)-C(21)	112.3(6)	111.9(10)
N(22)-C(22)-C(24)	123.2(6)	126.0(11)
C(13)-C(11)-C(12)	124.2(6)	122.3(11)
C(14)-C(12)-C(11)	124.4(6)	125.0(11)
C(23)-C(21)-C(22)	124.1(6)	126.8(11)
C(24)-C(22)-C(21)	124.4(6)	122.2(10)

^aThe atomic numbering of $\text{Co}(\text{H}_2\text{dmg}_2)(\text{an})_2\text{Cl}^{52}$ has been changed to correspond to that of compounds of this work.

Table 13 - continued - extended

$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{sulfa})^{46}$
 $[\text{Co}(\text{H}_2\text{dmg}_2)(\text{clan})_2]\text{Cl}$
 $[\text{Co}(\text{H}_2\text{dmg}_2)(\text{an})_2]\text{Cl}^{52}$

113.3(9)	112.2(2)	112.4(10)
125.0(10)	125.0(2)	124.6(16)
110.7(9)	112.5(2)	112.2(9)
124.0(10)	124.1(2)	125.0(16)
113.1(9)		
120.7(10)		
113.1(9)		
122.9(10)		
121.7(10)	122.9(2)	123.0(12)
125.3(10)	123.4(2)	122.9(13)
126.1(10)		
123.6(10)		

ligands. This is in contrast to results reported for various $\text{Co}(\text{H}_2\text{dmg}_2)$ complexes^{40,47,48,50,52} as well as for $\text{Fe}(\text{H}_2\text{dmg}_2)\text{--}(\text{imidazole})_2$,⁵⁵ $\text{Ni}(\text{H}_2\text{dmg}_2)$,⁵⁶ and $\text{Cu}(\text{H}_2\text{dmg}_2)$,⁵⁷ where either the hydrogen bridges were assumed to be equidistant from the two oxygen atoms or the ligands were monoprotonated. The assumption of a symmetrical bridge may have in part been based on the earlier IR spectroscopic work on $\text{M}(\text{H}_2\text{dmg}_2)$ complexes where the weak band due to an O-H vibration near 1725 cm^{-1} was assumed to indicate a very short and symmetrical O-H-O bridge.^{19,20} McFadden and McPhail⁵¹ reported the structure of $\text{Co}(\text{H}_2\text{dmg}_2)(\text{CH}_3)(\text{H}_2\text{O})$ in which both bridging hydrogen atoms if ordered are required crystallographically to be on one dmg ligand. No comment was made concerning the bridging hydrogen atoms.

Although both hydrogen bridges in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ appear to be shifted toward one dmg where the $\text{O}(21)\text{--H}(\text{B}2)$ and $\text{O}(22)\text{--H}(\text{B}1)$ distances are $1.16(10)$ and $1.17(15)\text{ \AA}$ while the $\text{O}(12)\text{--H}(\text{B}2)$ and $\text{O}(11)\text{--H}(\text{B}1)$ distances are $1.30(10)$ and $1.41(14)\text{ \AA}$, the experimental uncertainty is too large to show that result to be significant.

The hydrogen bridges in $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ are not symmetrical and each dmg is singly protonated. The $\text{O}(12)\text{--H}(\text{B}1)$ distance is $1.07(3)\text{ \AA}$ and the $\text{O}(11)\cdots\text{H}(\text{B}1)$ distance is $1.44(3)\text{ \AA}$. The gross structure is very similar to that of $[\text{Co}(\text{Hdmg})_2(\text{an})_2]\text{Cl}$.

Bowman et al.⁵⁵ suggested the N-O distance to be a sensitive indicator of the position of the bridging hydrogen.

Table 14
Deviations and Equations of Selected Least-Squares Planes
in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})^a$

(a) Deviations ($\text{\AA} \times 10^3$)

	Plane 1	Plane 2	Plane 3	Plane 4
Co	5	-1796	0*	72
O(11)	25		-2574	209
O(12)	-23		2533	80
N(11)	-2*		-1260	175
N(12)	2*		1218	140
C(11)	4*		-775	251
C(12)	-4*		682	220
C(13)	73		-1633	413
C(14)	41		1498	330
O(21)	34		2602	-22
O(22)	-79		-2548	-55
N(21)	48		1269	1*
N(22)	7		-1197	-1*
C(21)	113		795	-2*
C(22)	94		-673	2*
C(23)	230		1664	24
C(24)	143		-1482	-17
N(1)	2004	-41	0*	
C(1)	2752	-12*	0*	
C(2)	3092	5*	1197	
C(3)	3767	5*	1204	
C(4)	4105	-9*	18	
C(5)	3790	3*	-1193	
C(6)	3112	8*	-1204	
Cl(2)	4946	-28	5	
Cl(1)	-2252		-29	

(b) Coefficients of the Plane Equation⁵⁸
 $Ax + By + Cz = D$

Plane	A	B	C	D
1	0.8529	0.4975	0.1583	1.6954

Table 14 - continued

Plane	A	B	C	D
2	0.9995	0.0282	0.0142	1.6347
3	0.0208	-0.3098	0.9506	1.7440
4	0.8174	0.5536	0.1594	1.8108

^aThe deviations of atoms used to define the plane are marked with an asterisk.

Table 15
Deviations and Equations of Selected Least-Squares Planes
in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})^a$

(a) Deviations ($\text{\AA} \times 10^3$)

	Plane 1	Plane 2	Plane 3	Plane 4
Co	19	-1932	0*	29
O(11)	-56		1350	-101
O(12)	122		-2807	192
N(11)	17*		160	2
N(12)	-18*		-1881	24
C(11)	-30*		-945	-30
C(12)	30*		-2118	62
C(13)	-179		-1048	-195
C(14)	94		-3571	149
O(21)	-5			60
O(22)	-37			-87
N(21)	-43			-8*
N(22)	28			8*
C(21)	-9			13*
C(22)	-1			-13*
C(23)	93			133
C(24)	-58			-89
N(1)	1958	-148	0*	
C(1)	2755	-18*	0*	
C(2)	3166	4*	-1171	
C(3)	3843	16*	-1184	
C(4)	4069	-20*	10	
C(5)	3720	5*	1166	
C(6)	3076	14*	1205	
Cl(2)	4901	-1	-10	
Cl(1)	-2223		24	
C(1A)	676			
C(2A)	510			
C(3A)	-529			
C(4A)	-1417			
C(5A)	-1255			

Table 15 - continued

	Plane 1	Plane 2	Plane 3	Plane 4
C(1B)	1094			
C(2B)	1237			
C(3B)	427			
C(4B)	-641			
C(5B)	-821			
C(1C)				1232
C(2C)				1380
C(3C)				361
C(4C)				-734
C(5C)				-827
C(1D)				571
C(2D)				554
C(3D)				-230
C(4D)				-874
C(5D)				-858

(b) Coefficients of the Plane Equation⁵⁸
 $Ax + By + Cz = D$

Plane	A	B	C	D
1	0.1954	-0.9752	-0.1036	3.3476
2	-0.2301	-0.9634	0.1374	1.9549
3	0.5744	0.0297	0.8181	-7.1571
4	0.1976	-0.9769	-0.0813	3.2302

^aThe deviations of atoms used to define the plane are marked with an asterisk.

Table 16
Deviations and Equations of Selected Least Squares Planes
in $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}^{\text{a}}$

(a) Deviations ($\text{\AA} \times 10^{+3}$)

	Plane 1	Plane 2	Plane 3
Co	10	-1772	0*
O(11)	36		2519
O(12)	14		-523
N(11)	0*		1902
N(12)	0*		428
C(11)	1*		2567
C(12)	-1*		1677
C(13)	26		4046
C(14)	11		2173
N(1)	2009	-28	0*
C(1)	2799	-2*	0*
C(2)	3030	2*	1194
C(3)	3758	-1*	1208
C(4)	4257	0*	37
C(5)	4048	0*	-1168
C(6)	3312	1*	-1174
Cl(2)	5159	-33	53

(b) Coefficients of the Plane Equation⁵⁹
 $Ax + By + Cz = D$

Plane	A	B	C	D
1	-0.4938	0.6723	0.5515	-0.0101
2	-0.5672	0.8236	0.0096	1.7716
3	0.7336	0.6606	-0.1594	0.0000

^aThe deviations of atoms used to define the plane are marked with an asterisk.

Hydrogen Bonds with Estimated Standard Deviations Given in Parentheses.

Bond	Position of A	D-H	H...A	Distances (Å)	Angles (°)
D-H...A ^a				D...A	D-H...A
ClCo(H ₂ dmg ₂) (clan)					
O(21)-H(B2) ...O(12)	x, y, z	1.13(8)	1.36(8)	2.479(7)	166(7)
O(22)-H(B1) ...O(11)	x, y, z	1.16(8)	1.37(8)	2.497(7)	161(6)
N(1)-H(7) ...O(w1)	x, y, z	1.03(7)	1.92(7)	2.900(7)	157(6)
N(1)-H(8) ...O(w2)	x, y, z	0.83(6)	2.04(7)	2.849(7)	164(6)
O(w1)-H(w1) ...Cl(1)	1+x, y, z	0.70(8)	2.76(8)	3.284(6)	134(8)
O(w1)-H(w1') ...O(11)	1-x, 1-y, -z	0.80(13)	2.34(12)	2.823(7)	120(11)
O(w2)-H(w2) ...O(12)	1-x, 1-y, 1-z	0.79(7)	2.05(7)	2.813(6)	164(8)
O(w2)-H(w2') ...Cl(1)	1+x, y, z	0.71(7)	2.56(7)	3.226(5)	157(7)
[Co(H ₂ dmg ₂) (clan ₂)]Cl					
O(12)-H(B1) ...O(11)	-x, -y, -z	1.07(3)	1.44(3)	2.495(3)	170(3)
N(1)-H(7) ...O(11)	-1+x, y, z	0.88(2)	2.07(3)	2.918(3)	163(2)
N(1)-H(8) ...Cl(1)	x, y, z	0.94(2)	2.17(2)	3.100(2)	168(2)
ClCo(H ₂ dpg ₂) (clan)					
O(21)-H(B1) ...O(12)	x, y, z	1.16(10)	1.30(10)	2.460(12)	172(10)
O(22)-H(B2) ...O(11)	x, y, z	1.17(15)	1.41(14)	2.540(11)	159(13)
O(S1) ... O(22)	x, y, z			2.852(15)	

^a Donor-Hydrogen...Acceptor, D-H at x, y, z.

Dissimilar N-O bond lengths should indicate the hydrogen is not symmetrically located and is closer to the dmg with the longer bond. This holds true in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ where the N-O distances appear to be different. The N(21)-O(21) and N(22)-O(22) distances of 1.348(6) and 1.359(6) Å in the diprotonated dmg are longer than the N(12)-O(12) and N(11)-O(11) distances of 1.329(6) and 1.337(6) Å in the dianionic dmg. Using the significance test described by Cruickshank and Robertson⁶⁰ the N(21)-O(21) distance is possibly longer than the N(12)-O(12) with a t_o value of 2.24 and the N(22)-O(22) bond is significantly longer than the N(11)-O(11) bond with a t_o value of 2.59. Also, in $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ the N(12)-O(12) bond of 1.362(3) Å is significantly longer than the N(11)-O(11) bond of 1.340(3) Å, where the bridging hydrogen atom is bonded to O(12). Neither the N-O distances nor the bridging O-H distances in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ are significantly different. In $[\text{Co}(\text{Hdmg})_2(\text{an})_2]\text{Cl}$ where the hydrogen atoms are not significantly removed from a symmetrical position, the N(12)-O(12) distance is shorter than that of N(11)-O(11). The difference in these two bond lengths of 1.333(6) and 1.353(6) Å is of possible significance ($t_o = 2.36$). The sensitivity of the N-O bond as an indicator of the bridge position is questionable. The N-O bonds are not significantly different in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$ when both bridging hydrogen atoms are shifted to one dmg. In the closely related dimethyl(3,3'-trimethylenedinitrilo)bis-(butan-2-one-oximato)cobalt(III) complex the two N-O distances are equal

even though an asymmetric hydrogen bridge is clearly indicated by the difference Fourier syntheses.⁶¹ Although a difference in the N-O bond lengths as a function of protonation is reasonable, there are very few structures so precisely determined that this comparison can be made. Hence, no general conclusion may be made. However, when a significant difference in the N-O distances has been found and the bridging hydrogen atom has been precisely located, the hydrogen atom is associated with the longer N-O bond.

Another point in support of the formulation $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ is the difference in the Co-N bond lengths. The Co-N distances on the H_2dmg side are 1.908(5) and 1.906(5) Å compared to distances of 1.872(5) and 1.884(5) Å on the dmg side. The differences in the Co-N bond lengths are significant and the shorter distances involve the dianionic group. This holds true in the other cases where the presence of both H_2dmg and dmg ligands has been indicated. In $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$ ⁴⁶ and in $\text{Co}(\text{H}_2\text{dmg}_2)(\text{CH}_3)(\text{H}_2\text{O})$ ⁵¹ the distances from the cobalt atom to the dianionic ligand are shorter than the distances to the neutral H_2dmg ligand. This is not the case in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ where the distances from the cobalt atom to what would be the dpg dianionic ligand, 1.935(11) and 1.908(9) Å, appear to be longer than the corresponding distances to the H_2dpg ligand, 1.887(10) and 1.897(9) Å. These differences together with the apparent positions of the bridging hydrogen atoms (vide supra) in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ are of questionable significance.

For the mononegative ligands in $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ the Co-N distances are significantly different. However, N(12) which is bonded to the protonated oxygen atom is closer to the cobalt atom than is N(11) with distances of 1.889(2) and 1.906(2) Å, respectively. The same relationship holds in $\text{Fe}(\text{Hdmg})_2(\text{imidazole})_2$,⁵⁵ the only other $\text{M}(\text{Hdmg})_2$ complex whose X-ray structure precisely places one bridging hydrogen on each dmg and shows a significant difference in the metal to nitrogen distance.

An unsymmetrical hydrogen-bonding system involving two similar atoms may be fluxional.⁶² In such a system two equilibrium positions, i.e. potential wells, exist for the hydrogen atom. Each of these positions may be considered as having the hydrogen atom covalently bonded to one atom and hydrogen bonded to the other. For the system to be truly fluxional the energy barrier between the two positions must be thermally accessible. Depending on the relative depths of the potential wells, the energy barrier between them, and the thermal energy of the system the position of the hydrogen atom as indicated by X-ray diffraction experiments would vary. Because of the diffuse appearance of the bridging hydrogen atoms of the $\text{M}(\text{H}_2\text{dmg}_2)$ complexes in difference Fourier syntheses, a fluxional system with two potential wells of unequal depth seems reasonable. The relative populations of the two positions will depend somewhat on the depths of the potential wells. The experimentally determined position (or positions) of the hydrogen atom will reflect these populations. As the depths of the

potential wells approach equivalence and as the energy barrier between them becomes smaller the position of the hydrogen atom will become experimentally more uncertain. A fluxional system could, in part, account for the difficulty in precisely locating the bridging hydrogen atoms in $M(H_2dmg)_2$ complexes.

The orientation of the 4-chloroaniline ligand in the complexes of this study is quite intriguing. A projected view down the Co-N(1) bond for $ClCo(H_2dmg)(dmg)(clan)$ is shown in Figure 4. A similar view for $[Co(Hdmg)_2(clan)_2]Cl$ is given in Figure 5(a) and one for $ClCo(H_2dpg_2)(clan)$ is given in Figure 5(b). In $ClCo(H_2dmg)(dmg)(clan)$, as in $ClCo(H_2dmg)(dmg)(sulfa)$ ⁴⁶ the aromatic ring of the aniline is oriented over the dianionic dmg ligand. The orientation angle, i.e. the dihedral angle between the planes having Co-N(1) in common with one containing C(1) and the other containing the bisector of the angle N(11)-Co-N(12), for $ClCo(H_2dmg)(dmg)(clan)$ is 0.9° and for $ClCo(H_2dmg)(dmg)(sulfa)$ is 1.8° as given in Table 18. In $[Co(Hdmg)_2(clan)_2]Cl$ and in $[Co(Hdmg)_2(an)_2]Cl$ the benzene rings are skewed relative to the equatorial ligands with orientation angles of 53.9° and 58.3° , respectively. It seems significant that in the former pair of $Co(H_2dmg)(dmg)$ type complexes the rings align while in the latter pair of $Co(Hdmg)_2$ type complexes the rings are skewed. Although the benzene ring of the aniline is tipped from being parallel to the dmg plane by ca. 30° as in other similar complexes (see Table 18) the alignment and the distances between the two planes in $ClCo(H_2dmg)(dmg)(clan)$ suggest a π -type interaction. The

Figure 4
A projected view along Co-N(1) for $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$.

Figure 5

A projected view along Co-N(1) for (a) $[\text{Co}(\text{H}_2\text{mg})_2(\text{clan})_2]\text{Cl}$ and (b) $\text{ClCo}(\text{H}_2\text{dp}_2)(\text{clan})$.

(a)

(b)

Table 18
Dihedral Angles Formed by Selected Planes^a in Some Cobaloxime Complexes

Intersecting Planes	Angles (°)		
	$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{clan})$	$\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$	$\text{ClCo}(\text{H}_2\text{dmg}_2)(\text{sulfa})^{46}$
1-2	29.7	28.3	25.2
1-3	89.2	89.9	88.9
1-4	3.8	1.3	5.6
2-3	88.5	87.2	88.5
2-4	33.4	27.8	30.8
3-4	89.8	89.0	89.2
3-5	0.9	36.4	1.8

^aPlanes 1 to 4 are least-squares planes as defined in Tables 14-16. Plane 1 is defined by N(11), N(12), C(11), and C(12). Plane 2 is defined by the carbon atoms in the benzene ring of the aniline ligand. Plane 3 is defined by Co, N(1), and C(1). Plane 4 is defined by N(21), N(22), C(21), and C(22). Plane 5 contains Co, N(1), and the bisector of the angle N(11)-Co-N(12).

Table 18 - extended

Intersecting Planes	Angles (°)	
	$[\text{Co}(\text{H}_2\text{dmg}_2)(\text{clan})_2]\text{Cl}$	$[\text{Co}(\text{H}_2\text{dmg}_2)(\text{an})_2]\text{Cl}^{52}$
1-2	33.0	32.9
1-3	89.7	86.9
1-4	(180)	(180)
2-3	82.7	86.9
2-4		
3-4		
3-5	53.8	58.3

distances from the dmg plane to C(1), C(2), and C(6) given in Table 14 are substantially less than the 3.40 Å interplanar distance in graphite.⁶³ A proton transfer occurring from one Hdmg ligand to the other would increase the electron density within the π -system of the formed dianion. An interaction by which the filled π orbitals of the dmg overlap with the empty π^* orbitals of the aniline would enhance the basicity of the aniline ligand. The complex formed would be stronger than might be expected based on the K_b value alone. This same argument applies to $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$ ⁴⁶ which was the first example of ligand-induced proton shift in a molecular complex. While the positions of the bridging protons in $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ and $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ are well defined, the bridge in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ is ill defined and the orientation angle of 36.7° is an intermediate value (see Table 18). The O...O distances in this complex show more variation than those in other related complexes as shown in Table 12. The 0.08 Å difference in the O...O distances is the same as for the corresponding N...N distances. The N(12)...N(21) separation is 2.836(15) Å and the N(11)...N(22) distance is 2.914(13) Å. Concurring with these observed distances, the N(12)-Co-N(21) angle of 97.0(4)° is more acute than the N(11)-Co-N(22) angle of 100.0(4)°. None of the other compounds examined shows any significant differences in the corresponding distances and angles between the diglyoxime ligands.

A comparison of mean bonding distances for each of the reported $\text{Co}(\text{H}_2\text{dmg}_2)$ complexes may be made from Table 19. There appears to be little variation in the average Co-N distances or in the average dimensions within the equatorial dimethylglyoxime ligands as a function of the axial ligand.

Those complexes having chloride as an axial ligand show a definite variation with the nature of the trans ligand. The longest Co-Cl distance is found where tpp is the trans ligand. This is not surprising since phosphines are known to have a very large trans-influence⁶⁴ but the small influence the tpp ligand exerts on the trans-chlorine atom compared to that of an ammonia ligand is unexpected.⁴⁰ There is no significant difference in the Co-N(1) distance involving a clan ligand whether it is trans to a chlorine atom or trans to another clan ligand. The trans-influence appears to occur in $\text{Co}(\text{H}_2\text{dmg}_2)$ complexes but not to a large extent.

The Co-Y distances in the $\text{XCo}(\text{H}_2\text{dmg}_2)\text{Y}$ complexes where Y is a ligand with an sp^3 nitrogen, increase in the following order of Y: $\text{NH}_3 < \text{an} \sim \text{clan} < \text{sulfa}$ (see Table 19). This series can be rationalized in terms of the relative K_b 's for sulfa (2.3×10^{-12}),⁶⁵ clan (9.6×10^{-11}),⁶⁶ aniline (4.0×10^{-10}),⁶⁶ and ammonia (1.3×10^{-5}).⁶⁷ Brückner and Randaccio⁴⁰ did not consider the K_b 's of the different nitrogen donors in their argument of the trend in trans-influencing ligands, X, upon the Co-N bond. The same Co-N distances were used for NH_3 and aniline complexes in their argument for basing the extent of trans-influence on the σ -donor power of the trans

Table 19
 A Summary of the Average Bond Distances (Å) in $\text{XYCo}(\text{H}_2\text{dmg}_2)$ Complexes. a,b,c,d

X	Y	Co-X	Co-Y	Co-N	N-O
clan	Cl	1.999(6)	2.257(2)	1.893(5)	1.343(6)
clan	clan	2.003(2)		1.898(2)	1.351(3)
*clan	Cl	1.946(11)	2.244(4)	1.907(11)	1.333(12)
sulfa	Cl	2.023(8)	2.235(3)	1.889(8)	1.333(11)
NiH_3	Cl	1.965(4)	2.251(1)	1.890(5)	1.346(10)
tpp	Cl	2.327(4)	2.277(4)	1.89(1)	1.343(9)
SnPh_3	Cl	2.54(2)	2.25(2)	1.95(2)	
an	an	2.001(5)		1.887(6)	1.343(6)
CH_3	H_2O	1.990(5)	2.053(3)	1.890(3)	1.352(5)
C-py	P(<u>n</u> -But) ₃	1.979(1)	2.339(1)	1.876(3)	1.339(7)
$\text{CH}_2\text{COOCH}_3$	py	2.04	2.04	1.88	1.37
DDT	py	1.97(1)	2.04(1)	1.88(1)	1.35(2)

^aThe ligands X and Y are approximately normal to the plane of the two dmg groups.

^bThe entry marked with an asterisk contains Hdpq rather than Hdmg and the distance under C-CH₃ is C-C₆H₅.

^cThe values given in parentheses are usually the mean of the estimated standard deviations. They are presented only to indicate the precision of the original values in a most general sense.

^dC-py is a carbon-bonded pyridine and DDT is 1,1-bis(4-chlorophenyl)-2-chloroethylene.

Table 13 - extended

X	Y	C-N	C-C	C-CH ₃	O...O	Reference
clan	Cl	1.297(8)	1.463(9)	1.490(11)	2.488(7)	-
clan	clan	1.295(3)	1.477(4)	1.484(4)	2.495(3)	-
*clan	Cl	1.309(16)	1.469(16)	1.486(17)	2.500(12)	-
sulfa	Cl	1.291(14)	1.471(17)	1.498(17)	2.493(11)	46
NH ₃	Cl	1.282(4)	1.483(6)	1.50(2)	2.486(7)	40
tpp	Cl	1.300(14)	1.485(15)	1.501(8)	2.50(1)	40
SbPh ₃	Cl					49
an	an	1.294(6)	1.463(7)	1.479(12)	2.491(8)	52
Cl ₃	H ₂ O	1.302(5)	1.463(7)	1.494(7)	2.486(4)	51
C-py	P(n-But) ₃	1.295(7)	1.443(3)	1.499(3)	2.474(2)	48
CH ₂ COOCH ₃	py	1.28	1.46	1.50	2.50	47
DDT	py	1.30(2)	1.43(2)		2.50(11)	50

ligand as are presented here.

In comparing $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ with $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ the distances from the cobalt atom to the equatorial nitrogens in the H_2dpg complex are longer and the distances to the axial ligands are shorter in the same complex. Because the phenyl substituents are inductively more electron withdrawing than methyl groups, Hdpg should be a weaker Lewis base than Hdmg . The equatorial distances to the Hdpg should, therefore, be longer. From an electronic standpoint the cobalt ion in the Hdpg complex would be more positively charged and a better Lewis acid toward the axial ligands than in the Hdmg complex. From a steric point of view the axial ligands are afforded a wider path of approach and will, therefore, be closer to the central cobalt ion when the equatorial ligands are farther away.

The benzene rings in the clan ligands of $\text{ClCo}(\text{H}_2\text{dmg}_2)^-(\text{clan})$, $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$, and $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ are planar (see Tables 14-16) having average C-C values of 1.376(3), 1.380(10), and 1.378(3) Å, respectively, with individual values reported in Table 20. The phenyl rings of the Hdpg ligands of $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ are also planar with pertinent values and equations of least-squares planes given in Table 21.

The crystals of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ are held together by six hydrogen bonds where there are eight hydrogen atoms capable of hydrogen bonding. Relevant hydrogen-bonding data are presented in Table 17. Although the $\text{O-H}\cdots\text{O}$ bridges between the H_2dmg and dmg groups are not symmetrical, the O-H

Bond Distances and Bond Angles of Coordinated 4-Chloroaniline Molecules with Their Estimated Standard Deviations.

Distances (Å)	CℓCo(H ₂ dmg ₂) (clan)	CℓCo(H ₂ dp ₂) (clan)	[Co(H ₂ dmg ₂) (clan) ₂]Cl
N(1)-C(1)	1.461(3)	1.451(15)	1.443(3)
C(1)-C(2)	1.374(3)	1.380(19)	1.383(4)
C(2)-C(3)	1.364(10)	1.409(20)	1.377(4)
C(3)-C(4)	1.370(10)	1.362(20)	1.354(5)
C(4)-C(5)	1.388(10)	1.344(21)	1.378(6)
C(5)-C(6)	1.378(10)	1.376(20)	1.385(4)
C(6)-C(1)	1.379(9)	1.406(17)	1.380(4)
Cℓ(2)-C(4)	1.734(8)	1.724(15)	1.752(3)
Angles (°)			
N(1)-C(1)-C(2)	119.4(5)	122.0(12)	119.4(2)
N(1)-C(1)-C(6)	119.2(5)	120.7(11)	121.0(2)
C(1)-C(2)-C(3)	119.7(6)	122.4(13)	120.2(3)
C(2)-C(3)-C(4)	119.8(7)	117.9(13)	119.5(3)
C(3)-C(4)-C(5)	120.7(7)	120.8(14)	121.8(4)
C(4)-C(5)-C(6)	119.7(7)	122.3(14)	118.4(3)
C(5)-C(6)-C(1)	118.7(6)	119.4(12)	120.7(3)
C(6)-C(1)-C(2)	121.4(6)	117.2(12)	119.5(2)
Cℓ(2)-C(4)-C(3)	120.5(6)	117.7(11)	119.4(3)
Cℓ(2)-C(4)-C(5)	118.8(6)	121.3(11)	118.8(3)

Table 21

Bond Distances, Bond Angles, and Least-Squares Planes of the Phenyl Rings in $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ with Their Estimated Standard Deviations.

(a) Distances	n = 13 l = A	14 B	23 C	24 D
C(n)-C(1l)	1.363(18)	1.411(20)	1.370(19)	1.426(17)
C(n)-C(5l)	1.421(20)	1.396(20)	1.356(17)	1.458(18)
C(1l)-C(2l)	1.368(19)	1.371(20)	1.432(19)	1.385(19)
C(2l)-C(3l)	1.370(21)	1.367(20)	1.351(21)	1.401(20)
C(3l)-C(4l)	1.352(20)	1.391(23)	1.371(23)	1.397(20)
C(4l)-C(5l)	1.374(20)	1.390(20)	1.409(18)	1.397(18)
(b) Angles ($^\circ$)				
C(n-2)-C(n)-C(1l)	123.9(11)	119.3(12)	120.9(11)	121.7(11)
C(n-2)-C(n)-C(5l)	119.9(11)	120.9(12)	121.2(11)	120.6(11)
C(n)-C(1l)-C(2l)	122.8(13)	120.6(13)	122.3(12)	122.6(12)
C(1l)-C(2l)-C(3l)	119.5(13)	119.3(14)	117.0(13)	117.7(13)
C(2l)-C(3l)-C(4l)	120.5(13)	121.0(14)	122.2(14)	122.5(13)
C(3l)-C(4l)-C(5l)	120.0(14)	120.4(14)	118.7(13)	120.2(13)
C(4l)-C(5l)-C(n)	121.0(13)	118.4(14)	121.7(12)	119.0(12)
C(5l)-C(n)-C(1l)	116.2(12)	119.8(13)	117.9(12)	117.7(11)
(c) Deviations ($\text{\AA} \times 10^{+3}$) from Least-Squares Planes of Phenyl Rings				
C(n)	2	41	-3	3
C(1l)	-7	-14	8	-12
C(2l)	10	-31	15	24
C(3l)	-10	48	-29	-28
C(4l)	5	-20	3	20
C(5l)	-2	-24	19	-7
C(n-2)	-3	172	-16	20
(d) Coefficients of the Plane Equation $PX + QY + RZ = S$				
	P	Q	R	S
Phenyl A	-0.5815	0.5296	-0.6176	4.7459
Phenyl B	-0.4144	-0.7611	0.4990	3.1793
Phenyl C	-0.6482	0.3950	-0.6509	4.0341
Phenyl D	-0.1592	-0.8986	0.4088	1.3642

distances are longer than might be expected. The two hydrogen atoms on N(1) of the clan ligand both hydrogen bond to different water molecules. The hydrogen atoms of one water molecule, O(w2), form reasonably strong hydrogen bonds to O(12) and Cl(1). The hydrogen atoms on O(w1), however, have only short contacts with angles indicating only weak hydrogen bonds.

While $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ and $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ both exhibit the hydrogen bonding between the equatorial ligands, $\text{ClCo}(\text{H}_2\text{dpg}_2)(\text{clan})$ has no intermolecular hydrogen bonds. While the hydrogen atom on the solvent molecule was not located, a hydrogen bond may exist between O(S1) and O(22). Each molecule of $[\text{Co}(\text{Hdmg})_2(\text{clan})_2]\text{Cl}$ possesses two intermolecular hydrogen bonds. Each clan molecule shows a hydrogen bond from N(1) to the O(11) of another molecule. The other hydrogen on each N(1) is hydrogen bonded to the ionic chloride. Relevant hydrogen-bonding data for these two compounds are also presented in Table 17.

All intermolecular distances less than $3.6 \text{ \AA}$ were calculated and carefully examined. No unusually short intermolecular distances were found.

Ligand-induced proton shifts may be of biological significance. Since proton transfers in living systems are relatively common, the study presented here provides an important examination of orientation effects and enhanced stabilities which may be achieved by a small shift of one proton.

CHAPTER 5

A NOVEL BINUCLEATING LIGAND: THE CRYSTAL AND MOLECULAR STRUCTURES OF 1,4-DIHYDRAZINOPHTHALAZINEBIS(2-PYRIDINIUMCARBOXALDIMINE) NITRATE DIHYDRATE AND μ -CHLOROTETRAAQUA[1,4-DIHYDRAZINOPHTHALAZINEBIS(2-PYRIDINECARBOXALDIMINE)]DINICKEL(II) CHLORIDE DIHYDRATE

Binuclear complexes of chelating ligands have been of interest recently for their potential activation of other ligands at an accessible bridging site⁶⁸⁻⁷³ and for their magnetic properties.^{24,74-80} The structure of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3$ shows the planar chelating ligand, dhphpy, to be capable of binding two metal atoms simultaneously. In that complex, a bridging site between the nickel ions is occupied by a chloride ion. Therefore, at least one bridging ligand in addition to dhphpy may be accommodated by M_2dhphpy complexes.

While the study of magnetic interactions between metal ions through bridging atoms in such systems is convenient and theoretically significant, the catalytic possibilities of this type system are exceptional. The nitrogen-fixing enzyme nitrogenase has been considered to contain a polynuclear active site.^{6,7}

Although the mechanism of the reduction of N_2 to NH_3 by nitrogenase is not understood N_2 is believed to be coordinated to the metal ions of the enzyme.^{67,81,82} Nitrogenase has been shown to reduce a wide variety of small molecules which contain a triple bond.⁷ The distance between the metal

ions should be of importance in the activation of those molecules. In the complexes of Robson and coworkers⁶⁸⁻⁷³ and of Okawa *et al.*⁸³ the metal-metal distance is essentially controlled by a single bridging phenoxide ion. However, in dhphpy complexes the metal ion separation is fixed at a greater distance by the geometry of the chelating ligand. Therefore, larger molecules which are reduced in the presence of nitrogenase, e.g. N_2 , N_3^- , N_2O , C_2H_2 , and HCN ,⁷ should be suitable for incorporation as bridging molecules opposite the N-N bridge of dhphpy. The syntheses and X-ray structures of $H_2dhphpy(NO_3)_2 \cdot H_2O$ and $[Ni_2Cl(H_2O)_4(dhphpy)]Cl_3 \cdot 2H_2O$ were undertaken to examine the nature of the accessible bridging site in complexes of this type ligand.

Solution and Refinement of the Structure of $H_2dhphpy(NO_3)_2 \cdot 2H_2O$

The direct method of symbolic addition was used in which the signs of two hundred large L's were assigned. All fourteen nonhydrogen atoms of the ligand within the asymmetric unit were located in an E-map computed from the signed E values. Two Fourier syntheses were used to validate the selected model, locate the remaining nonhydrogen atoms, and refine the atomic parameters. The refinement is outlined in Table 5. The observed and calculated structure factors are given in Table B-3. The final positional and thermal parameters are presented in Tables 22 and 23.

Table 22
Final Atomic Parameters^a for the Nonhydrogen Atoms for H₂dhpmpy(NO₃)₂·2H₂O

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	378(2)	3536(3)	1603(3)	21(1)	80(4)	76(4)	0(3)	6(3)	-6(6)
C(2)	181(2)	2379(3)	2019(3)	21(1)	71(3)	83(4)	-1(3)	5(3)	8(6)
C(3)	354(2)	1293(3)	1534(3)	33(1)	74(4)	110(4)	3(3)	36(4)	-14(7)
C(4)	172(2)	240(3)	2015(4)	39(2)	73(4)	140(5)	-2(4)	43(4)	-13(7)
C(10)	1382(2)	4771(3)	-289(3)	24(1)	97(4)	86(4)	-1(3)	27(3)	-11(6)
C(11)	1579(2)	5947(3)	-658(3)	20(1)	86(4)	91(4)	-7(3)	9(3)	0(6)
C(12)	1968(2)	6072(4)	-1546(4)	27(1)	113(4)	108(4)	-8(4)	35(4)	2(7)
C(13)	2116(2)	7214(4)	-1912(4)	30(1)	142(5)	119(5)	-13(4)	43(4)	36(8)
C(14)	1883(2)	8189(4)	-1367(4)	30(1)	114(5)	148(5)	-15(4)	31(4)	44(8)
C(15)	1521(2)	8013(3)	-457(4)	28(1)	92(4)	140(5)	-9(4)	23(4)	8(8)
N(1)	200(1)	4549(2)	2064(2)	23(1)	77(3)	89(3)	4(3)	25(2)	-7(5)
N(2)	783(1)	3597(2)	753(3)	30(1)	77(3)	99(3)	-9(3)	36(3)	-6(5)
N(3)	972(1)	4712(2)	448(2)	25(1)	73(3)	95(3)	-4(3)	25(3)	1(5)
N(10)	1368(1)	6918(3)	-123(3)	27(1)	81(3)	111(3)	-5(3)	23(3)	7(5)
N(20)	1628(2)	1394(3)	-781(4)	68(2)	93(4)	223(6)	33(4)	148(5)	9(7)
O(1)	565(2)	6955(3)	1629(3)	53(1)	113(3)	162(4)	14(3)	62(3)	-50(6)
O(20)	1843(2)	1108(4)	-1701(5)	114(2)	169(5)	445(9)	15(5)	355(8)	-29(10)
O(21)	1086(2)	1953(3)	-974(3)	58(1)	123(3)	151(4)	34(3)	76(4)	-26(6)
O(22)	1861(2)	1062(4)	290(4)	89(2)	284(7)	285(7)	127(6)	56(6)	109(11)

^aAll values are $\times 10^4$. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$

Table 23
Final Parameters for the Hydrogen Atoms in $\text{H}_2\text{dhpPy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}^a$

Atom [Bonded to]	Distance	x	y	z	B
H(1) [O(1)]	0.78(5)	57(3)	629(4)	185(5)	12.5(1.5)
H(2) [O(1)]	0.88(4)	80(2)	737(4)	228(4)	10.1(1.3)
H(3) [C(3)]	1.00(3)	61(2)	129(3)	84(3)	6.2(0.9)
H(4) [C(4)]	1.01(4)	33(2)	-54(4)	171(3)	8.0(1.1)
H(10) [C(10)]	1.05(4)	157(2)	402(3)	-68(3)	6.5(1.0)
H(12) [C(12)]	1.02(3)	212(2)	533(3)	-196(3)	5.7(0.9)
H(13) [C(13)]	0.99(4)	235(2)	734(4)	-262(4)	9.4(1.3)
H(14) [C(14)]	0.91(4)	200(2)	895(4)	-152(4)	7.9(1.1)
H(15) [C(15)]	1.00(4)	136(2)	870(3)	-1(3)	6.6(1.0)
H(N2) [N(2)]	0.95(4)	85(2)	293(4)	26(4)	9.4(1.2)
H(PY) [N(10)]	1.21(6)	105(3)	682(5)	69(5)	15.9(1.8)

^aThe hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (in Å), the positional parameters ($\times 10^3$), and the isotropic thermal parameter (in Å²). The estimated standard deviations are given in parentheses.

Solution and Refinement of the Structure
of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$

The position of Ni(1) was determined from a sharpened three-dimensional Patterson function. The positions of the remaining atoms were determined in a manner analogous to that used with $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$. After the hydrogen atoms were located they were included in further refinement with each having an isotropic thermal parameter one unit higher than the refined isotropic value for the atom to which the hydrogen atom was bonded. A summary of the refinement is given in Table 5. The scattering factors for the nonhydrogen atoms were from Hanson *et al.*²⁹ and the hydrogen scattering factors from Stewart *et al.*³⁰ Lists of observed and calculated structure factors are given in Table B-4. The final positional and thermal parameters are listed in Tables 24 and 25.

Results and Discussion

The atomic numbering and thermal ellipsoids of $\text{H}_2\text{dhphpy} \cdot (\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ are shown in Figure 6 and those of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ are shown in Figure 7. Selected interatomic distances of both compounds are listed in Table 26 and corresponding angles are given in Tables 27 and 28. Both compounds crystallize with the cationic complexes, their anions, and water molecules linked in a three-dimensional hydrogen-bonded network. The postulated hydrogen bonds in the structures are listed in Table 29. Diagrams illustrating the pack-

Table 24
The Final Atomic Parameters^a of the Nonhydrogen Atoms for
[Ni₂Cl(H₂O)₄(dhphpy)]Cl₃·2H₂O

Atom	x	y	z	β_{11}
Ni (1)	11817 (7)	17289 (5)	9891 (3)	442 (5)
Ni (2)	11346 (6)	-4660 (5)	13854 (3)	407 (5)
Cl (1)	1046 (1)	315 (1)	650 (1)	63 (1)
Cl (2)	1196 (2)	4767 (1)	2115 (1)	86 (2)
Cl (3)	1297 (2)	-1548 (1)	3350 (1)	69 (1)
Cl (4)	1288 (2)	3725 (2)	4540 (1)	90 (2)
O (1)	-362 (4)	1864 (3)	639 (2)	55 (3)
O (2)	2743 (4)	1634 (3)	1329 (2)	55 (3)
O (3)	-423 (3)	-532 (3)	1026 (2)	48 (3)
O (4)	2664 (3)	-435 (4)	1708 (2)	48 (3)
O (5)	1626 (4)	-520 (4)	-194 (2)	54 (3)
O (6)	1072 (4)	5047 (5)	3678 (2)	74 (4)
N (1)	1178 (4)	1408 (3)	1690 (2)	50 (4)
N (2)	1153 (4)	576 (3)	1834 (2)	48 (4)
N (3)	1265 (4)	2854 (3)	1801 (2)	74 (5)
N (4)	1258 (4)	2873 (3)	1324 (2)	53 (4)
N (5)	1143 (4)	-469 (3)	2395 (2)	55 (4)
N (6)	1165 (4)	-1007 (3)	2025 (2)	45 (4)
N (10)	1234 (4)	2554 (4)	433 (2)	54 (4)
N (20)	1163 (4)	-1776 (4)	1227 (2)	55 (4)
C (1)	1233 (5)	2052 (4)	1992 (3)	42 (4)
C (2)	1251 (5)	1919 (4)	2495 (3)	36 (4)
C (3)	1280 (5)	2594 (5)	2826 (3)	50 (5)
C (4)	1300 (5)	2410 (5)	3302 (3)	56 (5)
C (5)	1288 (5)	1559 (5)	3450 (3)	51 (5)
C (6)	1260 (5)	887 (4)	3136 (2)	47 (5)
C (7)	1236 (4)	1057 (4)	2649 (2)	29 (4)
C (8)	1182 (4)	394 (4)	2288 (2)	29 (4)
C (10)	1281 (6)	3550 (4)	1076 (3)	71 (6)
C (11)	1291 (5)	3337 (5)	578 (3)	52 (5)

Table 24- extended

β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
273 (4)	106 (1)	-66 (8)	224 (5)	14 (4)
244 (3)	92 (1)	2 (8)	184 (4)	13 (4)
31 (1)	10 (0)	-10 (2)	26 (1)	-2 (1)
35 (1)	14 (0)	8 (2)	18 (1)	0 (1)
50 (1)	17 (0)	46 (2)	39 (1)	17 (1)
72 (1)	25 (1)	-58 (3)	26 (2)	-1 (1)
42 (3)	21 (1)	3 (5)	26 (3)	6 (3)
40 (2)	21 (1)	-6 (5)	29 (3)	2 (3)
58 (3)	18 (1)	-5 (5)	23 (3)	22 (3)
69 (3)	12 (1)	17 (5)	14 (3)	-2 (3)
62 (3)	17 (1)	1 (5)	26 (3)	-3 (3)
111 (5)	18 (1)	1 (7)	35 (4)	-6 (4)
23 (2)	11 (1)	-2 (5)	25 (3)	-1 (2)
24 (2)	11 (1)	-1 (5)	25 (3)	1 (2)
26 (2)	15 (1)	-14 (6)	38 (4)	-3 (3)
31 (3)	14 (1)	-12 (5)	29 (3)	3 (3)
25 (2)	9 (1)	1 (5)	19 (3)	1 (2)
26 (2)	11 (1)	-1 (5)	21 (3)	3 (2)
41 (3)	14 (1)	5 (5)	33 (3)	10 (3)
32 (3)	13 (1)	13 (5)	26 (3)	0 (3)
24 (3)	14 (1)	-9 (6)	26 (4)	0 (3)
30 (3)	13 (1)	-11 (6)	14 (4)	-6 (3)
37 (4)	14 (1)	-12 (7)	27 (4)	-10 (3)
44 (4)	14 (1)	-8 (7)	26 (4)	-17 (4)
55 (4)	12 (1)	-17 (7)	23 (4)	-11 (4)
40 (4)	9 (1)	-2 (6)	18 (4)	1 (3)
32 (3)	10 (1)	-8 (6)	15 (4)	-3 (3)
28 (3)	12 (1)	-5 (6)	20 (3)	-2 (3)
30 (3)	20 (2)	-7 (7)	41 (5)	7 (4)
36 (3)	17 (1)	-3 (7)	29 (4)	7 (4)

Table 24 - continued

Atom	x	y	z	β_{11}
C(12)	1343(6)	4055(5)	270(3)	83(7)
C(13)	1353(7)	3839(6)	-202(3)	86(7)
C(14)	1308(6)	2992(6)	-348(3)	73(6)
C(15)	1251(6)	2361(5)	-17(3)	59(6)
C(20)	1143(5)	-1829(4)	2053(3)	54(5)
C(21)	1147(5)	-2273(4)	1604(3)	48(5)
C(22)	1149(6)	-3175(5)	1577(3)	64(6)
C(23)	1165(6)	-3554(5)	1149(3)	77(6)
C(24)	1204(6)	-3048(5)	758(3)	76(6)
C(25)	1195(5)	-2157(5)	812(3)	55(5)

^aAll values are $\times 10^4$ except for those of Ni(1) and Ni(2) which are $\times 10^5$. The estimated standard deviations are given in parentheses. The temperature factors are of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$

Table 24 - extended - continued

β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
49(4)	20(2)	-19(9)	36(6)	19(4)
68(5)	17(2)	-27(10)	34(6)	21(5)
68(5)	20(2)	7(9)	47(6)	15(5)
60(5)	14(1)	-6(8)	27(5)	5(4)
29(3)	14(1)	0(6)	29(4)	6(3)
31(3)	14(1)	10(6)	25(4)	5(3)
32(3)	21(2)	6(7)	31(5)	3(4)
39(4)	21(2)	15(8)	33(5)	-6(4)
43(4)	19(2)	8(8)	24(5)	-13(4)
39(4)	16(1)	2(7)	24(5)	-6(4)

Table 25
Final Parameters for the Hydrogen Atoms in $[\text{Ni}_2\text{Cl}_2(\text{H}_2\text{O})_6(\text{dppp})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}^a$

Atom [Bonded to]	Distance	x	y	z	B
H(N3) [N(3)]	0.91	1397	3365	1972	4.6
H(N5) [N(5)]	0.97	1394	-703	2742	3.8
H(C3) [C(3)]	1.09	1271	3289	2781	4.8
H(C4) [C(4)]	1.05	1323	2949	3525	4.9
H(C5) [C(5)]	0.99	1316	1515	3799	4.8
H(C6) [C(6)]	1.02	1283	313	3312	4.2
H(10) [C(10)]	1.06	1379	4129	1286	5.0
H(12) [C(12)]	1.15	1514	4705	486	6.0
H(13) [C(13)]	1.10	1428	4364	-441	6.6
H(14) [C(14)]	1.04	1443	2797	-657	6.2
H(15) [C(15)]	1.04	1025	1751	-172	4.6
H(20) [C(20)]	1.05	993	-2163	2330	4.5
H(22) [C(22)]	1.04	1297	-3492	1907	5.3
H(23) [C(23)]	1.02	1313	-4180	1103	5.8
H(24) [C(24)]	1.17	972	-3299	327	6.4
H(25) [C(25)]	1.18	1233	-1547	570	5.4
H(1) [O(1)]	1.12	-793	1312	372	5.6
H(1') [O(1)]	0.95	-494	2465	576	5.6
H(2) [O(2)]	0.84	3145	1240	1479	5.5

Table 25 - continued

Atom [Bonded to]	Distance	x	y	z	B
H(2') [O(2)]	1.00	3228	2098	1520	5.5
H(3) [O(3)]	0.91	-793	-51	891	5.6
H(3') [O(3)]	0.73	-688	-756	1149	5.6
H(4) [O(4)]	0.92	3049	-428	2050	5.4
H(4') [O(4)]	0.85	2808	-935	1646	5.4
H(5) [O(5)]	0.86	1353	-476	14	5.7
H(5') [O(5)]	0.90	2283	-622	-50	5.7
H(6) [O(6)]	1.15	863	4328	3630	7.4
H(6') [O(6)]	1.13	1345	4724	4067	7.4

^aThe hydrogen atom is given followed by the atom to which it is bonded in brackets, the corresponding bond distance (in Å), the positional parameters ($\times 10^3$), and the isotropic thermal parameter (in Å²).

Figure 6

An ORTEP drawing of $\text{H}_2\text{dnpbp}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ showing the atomic numbering and thermal ellipsoids. The hydrogen atoms are isotropic and small relative to the 50% probability thermal ellipsoids for nonhydrogen atoms.

Figure 7

An ORTEP drawing of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\cdot 2\text{H}_2\text{O}$ showing atomic numbering and thermal ellipsoids. The hydrogen atoms and uncoordinated water molecules have been omitted.

Table 26

Selected Interatomic Distances for $\text{H}_2\text{dhpphy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ and $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$

(a) Distance ($\text{\AA}$) in the Coordination Sphere in

$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$			
Ni(1)-N(1)	2.074(5)	Ni(2)-N(2)	2.061(5)
Ni(1)-N(4)	1.999(5)	Ni(2)-N(6)	2.001(5)
Ni(1)-N(10)	2.074(6)	Ni(2)-N(20)	2.039(6)
Ni(1)-Cl(1)	2.374(2)	Ni(2)-Cl(1)	2.337(2)
Ni(1)-O(1)	2.098(6)	Ni(2)-O(3)	2.208(6)
Ni(1)-O(2)	2.117(6)	Ni(2)-O(4)	2.070(6)

(b) Distances ($\text{\AA}$) within the Ligand^a

$\text{H}_2\text{dhpphy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$		$[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_6(\text{dhpphy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$	
N(1)-N(1')	1.374(4)	N(1)-N(2)	1.363(7)
N(1)-C(1)	1.318(4)	N(1)-C(1)	1.302(8)
C(1)-C(2)	1.454(5)	C(1)-C(2)	1.447(10)
C(2)-C(3)	1.396(5)	C(2)-C(3)	1.402(10)
C(3)-C(4)	1.369(5)	C(3)-C(4)	1.383(10)
C(2)-C(2')	1.396(5)	C(2)-C(7)	1.414(9)
C(4)-C(4')	1.378(6)	C(4)-C(5)	1.390(11)
C(1)-N(2)	1.362(4)	C(1)-N(3)	1.370(8)
N(2)-N(3)	1.366(4)	N(3)-N(4)	1.366(8)
N(3)-C(10)	1.277(4)	N(4)-C(10)	1.278(9)
C(10)-C(11)	1.454(5)	C(10)-C(11)	1.457(11)
		N(2)-C(8)	1.313(8)
		C(7)-C(8)	1.439(9)
		C(6)-C(7)	1.407(9)
		C(5)-C(6)	1.368(10)
		C(3)-N(5)	1.382(8)
		N(5)-N(6)	1.364(7)
		N(6)-C(20)	1.279(8)
		C(20)-C(21)	1.464(10)

Table 26 - continued

μ_2 dhpppy(NO ₃) ₂ · 2H ₂ O	[Ni ₂ Cl(H ₂ O) ₆ (dhpppy)]Cl ₃ · 2H ₂ O
C(11)-C(12) 1.397(5)	C(11)-C(12) 1.388(11) C(21)-C(22) 1.402(10)
C(12)-C(13) 1.387(6)	C(12)-C(13) 1.400(13) C(22)-C(23) 1.370(12)
C(13)-C(14) 1.370(6)	C(13)-C(14) 1.373(13) C(23)-C(24) 1.392(12)
C(14)-C(15) 1.364(6)	C(14)-C(15) 1.392(12) C(24)-C(25) 1.393(11)
C(15)-N(10) 1.331(5)	C(15)-N(10) 1.339(10) C(25)-N(20) 1.349(10)
N(10)-C(11) 1.343(4)	N(10)-C(11) 1.351(9) N(20)-C(21) 1.339(9)
O(1)···N(3) 3.007(4)	
O(1)···O(1') 3.283(4)	Ni(1)···Ni(2) 3.603(1)

^aThe estimated standard deviations are given in parentheses.

Table 27

Selected Angles in $\text{H}_2\text{dhpppy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}^a$

Atoms	Angles (°)	Atoms	Angles (°)
N(1)-C(1)-N(2)	117.9(3)	C(1)-C(2)-C(3)	123.1(3)
N(1)-C(1)-C(2)	121.9(3)	C(2')-C(2)-C(3)	119.7(3)
C(1)-C(2)-C(2')	117.2(3)	C(1)-N(1)-N(1')	120.8(3)
C(2)-C(3)-C(4)	119.4(3)	C(2)-C(1)-N(2)	120.1(3)
C(3)-C(4)-C(4')	120.8(4)	N(2)-N(3)-C(10)	117.2(3)
C(1)-N(2)-N(3)	116.9(3)	C(10)-C(11)-N(10)	118.5(3)
N(3)-C(10)-C(11)	118.4(3)	C(11)-C(12)-C(13)	119.0(4)
C(10)-C(11)-C(12)	121.2(3)	C(13)-C(14)-C(15)	119.1(4)
C(12)-C(13)-C(14)	119.5(4)	C(14)-C(15)-N(10)	121.5(4)
C(15)-N(10)-C(11)	120.6(3)	N(10)-C(11)-C(12)	120.3(3)
N(1)···O(1)···N(10)	108.3(1)	O(20)-N(20)-O(21)	118.1(4)
N(20)-O(21)···N(2)	123.0(3)	O(20)-N(20)-O(22)	123.9(5)
O(21)-N(20)-O(22)	117.6(4)		

^aThe estimated standard deviations are given in parentheses.

Table 28

Selected Angles in $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_6(\text{dhpppy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}^a$

Atom	Angle	Atom	Angle
N(1)-Ni(1)-Cl(1)	98.0(2)	N(2)-Ni(2)-Cl(1)	97.8(2)
N(1)-Ni(1)-N(4)	76.8(2)	N(2)-Ni(2)-N(6)	76.5(2)
N(1)-Ni(1)-N(10)	155.7(2)	N(2)-Ni(2)-N(20)	154.8(2)
N(1)-Ni(1)-O(1)	91.1(2)	N(2)-Ni(2)-O(3)	93.1(2)
N(1)-Ni(1)-O(2)	90.3(2)	N(2)-Ni(2)-O(4)	89.5(2)
N(4)-Ni(1)-Cl(1)	174.6(2)	N(6)-Ni(2)-Cl(1)	174.1(2)
N(4)-Ni(1)-N(10)	78.9(2)	N(6)-Ni(2)-N(20)	78.2(2)
N(4)-Ni(1)-O(1)	87.8(2)	N(6)-Ni(2)-O(3)	90.4(2)
N(4)-Ni(1)-O(2)	91.1(2)	N(6)-Ni(2)-O(4)	91.2(2)
N(10)-Ni(1)-Cl(1)	106.3(2)	N(20)-Ni(2)-Cl(1)	107.5(2)
N(10)-Ni(1)-O(1)	88.5(2)	N(20)-Ni(2)-O(3)	88.3(2)
N(10)-Ni(1)-O(2)	89.6(2)	N(20)-Ni(2)-O(4)	89.8(2)
O(1)-Ni(1)-Cl(1)	90.9(2)	O(3)-Ni(2)-Cl(1)	88.2(2)
O(1)-Ni(1)-O(2)	178.0(2)	O(3)-Ni(2)-O(4)	177.2(2)
O(2)-Ni(1)-Cl(1)	90.3(2)	O(4)-Ni(2)-Cl(1)	90.5(2)
N(10)-C(11)-C(12)	122.2(7)	N(20)-C(21)-C(22)	121.9(7)
C(11)-C(12)-C(13)	117.8(8)	C(21)-C(22)-C(23)	118.7(7)
C(12)-C(13)-C(14)	120.3(9)	C(22)-C(23)-C(24)	120.2(8)
C(13)-C(14)-C(15)	118.4(8)	C(23)-C(24)-C(25)	117.7(8)
C(14)-C(15)-N(10)	122.3(8)	C(24)-C(25)-N(20)	122.6(7)
C(15)-N(10)-C(11)	119.1(7)	C(25)-N(20)-C(21)	118.8(6)
N(10)-C(11)-C(10)	116.2(7)	N(20)-C(21)-C(20)	116.7(6)
C(12)-C(11)-C(10)	121.6(7)	C(22)-C(21)-C(20)	121.4(7)
C(11)-C(10)-N(4)	114.7(7)	C(21)-C(20)-N(6)	113.8(6)
C(10)-N(4)-N(3)	125.9(6)	C(20)-N(6)-N(5)	123.4(6)
N(4)-N(3)-C(1)	115.8(6)	N(6)-N(5)-C(8)	113.8(5)
N(1)-C(1)-N(3)	115.7(6)	N(2)-C(8)-N(5)	116.3(6)
C(2)-C(1)-N(3)	122.7(6)	C(7)-C(8)-N(5)	121.8(6)
N(1)-C(1)-C(2)	121.6(6)	N(2)-C(8)-C(7)	121.8(6)
C(1)-N(1)-N(2)	121.8(6)	C(8)-N(2)-N(1)	120.8(5)
C(1)-C(2)-C(7)	116.8(6)	C(2)-C(7)-C(8)	117.0(6)

Table 28 - continued

Atom	Angle	Atom	Angle
C(1)-C(2)-C(3)	123.5(6)	C(6)-C(7)-C(8)	123.5(6)
C(2)-C(3)-C(4)	119.7(7)	C(5)-C(6)-C(7)	119.4(6)
C(3)-C(4)-C(5)	120.1(7)	C(4)-C(5)-C(6)	121.6(7)
Ni(1)-N(1)-N(2)	122.4(4)	Ni(2)-N(2)-N(1)	123.3(4)
Ni(1)-N(1)-C(1)	115.8(5)	Ni(2)-N(2)-C(8)	115.9(4)
Ni(1)-N(4)-N(3)	115.9(4)	Ni(2)-N(6)-N(5)	117.3(4)
Ni(1)-N(4)-C(10)	118.2(5)	Ni(2)-N(6)-C(20)	119.1(5)
Ni(1)-N(10)-C(11)	111.9(5)	Ni(2)-N(20)-C(21)	112.1(5)
Ni(1)-N(10)-C(15)	128.9(5)	Ni(2)-N(20)-C(25)	129.1(5)
Ni(1)-Cℓ(1)-Ni(2)	98.4(1)		

^aThe estimated standard deviations are given in parentheses.

Table 29
Hydrogen Bonds in $\text{H}_2\text{dhpppy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ and $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpppy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$

D-H...A ^a	Position of A	Distances (Å) ^b		Angles (°)	
		D-H	H...A	D...A	D-H...A
H ₂ dhpppy(NO ₃) ₂ ·2H ₂ O					
N(2)-H(N2)...O(21)	x, y, z	0.95(4)	1.85(4)	2.773(4)	163(4)
N(10)-H(PY)...O(1)	x, y, z	1.21(6)	1.57(6)	2.758(4)	167(5)
O(1)-H(1)...N(1)	x, y, z	0.78(5)	2.12(5)	2.855(4)	159(5)
O(1)-H(2)...O(21)	x, 1-y, 1/2+z	0.98(4)	1.98(4)	2.824(4)	160(4)
[Ni ₂ Cl(H ₃ O) ₄ (dhpppy)2Cl ₃ ·2H ₂ O					
N(3)-H(N3)...Cl(2)	x, y, z	0.91	2.26	3.119(6)	158
N(5)-H(N5)...Cl(3)	x, y, z	0.97	2.24	3.135(6)	153
O(1)-H(1)...O(5)	-x, -y, -z	1.12	1.75	2.735(8)	144
O(1)-H(1')...Cl(4)	-x, y, 1/2-z	0.95	2.24	3.150(6)	159
O(2)-H(2')...Cl(3)	1/2-x, 1/2+y, 1/2-z	1.00	2.20	3.121(6)	152
O(3)-H(3')...Cl(3)	-x, y, 1/2-z	0.73	2.36	3.075(6)	171
O(4)-H(4)...Cl(2)	1/2-x, 1/2+y, 1/2-z	0.92	2.16	3.067(5)	171
O(5)-H(5)...Cl(1)	x, y, z	0.86	2.41	3.185(6)	151
O(5)-H(5')...Cl(4)	1/2-x, 1/2+y, 1/2-z	0.90	2.25	3.098(6)	157
O(5)-H(6')...Cl(4)	x, y, z	1.23	2.09	3.121(7)	151

^aDonor-Hydrogen...Acceptor. D-H is at x, y, z.

^bThe estimated standard deviations are given in parentheses.

ing and hydrogen bonding in $\text{H}_2\text{dhpphy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ and in $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ are presented in Figures 8 and 9.

The most noticeable difference in the structures of the two dhpphy ligands is that $\text{H}_2\text{dhpphy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ contains a twofold rotation axis while the nickel complex does not. In both cases the ligand is approximately planar (see Table 30). The nickel atoms and the bridging chloride of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ lie slightly "below" the least-squares plane of the ligand (Plane 3) and both hydrazone portions are pivoted generally about an $\text{N}(3) \cdots \text{N}(5)$ axis with both $\text{C}(14)$ and $\text{C}(24)$ "above" the plane. However, in the protonated ligand one hydrazone is pivoted "upward" and the other "downward" as required by the twofold axis. Also, the hydrazone "arms" in the nickel complex are drawn toward each other compared to the protonated form as indicated by the bond angles within the "arms." All of the pyridine rings are rotated about the $\text{C}(n0)-\text{C}(n1)$ bond relative to the phthalazine plane with the pyridine nitrogen atoms tipped toward the coordinated species. In $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ the pyridine containing $\text{N}(10)$ is rotated to a much greater extent than that containing $\text{N}(20)$. This is shown by the deviations from plane 4 (Table 30) of $\text{N}(10)$ and $\text{C}(12)$, 0.124 and 0.222 Å, compared to the deviations of $\text{N}(20)$ and $\text{C}(22)$, 0.148 and 0.161 Å. The rings of the phthalazine fragment in each compound appear twisted relative to each other but by less than 2°.

Figure 8

A packing diagram of $\text{H}_2\text{dhp}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ with atoms at x, y, z and $\bar{x}, \bar{1}-y, \bar{1}-z$ labeled and those at $x, 1-y, 1/2+z$ and $\bar{x}, y, 1/2-z$ unlabeled. Proposed hydrogen bonds are indicated by broken lines.

Figure 9

A packing diagram of $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhp}_2\text{py})] \cdot 2\text{H}_2\text{O}$ where $\text{O}(6)$ is at x, y, z ; $\text{O}(6')$ is at $\bar{x}, \bar{y}, \bar{z}$; $\text{O}(6'')$ is at $1/2-x, 1/2+y, 1/2-z$; and $\text{O}(6''')$ is at $1/2+x, 1/2+y, z$. Proposed hydrogen bonds are indicated by broken lines.

Table 30
Deviations and Equations of Selected Least-Squares Planes in $\text{H}_2\text{dhpby}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$
and $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpby})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$
(a) Deviations ($\text{\AA} \times 10^{+3}$)^a
 $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpby})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$

Atom	Plane 1	Plane 2	Atom	Plane 3	Plane 4	Atom	Plane 3	Plane 4
N(1)	-13*	-2*	N(1)	-85*	-6*	N(2)	-92*	-15*
C(1)	-40*	15*	C(1)	-28*	13*	C(8)	-44*	-5*
C(2)	-2*	-13*	C(2)	6*	8*	C(7)	12*	11*
C(3)	-43*	-14*	C(3)	27*	-8*	C(6)	54*	13*
C(4)	52*	-4*	C(4)	63*	-12*	C(5)	74*	-4*
N(2)	-40*	119	N(3)	-9*	43	N(5)	-70*	-30
N(3)	-16*	200	N(4)	-24*	71	N(5)	-27*	53
C(10)	62*	376	C(10)	-14*	94	C(20)	-32*	56
C(11)	53*	429	C(11)	0*	155	C(21)	-18*	117
C(12)	5*	448	C(12)	47*	222	C(22)	13*	161
C(13)	-66*	472	C(13)	63*	283	C(23)	42*	233
C(14)	-63*	424	C(14)	27*	270	C(24)	76*	296
C(15)	36*	418	C(15)	-29*	192	C(25)	38*	242
N(10)	79*	407	N(10)	-54*	124	N(20)	-13*	148
O(1)	116	243	Ni(1)	-95	43	Ni(2)	-90	40
			Cl(1)	-239	-55			

Table 30 - continued
 (b) Coefficients of the plane equation $AX + BY + CZ = D$ ⁵⁸

Plane	A	B	C	D
$\text{H}_2\text{dhp}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$				
1	0.6518	-0.0289	0.7578	1.4465
2	0.7079	-0.0175	0.7061	1.3716
$\{\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhp})\}\text{Cl}_3 \cdot 2\text{H}_2\text{O}$				
3	0.8991	-0.0193	0.4374	1.6470
4	0.9121	-0.0276	0.4091	1.4216

^aThe entries marked with an asterisk were used to define the plane.

All bonding distances involving nonhydrogen atoms are normal. The N-N distances in both compounds range from 1.363(7) to 1.374(4) Å and are comparable to the N-N distance in 4-FPYTSC of 1.365(3) Å.⁸⁴ Since this distance in both the phthalazine and hydrazone groups is significantly shorter than the accepted N-N single bond distance, 1.44±4 Å,⁸⁵ and since the ligand is planar, a delocalized system is presumed to exist. In agreement with this assumption the C(n0)-N distances are longer than the pure C-N double bond distance and are all equivalent to the related C-N distance in 4-FPYTSC, 1.275(3) Å.⁸⁴ All other distances within the ligand are not significantly different from those in [Ni(dhph)(H₂O)₂Cl₄·2H₂O].⁸⁶

All Ni-N distances in [Ni₂Cl(H₂O)₄(dhphpy)]Cl₃·2H₂O are within the range of reported bonding distances of nickel(II) with aromatic nitrogen atoms (2.00 to 2.112 Å).⁸⁷

The bridging chloride is not symmetrically located between the two nickel atoms with Ni-Cl distances of 2.374(2) and 2.387(2) Å. The appearance of this bridge is remarkably similar to that in di-μ-chloro-sym-trans-dichlorobis-(2,9-dimethyl-1,10-phenanthroline)dinickel(II) · 2chloroform⁸⁸ where the Ni-C distances are 2.378(3) and 2.394(3) Å. Also, the Ni···Ni distance, 3.602(2) Å, and Ni-Cl-Ni angle, 98.0(1)°, in that compound are equivalent to the 3.603(1) Å separation and 98.36(7)° angle in [Ni₂Cl(H₂O)₆(dhphpy)]Cl₃·2H₂O. This distance between the nickel atoms is somewhat shorter than

the 3.791(4) Å distance found in the $[\text{Ni}(\text{dhph})(\text{H}_2\text{O})_2]\text{Cl}_4 \cdot 2\text{H}_2\text{O}$ complex reported by Andrew and Blake⁸⁶ where both bridges are phthalazine nitrogen atoms. The separation between the nickel atoms in the dhphpy complex, however, is substantially longer than the Ni...Ni distance of 2.879 Å in the doubly oxo-bridged complex of Hoskins, Robson, and Schaap.⁷⁰ All these inter-nickel distances are much greater than twice the covalent radius of nickel and must be a function of the bridging atoms.

The distorted octahedral coordination geometry about each nickel atom in $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$ is completed by two water molecules which lie on a line almost perpendicular to the ligand plane. The Ni-O bond distances are typical⁸⁷ for water coordinated to nickel(II) ranging from 2.070(6) to 2.117(6) Å.

A degree of uncertainty exists concerning the positions of hydrogen atoms about O(1) in $\text{H}_2\text{dhphpy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$. The O(1)-H(1) distance appears to be very short, 0.78 Å, while the N(10)-H(py) distance appears to be very long, 1.21 Å. Although the locations presented for the hydrogen atoms are the most reasonable interpretation of the difference map in terms of peak heights, distances, and H-O-H angles, other areas of positive density exist about the N(1), O(1), and N(10) positions. Disorder may exist with alternate forms having N(1) protonated or having a "coordinated hydronium ion."

Complexes of dhphpy structurally provide a promising

uni-molecular system for the incorporation of a small molecule at a bridging position. Dinitrogen has been reported as a bridging ligand connecting two metal complexes in the μ -dinitrogen-bis{[1,2-bis(dimethylphosphino)ethane]hydrido-[η -(1,3,5-trimethylbenzene)]molybdenum} cation and similar compounds.⁸⁹ No complex has been reported which could retain its structural integrity after the removal of a bridging dinitrogen. The structures presented here suggest complexes of ligands similar to dhphpy may have such a capacity.

CHAPTER 6

MODELS OF PROPOSED INTERMEDIATES FOR THE CATALYZED CYCLIZATION OF ACETYLENES: THE CRYSTAL AND MOLECULAR STRUCTURES OF 1-(π -CYCLOPENTADIENYL)-1-TRIPHENYLPHOSPHINE-2,3,4,5-TETRAKIS(PENTAFLUOROPHENYL)COBALTOLE AND 1-(π -CYCLOPENTADIENYL)-1-TRIPHENYLPHOSPHINE-2,3,4,5-TETRAKIS(PENTAFLUOROPHENYL)RHODOLE

The catalysis of the oligomerization of acetylenes by transition metal complexes has been extensively studied.⁹⁰ A reaction mechanism involving a metallo-cyclopentadiene intermediate has been suggested⁸⁻¹³ for the trimerization of two molecules of acetylene with one of olefin in the presence of $\text{NiBr}_2(\text{tpp})_2$, $\text{Ni}(\text{CO})_2(\text{tpp})_2$, and other nickel catalysts. Metal-containing heterocycles, metallocycles, have been implicated^{14,91-93} as intermediates in the reactions of acetylenes with π -cyclopentadienyldicarbonyl-metal complexes in which the metal was cobalt, rhodium, or iridium. Yamazaki *et al.*⁹⁴⁻⁹⁶ on the basis of chemical reactions assigned a metallocyclic structure to a phosphine-containing cobalt complex isolated from the reaction of diphenylacetylene with $\text{Co}(\text{cp})(\text{tpp})\text{I}_2$ and isopropylmagnesium bromide. They also isolated the same product from the reaction of excess diphenylacetylene with $\text{Co}(\text{cp})(\text{tpp})_2$. A preliminary report of the structure of a cobaltacycle formed by the reaction of $\text{Co}(\text{cp})(\text{tpp})(\text{PhC}\equiv\text{CCO}_2\text{Me})$ with dimethyl maleate has been reported.⁵⁷

Rausch and Gastinger¹⁵ prepared $C_4(fph)_4Co(cp)(tpp)$ by the reaction of bis(pentafluorophenyl)acetylene with π -cyclopentadienylcarbonyltriphenylphosphinecobalt. The analogous rhodium compound was prepared by the reaction of the corresponding rhodium compound.¹⁵

Except for one preliminary report⁹⁷ no structural data have been available for cobaltacyclopentadiene metallocycles. Therefore, the X-ray diffraction structural analysis of $C_4(fph)_4Co(cp)(tpp)$ was undertaken. The corresponding rhodacycle was studied for comparison with this cobaltacycle and related compounds.

Structure Solution and Refinement for $C_4(fph)_4Co(cp)(tpp)$

The heavy atom method was used in which the positions of the cobalt and phosphorus atoms were estimated from a sharpened Patterson function. A Fourier synthesis based on these atoms was used to estimate the positions of eighteen additional atoms. Successive Fourier syntheses revealed the locations of all nonhydrogen atoms in the compound. A difference Fourier synthesis at that point revealed a region between the cobaltacycles which was of relatively high electron density. Because this density was diffuse no additional atomic positions were estimated before starting refinement, $R = 0.27$. Three cycles of least-squares refinement with individual isotropic thermal parameters reduced R to 0.14. A difference Fourier synthesis again revealed relatively high elec-

tron density in the same location as before.

Because of the discrepancy of the calculated density (1.423 g/cm^3) from the measured density (1.59 g/cm^3), solvent molecules were presumed to be in the crystal. The deep red crystals of the compound were grown from Skelly C¹⁴ which is a saturated hydrocarbon fraction boiling between 88 and 98°C and consisting mainly of n-heptane, C_7H_{16} . If two solvent molecules were in the unit cell the calculated density would be much nearer the measured value at 1.55 g/cm^3 . Several maxima were observed in the difference Fourier synthesis within the region of high electron density. The distances between these points and the angles made by lines connecting them did not reasonably approximate a hydrocarbon chain.

The thermal parameters were converted to their anisotropic equivalent and nine least-squares cycles using a block approximation to the matrix reduced R to 0.077. The shifts of all parameters during the final cycle were less than one-tenth of their respective estimated standard deviations. A difference Fourier synthesis calculated at this stage again suggested the presence of an ill-defined solvent molecule. Although the distribution of the peaks, which were not well resolved, suggested a C_7 or C_8 chain, a closer examination of the distances and angles within the group showed them not to reasonably approximate a hydrocarbon chain.

Six peaks were selected which closely retained their positions in the final Fourier summation before refinement and in the difference Fourier syntheses just discussed and

which seemed the most reasonable in approximately a hydrocarbon chain. These locations were used isotropically as carbon atoms together with the seventy-three refined positions from the third full-matrix least-squares cycle used anisotropically in a structure factor calculation and in three cycles of block approximation least-squares refinement. Although almost all the poorly matched reflections ($|F_{\text{obs}} - F_{\text{calc}}| > 20$) improved, a Fourier synthesis revealed peaks at positions shifted to a less reasonable distribution from the linear hydrocarbon approximation used. The refinement was terminated at this point. An outline of the refinement is presented in Table 5.

Scattering factors for cobalt, phosphorus, fluorine, oxygen, and carbon were taken from Hanson *et al.*²⁹ A list of observed and calculated structure factors is available.¹⁴

Structure Solution and Refinement: for $C_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$

The method of isomorphous replacement was used for the solution of the structure of $C_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$. The cell constants of $C_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$ and $C_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$ as reported in Table 4 are very similar with differences of less than one percent. The positional parameters from the third cycle of full-matrix least-squares refinement for the non-hydrogen atoms in the isomorphous compound $C_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$ were used in a structure factor calculation and a difference Fourier synthesis with the $C_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$ data. The structure factor calculation resulted in an R of 0.17 and the

difference Fourier synthesis revealed no major structural differences in the two compounds. The same positional parameters were used in an isotropic least-squares refinement of the $C_4(fph)_4Rh(cp)(tpp)$ data. A summary of further refinement is given in Table 5.

A difference Fourier synthesis after refinement suggested the presence of an ill-defined solvent molecule. As in the case of the cobaltacycle the calculated density, 1.479 g/cm^3 , is significantly less than the density of 1.60 g/cm^3 obtained from flotation measurements of the yellow crystals. If two molecules of *n*-heptane are assumed within the unit cell the calculated density would be 1.60 g/cm^3 .

An attempt to fit a linear molecule to peaks in the difference Fourier synthesis was also unsuccessful and was not pursued.

The scattering factors used were taken from Hanson et al.²⁹ The observed and calculated structures are listed in Table B-5.

Results and Discussion for $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$

The final positional and thermal parameters for the nonhydrogen atoms of both $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$ are listed in Table 31. The atomic numbering and thermal ellipsoids of the cobaltacycle are shown in Figure 10. The atomic numbering of the rhodacycle is analogous. Selected bond distances and angles for the two compounds are listed

Table 31

Final Atomic Parameters ($\times 10^4$) for the Nonhydrogen Atoms in $C_4(fph)_2Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$ with Estimated Standard Deviations Given in Parentheses.^a

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co	482(1)	4958(1)	2130(1)	65(1)	64(1)	24(0)	55(2)	32(1)	46(1)
Rh	453(1)	4917(1)	2125(0)	62(1)	63(1)	25(0)	54(1)	29(1)	44(1)
C(1)	1469(8)	4004(8)	2096(5)	78(10)	71(8)	27(3)	70(15)	32(10)	52(9)
	1546(9)	4003(8)	2101(5)	96(11)	71(8)	26(3)	77(16)	36(10)	49(9)
C(2)	2439(8)	4318(8)	1903(5)	89(10)	78(8)	26(3)	95(16)	51(10)	53(9)
	2531(9)	4307(8)	1901(5)	87(10)	61(8)	26(3)	63(15)	41(10)	43(9)
C(3)	2748(3)	5385(7)	1870(5)	72(9)	71(8)	27(3)	84(15)	48(10)	51(9)
	2825(8)	5370(8)	1872(5)	70(9)	68(8)	26(3)	66(15)	34(9)	48(9)
C(4)	1955(8)	5881(7)	2001(5)	78(10)	69(8)	23(3)	52(15)	25(9)	51(9)
	2016(8)	5864(8)	2003(5)	72(9)	75(8)	26(3)	57(15)	27(9)	56(9)
C(11)	1050(9)	2894(8)	2093(5)	82(10)	72(8)	38(4)	80(16)	60(11)	68(10)
	1091(9)	2877(8)	2092(6)	89(11)	73(9)	37(4)	84(16)	52(11)	63(10)
C(12)	1267(9)	2877(8)	2792(6)	89(11)	79(9)	39(4)	76(16)	45(11)	67(10)
	1298(10)	2836(9)	2781(6)	94(11)	89(10)	42(4)	84(17)	55(12)	83(11)
C(13)	889(10)	1830(9)	2778(6)	135(14)	116(11)	51(5)	134(21)	89(14)	117(13)
	902(11)	1800(10)	2759(7)	127(14)	112(11)	56(5)	115(21)	80(14)	117(14)
C(14)	263(12)	754(9)	2043(7)	168(16)	87(10)	68(6)	135(22)	117(17)	107(14)
	273(12)	735(10)	2027(8)	166(16)	83(10)	78(7)	131(22)	122(13)	125(15)
C(15)	19(11)	736(9)	1333(6)	151(15)	80(10)	47(5)	116(20)	97(14)	60(11)
	35(12)	725(9)	1327(7)	147(15)	74(10)	57(6)	81(20)	92(16)	65(13)
C(16)	445(10)	1799(8)	1379(6)	126(13)	80(9)	43(4)	110(18)	87(13)	78(11)
	438(11)	1777(9)	1363(6)	132(13)	82(9)	44(5)	109(19)	84(13)	75(11)

Table 31 - continued

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
F(12)	1875(6) 1952(6)	3866(5) 3850(5)	3516(3) 3520(3)	148(8) 153(8)	97(5) 98(6)	34(2) 38(2)	91(11) 96(11)	53(7) 54(7)	67(6) 72(6)
F(13)	1138(7) 1163(8)	1855(6) 1809(7)	3474(4) 3446(4)	215(10) 210(11)	147(7) 160(8)	64(3) 68(4)	164(14) 152(16)	113(10) 101(10)	157(9) 169(10)
F(14)	-138(8) -143(9)	-275(6) -293(6)	2022(5) 1990(5)	272(12) 263(13)	103(7) 100(7)	90(4) 101(5)	182(15) 162(16)	178(13) 158(14)	145(9) 149(10)
F(15)	-612(7) -610(9)	-301(5) -305(6)	622(4) 602(5)	239(11) 249(12)	78(6) 72(6)	65(3) 70(4)	112(13) 86(14)	132(10) 138(12)	62(7) 52(8)
F(16)	198(6) 188(7)	1719(5) 1725(5)	670(3) 667(3)	182(8) 188(9)	37(5) 36(6)	37(2) 39(3)	106(11) 94(12)	88(8) 79(8)	54(6) 50(6)
C(21)	3171(9) 3231(9)	3601(8) 3588(8)	1668(5) 1667(5)	106(11) 87(10)	71(8) 74(9)	33(4) 35(4)	87(16) 86(16)	56(11) 51(11)	58(10) 58(10)
C(22)	4034(10) 4056(10)	3453(9) 3435(9)	2197(6) 2182(6)	123(13) 118(13)	95(10) 86(10)	42(4) 41(5)	135(19) 113(19)	68(13) 60(13)	67(11) 62(11)
C(23)	4718(12) 4706(11)	2839(11) 2768(11)	1981(7) 1945(8)	145(15) 123(14)	140(13) 114(12)	59(6) 63(6)	190(25) 157(22)	75(16) 67(15)	103(15) 99(15)
C(24)	4545(12) 4517(12)	2345(11) 2266(11)	1201(8) 1170(8)	154(16) 137(15)	126(13) 113(12)	78(7) 65(6)	198(25) 173(23)	128(18) 98(16)	99(16) 77(15)
C(25)	3682(11) 3684(12)	2460(9) 2412(10)	647(6) 635(7)	159(15) 156(15)	98(11) 91(11)	48(5) 45(5)	123(22) 109(21)	107(15) 100(15)	58(12) 50(12)
C(26)	3020(12) 3043(10)	3081(8) 3059(9)	825(6) 876(6)	112(12) 100(11)	84(9) 83(9)	42(4) 41(4)	103(19) 95(17)	68(13) 65(12)	69(11) 66(11)
F(22)	4250(7) 4288(7)	2923(6) 3912(6)	2967(4) 2963(4)	188(9) 170(9)	145(7) 147(7)	47(3) 46(3)	216(14) 204(14)	75(8) 68(3)	100(5) 101(3)
F(23)	5532(8) 5526(9)	2681(8) 2636(8)	2501(5) 2478(5)	237(12) 228(12)	215(10) 205(11)	81(4) 80(4)	346(20) 337(20)	104(12) 98(12)	152(11) 144(12)

Atom	z	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
F(24)	5233(9) 5155(9)	1775(8) 1657(8)	972(5) 926(6)	261(13) 233(13)	200(10) 179(10)	102(5) 101(5)	359(20) 310(20)	197(14) 180(14)	134(12) 120(12)
F(25)	3500(8) 3478(8)	1971(6) 1910(7)	-124(4) -144(4)	251(12) 238(12)	151(8) 148(8)	65(4) 63(4)	210(16) 200(17)	176(11) 164(11)	97(9) 90(9)
F(26)	2165(6) 2223(6)	3179(5) 3177(6)	329(3) 332(3)	177(9) 167(9)	111(6) 118(6)	37(2) 38(2)	143(12) 150(13)	79(8) 77(8)	71(7) 75(7)
C(31)	3869(9) 3949(9)	5823(7) 5834(8)	1701(5) 1710(5)	92(10) 94(11)	63(8) 68(8)	33(4) 34(4)	77(15) 85(16)	50(11) 51(11)	56(9) 54(10)
C(32)	3655(9) 3746(10)	5820(8) 5826(9)	992(6) 1002(6)	103(12) 108(12)	84(9) 89(10)	37(4) 37(4)	87(17) 91(18)	57(12) 61(12)	61(11) 69(11)
C(33)	4687(11) 4764(12)	6121(10) 6138(10)	789(7) 805(7)	161(15) 153(15)	119(12) 106(11)	55(5) 51(5)	151(22) 125(22)	135(16) 114(15)	110(14) 96(13)
C(34)	5991(11) 6049(11)	6489(10) 6498(10)	1326(7) 1334(7)	113(13) 123(13)	125(12) 112(11)	73(6) 69(6)	123(21) 136(21)	132(16) 144(16)	118(15) 109(14)
C(35)	6264(9) 6328(10)	6524(9) 6544(10)	2038(7) 2048(7)	80(11) 81(11)	109(11) 100(10)	63(6) 60(5)	108(19) 104(18)	80(14) 73(13)	92(13) 87(13)
C(36)	5234(9) 5288(10)	6200(9) 6213(9)	2213(6) 2221(6)	104(11) 94(11)	92(10) 90(10)	39(4) 37(4)	111(18) 84(18)	59(12) 42(12)	72(11) 63(11)
F(32)	2390(6) 2468(6)	5458(5) 5439(6)	454(3) 459(3)	127(7) 122(7)	147(7) 147(7)	43(3) 40(3)	129(12) 125(12)	63(7) 56(7)	107(7) 104(7)
F(33)	4392(7) 4482(8)	6050(7) 6073(7)	81(4) 94(4)	225(11) 212(11)	199(9) 194(10)	67(4) 65(4)	212(17) 204(17)	174(11) 166(11)	169(10) 158(10)
F(34)	6973(7) 7059(8)	6763(7) 6827(8)	1127(5) 1164(6)	178(10) 164(10)	213(10) 208(10)	111(5) 111(5)	200(17) 198(17)	224(13) 207(13)	206(12) 203(13)
F(35)	7531(6) 7607(6)	6879(7) 6928(7)	2557(5) 2567(5)	100(7) 88(7)	181(9) 163(8)	93(4) 84(4)	158(13) 127(13)	99(9) 76(9)	154(10) 124(10)

Table 31 - continued

Atom	z	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
F(36)	5552(5) 5597(6)	5243(6) 5265(6)	2923(3) 2930(4)	106(7) 107(7)	157(7) 152(7)	47(3) 46(3)	125(12) 127(12)	48(7) 47(7)	112(8) 105(8)
C(41)	2261(9) 2290(9)	7041(8) 7009(8)	2072(5) 2054(5)	91(10) 80(10)	75(8) 72(8)	33(4) 32(4)	95(16) 76(15)	64(11) 53(10)	61(10) 59(9)
C(42)	1472(9) 1474(10)	7178(8) 7113(9)	1482(5) 1470(6)	107(11) 98(11)	90(9) 83(9)	31(4) 34(4)	104(18) 88(17)	50(11) 45(11)	65(10) 67(10)
C(43)	1764(10) 1711(12)	8273(9) 8169(10)	1579(6) 1549(7)	137(14) 150(15)	109(11) 118(12)	49(5) 50(5)	150(21) 157(22)	81(14) 84(15)	109(13) 115(14)
C(44)	2816(11) 2786(12)	9268(9) 9217(10)	2269(7) 2252(7)	143(14) 144(14)	79(9) 91(11)	61(6) 68(6)	110(20) 128(21)	106(15) 111(16)	95(13) 113(14)
C(45)	3644(10) 3630(10)	9168(8) 9135(9)	2845(6) 2818(6)	105(12) 103(12)	79(9) 84(10)	45(5) 45(5)	54(18) 51(18)	70(13) 64(13)	57(11) 54(11)
C(45)	3377(8) 3405(9)	8056(8) 8064(8)	2729(5) 2722(6)	78(10) 94(11)	68(8) 73(9)	32(4) 37(4)	54(15) 72(16)	39(10) 56(11)	52(9) 65(10)
F(42)	388(5) 402(6)	6210(5) 6129(5)	778(3) 785(3)	129(7) 127(7)	110(6) 107(6)	35(2) 38(2)	99(11) 96(11)	34(7) 30(7)	78(6) 78(6)
F(43)	970(7) 887(8)	8332(6) 8225(7)	985(4) 964(5)	213(10) 198(11)	152(8) 165(3)	74(4) 79(4)	214(15) 204(16)	100(10) 92(11)	166(9) 179(10)
F(44)	3063(8) 3005(8)	10324(6) 10263(6)	2369(5) 2332(5)	236(11) 236(12)	96(6) 98(7)	93(4) 100(5)	155(14) 172(15)	133(12) 144(13)	131(9) 137(10)
F(45)	4746(6) 4715(7)	10156(5) 10148(5)	3532(4) 3495(4)	162(9) 164(9)	81(6) 73(6)	61(3) 64(3)	35(11) 31(12)	75(9) 79(9)	55(7) 47(7)
F(46)	4247(5) 4296(5)	8032(5) 8055(5)	3315(3) 3305(3)	100(6) 100(6)	94(5) 93(5)	38(2) 37(2)	68(10) 64(10)	34(6) 29(6)	63(6) 59(6)
C(51)	-1476(9) -1641(9)	4842(10) 4744(11)	1969(6) 1924(6)	53(10) 63(10)	125(11) 133(13)	40(4) 43(5)	70(18) 72(19)	22(11) 27(12)	77(12) 77(13)

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(52)	-1486(9)	3709(9)	1766(6)	64(10)	112(11)	50(5)	26(18)	25(12)	90(13)
	-1672(10)	3638(11)	1750(7)	66(11)	125(13)	56(6)	6(19)	16(13)	103(14)
C(53)	-1196(10)	3326(9)	1116(6)	99(12)	84(10)	34(4)	61(18)	10(12)	41(11)
	-1403(10)	3198(10)	1083(7)	77(11)	90(10)	48(5)	29(18)	1(12)	54(12)
C(54)	-929(9)	4195(8)	911(5)	88(11)	89(9)	29(4)	81(17)	21(11)	40(10)
	-1161(10)	4034(10)	847(6)	81(11)	108(11)	30(4)	73(18)	10(11)	41(11)
C(55)	-1115(9)	5132(9)	1426(6)	77(11)	111(10)	35(4)	80(18)	19(11)	73(11)
	-1339(9)	4970(10)	1355(6)	71(10)	104(11)	41(4)	62(17)	16(11)	69(12)
P	1381(2)	6265(2)	3462(1)	72(3)	71(2)	26(1)	61(4)	39(3)	52(2)
	1433(2)	6288(2)	3493(1)	71(3)	72(2)	26(1)	62(4)	38(3)	53(2)
C(60)	174(9)	5972(8)	3855(5)	77(10)	97(10)	30(4)	67(16)	44(10)	61(10)
	188(9)	5980(9)	3869(6)	82(10)	108(10)	30(4)	75(17)	52(11)	71(11)
C(61)	-309(10)	4875(10)	3800(6)	118(13)	117(11)	53(5)	95(20)	87(14)	109(13)
	-282(11)	4899(10)	3822(7)	126(14)	123(12)	50(5)	99(22)	88(14)	111(14)
C(62)	-1268(12)	4596(11)	4068(8)	143(15)	158(15)	66(6)	103(25)	119(17)	140(17)
	-1248(13)	4597(12)	4062(8)	162(17)	146(15)	67(7)	124(26)	124(18)	130(17)
C(63)	-1740(12)	5396(12)	4382(8)	160(17)	160(15)	65(6)	126(26)	134(18)	121(17)
	-1735(14)	5371(14)	4357(9)	159(18)	171(17)	74(7)	132(29)	136(20)	137(19)
C(64)	-1260(14)	6475(12)	4438(8)	206(20)	158(16)	80(8)	182(30)	202(22)	129(19)
	-1248(15)	6446(14)	4401(10)	188(20)	184(18)	91(9)	213(33)	196(23)	156(22)
C(65)	-281(11)	6770(10)	4179(7)	156(15)	130(12)	59(6)	161(23)	140(16)	105(14)
	-311(12)	6748(11)	4152(7)	135(15)	137(13)	60(6)	147(24)	128(16)	99(15)
C(70)	2931(9)	6458(8)	4204(5)	93(11)	67(8)	30(4)	53(16)	30(11)	53(10)
	2953(9)	6484(8)	4230(5)	73(10)	72(8)	29(4)	60(15)	26(10)	53(9)
C(71)	3110(10)	6734(9)	4984(6)	130(13)	96(10)	33(4)	76(19)	47(12)	72(11)
	3141(11)	6760(10)	5001(6)	111(13)	118(12)	35(4)	70(20)	36(12)	81(12)

Table 31 - continued

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(72)	4288(11) 4315(12)	6884(10) 6902(12)	5544(6) 5555(7)	121(14) 123(14)	122(12) 145(14)	42(5) 42(5)	56(21) 77(23)	24(13) 26(14)	92(13) 102(14)
C(73)	5256(11) 5271(12)	6731(10) 6770(11)	5313(7) 5344(7)	113(14) 116(14)	128(13) 130(13)	54(5) 52(6)	81(22) 84(23)	22(14) 25(14)	102(14) 101(15)
C(74)	5079(10) 5119(11)	6465(10) 6504(11)	4545(6) 4572(7)	102(13) 109(14)	116(12) 118(13)	46(5) 52(6)	92(20) 81(22)	27(13) 20(14)	74(13) 78(14)
C(75)	3935(9) 3938(9)	6342(8) 6368(9)	3993(6) 4025(6)	76(10) 79(11)	85(9) 91(10)	38(4) 37(4)	72(16) 72(17)	32(11) 22(11)	58(10) 59(11)
C(80)	1783(9) 1836(9)	7786(8) 7791(8)	3738(5) 3744(5)	101(11) 91(11)	77(9) 85(9)	31(4) 32(4)	84(16) 90(16)	66(11) 56(11)	58(10) 66(10)
C(81)	857(9) 938(10)	7958(8) 7945(9)	3226(6) 3225(6)	109(12) 117(13)	93(10) 91(10)	41(4) 37(4)	115(18) 109(19)	77(12) 65(12)	75(11) 67(11)
C(82)	1115(11) 1146(12)	9122(10) 9094(10)	3449(7) 3420(7)	144(14) 150(15)	112(11) 91(15)	54(5) 53(5)	154(21) 135(21)	107(15) 94(15)	100(13) 89(13)
C(83)	2298(11) 2317(13)	10114(10) 10102(10)	4154(7) 4129(2)	143(13) 158(16)	99(11) 98(11)	53(6) 53(6)	109(21) 115(23)	193(16) 101(17)	81(13) 76(14)
C(84)	3216(11) 3211(12)	9918(9) 9921(10)	4656(7) 4638(7)	127(14) 133(15)	84(10) 91(11)	53(5) 55(6)	80(20) 85(21)	81(15) 67(15)	69(12) 70(13)
C(85)	2962(10) 2980(10)	8774(9) 8797(9)	4448(6) 4458(6)	113(12) 105(12)	83(10) 81(10)	38(4) 42(5)	65(18) 69(18)	53(12) 54(12)	58(11) 57(11)

^aThe coordinates of the atoms in each structure are listed in order of the metal atom.

Figure 10

An ORTEP drawing of $C_4(fph)_4Co(cp)(tpp)$ showing the atomic numbering and thermal ellipsoids. The fph rings are numbered 1-4 and the fluorines have been omitted for clarity. Similarly, the three phenyl rings of the tpp ligand have been omitted with only the first atoms C(60), C(70), and C(80) shown.

in Tables 32 and 33. Least-squares planes and deviations are given in Table 34.

The molecules are metallocycles with the metal atom also bonded to the cyclopentadienyl ring and to the triphenylphosphine ligand. The C(1) to C(4) fragment in both compounds is planar with the largest deviation from the best plane being 0.015 Å in the cobalt compound and 0.017 Å in the rhodium compound. The metal atoms, however, are significantly displaced from the plane in the direction of the cp ring by -0.203 and -0.239 Å. This perpendicular displacement is similar to that found in other similar metallocycles. ⁹⁸

The metallocycles may be considered as a delocalized diene with the metal atom σ -bonded to the two carbon atoms of the ring, C(1) and C(4). The Co-C bond distances, 1.995(11) and 1.993(11) Å, and the Rh-C bond distances, 2.060(12) and 2.067(11) Å, are similar to various values given by Churchill.⁹⁹ Values of 1.979(1) Å⁴⁸ and 1.990(5) Å⁵¹ have more recently been reported for Co-C bonds in cobaloxime complexes. Mague^{100,101} has reported structures of similar rhodacycles in which the Rh-C distances are 2.000(11), 1.964(11), 2.047(16), and 1.998(16) Å. Also, Cotton and Norman¹⁰² report a single-bond covalent radius of 1.39 Å for Rh(III). When this value is added to half the 1.485 Å suggested length for a single-bond between sp^2 carbon atoms¹⁰³ the Rh-C distance is predicted to be 2.13 Å. The observed Rh-C distances where rhodium has a formal oxidation number of +1 are shorter than the above predicted single-bond distance. This differ-

Table 32
 Selected Bond Distances (Å) of $C_4(fph)_4M(cp)(tpp)$ (M=Co, Rh)
 with Their Estimated Standard Deviations in Parentheses.

	M = Co	Rh
M - C(1)	1.995(11)	2.060(12)
M - C(4)	1.993(11)	2.067(11)
M - P	2.234(3)	2.293(2)
M - C(51)	2.157(12)	2.286(13)
M - C(52)	2.121(13)	2.261(14)
M - C(53)	2.119(11)	2.250(13)
M - C(54)	2.104(9)	2.238(10)
M - C(55)	2.133(12)	2.268(12)
C(1)-C(2)	1.326(15)	1.343(16)
C(2)-C(3)	1.467(16)	1.457(16)
C(3)-C(4)	1.335(15)	1.354(15)
C(1)-C(11)	1.487(16)	1.498(17)
C(2)-C(21)	1.523(16)	1.497(16)
C(3)-C(31)	1.481(15)	1.478(16)
C(4)-C(41)	1.493(16)	1.492(17)
P-C(60)	1.848(11)	1.858(12)
P-C(70)	1.843(11)	1.821(10)
P-C(80)	1.834(12)	1.820(13)
C(51)-C(52)	1.463(20)	1.429(22)
C(52)-C(53)	1.400(16)	1.420(17)
C(53)-C(54)	1.426(18)	1.424(20)
C(54)-C(55)	1.433(16)	1.422(17)
C(55)-C(51)	1.457(17)	1.431(18)

Table 33

Selected Bond Angles ($^{\circ}$) of $C_4(fph)_4M(cp)(tpp)$ with Their
Estimated Standard Deviations Given in Parentheses. (M=Co, Rh)

	M = Co	Rh
M-C(1)-C(2)	112.1(8)	115.5(8)
C(1)-C(2)-C(3)	116.8(9)	114.9(9)
C(2)-C(3)-C(4)	114.8(9)	115.5(9)
M-C(4)-C(3)	113.1(7)	114.8(8)
C(1)-M-C(4)	82.4(4)	78.3(4)
P-M-C(1)	103.0(3)	101.6(3)
P-M-C(4)	95.2(3)	93.3(3)
C(11)-C(1)-M	127.0(7)	123.3(8)
C(11)-C(1)-C(2)	119.6(9)	119.4(10)
C(21)-C(2)-C(1)	123.9(9)	124.1(10)
C(21)-C(2)-C(3)	119.2(9)	120.9(9)
C(31)-C(3)-C(2)	119.7(9)	119.7(9)
C(31)-C(3)-C(4)	125.5(9)	124.9(10)
C(41)-C(4)-C(3)	119.8(9)	120.3(9)
C(41)-C(4)-M	127.0(7)	124.9(7)
C(51)-C(52)-C(53)	108.1(11)	108.3(12)
C(52)-C(53)-C(54)	109.8(10)	108.8(11)
C(53)-C(54)-C(55)	107.7(10)	106.9(11)
C(54)-C(55)-C(51)	108.0(10)	109.3(11)
C(55)-C(51)-C(52)	106.3(10)	106.8(11)

Table 34

Deviations from and Equations of Some Least-Squares Planes of $C_4(fph)_4Co(cp)(tpp)$ and $C_4(fph)_4Rh(cp)(tpp)$.^a

(a) Deviations ($\text{\AA} \times 10^{+3}$)				
Atom	Plane 1	Plane 2	Plane 3	Plane 4
Co	-203		1741	
Rh		-239		1908
C(1)	8*	9*		
C(2)	-15*	-17*		
C(3)	14*	17*		
C(4)	-8*	-9*		
C(51)	-931	-1058	-7*	2*
C(52)	-1211	-1307	15*	6*
C(53)	-2043	-2168	-16*	-12*
C(54)	-2265	-2437	11*	13*
C(55)	-1598	-1774	-2*	-9*
P	1884	1922	3025	3241

(b) Coefficients of the Plane ⁵⁹ $AX + BY + CZ = D$				
Plane	A	B	C	D
1	0.2201	0.0627	0.9735	3.2807
2	0.2193	0.0672	0.9733	3.3160
3	0.7356	0.1345	0.6639	-0.8420
4	0.7474	0.1591	0.6450	-1.0481

^aThe entries marked with an asterisk were used to define the plane.

ence could be indicative of multiple bonding between the terminal carbon atoms of the diene and the metal atom. The C-C distances in the metallocycle rings fall into two groups. The C(1)-C(2) and C(3)-C(4) distances are equal within experimental error to the accepted value of $1.337(6) \text{ \AA}$ for a simple C-C double bond.¹⁰⁴ The C(2)-C(3) distances are indicative of a C-C single bond between two double bonds.¹⁰⁴ The observations of Mague^{100,101} on two rhodacycles suggested a double-bond system similar to those in $C_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$ and $C_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$.

The cp rings in the compounds are planar with the maximum deviations from the least-squares planes of -0.016 and $-0.012 \text{ \AA}$. The distances from the cp ring atoms to the metal atom show that the metal atom is slightly displaced from the center of the cp ring. The range of the Co-C(cp ring) distances is from $2.104(9)$ to $2.157(12) \text{ \AA}$ with a mean of $2.127(9) \text{ \AA}$. These values are similar to those in other Co-cp complexes.^{105,106}

In both the cobalt and rhodium compounds the longest metal-C(cp ring) distance involves C(51), the carbon atom nearest the phosphine ligand. The mean Rh-C(cp ring) distance is $2.286(13) \text{ \AA}$. This value is equivalent to the mean distance of $2.246(9) \text{ \AA}$ in $\text{Rh}(\text{C}_2\text{F}_5)(\text{cp})\text{I}(\text{CO})$ ¹⁰⁷ and falls within the 2.19 to $2.26 \text{ \AA}$ range reported for corresponding mean values for other cp-rhodium complexes.¹⁰⁸

The C-C bond distances within the cp rings range from $1.400(16)$ to $1.463(20) \text{ \AA}$ with a mean of $1.436(11) \text{ \AA}$ in the

cobalt compound and a range from 1.420(17) to 1.431(18) Å with a mean of 1.425 Å in the rhodium compound. These C-C distances are comparable to those found in other cp complexes.^{105,106,109} The cp rings are tipped relative to the C(1) to C(4) planes by 35.3° and 36.6°.

The Co-P distance of 2.234(3) Å is similar to the Co-P distance in five-coordinate complexes of cobalt where the range is reported¹¹⁰ to be from 2.192(6) to 2.27(1) Å. Also, in cobalt-carbonyl complexes such as $\text{Co}_4(\text{CO})_{10}(\text{Ph}_2\text{P}=\text{CCF}_3)_2$ and $\text{Co}(\text{CO})_2(\text{NO})(\text{tpp})$ the Co-P distances are 2.236 and 2.229 Å¹¹¹ in the former and 2.224(3) and 2.230(3) Å¹¹² in the latter. The Rh-P distance of 2.293(3) Å is similar to those in phosphine complexes of rhodium(I).¹¹³ The metal to phosphine distance in metal-oxime complexes have been found to be somewhat longer.^{40,97} The Co-P distance in cobaloxime complexes has been reported as 2.327(4) Å⁴⁰ and 2.339(1) Å.⁴⁸ The Rh-P distance in $\text{RhCl}(\text{Hdmg})_2(\text{tpp})$ was reported to be 2.327(1) Å.¹⁰² Since the distances in oxime complexes in both cobalt and rhodium are equivalent, the phosphorus atom may be in the position of closest approach to the metal atom as limited by the steric constraints of the oxime ligands.

The distances in the fph rings have been summarized in Table 35. The individual values for the distances and angles in the fph rings on the metallocycles and the phenyl rings of the phosphines are given in Tables 36-38. The dimensions are not unusual and are in agreement with expected values.

Table 35
Average C-F and C-C Distances for the Pentafluorophenyl Groups in $C_4(fph)_4M(cp)(tpp)$ with Estimated Standard Deviations^a Given in Parentheses (M=Co,Rh).

M =	(a) C-F Distances (Å)		(b) C-C Distances (Å)	
	Co	Rh	Co	Rh
All Rings	1.344(2)	1.344(2)	1.378(3)	1.373(3)
Ring 1	1.342(6)	1.340(3)	1.385(1)	1.376(4)
Ring 2	1.345(4)	1.347(4)	1.373(4)	1.371(9)
Ring 3	1.340(3)	1.345(3)	1.384(8)	1.375(6)
Ring 4	1.348(4)	1.346(3)	1.372(8)	1.371(7)

^aStandard deviations were estimated using the equation:

$$\sigma = \left[\sum_{i=1}^N (x_i - \bar{x})^2 / N(N-1) \right]^{1/2}$$

Table 36
Bond Distances and Bond Angles of Pentafluorophenyl Groups
in $C_4(fph)_4Rh(cp)(tpp)$.

(a) Distances ($\text{\AA}$)

n =	1	2	3	4
Cn1-Cn2	1.384 (15)	1.342 (16)	1.392 (15)	1.385 (15)
Cn2-Cn3	1.364 (20)	1.400 (20)	1.374 (20)	1.351 (20)
Cn3-Cn4	1.375 (18)	1.358 (18)	1.357 (19)	1.389 (18)
Cn4-Cn5	1.367 (19)	1.365 (20)	1.368 (18)	1.355 (19)
Cn5-Cn6	1.372 (20)	1.373 (19)	1.367 (18)	1.362 (19)
Cn6-Cn1	1.393 (15)	1.389 (14)	1.389 (16)	1.386 (14)
Cn2-Fn2	1.347 (12)	1.354 (12)	1.351 (13)	1.344 (12)
Cn3-Fn3	1.339 (15)	1.341 (18)	1.349 (15)	1.348 (16)
Cn4-Fn4	1.338 (18)	1.337 (19)	1.335 (18)	1.340 (18)
Cn5-Fn5	1.343 (15)	1.358 (14)	1.338 (15)	1.357 (14)
Cn6-Fn6	1.331 (13)	1.343 (14)	1.351 (13)	1.342 (13)

(b) Angles ($^\circ$)

Cn1-Cn2-Cn3	123.1 (11)	122.4 (12)	123.7 (11)	122.9 (11)
Cn2-Cn3-Cn4	119.6 (13)	119.3 (13)	118.8 (13)	120.2 (13)
Cn3-Cn4-Cn5	119.6 (13)	119.3 (14)	120.8 (13)	117.9 (13)
Cn4-Cn5-Cn6	119.8 (13)	120.6 (13)	119.0 (12)	121.4 (12)
Cn5-Cn6-Cn1	122.6 (12)	121.1 (11)	123.6 (11)	122.0 (11)
Cn6-Cn1-Cn2	115.3 (11)	117.3 (11)	114.1 (10)	115.4 (10)
Cn -Cn1-Cn2	124.2 (10)	123.9 (10)	123.1 (10)	124.1 (10)
Cn -Cn1-Cn6	120.5 (10)	118.8 (10)	122.5 (10)	120.5 (10)
Fn2-Cn2-Cn1	120.2 (10)	121.3 (11)	118.2 (10)	119.4 (10)
Fn2-Cn2-Cn3	116.7 (11)	116.4 (11)	118.0 (11)	117.7 (11)
Fn3-Cn3-Cn2	120.9 (12)	120.7 (13)	120.3 (12)	120.8 (12)
Fn3-Cn3-Cn4	119.5 (12)	120.0 (13)	120.9 (12)	119.0 (12)
Fn4-Cn4-Cn3	120.7 (13)	121.3 (14)	119.9 (13)	119.9 (12)
Fn4-Cn4-Cn5	119.7 (13)	119.4 (13)	119.3 (13)	122.1 (13)
Fn5-Cn5-Cn4	120.9 (13)	120.1 (13)	119.6 (12)	118.8 (12)

Table 36 - continued

	n = 1	2	3	4
Fn6-Cn6-Cn5	115.7(10)	118.3(11)	117.6(10)	117.2(9)
Fn6-Cn6-Cn1	120.4(10)	118.8(10)	118.5(10)	119.7(9)

Table 37
Bond Distances and Bond Angles of Pentafluorophenyl Groups
in $C_4(fph)_4Co(cp)(tpp)$.

(a) Distances ($\text{\AA}$)				
n =	1	2	3	4
Cn1-Cn2	1.387(14)	1.372(16)	1.394(14)	1.403(15)
Cn2-Cn3	1.388(19)	1.368(20)	1.398(19)	1.358(19)
Cn3-Cn4	1.387(17)	1.374(18)	1.370(18)	1.348(16)
Cn4-Cn5	1.382(17)	1.374(20)	1.372(18)	1.370(17)
Cn5-Cn6	1.382(18)	1.363(19)	1.362(18)	1.384(17)
Cn6-Cn1	1.385(14)	1.389(14)	1.408(15)	1.367(14)
Cn2-Fn2	1.322(11)	1.341(12)	1.339(13)	1.358(11)
Cn3-Fn3	1.350(14)	1.338(17)	1.339(14)	1.338(14)
Cn4-Fn4	1.360(17)	1.339(19)	1.334(17)	1.335(16)
Cn5-Fn5	1.336(13)	1.354(13)	1.330(14)	1.361(13)
Cn6-Fn6	1.341(12)	1.355(13)	1.356(12)	1.348(12)
(b) Angles ($^\circ$)				
Cn1-Cn2-Cn3	122.4(11)	122.9(12)	123.4(11)	122.6(10)
Cn2-Cn3-Cn4	119.7(12)	119.2(13)	118.9(12)	120.5(12)
Cn3-Cn4-Cn5	119.6(12)	120.1(14)	120.2(13)	118.7(12)
Cn4-Cn5-Cn6	118.7(12)	119.0(12)	119.8(12)	120.4(11)
Cn5-Cn6-Cn1	123.9(11)	122.9(11)	123.8(11)	123.0(10)
Cn6-Cn1-Cn2	115.6(10)	116.0(10)	113.9(10)	114.5(10)
Cn -Cn1-Cn2	123.3(10)	123.8(10)	122.9(9)	124.2(9)
Cn -Cn1-Cn6	121.0(10)	120.2(10)	123.0(9)	121.3(9)
Fn2-Cn2-Cn1	121.4(10)	120.5(10)	119.1(10)	119.8(9)
Fn2-Cn2-Cn3	116.2(10)	116.6(11)	117.5(10)	117.7(10)
Fn3-Cn3-Cn3	120.4(11)	122.0(13)	119.9(11)	119.1(11)
Fn3-Cn3-Cn4	119.9(11)	118.8(13)	121.2(12)	120.4(11)
Fn4-Cn4-Cn3	120.0(12)	121.2(13)	118.9(12)	120.1(11)
Fn4-Cn4-Cn5	120.4(12)	118.7(13)	120.9(12)	121.2(11)
Fn5-Cn5-Cn4	119.7(11)	120.5(12)	119.9(12)	119.8(11)
Fn5-Cn5-Cn6	121.6(11)	120.5(12)	120.3(11)	119.8(10)

Table 37 - continued

n =	1	2	3	4
Fn5-Cn5-Cn6	119.4 (12)	119.3 (12)	121.4 (12)	119.8 (11)
Fn6-Cn6-Cn5	117.7 (11)	119.0 (11)	117.6 (11)	117.9 (10)
Fn6-Cn6-Cn1	119.7 (11)	119.9 (10)	118.9 (10)	120.1 (10)

Table 38
Bond Distances and Bond Angles of Triphenylphosphine in $C_4(fph)_4M(cp)(tpp)$.
(a) Distances (Å)

M =	n = 6			7			8		
	Co	Rh	Co	Co	Rh	Co	Rh	Co	Rh
P-C(n0)	1.848(11)	1.858(12)	1.843(11)	1.821(10)	1.820(12)	1.834(12)	1.820(13)		
C(n0)-C(n1)	1.419(19)	1.400(20)	1.411(14)	1.387(14)	1.387(16)	1.416(16)	1.395(16)		
C(n1)-C(n2)	1.414(20)	1.382(22)	1.394(17)	1.399(19)	1.413(19)	1.413(20)	1.413(20)		
C(n2)-C(n3)	1.397(22)	1.379(25)	1.386(19)	1.347(21)	1.416(17)	1.416(19)	1.413(19)		
C(n3)-C(n4)	1.394(25)	1.396(30)	1.390(17)	1.405(18)	1.422(19)	1.406(21)	1.406(21)		
C(n4)-C(n5)	1.423(23)	1.367(25)	1.376(16)	1.403(18)	1.391(19)	1.380(21)	1.380(21)		
C(n5)-C(n0)	1.337(18)	1.377(20)	1.394(16)	1.368(16)	1.413(14)	1.404(15)	1.404(15)		
(b) Angles (°)									
P-C(n0)-C(n1)	117.7(8)	117.4(9)	120.3(8)	121.4(9)	118.3(8)	118.5(9)	118.5(9)		
P-C(n0)-C(n5)	122.2(9)	122.2(10)	119.6(8)	119.5(8)	121.8(8)	122.3(9)	122.3(9)		
C(n0)-C(n1)-C(n2)	119.7(12)	120.1(13)	119.9(11)	120.3(12)	119.5(11)	121.0(11)	121.0(11)		
C(n1)-C(n2)-C(n3)	120.0(13)	119.7(15)	119.0(12)	120.3(14)	120.7(12)	119.5(12)	119.5(12)		
C(n2)-C(n3)-C(n4)	120.2(14)	119.2(16)	120.8(13)	120.8(14)	118.7(12)	118.2(13)	118.2(13)		
C(n3)-C(n4)-C(n5)	120.2(14)	121.8(17)	120.8(12)	118.2(13)	120.8(12)	122.0(13)	122.0(13)		
C(n4)-C(n5)-C(n0)	119.8(13)	118.8(14)	119.2(11)	121.3(11)	120.3(11)	120.1(12)	120.1(12)		
C(n5)-C(n0)-C(n1)	120.0(11)	120.4(12)	120.1(10)	119.1(11)	119.9(10)	119.1(11)	119.1(11)		

Table 38 - continued

	M = Co	Rh
C(60)-P-C(70)	102.7(5)	103.5(5)
C(60)-P-C(80)	100.9(5)	101.8(5)
C(70)-P-C(80)	103.0(5)	103.8(5)

The fluorinated metallocycles resist thermal decomposition better than the hydrocarbon analogs.^{14,15} Enhanced thermal stabilities have been observed in other highly fluorinated metallocycles relative to their hydrocarbon analogs.¹¹⁴ In the compounds of this study the triphenylphosphine ligand and the four fph rings provide an effective shield for the two double bonds in the metallocycles. Although the fluorine atoms of the fph rings and the phenyl rings of the tpp were omitted from Figure 10, the sterically hindered nature of the metallocycle may easily be seen. The lack of a convenient path for an attacking acetylene together with the enhanced thermal stability of the fluorinated derivatives may have allowed the isolation of these intermediate metallocycles. Metallocycles of cobalt and rhodium of the type presented are reasonable intermediates in the catalyzed oligomerization of acetylenes.

CHAPTER 7

CONCLUDING REMARKS

The structure of $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{clan})$ shows the same LIPS phenomenon as $\text{ClCo}(\text{H}_2\text{dmg})(\text{dmg})(\text{sulfa})$.⁴⁶ These two compounds exhibit the unusual feature of containing both neutral and dianionic dimethylglyoxime groups. Also, the orientation of the benzene ring of the sulfa and clan group in the respective compounds is over the dianionic dmg. The various distances and the relative orientation of the axial ligand in both compounds suggest a π -type interaction. LIPS supports the contention that "hydrophobic forces" are important in enzymic processes.³ The bis(diglyoximato)cobalt(III) complexes of aniline derivatives have here been shown to be useful models for the examination of this type interaction. An extension of X-ray structural determinations to similar compounds with other aniline derivatives and with other diglyoximes is suggested. Low-temperature X-ray studies could effect better resolution of the inter-dmg bridge structure and the N-O distances.

An investigation of the fluorescence spectra of these compounds could reveal additional information concerning the interaction between the equatorial and axial ligands. The fluorescence of 5-dimethylaminonaphthalene-1-sulfonamide was observed to be enhanced while the fluorescence of carbonic

anhydrase was diminished when a 1:1 complex of the two was formed.⁵¹ Although the major contribution to this observation is believed to be the ionization of the sulfonamide, a portion of the change is attributed to a hydrophobic interaction.^{51,115} The fluorescence spectra of cobaloxime complexes with aniline derivatives should help reveal the nature of the interligand interaction as a function of the orientation angle.

The novel ligand dhpphy has been demonstrated as a binucleating ligand. The bridging site occupied by a chlorine atom in $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4(\text{dhpphy})]\text{Cl}_3$ clearly is accessible and of convenient dimensions to accommodate a molecule such as dinitrogen. Further development of this system as a possible model for nitrogenase should include use of molybdenum salts and work with the exclusion of oxygen. Synthesis of similar ligands with saturated "side arms" is also suggested.

The compounds $\text{C}_4(\text{fph})_4\text{Co}(\text{cp})(\text{tpp})$ and $\text{C}_4(\text{fph})_4\text{Rh}(\text{cp})(\text{tpp})$ contain a butadiene fragment with each end bound to a metal atom. The metal to carbon bonds are shorter than expected for the single-bonded distance. The metallocycles are, therefore, believed to contain a delocalized π -bonding system. While metallocycles should be highly susceptible to nucleophilic attack and thermal decomposition the two compounds studied here are very stable. The enhancement of thermal stability by the fluorinated substituents may be at least partially responsible. Also, the presence of the four fph rings

along with the tpp and cp ligands provides a shield from attack for the metallocycle.

The understanding of catalytic processes should improve the efficiency of our existence. Hopefully, enzymic processes occurring in nature can be duplicated in the laboratory by suitable models. These model enzyme systems may then be applied to cure the diseased and feed the hungry.

APPENDIX A BOOTHIT1

A listing of the FORTRAN language computer program BOOTHIT1 follows. This program was designed to interpolate atomic positional parameters by Booth's method¹¹⁶ from the values of a Fourier synthesis calculation. The Fourier synthesis program written by Dr. Gus J. Palenik was modified to store the calculated values on a magnetic disk. After supplying BOOTHIT1 with input data of the approximate position of each atom, the stored values are retrieved. The program estimates the position of maximum electron density for each atom from these Fourier synthesis values. The positional parameters may be translated to equivalent positions and may be passed to a bond distance and angle program. The resulting fractional coordinates are punched into IBM cards in the format required for their input into the Fourier synthesis and least-squares refinement programs.

BOOTH11

THIS IS A PROGRAM TO BOOTH VALUES FOR ATOMIC POSITIONS DIRECTLY
FROM FOURIER CALCULATIONS STORED ON DISK

SUMMARY OF INPUT CARDS FOLLOWS

CARD 1. TITLE

CARD 2. NFO; NACK, IF, IS, IT, ISEL, ICENT, NMUD, IDUMP AS IN
FOURIER, THEN ATMPAS. IF ATMPAS IS GREATER THAN ZERO, THE
ATOMIC PARAMETERS WILL BE WRITTEN ONTO UNIT 04 TO BE PASSED ON
TO THE BOND ANGLES PROGRAM. THEY WILL BE IN THE SAME ORDER
AS THEY WERE READ.

CARD(5) 3. EQUIVALENT POSITIONS CARDS. (MAY NEED MORE FOR
TRANSLATIONS THAN WERE NEEDED FOR FOURIER.)

CARD 4. NV, NU, JORGX FOR H, K, & L FOLLOWED BY NATOMS AND IDISK
WHERE IDISK IS THE UNIT ON WHICH THE FOURIER IS STORED,
THE NORMAL CPIGIN IS -1, -1, -1.

CARD(5) 5. FORMAT(G14, OF8.5, I2, I3, A3)
IPIC(X),(Y),&(Z) ARE THE DIVISIONAL COORDINATES, NTRX, NTRY, AND


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11 FORMAT(1H ,6F10.5,2I5,A3)
12 FORMAT(2H1 ,20A4)
13 FORMAT(2H0 ,A3, ' WAS NOT BOOTHED. (IPIC(3RD SUMMED) MAY BE TOO ',
1' LARG...GUESS AGAIN..... ' )
15 FORMAT(2H0 , 'ECC TH VALUES:  NO  ATCM  1ST SUMMED  2ND ',
1'SUMMED  3RD SUMMED  MAX')
27 FORMAT ( 'P0 ,9F3.0,3F10.5,5A4,AJ)
351 FORMAT(//,30X, ' FINAL FRACTIONAL COORDINATES PUNCHED AS FOLLOWS.')
357 FORMAT(2H0, ' THIS PROGRAM FINISHED NORMALLY')
375 FORMAT (2H0 , 'NC,2X,'ATCM',T14,'X',T24,'Y',T34,'Z',T44,'B11',
1 T54,'B22',T64,'B33',T74,'B12',T84,'B13',T94,'B23',T102,'TABLEN',
2//)
READ(05,06)ITITLE
WRITE(06,12) ITITLE
READ(05,03)NEG,NAIR,IF,IS,IT,ISEL,ICENT,NMOD,IDUMP,ATNPAS
WRITE(06,04) NEG,NAIR,IF,IS,IT,ISEL,ICENT,NMOD,IDUMP,ATNPAS
READ(05,05) ((PTM(M,N),M=1,12), (IDENT(M,N),M=1,6), N=1,NEG)
WRITE(06,27) ((PTM(M,N),M=1,12), (IDENT(M,N),M=1,6), N=1,NEG)
READ(05,02) NV,NV,IORGN,NATOMS,IDISK
WRITE(6,07) NV,NV,IORGN,NATOMS,IDISK
READ(05,01) (IPIC(1,1),IPIC(1,2),IPIC(1,3),NTRX(1),NTRY(1),NTRZ(1),
1,B11(1),B22(1),B33(1),B12(1),B13(1),B23(1),LFT(1),NREQ(1),CODW(1),
2I=1,NATOMS)
WRITE(05,11)(IPIC(1,1),IPIC(1,2),IPIC(1,3),NTRX(1),NTRY(1),NTRZ(1),
1,B11(1),B22(1),B33(1),B12(1),B13(1),B23(1),LFT(1),NREQ(1),CODW(1),
2I=1,NATOMS)
REWIND IDISK
IVF=IORGN(IF)
IVS=IORGN(IS)
IVI=IORGN(IT)

NF = NV(IF)
NS = NV(IS)
NT = NV(IT)
NVF = NV(IVF)

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NVS = NU(IS)
NVT = NU(IT)
READ(IDISK)      IRT,((PFS1(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
READ(IDISK)      IPT,((PFS2(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
READ(IDISK)      IRT,((PFS3(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
WRITE(06,15)
NVT = NVT - 2
MVIT = NVT + IVT
IF(MVIT.GT.NT) MVIT = MVIT - NT
DO 200 JLEVEL = 1,NVT
  MLEVEL = IRT - 1
  IF (MLEVEL.GE.NT) MLEVEL = MLEVEL - NT
  DO 198 NATS = 1,NATOMS
    IF(IPIC(NATS,IT).GT.MVIT) IPIC(NATS,IT) = MVIT
    IF (IPIC(NATS,IT).EQ.MLEVEL) GO TO 150
  GO TO 198
150 CALL LOOK
    IF (1/(NATS)-NE.MLEVEL) GO TO 198
    CALL BOOTP
198 CONTINUE
    IF (JLEVEL.EQ.NVT) GO TO 200
    DO 199 IRS = 1,NVS
      DO 199 IRF = 1,NVF
        PFS1(IRS,IRF) = PFS2(IRS,IRF)
        PFS2(IRS,IRF) = PFS3(IRS,IRF)
199 CONTINUE
    READ(IDISK)  IRT,((PFS3(IRS,IRF),IRS=1,NVS),IRF=1,NVF)
200 CONTINUE
    WRITE(06,07) IPT,MLEVEL,JLEVEL
    WRITE(06,275)
    WRITE(06,10)  (1,CORR(I),FC(I,1),FC(I,2),FC(I,3),B11(I),B22(I),
1 B33(I),B12(I),B13(I),B23(I),LFT(I), I=1,NATOMS)
    DO 40 I = 1,NATOMS
      IF (IMAX(I).LE.C.0) WRITE(06,13) CORR(I)
      X(I) = FC(I,1) / NV(I)

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Y(1) = FC(1,2) / NV(2)
Z(1) = FC(1,3) / NV(3)
40 CONTINUE
WRITE(06,375)
WRITE(06,10) (1,CODW(I),X(I),Y(I),Z(I),B11(I),B22(I),B33(I),
1 B12(I),B13(I),B23(I),LFT(I),I = 1,NATOMS)
DO 60 I = 1,NATOMS
IF(NRLQ(I).EQ.0) GO TO 554
N = IABS(NREQ(I))
ICI = I
IF (NREQ(I)) 545,550,550
545 ICI = -I
550 CONTINUE
X(1) = ICI * (X(1) * PTW(1,N) + PTW(10,N)) + NTRX(1)
Y(1) = ICI * (Y(1) * PTW(5,N) + PTW(11,N)) + NTRY(1)
Z(1) = ICI * (Z(1) * PTW(9,N) + PTW(12,N)) + NTRZ(1)
GO TO 60

554 CONTINUE
X(1) = X(1) + NTRX(1)
Y(1) = Y(1) + NTRY(1)
Z(1) = Z(1) + NTRZ(1)
60 CONTINUE
349 CONTINUE
WRITE(06,351)
WRITE(06,375)
WRITE(06,10) (1,CODW(I),X(I),Y(I),Z(I),B11(I),B22(I),B33(I),
1 B12(I),B13(I),B23(I),LFT(I),I = 1,NATOMS)
WRITE(07,09) (X(1),Y(1),Z(1),B11(I),B22(I),B33(I),B12(I),
1 B23(I),LFT(I),CODW(I), I = 1,NATOMS)
IF (AIMPAS.LE.0) GO TO 50
REWIND 04
WRITE(04,09) (X(1),Y(1),Z(1),B11(I),B22(I),B33(I),B12(I),
1 B23(I),LFT(I),CODW(I), I = 1,NATOMS)
50 CONTINUE
WRITE(06,357)

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154 TRY = PFS2(IP02,IP01)
    IPD3 = MLEVEL
    GO TO 160

156 TRY = PFS1(IP02,IP01)
    IPD3 = MLEVEL - 1
160 IF (TMAX(NATS) - TRY) 175,180,180
175 TMAX(NATS) = TRY
    IV(NATS) = IPD3 + IVS - 1
    IU(NATS) = IPD1 + IVF - 1
    IW(NATS) = IPD3
180 CONTINUE
    IF (IW(NATS).GT.MLEVEL) IPIC(NATS,IT) = IW(NATS)
    IF (IW(NATS).LI.MLEVEL) GO TO 190
    GO TO 191

190 IV(NATS) = 0
    IW(NATS) = 0
    IU(NATS) = 0
    TMAX(NATS) = 0.0
    FC(NATS,1) = 0.0
    FC(NATS,2) = 0.0
    FC(NATS,3) = 0.0
191 CONTINUE
    IF (IU(NATS).GE.NF) IU(NATS) = IU(NATS) - NF
    IF ( IV(NATS).GE.NS) IV(NATS) = IV(NATS) - NS
    IF (IW(NATS).GE.NT) IW(NATS) = IW(NATS) - NT
    RETURN
    END

```

C
C

C SUBROUTINE BOOTH
C THE PURPOSE OF THIS SUBROUTINE IS TO DETERMINE THE MAXIMUM F IN
C THREE DIMENSIONS.
C DIMENSION IU(99), IV(99), IW(99), PFS1(60,120), PFS2(60,120),
1 PFS3(60,120), FC(99,3), IPIC(99,3), TMAX(99), CODW(99)
COMMON IPIC,NATS,IF,IS,IT,IVF,IVS,IVT,TMAX,IU,IV,IW,PFS1,PFS2,

```

: PFS3, NF, NS, NT, FC, MLEVEL, NVS, NVF, COD%
LIF = IU(NATS) - IVF + 1
IF (LIF.LE.0) LIF = LIF + NF
LIS = IV(NATS) - IVS + 1
IF (LIF.LE.0) LIS = LIS + NS
TMID = PFS2(LIS,LIF)
TUPF = PFS3(LIS,LIF)
TDNT = PFS1(LIS,LIF)
TUPS = PFS2(LIS+1,LIF)
TDNS = PFS2(LIS-1,LIF)
TUPF = PFS2(LIS,LIF+1)
TDNF = PFS2(LIS,LIF-1)
IF (TUPF.GT.TDNF) GO TO 330
TMAXF = TDNF
TMINF = TUPF
MINDF = LIF + IVF
GO TO 335
330 TMAXF = TUPF
TMINF = TDNF
MINDF = LIF + IVF - 2
335 IF (MINDF.GT.NF) MINDF = MINDF - NF
IF (TUPS.GT.TDNS) GO TO 340
TMAXS = TDNS
TMINs = TUPS
MINDS = LIS + IVS
GO TO 345
340 TMAXS = TUPS
TMINs = TDNS
MINDS = LIS + IVS - 2
345 IF (MINDS.GT.NS) MINDS = MINDS - NS
IF (TUPF.GT.TDNT) GO TO 350
TMAXI = TDNT
TMINI = TUPF
MINDI = IW(NATS) + 1
GO TO 355

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350 TMAXI = TUPT
   TMINT = TDNT
   MINDI = I*(NATS) - 1
355 IF (MINDI.GT.NI) MINDI = MINDI - NI
   RTBF = (TMAXI - TMINF) / (TMID - TMINF)
   RTJS = (TMAXS - TMINS) / (TMID - TMINS)
   RTUF = (TMAXT - TMINT) / (TMID - TMINT)
   BCOF = (RTBF - 4) / (2*RTBF - 4)
   BUUS = (RTJS - 4) / (2*RTJS - 4)
   ECOT = (RTUF - 4) / (2*RTUF - 4)
   IF (BCOF.LT.1.0.OR.BCOF.GT.1.5) TMAX(NATS) = 0.0
   IF (BUUS.LT.1.0.OR.BUUS.GT.1.5) TMAX(NATS) = 0.0
   IF (ECOT.LT.1.0.OR.ECOT.GT.1.5) TMAX(NATS) = 0.0
14 FORMAT(1H ,14X,15,3X,A3,15,F10.5, /',15,F10.5,
12X,F10.1)
   WRITE(06,14)NATS,CUDW(NATS),IU(NATS),BCOF,IU(NATS),BUUS,I*(NATS),
1BOUT,TMAX(NATS)
   FC1 = MINDF + FCOF
   FC2 = MINDS + BUUS
   FC3 = MINDT + ECOT
   IF (MINDF.GT.IU(NATS)) FC1 = MINDF - BCOF
   IF (MINDS.GT.IV(NATS)) FC2 = MINDS - BUUS
   IF (MINDT.GT.IW(NATS)) FC3 = MINDT - ECOT
   FC(NATS,1F) = FC1
   FC(NATS,IS) = FC2
   FC(NATS,IT) = FC3
   RETURN
   END

```

APPENDIX B

OBSERVED AND CALCULATED STRUCTURE FACTORS

Table B-1
Observed and Calculated Structure Factors for $\text{ClCo}(\text{H}_2\text{dpg}_2) \cdot \text{(clan)} \cdot \text{C}_2\text{H}_5\text{OH}$

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	0, K=	0	19	-141	-100	11	-136	70	2	-142	100
2	2949	-3137	H=	0, K=	4	12	292	270	3	-146	-138
4	398	-473	0	1749	1724	13	-137	-48	4	-144	-10
6	-108	-115	1	2748	-2742	14	413	-407	5	-145	-64
8	461	485	2	211	-263	15	288	-282	6	278	18
10	-112	46	3	694	706	16	271	270	7	246	139
12	427	-435	4	559	-557	H=	0, K=	8	8	-150	67
14	530	556	5	181	-195	0	-123	-23	H=	0, K=	13
16	-133	86	6	303	-279	1	-123	12	1	-146	-10
18	-131	-65	7	210	-55	2	265	263	2	-146	-11
H=	0, K=	1	8	245	-234	3	-129	79	3	-146	121
1	485	649	9	-116	58	4	-128	-152	4	-153	-55
2	1334	1255	10	287	371	5	439	-418	H=	1, K=	0
3	440	-313	11	267	235	6	211	-107	1	1980	-2098
4	1079	1074	12	239	-203	7	-135	-66	2	844	833
5	-111	100	13	267	289	8	241	217	3	419	442
6	1139	1080	14	-136	152	9	-139	175	4	1784	-1783
7	-107	127	15	243	-247	10	-142	-61	5	996	1025
8	335	-347	16	-134	139	11	234	-134	6	-113	0
9	189	-175	17	-135	-39	12	-141	113	7	-124	179
10	-112	-16	18	247	-216	13	223	323	8	282	350
11	269	209	H=	0, K=	5	14	223	-137	9	211	-303
12	267	297	1	923	890	15	-141	-109	10	310	339
13	459	-459	2	228	151	H=	0, K=	9	19	-140	60
14	694	-701	3	1038	-1034	1	-130	168	17	192	-158
15	379	357	4	-112	96	2	-131	-120	18	615	614
16	542	530	5	-111	14	3	-133	-55	19	690	-696
17	-135	50	6	228	209	4	-134	40	20	160	3
18	-135	53	7	593	-601	5	196	41	21	358	-450
19	-142	30	8	-117	87	6	232	-132	22	-164	-177
H=	0, K=	2	9	337	326	7	-140	-55	23	867	861
0	2055	-2207	10	448	-407	8	247	198	24	1438	-1533
1	1523	1485	11	-126	-45	9	-143	-172	25	2644	1892
2	461	334	12	-132	-52	10	-127	-81	H=	1, K=	1
3	195	-177	13	401	-441	11	-139	24	0	504	576
4	255	76	14	240	19	12	-140	47	1	1595	1364
5	-111	48	15	658	676	13	235	57	2	-98	50
6	-108	55	16	-137	6	14	-147	147	3	1698	-1695
7	464	448	17	344	-306	H=	0, K=	10	4	1269	1259
8	164	99	18	-144	72	0	428	433	5	-114	16
9	-108	24	H=	0, K=	6	1	274	225	6	557	-543
10	401	379	0	629	622	2	216	-251	7	554	-547
11	-116	-20	1	1151	1149	3	-140	-105	8	-111	-40
12	287	202	2	424	-433	4	-141	133	9	-111	-151
13	301	-255	3	538	-535	5	229	169	10	-116	154
14	492	-512	4	-115	-147	6	-144	-152	11	259	-277
15	-137	172	5	437	445	7	-142	101	12	200	-195
16	229	15	6	275	226	8	-143	-150	13	639	-656
17	-133	-35	7	377	369	9	212	-148	14	471	512
18	-135	-21	8	-123	-37	10	283	299	15	716	685
19	-143	19	9	439	-445	11	-145	-54	16	-136	-185
H=	0, K=	3	10	297	299	12	222	-215	17	231	-210
1	638	-561	11	244	184	13	234	0	18	-138	68
2	982	-984	12	261	-173	H=	0, K=	11	19	-142	91
3	634	-828	13	350	-368	0	428	433	20	-133	103
4	218	-105	14	-136	-87	1	274	225	21	-138	-67
5	333	340	15	-138	130	2	216	-251	22	-135	-133
6	192	191	16	-140	-134	3	-140	-105	23	295	297
7	312	272	17	230	225	4	-141	133	24	571	582
8	222	-229	H=	0, K=	7	5	229	169	25	281	-252
9	-111	-27	1	572	-596	6	-144	-152	26	217	-142
10	189	189	2	-119	-120	7	-142	101	27	-124	-175
11	-119	-106	3	318	328	8	-143	-150	28	-116	43
12	185	72	4	554	-561	9	212	-148	29	175	-216
13	196	123	5	201	-187	10	283	299	30	347	372
14	210	150	6	488	539	11	-145	-54	31	403	-403
15	376	-359	7	-125	104	12	222	-215	32	1168	-1156
16	207	-130	8	295	-323	13	234	0	33	843	861
17	-135	217	9	-133	159	H=	0, K=	12	34	487	480
18	212	-67	10	-135	70	0	-139	-115	35	1279	-1215
						1	-143	170	36	354	-326
									37	-96	107

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-1	585	-563	-7	358	330	-10	-125	-36	-7	369	-414
H=	1, K=	2	-6	-112	-72	-9	-119	-147	-6	-126	-108
0	-101	-17	-5	385	-327	-8	404	-403	-5	722	740
1	1167	1077	-4	750	763	-7	-114	56	-4	515	516
2	-107	-48	-3	474	502	-6	1334	1319	-3	251	-270
3	1256	1165	-2	315	-280	-5	163	-54	-2	840	-839
4	415	404	-1	2463	-2419	-4	821	-858	-1	518	-570
5	436	435	H=	1, K=	4	-3	426	-412	H=	1, K=	8
6	-110	10	0	981	-1005	-2	563	-594	0	-126	0
7	-112	123	1	-115	-169	-1	1052	1033	1	-126	61
8	452	-474	2	844	828	H=	1, K=	6	2	-124	38
9	-113	15	3	501	-490	0	1459	1489	3	-126	57
10	-115	46	4	-112	51	1	178	-4	4	-132	0
11	-118	78	5	206	-153	2	301	-321	5	-138	-138
12	-123	78	6	499	-490	3	-117	150	6	-136	-54
13	489	-457	7	584	-571	4	-121	-239	7	-138	-30
14	-135	-66	8	541	521	5	-116	-5	8	-142	61
15	-137	-112	9	228	218	6	514	501	9	-144	-216
16	-134	12	10	-123	-112	7	268	-276	10	-142	108
17	-134	75	11	-129	-194	8	620	-616	11	257	235
18	-135	3	12	238	105	9	351	353	12	241	154
19	-147	5	13	199	171	10	438	428	13	-139	-91
-19	246	-96	14	-138	-71	11	223	-60	14	-146	-118
-18	-139	-120	15	-139	147	12	251	-289	15	-146	12
-17	215	148	16	-134	-113	13	-140	49	-16	221	54
-16	-136	-203	17	310	-265	14	-135	48	-15	-144	-147
-15	451	-404	18	238	74	15	-136	-81	-14	-141	-141
-14	332	368	19	-146	15	16	-145	204	-13	270	297
-13	491	490	-18	-138	-84	17	-146	3	-12	-138	17
-12	268	-255	-17	-134	-44	-17	-143	-42	-11	-138	-157
-11	512	518	-16	-139	194	-16	-142	-73	-10	-139	55
-10	-114	65	-15	-135	141	-15	-136	180	-9	-142	-38
-9	546	-543	-14	580	-582	-14	338	347	-8	-141	-68
-8	627	-594	-13	-134	-94	-13	255	-239	-7	-137	-60
-7	374	388	-12	-134	199	-12	411	-384	-6	219	217
-6	-109	-66	-11	213	159	-11	388	450	-5	-131	93
-5	204	96	-10	440	415	-10	232	273	-4	216	-205
-4	-114	-55	-9	333	-324	-9	258	-308	-3	259	320
-3	2196	2056	-8	-113	-119	-8	-125	-46	-2	-129	75
-2	1663	-1663	-7	221	146	-7	184	232	-1	366	-440
-1	2235	-2404	-6	335	276	-6	387	-410	H=	1, K=	9
H=	1, K=	3	-5	610	614	-5	-116	14	0	-135	-111
0	2381	-2335	-4	563	-534	-4	555	1028	1	-135	22
1	1050	1038	-3	340	-370	-3	492	-510	2	-134	-41
2	-118	-56	-2	322	328	-2	1315	-1314	3	-134	46
3	806	-823	-1	621	591	-1	277	282	4	-141	148
4	1758	1710	H=	1, K=	5	H=	1, K=	7	5	-145	-152
5	-112	-144	0	574	538	0	250	292	6	-145	-215
6	228	-225	1	212	-190	1	534	552	7	-146	109
7	-111	-13	2	868	-886	2	-118	-150	8	-144	-59
8	754	-729	3	-112	-85	3	212	-258	9	207	-150
9	707	702	4	671	672	4	317	289	10	220	174
10	-117	29	5	-114	122	5	184	202	11	-145	-225
11	-123	-179	6	683	-705	6	265	238	12	-143	-106
12	-136	234	7	343	341	7	304	-268	13	230	301
13	-134	259	8	222	81	8	-135	47	14	-145	96
14	349	-359	9	389	-386	9	-136	102	-14	-142	19
15	252	-317	10	191	193	10	343	-351	-13	-139	-44
16	289	200	11	-132	25	11	248	243	-12	267	-206
17	-139	-83	12	323	-314	12	258	256	-11	249	201
18	197	-206	13	-139	35	13	312	-202	-10	-140	95
19	-141	-32	14	589	587	14	256	-266	-9	305	-257
-19	-145	-189	15	257	-156	15	283	255	-8	-142	-21
-18	228	47	16	342	-374	16	211	161	-7	377	393
-17	-138	58	17	230	171	-17	221	-220	-6	365	338
-16	-136	-155	18	-143	70	-16	-145	-169	-5	-137	-116
-15	229	-237	-18	323	-258	-15	-142	132	-4	324	-334
-14	244	215	-17	-133	-6	-14	-134	0	-3	-138	-169
-13	-130	-122	-16	456	442	-13	-137	-115	-2	-136	55
-12	182	84	-15	-137	113	-12	273	246	-1	195	204
-11	-117	65	-14	362	-423	-11	-137	63	H=	1, K=	10
-10	-116	-29	-13	-136	133	-10	401	-410	0	251	176
-9	386	-417	-12	-131	-123	-9	-133	67			
-8	-112	-163	-11	-130	-23	-8	231	239			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 2, K= 6			0	195	-153	11	-146	-15	9	494	-493
0	269	-293	1	-133	300	12	-146	55	11	273	-247
1	646	-625	2	-130	-4	-13	-147	-88	13	408	429
2	584	-576	3	285	290	-12	-144	111	15	714	-729
3	-119	-168	4	-134	-124	-11	-144	-55	17	254	304
4	203	79	5	-135	-142	-10	-142	5	19	254	-155
5	748	786	6	-141	198	-9	-140	206	-19	-136	-64
6	197	-204	7	-142	-89	-8	-140	-98	-17	613	634
7	541	-542	8	-141	56	-7	-141	-74	-15	531	-542
8	258	275	9	217	-162	-6	-139	-25	-13	497	493
9	337	334	10	213	127	-5	-148	-148	-11	440	-436
10	319	-305	11	-141	7	-4	370	-355	-9	356	-310
11	-133	13	12	-139	-131	-3	-143	19	-7	1011	1026
12	-145	-5	13	-144	-6	-2	488	487	-5	1442	-1403
13	-141	-120	14	-141	-9	-1	201	226	-3	203	221
14	-135	56	15	-144	121	H= 2, K= 11			-1	1290	-1240
15	-137	81	-16	281	-187	0	-144	158	H= 3, K= 1		
16	-139	-58	-15	-148	-45	1	-143	-73	0	551	-573
-17	-145	-117	-14	-143	128	2	330	-352	1	289	-216
-16	-137	208	-13	-137	60	3	-143	62	2	1756	1738
-15	347	344	-12	-136	-88	4	307	324	3	281	-271
-14	-141	-253	-11	-141	152	5	-143	-185	4	583	-589
-13	310	-308	-10	-145	181	6	-144	-73	5	241	-271
-12	421	416	-9	-147	-284	7	-145	177	6	754	-771
-11	204	210	-8	-140	-161	8	-146	-112	7	510	-492
-10	360	-358	-7	380	415	9	-149	-29	8	-114	124
-9	-128	58	-6	-134	-34	10	327	240	9	716	708
-8	199	256	-5	-134	-85	-11	322	153	10	-121	-169
-7	262	-294	-4	481	499	-10	-152	230	11	796	-805
-6	-122	-92	-3	260	304	-9	-144	-146	12	343	389
-5	-120	246	-2	-129	-129	-8	292	-355	13	446	432
-4	532	-517	-1	425	-431	-7	-144	119	14	307	-268
-3	609	-601	H= 2, K= 9			-6	331	270	15	199	-127
-2	1065	1096	0	291	-369	-5	-142	-102	16	215	-187
-1	1220	1224	1	-137	-52	-4	-143	13	17	-136	-102
H= 2, K= 7			2	-141	145	-3	-140	-26	18	-141	27
0	601	579	3	-137	79	-2	-144	-220	19	-146	150
1	206	210	4	-137	0	-1	-142	105	-19	-144	-179
2	394	-435	5	231	241	H= 2, K= 12			-18	213	130
3	375	-341	6	-143	-42	0	-144	126	-17	-137	232
4	449	405	7	-146	-126	1	-145	-6	-16	-135	-103
5	-130	151	8	-144	-38	2	-147	-35	-15	-138	190
6	-132	-277	9	-142	183	3	214	-107	-14	-129	-88
7	-136	-152	10	-138	-31	4	-149	-163	-13	412	-424
8	-133	60	11	-143	-271	5	-149	224	-12	-125	194
9	-138	-139	12	236	223	6	254	144	-11	885	870
10	222	226	13	-151	138	7	226	-246	-10	270	-286
11	335	347	14	-149	-72	8	223	-42	-9	453	-438
12	572	-601	-14	-139	-8	9	223	-42	-8	624	615
13	255	-188	-13	-143	-66	-8	-151	-17	-7	282	241
14	306	308	-12	-141	34	-7	-149	-29	-6	333	-399
15	-147	152	-11	313	257	-6	-153	-122	-5	-110	179
16	215	-71	-10	224	-310	-5	-151	251	-4	505	-520
-17	-146	-97	-9	252	-228	-4	225	277	-3	-112	48
-16	-143	89	-8	-140	25	-3	335	-359	-2	393	323
-15	200	16	-7	-140	117	-2	-145	-177	-1	1687	1683
-14	-136	85	-6	-140	71	H= 2, K= 13			H= 3, K= 2		
-13	219	126	-5	285	-275	0	282	223	0	450	-470
-12	-138	-170	-4	-138	-68	1	-149	53	1	413	385
-11	219	-257	-3	509	507	2	-150	104	2	822	849
-10	457	455	-2	263	377	3	-148	15	3	222	-194
-9	403	441	-1	301	-252	4	-148	-71	4	852	831
-8	476	-503	H= 2, K= 10			5	-150	-59	5	1072	1074
-7	240	-315	0	276	-243	6	-151	52	6	635	-636
-6	437	459	1	-142	-146	7	-151	-6	7	428	-421
-5	185	-150	2	-146	-77	8	-151	-6	8	428	446
-4	-124	72	3	-143	-99	9	278	-188	9	190	238
-3	-122	153	4	-147	188	H= 3, K= 0			10	-117	-94
-2	382	-410	5	-145	153	1	586	-564	11	-122	-173
-1	299	-221	6	300	-262	2	799	-756	12	184	-116
H= 2, K= 8			7	-141	-3	3	1501	-1510	13	-134	-217
0	195	-153	8	-145	196	4	1092	1061	14	337	359
1	-133	300	9	-143	81				15	-141	251
2	-130	-4	10	-149	-216				16	286	-219

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
17	-136	-185	13	248	179	11	-140	51	-15	-146	82
16	285	127	14	281	-300	12	256	-230	-14	-138	2
-19	-140	95	15	-136	-189	12	373	378	-13	-137	101
-18	242	-216	16	-145	166	14	374	318	-12	236	142
-17	225	-273	17	-147	192	15	-144	-177	-11	-141	-125
-16	-136	160	18	-145	-165	16	-150	-210	-10	385	-390
-15	421	420	-19	-143	75	-17	-147	129	-9	-139	116
-14	302	-229	-18	278	244	-16	324	307	-8	-140	207
-13	-129	-197	-17	-138	-25	-15	-137	49	-7	-136	-110
-12	416	449	-16	421	-406	-14	378	-337	-6	-135	-22
-11	402	-409	-15	-135	-34	-13	-138	19	-5	-138	258
-10	-114	49	-14	255	267	-12	271	314	-4	260	280
-9	516	522	-13	-130	94	-11	-136	-196	-3	590	-574
-8	554	-529	-12	220	24	-10	236	192	-2	447	-490
-7	172	-156	-11	-125	-8	-9	-124	-7	-1	-129	84
-6	553	547	-10	-121	-121	-8	525	-500	H= 3, K= 9		
-5	267	-220	-9	-119	-224	-7	538	523			
-4	-112	-16	-8	598	608	-6	-120	191	0	-137	-79
-3	210	-161	-7	245	283	-5	407	-407	1	228	102
-2	654	610	-6	248	233	-4	573	-582	2	-141	131
-1	369	-330	-5	232	-186	-3	316	314	3	-139	-82
H= 3, K= 3			-4	-110	-36	-2	593	920	4	-137	-36
			-3	579	603	-1	-114	44	5	-144	93
0	-115	-9	-2	738	-778	H= 3, K= 7			6	266	-323
1	331	-281	-1	858	-858				7	241	75
2	1146	1182	H= 3, K= 5			0	633	626	8	221	213
3	298	-331				1	466	-456	9	232	-157
4	485	-444	0	587	-574	2	268	253	10	-144	-67
5	428	428	1	219	47	3	443	472	11	-145	67
6	-112	55	2	940	967	4	-123	-11	12	217	273
7	162	72	3	-113	-47	5	-126	-38	13	-151	-70
8	217	244	4	710	-718	6	-130	29	-14	222	147
9	-117	-29	5	-118	-152	7	183	-102	-13	-144	6
10	328	260	6	286	-277	8	-135	-83	-12	-140	-41
11	257	256	7	181	-153	9	-141	22	-11	-140	-66
12	335	-309	8	386	398	10	203	156	-10	-141	-128
13	221	-222	9	187	228	11	242	-235	-9	-141	130
14	-138	193	10	380	-379	12	353	-377	-8	-144	-9
15	-137	199	11	-134	34	13	-143	154	-7	-142	101
16	-132	159	12	636	638	14	-140	155	-6	263	198
17	-139	-83	13	-137	64	15	-143	-16	-5	-139	-170
18	-143	-74	14	218	-210	16	-144	-2	-4	254	-245
-19	-140	89	15	-140	-214	-16	-143	-33	-3	265	329
-18	-138	13	16	-137	-97	-15	-139	-9	-2	-138	43
-17	-135	-80	17	-140	-8	-14	-136	39	-1	352	-366
-16	-135	-193	-18	273	247	-13	-135	-57	H= 3, K= 10		
-15	-133	-97	-17	254	220	-12	243	-204			
-14	-132	99	-16	-136	-48	-11	318	248	0	266	-172
-13	315	324	-15	223	-246	-10	314	287	1	-147	-10
-12	336	-228	-14	-136	-162	-9	561	-558	2	-147	60
-11	496	-505	-13	-140	181	-8	-134	163	3	-145	91
-10	636	649	-12	-135	162	-7	-123	110	4	-147	-29
-9	352	367	-11	-132	-27	-6	274	-148	5	315	-292
-8	-112	-34	-10	628	-629	-5	-126	66	6	-148	10
-7	-109	-78	-9	-119	39	-4	294	350	7	239	253
-6	516	-555	-8	969	954	-3	447	-470	8	-147	-136
-5	-110	-103	-7	-115	7	-2	646	-672	9	-149	-48
-4	275	-270	-6	200	53	-1	524	546	10	-145	35
-3	557	566	-5	-115	-7	H= 3, K= 8			11	-152	50
-2	411	-380	-4	358	-339				12	-152	52
-1	849	-841	-3	-113	91	0	330	412	-13	-152	87
H= 3, K= 4			-2	1008	1015	1	194	46	-12	-154	244
			-1	293	-268	2	-134	4	-11	-151	-146
0	199	-205	H= 3, K= 6			3	-133	-170	-10	-146	-78
1	549	535				4	257	-131	-9	-145	-37
2	-109	-23	0	-118	96	5	247	208	-8	278	-159
3	-112	-7	1	302	280	6	-137	164	-7	-152	284
4	504	-510	2	531	-538	7	-140	-178	-6	-144	64
5	529	-560	3	268	264	8	-145	242	-5	357	-379
6	359	389	4	659	651	9	-142	65	-4	-151	-68
7	-117	85	5	678	-694	10	-142	-79	-3	349	386
8	208	-160	6	847	-851	11	-137	1	-2	262	327
9	246	319	7	372	398	12	205	-52	-1	-145	-134
10	205	53	8	413	451	13	-141	-196			
11	288	-231	9	290	-288	14	-144	18			
12	-137	140	10	-135	-166	15	250	57			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 3, K= 11			0	237	-227	-1	-113	105	-3	-110	-53
0	-147	-69	1	-114	-135	H= 4, K= 3			-2	-109	-58
1	-156	-318	2	629	599	0	-111	-61	-1	241	224
2	-146	86	3	270	-273	1	-111	-114	H= 4, K= 5		
3	-151	151	4	-109	83	2	643	633	0	245	-328
4	-147	-126	5	401	389	3	430	395	1	255	348
5	266	25	6	252	-205	4	458	-449	2	-114	89
6	-150	146	7	535	520	5	-112	6	3	-117	94
7	-153	-226	8	1196	1187	6	360	363	4	-118	-92
8	-149	-32	9	505	-487	7	588	-618	5	254	-238
9	-161	248	10	844	-824	8	364	-375	6	-121	130
10	-155	-109	11	333	334	9	374	354	7	389	364
-11	-153	3	12	432	463	10	266	289	8	-129	-168
-10	-150	-43	13	-132	23	11	288	-243	9	724	-735
-9	-149	-41	14	192	46	12	-132	-89	10	-134	-14
-8	-149	186	15	-137	-201	13	-133	-118	11	690	729
-7	-148	-51	16	-138	127	14	265	292	12	-137	84
-6	-150	-52	17	-140	54	15	-136	23	13	-139	-103
-5	-146	-47	18	294	191	16	200	-127	14	-139	-176
-4	379	-395	-19	-143	74	17	-140	39	15	-140	-131
-3	296	-279	-18	-142	-85	18	-145	-66	16	-142	112
-2	299	333	-17	-140	-74	-19	-145	-63	17	222	168
-1	521	524	-16	201	23	-18	-139	-56	-18	-140	24
H= 3, K= 12			-15	-131	26	-17	-137	-211	-17	-137	-66
0	-151	-123	-14	562	-602	-16	259	157	-16	-138	-199
1	-147	-33	-13	287	298	-15	306	286	-15	-135	-92
2	-153	-44	-12	680	709	-14	226	8	-14	-136	166
3	-149	3	-11	269	-282	-13	-135	-111	-13	331	352
4	-155	115	-10	615	-623	-12	230	-204	-12	-136	-141
5	238	160	-9	455	458	-11	271	301	-11	480	-451
6	291	-195	-8	221	184	-10	-119	218	-10	183	-26
7	-151	-119	-7	257	-179	-9	351	-328	-9	400	411
-8	-158	-93	-6	-107	105	-8	386	390	-8	537	545
-7	-158	-70	-5	-109	57	-7	172	-160	-7	313	-346
-6	312	281	-4	741	-773	-6	-110	-124	-6	-118	3
-5	288	249	-3	391	393	-5	670	694	-5	249	-202
-4	422	-434	-2	271	226	-4	655	640	-4	651	-648
-3	495	-441	-1	343	-367	-3	164	171	-3	661	678
-2	316	337	H= 4, K= 2			-2	-113	135	-2	-114	134
-1	-152	117	0	726	-734	-1	556	-533	-1	-112	-86
H= 3, K= 13			1	243	-172	H= 4, K= 4			H= 4, K= 6		
0	-161	229	2	-112	-227	0	-111	-175	0	376	-431
1	223	-56	3	-112	-113	1	197	145	1	246	-213
2	-159	-113	4	201	-147	2	-113	198	2	367	335
-3	-159	95	5	489	-517	3	440	-446	3	861	898
-2	-161	-234	6	-110	-23	4	191	-260	4	414	-446
-1	-151	-109	7	226	225	5	559	532	5	1018	-1014
H= 4, K= 0			8	-113	7	6	755	730	6	727	699
0	806	-804	9	285	311	7	202	-209	7	383	375
2	2426	2359	10	-124	101	8	315	-379	8	219	-346
4	510	-456	11	240	-257	9	-123	4	9	-134	190
6	877	891	12	414	-422	10	234	-222	10	-142	-136
8	670	-664	13	353	339	11	302	304	11	241	-272
10	-123	-238	14	-138	153	12	218	293	12	-139	179
12	817	816	15	-133	-51	13	268	-158	13	-140	174
14	408	-463	16	-137	6	14	-133	-55	14	-138	-168
16	-137	62	17	-144	196	15	245	69	15	298	-224
18	-153	-237	18	-141	62	16	225	186	16	-143	108
-18	-143	87	-19	256	-95	17	215	-184	-17	295	277
-16	369	-414	-18	-150	-83	18	-140	158	-16	-140	14
-14	646	646	-17	-137	89	-17	-144	-200	-15	-140	-212
-12	-124	77	-16	-137	61	-16	234	-204	-14	-134	-218
-10	781	-809	-15	-137	56	-15	-137	176	-13	-136	20
-8	886	888	-14	284	210	-14	314	330	-12	-136	56
-6	847	-842	-13	195	-146	-13	226	130	-11	251	197
-4	1443	1431	-12	293	-378	-12	234	-224	-10	377	-377
-2	698	-670	-11	-126	229	-11	387	-373	-9	349	-354
H= 4, K= 1			-10	333	359	-10	-126	-193	-8	347	321
0			-9	186	-183	-9	726	750	-7	617	648
2			-8	924	-907	-8	-116	53	-6	281	-206
4			-7	460	485	-7	681	-691	-5	738	-750
6			-6	840	856	-6	292	-265	-4	878	892
8			-5	413	-423	-5	830	848	-3	184	224
10			-4	-110	121	-4	189	150	-2	308	-315
12			-3	757	762						
14			-2	1159	-1135						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-1	172	-145	6	-140	92	3	-152	178	1	-109	-160
H=	4, K=	7	7	-141	65	4	263	131	2	561	564
0	314	-242	8	-142	-77	5	223	-240	3	511	499
1	-122	-47	9	237	-23	6	-149	-75	4	660	-665
2	225	231	10	-140	99	-7	-154	94	5	206	189
3	201	-240	11	-143	34	-6	-150	123	6	371	399
4	-132	-85	12	-145	-58	-5	223	-139	7	256	230
5	455	464	13	-150	-131	-4	-149	-44	8	264	235
6	365	-310	-14	-148	97	-3	-145	156	9	428	451
7	397	-388	-13	-145	-36	-2	-146	123	10	397	-394
8	399	413	-12	-138	-85	-1	-142	13	11	357	-364
9	-143	192	-11	-138	79	H=	5, K=	0	12	-132	17
10	325	-259	-10	-137	-98	1	569	561	13	-140	-249
11	313	-238	-9	-139	136	3	2366	-2345	14	-140	190
12	-140	-15	-8	222	6	5	1318	1326	15	-138	49
13	330	324	-7	-142	-43	7	-105	60	16	-135	146
14	-145	146	-6	-141	-93	9	656	-661	17	-122	20
15	-147	-114	-5	321	-354	11	672	674	18	-147	67
-16	-146	75	-4	-143	111	13	304	311	-19	269	-293
-15	-136	-14	-3	404	420	15	-126	35	-18	-144	220
-14	-140	-44	-2	313	-261	17	-137	-11	-17	245	37
-13	-138	52	-1	-142	-245	-19	416	371	-16	-133	-43
-12	-140	-20	H=	4, K=	10	-17	259	284	-15	-137	-115
-11	-141	115	0	-145	-133	-15	-137	-261	-14	269	-291
-10	-142	-207	1	-145	54	-13	-132	-160	-13	262	-200
-9	226	-232	2	-141	148	-11	537	-535	-12	339	324
-8	206	212	3	257	141	-9	1210	1201	-11	762	735
-7	202	-234	4	287	-356	-7	1254	-1269	-10	315	-295
-6	-132	-177	5	-143	-65	-5	367	348	-9	211	-157
-5	687	715	6	332	335	-3	-109	-47	-8	-113	140
-4	414	-414	7	-142	-129	-1	208	172	-7	-113	51
-3	360	-231	8	-142	-85	H=	5, K=	1	-6	555	-545
-2	673	711	9	-142	171	0	855	880	-5	415	366
-1	-123	119	10	-148	-158	1	-111	90	-4	456	471
H=	4, K=	8	11	-149	-29	2	253	-276	-3	392	-367
0	-135	-257	-12	206	23	3	737	736	-2	192	-44
1	-135	-104	-11	-147	-160	4	482	-495	-1	-109	53
2	-134	59	-10	-142	-95	5	1330	-1323	H=	5, K=	3
3	-135	-61	-9	-141	145	6	601	591	0	781	758
4	475	481	-8	-144	222	7	662	644	1	502	-492
5	-141	171	-7	-143	76	8	375	-386	2	738	-759
6	-144	-310	-6	354	-365	9	613	-634	3	627	-623
7	-143	-9	-5	-143	-106	10	272	385	4	259	-310
8	-143	11	-4	275	290	11	292	366	5	500	492
9	334	-248	-3	-146	23	12	-132	64	6	201	163
10	-142	161	-2	272	-183	13	404	-409	7	326	-363
11	-144	94	-1	-143	-162	14	-134	-48	8	520	508
12	-140	-164	H=	4, K=	11	15	-137	113	9	383	434
13	-143	-185	0	281	-304	16	-136	56	10	258	-250
14	-148	101	1	-141	99	17	407	461	11	-120	63
-15	-145	111	2	-144	93	18	-148	-185	12	156	-174
-14	-144	111	3	-144	17	-19	-126	-67	13	-145	274
-13	-140	50	4	-142	71	-18	-138	-160	14	276	-54
-12	-137	-185	5	-144	-57	-17	-132	122	15	158	-65
-11	-141	-176	6	267	-246	-16	208	139	16	-137	-46
-10	-143	219	7	-148	56	-15	-137	107	17	-142	-141
-9	-145	243	8	214	232	-14	-123	11	-15	205	145
-8	546	-498	9	-153	-32	-13	609	590	-18	-139	-39
-7	-139	-276	-10	-151	-131	-12	-127	-61	-17	-137	-143
-6	386	443	-9	-146	-13	-11	518	-523	-16	-133	15
-5	-137	-160	-8	-146	214	-10	643	662	-15	226	-196
-4	-135	-43	-7	-142	-1	-9	-113	17	-14	-125	-10
-3	242	275	-6	-139	6	-8	369	-344	-13	224	-126
-2	-131	6	-5	-144	-8	-7	551	554	-12	334	334
-1	-132	-47	-4	363	-223	-6	448	-403	-11	-122	32
H=	4, K=	9	-3	360	352	-5	557	-560	-10	184	237
0	-143	-6	-2	364	377	-4	606	617	-9	-119	-85
1	-142	175	-1	495	-401	-3	729	722	-8	297	-256
2	-144	162	H=	4, K=	12	-2	-110	33	-7	264	-288
3	-141	-140	0	-145	-38	-1	-111	-85	-6	-111	220
4	-142	-59	1	-148	-66	0	-110	55	-5	967	948
5	-146	32	2	-147	-41	H=	5, K=	2	-4	639	-678
									-3	272	-278
									-2	220	179
									-1	159	257

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 5, K= 4			H= 5, K= 6			H= 5, K= 9			H= 5, K= 12		
0	-116	-147	0	-121	-256	0	223	228	0	-151	-190
1	-113	94	1	301	304	1	-145	166	1	217	-180
2	724	-728	2	521	548	2	-146	-128	2	-150	236
3	-113	-37	3	378	-398	3	225	-113	3	-147	107
4	901	910	4	505	-484	4	-147	-150	4	355	-297
5	472	-451	5	378	392	5	-150	221	5	-154	-19
6	-118	-134	6	240	173	6	-145	89	6	-153	100
7	474	-456	7	-130	152	7	-141	-176	7	-152	-140
8	450	-470	8	-134	151	8	260	-157	8	-144	62
9	-128	-39	9	-140	-248	9	-142	88	9	-146	54
10	383	375	10	462	-462	10	-144	66	10	-153	-157
11	-137	104	11	257	247	11	212	-124	11	-151	93
12	-138	186	12	291	287	12	-144	65	12	-149	79
13	235	-153	13	-138	-76	13	-148	123	13	1064	1071
14	-137	-98	14	299	-291	14	232	-82	14	-132	-21
15	-141	58	15	-146	72	15	-146	-84	15	-135	66
16	-140	-16	16	-149	160	16	-141	132	16	-139	-46
17	-143	41	17	308	-179	17	-141	69	17	334	-321
18	210	-237	18	-139	-166	18	-141	-20	18	-130	42
19	235	-17	19	-138	-168	19	-144	-36	19	-136	-102
20	-139	-105	20	-140	-248	20	-143	-55	20	715	-744
21	232	353	21	-149	160	21	-143	-37	21	832	850
22	237	188	22	-179	-179	22	-144	243	22	-112	-158
23	587	-610	23	-166	-166	23	-141	37	23	1003	988
24	342	-382	24	-168	-168	24	-141	-249	24	-109	119
25	215	119	25	-179	-179	25	-138	24	25	-108	-49
26	438	430	26	-166	-166	26	-141	-82	26	107	-7
27	322	300	27	-166	-166	27	-141	-82	27	301	-322
28	208	-179	28	-166	-166	28	-141	-82	28	1098	1084
29	222	-371	29	-166	-166	29	-141	-82	29	156	-137
30	605	611	30	-166	-166	30	-141	-82	30	2108	-2038
31	390	-410	31	-166	-166	31	-141	-82	31	323	269
32	-114	56	32	-166	-166	32	-141	-82	32	605	615
33	403	364	33	-166	-166	33	-141	-82	33	181	-111
34	-111	-33	34	-166	-166	34	-141	-82	34	248	-337
35	-114	168	35	-166	-166	35	-141	-82	35	264	336
H= 5, K= 5			H= 5, K= 7			H= 5, K= 10			H= 6, K= 1		
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1	689	662	1	-129	-53	1	-146	232	1	301	-322
2	261	-301	2	195	-88	2	-143	101	2	1098	1084
3	319	352	3	-132	-24	3	325	-328	3	156	-137
4	890	-895	4	231	333	4	202	-57	4	2108	-2038
5	269	-132	5	281	-291	5	282	226	5	323	269
6	1020	1068	6	381	-393	6	-144	159	6	605	615
7	-125	48	7	440	499	7	-142	-43	7	181	-111
8	1006	-1040	8	514	507	8	-142	-66	8	248	-337
9	-132	0	9	408	-284	9	-147	-103	9	264	336
10	525	524	10	237	-80	10	-150	-85	10	261	252
11	-137	72	11	-135	62	11	-154	289			
12	384	-297	12	-136	-165	12	209	-52			
13	-136	-145	13	-137	148	13	354	-320			
14	205	212	14	-143	-125	14	-143	-8			
15	-138	60	15	-146	-141	15	-143	-8			
16	-145	35	16	-149	76	16	-143	-8			
17	-148	163	17	-145	-152	17	-143	-8			
18	-138	-10	18	-136	-41	18	-143	-8			
19	-139	-155	19	-131	58	19	-143	-8			
20	-133	-10	20	-132	109	20	-143	-8			
21	-141	159	21	-135	-85	21	-143	-8			
22	219	218	22	-137	-47	22	-143	-8			
23	573	-598	23	-136	82	23	-143	-8			
24	-133	-97	24	-136	82	24	-143	-8			
25	570	563	25	-136	82	25	-143	-8			
26	-128	2	26	-136	82	26	-143	-8			
27	-125	-155	27	-136	82	27	-143	-8			
28	197	-137	28	-136	82	28	-143	-8			
29	866	-888	29	-136	82	29	-143	-8			
30	550	561	30	-136	82	30	-143	-8			
31	747	784	31	-136	82	31	-143	-8			
32	167	-129	32	-136	82	32	-143	-8			
33	-115	-60	33	-136	82	33	-143	-8			
34	213	-273	34	-136	82	34	-143	-8			
35			35	-136	82	35	-143	-8			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	
H= 6, K= 10			H= 7, K= 1			H= 7, K= 3			H= 7, K= 6			
0	-144	258	0	524	-538	0	385	-442	0	538	559	
1	-143	77	1	673	654	1	269	-305	1	206	-199	
2	208	-179	2	581	-597	2	370	323	2	361	-357	
3	-143	-43	3	971	-971	3	-115	160	3	-132	147	
4	-141	113	4	613	569	4	-116	-21	4	-132	129	
5	-138	54	5	-118	151	5	253	-287	5	249	135	
6	-144	-30	6	294	-363	6	-119	26	6	-134	-25	
7	-147	-189	7	263	-277	7	-124	106	7	-140	-164	
8	-146	-131	8	-126	132	8	229	193	8	322	-341	
9	-147	92	9	-132	-55	9	-133	-64	9	223	209	
10	254	266	10	252	-269	10	-134	-20	10	578	559	
-11	-150	22	11	484	507	11	294	-285	11	268	-290	
-10	384	311	12	-139	106	12	-139	24	12	-139	-98	
-9	-142	-152	13	318	-308	13	-136	-7	13	257	221	
-8	-142	-107	14	-138	70	14	-138	125	14	-143	-168	
-7	-140	-51	15	-137	83	15	-137	-63	15	-141	-146	
-6	-136	105	16	-139	-106	16	-142	111	16	-141	-91	
-5	-147	174	17	-139	-127	17	212	119	17	310	248	
-4	-143	-13	18	248	-127	18	-138	72	18	-137	87	
-3	-141	-38	19	-139	-52	19	-138	-2	19	382	-389	
-2	-144	-254	20	200	186	20	258	148	20	-11	321	329
-1	-140	-81	21	-134	-158	21	-137	-79	21	405	402	
H= 6, K= 11			H= 7, K= 2			H= 7, K= 4			H= 7, K= 7			
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1	-143	33	1	185	236	1	750	-763	1	-133	165	
2	-147	-32	2	288	-264	2	-116	-97	2	-139	244	
3	-143	-24	3	249	-272	3	652	638	3	393	-397	
4	278	-179	4	190	209	4	271	289	4	-138	-92	
5	-147	59	5	-117	-66	5	329	-275	5	336	362	
6	-155	215	6	-118	165	6	351	-324	6	-144	119	
7	-150	-76	7	464	471	7	-127	48	7	-141	-63	
8	-149	3	8	300	-342	8	230	128	8	-136	9	
9	-151	110	9	422	-415	9	-132	-15	9	201	204	
-10	-148	-56	10	335	305	10	-132	-15	-10	-127	-82	
-11	-148	-219	11	-134	-23	11	-136	176	-11	497	-522	
-12	250	-219	12	-140	-268	12	229	227	-12	271	353	
-13	-148	73	13	-137	237	13	-139	-238	H= 7, K= 7			
-14	266	245	14	-140	-16	14	-136	-6	0	416	-461	
-15	-145	-61	15	-139	90	15	-145	-9	1	-133	165	
-16	-142	-62	16	-140	68	16	-150	-25	2	-139	244	
-17	-146	9	17	-145	8	17	-144	-30	3	393	-397	
H= 6, K= 12			H= 7, K= 0			H= 7, K= 5			4	-138	-92	
0	226	-74	0	1005	-1026	0	215	-236	5	336	362	
1	238	189	1	-110	25	1	750	-763	6	-144	119	
2	267	179	2	240	270	2	-116	-97	7	-141	-63	
3	226	-168	3	568	-555	3	652	638	8	-136	9	
4	-150	-87	4	889	906	4	271	289	9	201	204	
5	-153	-1	5	557	-576	5	329	-275	-10	-127	-82	
6	252	-23	6	266	238	6	351	-324	-11	497	-522	
7	-144	29	7	-137	-144	7	-127	48	-12	271	353	
8	-150	95	8	-140	-16	8	230	128	H= 7, K= 7			
-1	-148	-118	9	-139	90	9	-132	-15	0	416	-461	
H= 7, K= 0			10	-140	68	10	-139	-238	1	-133	165	
1	1005	-1026	11	-145	8	11	-136	176	2	-139	244	
3	-110	25	12	-141	75	12	229	227	3	393	-397	
5	240	270	13	-135	-7	13	-139	-238	4	-138	-92	
7	568	-555	14	-140	-16	14	-136	-6	5	336	362	
9	889	906	15	-145	8	15	-145	-9	6	-144	119	
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13	266	238	17	-135	-7	17	-136	176	8	-136	9	
15	-137	-144	18	-140	68	18	-139	-238	H= 7, K= 7			
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-17	-143	84	20	-141	75	20	-139	22	1	-133	165	
-15	-137	-117	21	-135	-7	21	-136	176	2	-139	244	
-13	220	-208	22	-140	-16	22	229	227	3	393	-397	
-11	651	653	23	-145	8	23	-136	176	4	-138	-92	
-9	380	-346	24	-141	75	24	-139	-238	5	336	362	
-7	-117	-155	25	-145	8	25	-145	-9	6	-144	119	
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-3	799	-810	27	-135	-7	27	-136	176	8	-136	9	

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
12	-137	-59	-5	-139	-108	-2	-145	136	2	-124	-15
13	351	337	-4	-136	-170	-1	-138	-46	3	415	-444
14	-142	3	-3	-134	57				4	264	216
-16	-138	-84	-2	-138	59	H=	8, K=	11	5	-127	93
-15	-138	-13	-1	-138	-114	0	-155	201	6	-131	-61
-14	-129	66				1	-153	-184	7	-130	-127
-13	237	-163	H=	8, K=	8	2	316	-276	8	-135	228
-12	-134	69	0	205	106	3	-151	107	9	-142	189
-11	281	320	1	-143	1	4	-153	237	10	-126	-55
-10	-139	-113	2	-141	50	-7	-152	106	11	-131	29
-9	229	-150	3	-138	65	-6	-157	235	12	-137	-27
-8	-136	-7	4	212	-197	-5	214	-59	13	275	-244
-7	429	435	5	-139	-154	-4	-147	-79	14	-141	83
-6	-130	200	6	269	325	-3	-147	-52	15	-151	207
-5	579	-544	7	-141	178	-2	-151	12	-17	255	-325
-4	-123	-59	8	-141	-174	-1	-149	133	-16	377	215
-3	-125	168	9	-143	42	H=	9, K=	0	-15	397	423
-2	198	-94	10	-148	-21	1	-118	-92	-14	236	-254
-1	-129	250	11	-141	-101	2	472	454	-13	265	-268
H=	8, K=	6	-13	-147	77	3	222	-243	-12	-135	132
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1	-137	-186	-11	-135	-88	5	225	294	-10	-135	-10
2	-134	-76	-10	219	33	7	267	-256	-9	190	194
3	-132	-95	-9	-136	94	9	-137	-150	-8	-128	117
4	-137	72	-8	-143	210	11	395	373	-7	289	-306
5	342	344	-7	217	147	13	500	-493	-6	-124	158
6	318	-218	-6	419	-453	15	243	322	-5	723	720
7	514	-552	-5	-140	-231	-17	224	-211	-4	447	-425
8	426	419	-4	-145	145	-15	198	208	-3	163	-23
9	393	328	-3	-142	107	-13	-140	-280	-2	229	226
10	313	-344	-2	-141	13	-11	-128	32	-1	311	-223
11	-142	-86	-1	-147	-100	-9	-126	175	H=	9, K=	3
12	-142	212	H=	8, K=	9	-7	569	-554	0	419	435
13	-146	-38	0	387	-393	-3	-116	107	1	383	411
-16	-146	37	1	-138	-44	-1	489	-474	2	190	-168
-15	-143	135	2	-141	202	H=	9, K=	1	3	-125	-89
-14	-138	-103	3	-140	115	0	-119	-157	4	-123	-30
-13	361	-305	4	-138	-45	1	683	-680	5	-133	-127
-12	227	152	5	-146	-224	2	571	553	6	-131	34
-11	387	331	6	-138	38	3	295	250	7	-131	58
-10	214	-1	7	-140	31	4	360	-371	8	243	-140
-9	-141	-122	8	-147	62	5	-124	-84	9	-138	-184
-8	-136	78	9	-147	-6	6	236	76	10	-142	229
-7	342	-292	10	-151	33	7	180	-44	11	265	266
-6	196	188	-12	-154	156	8	-136	3	12	-136	-149
-5	365	334	-11	-145	-35	9	523	523	13	-138	-93
-4	-136	-146	-10	-146	-180	10	428	-418	14	-142	156
-3	-133	-17	-9	-143	0	11	524	-514	-17	-148	87
-2	278	212	-8	-141	102	12	287	322	-16	-140	19
-1	-129	76	-7	-144	89	13	354	310	-15	-135	-25
H=	8, K=	7	-6	-137	-77	14	-139	-151	-14	376	367
0	410	454	-5	-136	20	15	-142	-134	-13	195	177
1	486	487	-4	-138	-12	-17	253	131	-12	483	-443
2	453	-460	-3	259	-223	-16	-140	-126	-11	197	-142
3	336	-373	-2	-141	153	-15	-139	101	-10	-135	0
4	-143	229	-1	-143	160	-14	-130	-24	-9	-131	-40
5	-139	111	H=	8, K=	10	-13	409	-395	-8	-131	63
6	-141	-214	0	-144	-22	-12	-138	136	-7	183	-187
7	-139	177	1	-138	-85	-11	613	610	-6	219	59
8	276	223	2	-141	-35	-10	311	-295	-5	-125	-74
9	-137	-109	3	-149	127	-9	-130	-68	-4	373	401
10	-139	-61	4	-145	69	-8	324	244	-3	240	272
11	-141	-39	5	-146	58	-7	-121	7	-2	585	-586
12	-143	-43	6	307	-263	-6	226	-253	-1	203	-265
-15	265	-128	7	226	-98	-5	-118	156	H=	9, K=	4
-14	233	-132	-10	-152	-121	-4	326	309	0	-124	-18
-13	-143	193	-9	268	-232	-3	251	-208	1	-123	-8
-12	-135	20	-8	-142	27	-2	367	-352	2	239	221
-11	-140	-259	-7	236	162	-1	335	371	3	-129	158
-10	-137	99	-6	-144	107	H=	9, K=	2	4	-129	-42
-9	390	401	-5	-142	-61	0	194	106	5	-132	-43
-8	304	-305	-4	-148	-209	1	368	266	6	-134	168
-7	249	-252	-3	-138	52				7	-135	136
-6	369	375							8	-143	-171

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
9	579	-591	-8	-138	-174	-8	-142	149	-12	-137	190
10	210	-145	-7	-139	153	-7	-143	-24	-11	-134	141
11	254	764	-6	451	473	-6	-144	-180	-10	-133	-300
12	269	190	-5	208	-205	-5	252	-28	-9	-132	99
13	-144	107	-4	466	-456	-4	-141	74	-8	216	191
14	-148	-213	-3	210	258	-3	299	275	-7	368	-392
-16	391	-298	-2	275	302	-2	-141	96	-6	-124	142
-15	-136	-56	-1	361	-368	-1	362	-366	-5	-126	100
-13	237	211							-4	597	-611
-13	212	302	H=	9, K=	7	H=	9, K=	10	-3	291	281
-12	-134	-59							-2	678	700
-11	221	-53	0	423	398	0	-140	11	-1	299	-314
-10	-136	-11	1	450	-458	1	-151	-48			
-9	-133	2	2	325	-327	2	251	-4	H=	10, K=	2
-8	186	224	3	204	206	3	292	257			
-7	-127	62	4	-140	65	4	-151	-21	0	494	513
-6	473	-482	5	241	-232	5	-147	-104	1	-121	5
-5	-130	65	6	-141	161	6	-150	-35	2	453	-419
-4	252	223	7	-138	-141	-6	-147	256	3	-131	112
-3	205	78	8	-142	-55	-7	-148	196	4	156	171
-2	-122	43	9	281	227	-6	-142	-76	5	293	-281
-1	-130	-208	10	-144	115	-5	-147	-142	6	-137	55
			11	249	-155	-4	-148	2	7	-136	156
H=	9, K=	5	-14	247	226	-3	254	164	8	-135	-83
0	547	-537	-13	-142	-65	-2	-140	-15	9	-136	100
1	195	-50	-12	-144	-125	-1	257	-187	10	-134	59
2	683	725	-11	-143	32				11	-139	-120
3	-131	137	-10	-135	-55	H=	9, K=	11	12	218	-249
4	-135	-203	-9	-138	-46				13	279	234
5	-137	133	-8	-136	-104	0	324	-235	14	-149	227
6	-136	-20	-7	-137	48	1	340	-355	-16	-139	176
7	-137	178	-6	-144	121	2	284	231	-15	-138	-102
8	-140	286	-5	-141	-145	-4	-147	20	-14	-132	83
9	227	-182	-4	362	336	-3	-144	-76	-13	-134	91
10	261	-305	-3	-140	-141	-2	-147	86	-12	-132	32
11	-140	50	-2	478	-494	-1	258	250	-11	-136	206
12	366	302	-1	216	290				-10	344	319
13	-148	-102	H=	9, K=	8	H=	10, K=	0	-9	276	-189
-16	-146	-38				0	-118	121	-8	454	-502
-15	-139	-81	0	290	-282	2	-126	100	-7	203	185
-14	-137	-132	1	-143	163	4	364	-328	-6	-130	28
-13	-139	175	2	-143	175	6	472	488	-5	-127	-48
-12	-141	187	3	-142	-169	8	378	-353	-4	-127	196
-11	-135	-41	4	239	-200	10	-136	-120	-3	254	201
-10	-138	-190	5	-136	83	12	368	416	-2	274	-219
-9	-136	29	6	-139	73	14	486	-489	-1	211	-223
-8	290	237	7	-140	-106	-16	340	-337	H=	10, K=	3
-7	-134	118	8	-141	-126	-14	-131	106	0	-129	187
-6	-130	-17	9	-144	64	-12	-136	130	1	246	-216
-5	-133	-174	10	-141	-2	-10	212	-158	2	233	188
-4	156	-66	-12	-143	-34	-8	219	253	3	-130	-158
-3	277	217	-11	-150	-85	-6	506	-517	4	-128	32
-2	-124	-105	-10	225	-123	-4	678	681	5	-134	254
-1	-130	78	-9	-143	164	-2	178	-234	6	210	291
			-8	-141	172				7	273	-321
H=	9, K=	6	-7	-138	-118	H=	10, K=	1	8	212	-179
0	-131	-56	-6	-140	-205	0	154	-255	9	-134	119
1	-134	76	-5	-142	214	1	221	185	10	264	271
2	333	-251	-4	-141	-190	2	226	155	11	-132	-159
3	205	190	-3	236	-153	3	123	-107	12	-139	-193
4	-149	160	-2	462	448	4	-135	73	13	-141	51
5	-141	-98	-1	207	-5	5	-125	106	-16	-143	-125
6	248	-242	H=	9, K=	9	6	227	-259	-15	294	266
7	-141	178				7	-135	73	-14	243	216
8	248	286	0	252	-261	8	232	314	-13	201	-240
9	-138	102	1	340	352	9	-134	-62	-12	200	-164
10	-143	-134	2	-146	236	10	299	-271	-11	381	356
11	-142	175	3	-146	-123	11	-135	168	-10	-127	130
12	-145	-79	4	-139	14	12	211	168	-9	-136	-197
-15	-146	-62	5	-144	0	13	-142	-189	-8	299	294
-14	301	-237	6	-143	23	14	-143	-44	-7	-133	-111
-13	-139	54	7	-146	2	-17	-141	13	-6	-129	-79
-12	-139	116	8	-149	-98	-16	275	256	-5	234	266
-11	-133	-3	-11	-148	-133	-15	-136	0	-4	223	221
-10	-138	63	-10	-141	-54	-14	-136	-187	-3	-125	-142
-9	-137	-173	-9	-142	140	-13	-131	-89	-2	369	-430

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-1	527	505	10	213	-179	-9	-147	62	1	315	-331
H= 10, K= 4			11	-142	-235	-8	-142	70	2	286	227
0	272	-235	-14	-141	75	-7	-140	-94	3	207	235
1	279	252	-13	-138	66	-6	-144	-150	4	-132	-104
2	-130	-77	-12	-137	94	-5	-144	71	5	-137	-112
3	-132	19	-11	-134	-113	-4	-144	162	6	-134	165
4	-135	-84	-10	-135	36	-3	243	53	7	-135	-102
5	-137	224	-9	217	-99	-2	-145	-268	8	-133	23
6	-139	272	-8	192	29	-1	-137	59	9	-134	38
7	-136	-54	-7	206	222	H= 10, K= 10			10	-136	-1
8	-133	-197	-6	-136	-90	0	-146	-46	11	-139	-137
9	-131	-29	-5	281	-254	1	-150	63	12	-141	160
10	253	257	-4	-143	155	2	-144	112	13	310	293
11	251	223	-3	-134	71	3	-146	-46	-10	-145	-147
12	-138	-25	-2	268	-286	4	-147	-56	-15	-139	-6
13	256	-249	-1	-139	188	-6	-155	-222	-14	-138	70
-16	229	-56	H= 10, K= 7			-5	-145	-2	-13	-137	-168
-15	-143	245	0	461	-478	-4	220	240	-11	-137	44
-14	-139	126	1	-128	-38	-3	-145	45	-10	-136	-17
-13	-134	48	2	336	360	-2	234	-103	-9	340	-312
-12	335	-467	3	-135	-172	-1	-150	-51	-8	373	295
-11	-134	-233	4	-131	-41	H= 11, K= 0			-7	232	282
-10	-139	201	5	211	174	1	609	633	-6	-133	-196
-9	-137	195	6	-138	-212	3	258	-354	-5	226	-59
-8	-137	-10	7	245	-220	5	378	395	-4	-130	78
-7	-136	-250	8	-141	246	7	-132	-54	-3	433	-476
-6	300	-220	9	234	239	9	246	243	-2	230	159
-5	296	334	10	312	-238	11	193	132	-1	904	890
-4	218	236	-13	217	-190	13	534	-476	H= 11, K= 3		
-3	204	-227	-12	-137	43	-15	-141	124	0	-129	-92
-2	-130	184	-11	-134	141	-13	-133	-88	1	-132	44
-1	-129	-67	-10	235	-67	-11	-129	28	2	206	-202
H= 10, K= 5			-9	-131	134	-9	438	426	3	199	1
0	-133	35	-8	-128	115	-7	-130	-38	4	259	292
1	314	290	-7	-135	-253	-5	-126	130	5	287	250
2	-134	41	-6	-127	24	-3	-124	-26	6	245	-192
3	273	-178	-5	191	13	-1	652	-661	7	208	-160
4	-135	-104	-4	-128	60	H= 11, K= 1			8	-131	71
5	-135	-22	-3	-137	-295	0	619	637	9	-136	-17
6	-136	68	-2	281	283	1	-130	140	10	-137	48
7	-135	178	-1	380	345	2	-131	-183	11	-138	-48
8	-133	-8	H= 10, K= 8			3	-129	11	12	-138	-8
9	332	-310	0	-139	140	4	-129	20	-15	238	234
10	-133	-120	1	379	435	5	409	-420	-14	264	-278
11	271	308	2	272	-248	6	-134	64	-13	-135	-113
12	-144	86	3	-138	-79	7	297	253	-12	-137	-132
-15	301	-268	4	-136	88	8	-137	-161	-11	224	183
-14	-137	71	5	-135	-22	9	-133	62	-10	-135	108
-13	-139	189	6	-134	104	10	-135	131	-9	-137	-132
-12	-133	-12	7	-141	-148	11	-138	131	-8	-136	-185
-11	233	-45	8	-145	9	12	-135	-82	-7	-135	-189
-10	211	-157	9	-143	81	13	-144	143	-6	-129	84
-9	-136	138	-11	-142	-58	-16	-145	-6	-5	-129	75
-8	-138	23	-10	-135	114	-15	272	-307	-4	466	-470
-7	243	-190	-9	213	180	-14	-139	57	-3	-131	-101
-6	-138	-213	-8	220	-231	-13	-137	74	-2	515	555
-5	226	-199	-7	-136	-124	-12	-135	-57	-1	-136	-228
-4	-135	156	-6	-138	75	-11	-135	52	H= 11, K= 4		
-3	608	641	-5	-135	200	-10	214	210	0	311	337
-2	224	-212	-4	-136	-48	-9	-135	-74	1	293	250
-1	746	-734	-3	-135	57	-8	-132	58	2	340	-318
H= 10, K= 6			-2	-140	122	-7	156	226	3	358	-340
0	-135	63	-1	550	-591	-6	-130	177	4	336	245
1	219	-30	H= 10, K= 9			-5	-123	-211	5	-135	102
2	239	-76	0	273	169	-4	-131	-229	6	-132	-46
3	-140	34	1	-143	-67	-3	750	750	7	-130	-43
4	-138	-151	2	-146	-63	-2	220	-220	8	-134	-65
5	217	-274	3	-138	14	-1	504	-531	9	199	57
6	-136	75	4	-148	-130	H= 11, K= 2			10	-137	46
7	-137	232	5	207	-10	0	-132	-165	11	-135	-83
8	-133	43	6	-152	184	-15	-140	-8	12	266	-252
9	-135	24	7	-148	134	-14	-143	7	-15	-140	-8

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-13	203	-105	6	320	-248	6	240	242	-2	-135	148
-12	-131	-75	7	227	227	7	-133	-67	-1	-137	-214
-11	-137	128	8	-149	112	8	164	10			
-10	347	365	9	243	-167	9	-143	145	H=	12, K=	4
-9	-131	-11	-12	-143	78	10	-137	-36	0	-138	-58
-8	335	-375	-11	-144	-25	11	-141	-34	1	346	-508
-7	-135	66	-10	-143	23	-15	-135	62	2	-135	13
-6	-134	-17	-9	-140	22	-14	-141	65	3	-135	77
-5	199	179	-8	-137	-138	-13	-133	22	4	-134	215
-4	-133	50	-7	-137	-47	-12	-138	-24	5	-131	-6
-3	-137	-197	-6	238	228	-11	-136	86	6	-132	-90
-2	365	-394	-5	-137	5	-10	-132	-111	7	-136	-32
-1	-136	-193	-4	228	-164	-9	264	-278	8	220	-54
H=	11, K=	5	-3	-136	-3	-8	240	247	9	-135	5
0	421	372	-2	-140	33	-7	-133	71	10	-142	142
1	-136	-110	-1	-140	-207	-6	260	-222	-14	-145	17
2	-138	-116	H=	11, K=	8	-5	-140	175	-13	267	-86
3	269	-250	0	239	210	-4	341	258	-12	-139	60
4	-139	-125	1	-141	-154	-3	-134	-151	-11	-139	100
5	-136	127	2	-144	-116	-2	622	-656	-10	-137	-75
6	-136	170	3	-144	24	H=	12, K=	2	-9	-136	-193
7	-133	88	4	-145	113	0	835	-825	-8	305	-228
8	-138	-184	5	-143	-39	1	-135	227	-7	-134	47
9	-142	-53	6	-149	120	2	-132	40	-6	311	270
10	-147	158	7	-148	-58	3	-134	-173	-5	-139	214
11	274	107	-10	-145	97	4	-139	169	-4	-140	-208
-14	234	170	-9	226	-120	5	-131	34	-3	408	-449
-13	-143	-5	-8	-146	-124	6	151	-155	-2	-138	-41
-12	253	-219	-7	264	194	7	-136	-44	-1	794	810
-11	-137	-137	-6	-138	-25	8	-136	107	H=	12, K=	5
-10	-138	192	-5	-138	-64	9	-134	0	0	225	161
-9	-137	172	-4	-142	91	10	-145	-106	1	-134	72
-8	-140	63	-3	-140	-75	11	270	208	2	-137	-190
-7	-134	-105	-2	-141	-69	-15	-142	-33	3	-135	-69
-6	-133	55	-1	-140	125	-14	-142	-144	4	-131	45
-5	-132	-5	H=	11, K=	9	-13	-139	5	5	-137	176
-4	-134	159	0	-145	-104	-12	-137	118	6	-142	-95
-3	-137	-3	1	-142	-48	-11	-134	-6	7	279	-250
-2	698	-666	2	-146	123	-10	-133	-83	8	-137	46
-1	431	426	3	-146	-97	-9	-133	11	9	-150	112
H=	11, K=	6	4	-148	-61	-8	-134	-86	-13	-149	19
0	548	-523	-7	-149	-154	-7	-134	-61	-12	-141	0
1	262	249	-6	-146	-22	-6	-134	153	-11	-136	-39
2	363	354	-5	242	226	-5	-130	2	-10	201	107
3	-139	-86	-4	-141	-15	-4	218	-167	-9	-136	-1
4	314	-336	-3	214	-151	-3	-134	49	-8	219	-85
5	-136	9	-2	-143	-29	-2	808	817	-7	-136	-166
6	-138	195	-1	-144	190	-1	557	-551	-6	-136	128
7	225	-96	H=	12, K=	0	H=	12, K=	3	-5	-136	222
8	-140	-53	0	947	991	0	-138	139	-4	-138	-10
9	-143	-51	2	-133	-134	1	212	-179	-3	271	-337
10	-149	6	4	-138	333	2	-141	-79	-2	369	-351
-13	-142	-103	6	250	-218	3	-136	-30	-1	356	257
-12	-143	63	8	-137	3	4	-135	57	H=	12, K=	6
-11	-135	-3	10	-143	186	5	-137	-101	0	-135	-72
-10	-136	-58	12	294	-357	6	-133	-41	1	350	397
-9	-138	80	-14	-135	43	7	192	46	2	-135	-126
-8	-134	35	-12	195	137	8	-136	-61	3	207	-195
-7	-135	-67	-10	-128	-1	9	-135	-9	4	-138	141
-6	211	-131	-8	-135	-158	10	-139	10	5	-141	30
-5	-131	-41	-6	-131	59	11	-146	-162	6	289	-158
-4	-136	176	-4	380	369	-14	-144	-119	7	-147	118
-3	-138	-128	-2	1112	-1095	-13	203	173	8	-148	-68
-2	326	251	H=	12, K=	1	-12	-134	3	-12	-143	-10
-1	-137	-53	0	-130	104	-11	-138	-6	-11	-139	-61
H=	11, K=	7	1	-131	-62	-10	-129	78	-10	-140	11
0	253	256	2	-131	49	-9	309	-273	-9	214	208
1	-137	170	3	-136	112	-8	-139	-153	-8	208	-123
2	290	-300	H=	12, K=	1	-7	317	337	-7	-139	0
3	-139	5	0	-130	104	-6	-137	174	-6	-145	265
4	-137	145	1	-131	-62	-5	-136	-207	-5	-134	-154
5	-140	-124	2	-131	49	-4	350	-261	-4	-134	32
			3	-136	112	-3	421	423	-3	-137	36

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-2	192	73	H=	13, K=	0	5	-134	-177	2	-135	-41
-1	304	-263				6	-139	-16	3	-140	-20
H=	12, K=	7	1	-136	-86	7	259	292	4	195	124
0	193	128	3	202	98	8	-138	-51	5	230	-13
1	200	-196	5	-135	167	9	223	-158	6	-141	-206
2	-143	127	7	207	-190	10	-143	46	7	-141	-77
3	205	135	9	212	160	-13	-138	116	8	-144	125
4	-142	-67	-13	-140	32	-12	-143	-126	9	-143	46
5	-143	-48	-11	-136	38	-11	198	-168	-12	-145	100
6	-146	141	-9	-134	-106	-10	-133	187	-11	-140	44
7	-146	-16	-7	-134	0	-9	-138	99	-10	-140	-153
-10	-144	7	-5	-138	36	-8	-136	-150	-9	264	204
-9	-147	-184	-3	683	-674	-7	-134	99	-8	-136	70
-8	-140	17	-1	430	442	-6	-136	35	-7	194	-20
-7	209	270	H=	13, K=	1	-5	390	-370	-6	-133	154
-6	-140	-100	0	-132	-139	-4	233	143	-5	-140	-245
-5	-143	-109	1	-133	117	-3	505	552	-4	400	-404
-4	-139	144	2	-130	65	-2	344	-286	-3	230	106
-3	201	164	3	285	-284	-1	-138	-173	-2	406	428
-2	-134	-102	4	-135	19	H=	13, K=	3	-1	268	195
-1	-137	-72	5	298	294	0	202	-223	I=	13, K=	5
H=	12, K=	8	6	-138	-179	1	-133	-117	0	-135	-99
0	298	-195	7	-135	-128	2	-137	150	1	-139	-143
1	232	-135	8	209	111	3	-136	29	2	-139	54
2	-147	63	9	-138	24	4	258	-245	3	-138	153
3	-141	28	10	-146	-37	5	-134	-74	4	240	228
4	-144	-42	-14	-146	-83	6	213	246	5	-138	-80
5	-150	171	-13	-139	55	7	-140	-160	6	290	-298
-8	254	143	-12	-139	106	8	-141	65	7	-143	111
-7	-144	-108	-11	-136	-195	9	-144	64	8	257	99
-6	-143	28	-10	-133	-16	-13	-138	-33	-11	-142	-12
-5	-140	144	-9	266	298	-12	-139	123	-10	-141	149
-4	-144	-194	-8	-130	-8	-11	-141	109	-9	-140	66
-3	276	-102	-7	-130	-116	-10	-139	-137	-8	-143	-264
-2	-148	195	-6	-132	-2	-9	353	-284	-7	-142	60
-1	253	184	-5	271	169	-8	-135	210	-6	318	293
H=	12, K=	9	-4	218	-310	-7	-130	182	-5	-134	121
0	-151	55	-3	258	-257	-6	240	-274	-4	241	-221
1	-145	-74	-2	220	270	-5	410	-417	-3	-138	-207
-4	-151	-90	-1	277	-156	-4	-135	69	-2	-135	140
-3	-144	-90	H=	13, K=	2	-3	547	525	-1	315	287
-2	-150	28	0	210	78	-2	-143	273	I=	13, K=	6
-1	-146	81	1	226	-193	-1	-136	-252	-10	-142	16
			2	-131	-64	H=	13, K=	4	-9	-141	-123
			3	-136	29	0	210	-248	-8	-143	39
			4	-132	89	1	-136	-15			

Table B-2
Observed and Calculated Structure Factors for $[\text{Co}(\text{Hdmg})_2^-$
 $(\text{clan})_2]\text{Cl}$

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	0, K=	0	0	155	-142	H=	0, K=	6	6	15	-6
1	765	730	1	134	-126	0	262	263	7	238	230
2	469	420	2	40	35	1	371	379	8	241	254
3	137	121	3	95	-88	2	299	295	9	64	62
4	202	177	4	28	30	3	247	258	10	229	234
5	437	405	5	116	-113	4	195	197	11	126	131
6	48	35	6	295	270	5	128	131	12	197	199
7	357	342	7	140	137	6	172	172	-13	122	128
8	75	73	8	135	131	7	43	44	-12	42	41
9	229	219	9	184	184	8	70	74	-11	147	155
10	55	58	10	60	61	9	68	63	-10	195	194
11	230	229	11	95	95	-10	131	136	-9	111	110
12	103	108	12	-12	-10	-9	92	91	-8	385	367
13	43	39	-12	66	69	-8	101	99	-7	231	223
H=	0, K=	1	-11	-12	-16	-7	75	70	-6	414	384
0	651	638	-10	42	-44	-6	140	141	-5	24	25
1	426	409	-9	135	133	-5	206	204	-4	311	300
2	345	309	-8	117	117	-4	178	178	-3	30	-21
3	177	164	-7	116	113	-3	228	228	-2	43	45
4	235	-217	-6	15	23	-2	190	188	-1	653	627
5	172	161	-5	234	238	-1	185	189	H=	1, K=	1
6	315	-270	-4	173	163	H=	0, K=	7	0	238	-229
7	226	191	-3	41	29	0	76	78	1	99	94
8	101	105	-2	304	-292	1	27	28	2	315	-301
9	66	54	-1	239	-225	2	59	58	3	110	-115
10	190	193	H=	0, K=	4	3	124	123	4	343	330
11	81	83	0	211	199	4	97	100	5	72	-61
12	174	177	1	194	191	5	54	48	6	223	217
13	27	21	2	333	332	6	-11	0	7	34	32
-13	53	57	3	235	224	7	32	37	8	287	281
-12	44	-48	4	202	201	8	110	112	9	-11	11
-11	101	103	5	328	329	-9	-12	2	10	127	127
-10	-14	15	6	132	131	-8	-11	10	11	17	32
-9	67	-62	7	204	199	-7	-11	-2	12	-12	-4
-8	-12	-8	8	68	67	-6	-11	-7	-13	-12	14
-7	31	1	9	138	136	-5	69	68	-12	60	60
-6	555	519	10	60	58	-4	214	211	-11	100	99
-5	231	216	11	132	137	-3	242	247	-10	144	140
-4	349	337	-12	104	107	-2	126	128	-9	175	-173
-3	103	-103	-11	104	105	-1	61	64	-8	166	177
-2	84	-73	-10	146	147	H=	0, K=	8	-7	55	53
-1	443	431	-9	224	230	0	104	111	-6	88	69
H=	0, K=	2	-8	75	78	1	67	66	-5	164	-164
0	475	-471	-7	194	190	2	93	99	-4	399	-370
1	394	367	-6	160	155	3	111	112	-3	285	292
2	299	279	-5	210	214	4	103	106	-2	176	-174
3	204	188	-4	283	285	5	54	57	-1	426	421
4	146	131	-3	31	30	6	90	90	H=	1, K=	2
5	40	-36	-2	21	19	-7	83	83	0	413	394
6	487	484	-1	112	-102	-6	51	52	1	59	53
7	269	256	H=	0, K=	5	-5	79	78	2	411	392
8	320	303	0	-10	8	-4	193	194	3	81	85
9	115	114	1	271	266	-3	280	282	4	284	260
10	297	291	2	193	190	-2	273	276	5	37	38
11	74	78	3	89	94	-1	192	193	6	241	225
12	91	87	4	58	54	H=	0, K=	9	7	194	188
-13	34	38	5	138	140	0	-11	5	8	213	204
-12	52	47	6	93	91	1	-11	17	9	322	323
-11	36	38	7	21	28	2	26	30	10	81	79
-10	102	103	8	59	-61	-3	26	24	11	70	72
-9	-14	21	9	51	-49	-2	45	45	12	73	-78
-8	238	241	10	28	26	-1	26	29	-13	74	74
-7	67	73	-11	92	94	H=	1, K=	0	-12	145	151
-6	486	472	-12	195	196	0	699	676	-11	110	113
-5	547	512	-9	90	93	1	250	242	-10	28	-27
-4	476	450	-8	16	-9	2	45	40	-9	146	144
-3	458	450	-7	20	-16	3	671	651	-8	126	132
-2	235	228	-6	61	60	4	337	324	-7	269	266
-1	673	668	-5	60	53	5	520	491	-6	140	143
H=	0, K=	3	-4	34	-30	H=	0, K=	6	-5	159	160
0	475	-471	-3	73	-72	0	262	263	-4	44	-37
1	394	367	-2	36	42	1	371	379	-3	306	323
2	299	279	-1	25	-19	2	299	295	-2	300	296
3	204	188	H=	0, K=	4	3	247	258	-1	302	284
4	146	131	0	155	-142	4	195	197			
5	40	-36	1	134	-126	5	128	131			
6	487	484	2	40	35	6	172	172			
7	269	256	3	95	-88	7	43	44			
8	320	303	4	28	30	8	70	74			
9	115	114	5	116	-113	9	68	63			
10	297	291	6	295	270	-10	131	136			
11	74	78	7	140	137	-9	92	91			
12	91	87	8	135	131	-8	101	99			
-13	34	38	9	184	184	-7	75	70			
-12	52	47	10	60	61	-6	140	141			
-11	36	38	11	95	95	-5	206	204			
-10	102	103	12	-12	-10	-4	178	178			
-9	-14	21	-12	66	69	-3	228	228			
-8	238	241	-11	-12	-16	-2	190	188			
-7	67	73	-10	42	-44	-1	185	189			
-6	486	472	-9	135	133						
-5	547	512	-8	117	117						
-4	476	450	-7	116	113						
-3	458	450	-6	15	23						
-2	235	228	-5	234	238						
-1	673	668	-4	173	163						
			-3	41	29						
			-2	304	-292						
			-1	239	-225						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	1, K=	3	H=	1, K=	6	-6	127	135	0	244	232
0	156	159	0	221	225	-5	175	175	1	408	166
1	237	-231	1	154	182	-4	193	187	2	395	384
2	146	140	2	166	166	-3	166	173	3	437	427
3	247	239	3	176	172	-2	104	107	4	184	186
4	33	37	4	188	177	-1	63	65	5	116	119
5	130	127	5	244	233	H=	1, K=	-7	6	103	105
6	146	-142	6	144	151	0	22	24	7	177	181
7	157	150	7	37	34	1	30	33	8	111	113
8	-11	-12	8	102	104	2	63	63	9	126	117
9	129	123	-10	105	104	3	107	107	10	75	68
10	66	68	-9	72	69	4	33	29	11	77	26
11	-11	9	-8	30	28	5	16	-12	-12	105	109
-13	96	92	-7	113	110	6	38	42	-11	114	115
-12	101	102	-6	260	252	7	100	102	-10	71	75
-11	-11	10	-5	309	314	8	99	104	-9	170	168
-10	108	-109	-4	246	240	-8	93	93	-8	133	134
-9	133	137	-3	176	175	-7	41	42	-7	-11	-2
-8	50	47	-2	160	158	-6	40	35	-6	262	251
-7	96	96	-1	152	153	-5	36	35	-5	245	229
-6	-10	15	H=	1, K=	7	-4	52	56	-4	350	354
-5	29	28	0	53	59	-3	45	48	-3	214	207
-4	257	249	1	16	-14	-2	46	-47	-2	194	193
-3	131	-132	2	-11	-5	-1	22	-11	-1	381	380
-2	186	178	3	47	47	H=	1, K=	-6	H=	1, K=	-3
-1	183	177	4	52	52	0	134	141	0	629	-617
H=	1, K=	4	5	56	58	1	229	225	1	71	66
0	298	295	6	-12	0	2	242	243	2	198	192
1	405	400	7	98	101	3	165	165	3	375	361
2	233	230	-9	-12	15	4	124	127	4	314	297
3	294	284	-8	-12	-17	5	120	118	5	59	-53
4	246	244	-7	30	-28	6	59	101	6	70	67
5	208	203	-6	22	-20	7	113	114	7	36	36
6	142	136	-5	36	35	8	112	111	8	159	162
7	113	110	-4	79	80	9	82	86	9	-11	3
8	28	24	-3	68	64	10	134	136	10	-11	-9
9	25	22	-2	62	82	-10	113	112	11	-11	-19
10	148	151	-1	77	75	-9	83	85	12	26	25
-12	83	86	H=	1, K=	8	-8	97	94	-12	62	62
-11	65	64	0	95	98	-7	121	123	-11	18	-21
-10	128	127	1	114	116	-6	78	72	-10	102	105
-9	127	127	2	114	115	-5	114	117	-9	-11	-17
-8	228	232	3	104	107	-4	141	141	-8	79	82
-7	266	267	-7	82	80	-3	129	125	-7	40	36
-6	283	291	-6	63	63	-2	73	70	-6	231	219
-5	254	251	-5	54	52	-1	75	76	-5	196	193
-4	231	240	-4	84	87	H=	1, K=	-5	-4	439	421
-3	114	117	-3	149	145	0	99	98	-3	562	567
-2	320	319	-2	119	122	1	55	55	-2	289	268
-1	495	489	-1	82	83	2	145	143	-1	265	261
H=	1, K=	5	H=	1, K=	-9	3	15	17	H=	1, K=	-2
0	152	140	0	66	68	4	-10	3	0	106	-102
1	314	313	1	118	119	5	62	61	1	411	392
2	136	135	2	84	83	6	40	38	2	345	328
3	39	44	3	21	15	7	28	32	3	183	184
4	135	132	-3	36	33	8	37	-42	4	503	482
5	95	94	-2	34	37	9	68	66	5	283	270
6	183	179	-1	25	24	10	77	79	6	405	396
7	99	-105	H=	1, K=	-8	11	37	40	7	118	116
8	46	-44	0	109	110	-11	116	124	8	191	189
9	56	54	1	147	154	-10	48	44	9	204	204
-11	38	37	2	174	177	-9	71	68	10	31	29
-10	71	76	3	180	186	-8	-11	-7	11	76	73
-9	-11	0	4	138	139	-7	41	-41	12	41	45
-8	55	53	5	100	101	-6	75	-68	-13	35	35
-7	179	175	6	122	123	-5	72	69	-12	166	168
-6	298	302	7	131	131	-4	-10	-2	-11	57	57
-5	244	241	H=	1, K=	-4	-3	17	-15	-10	206	201
-4	20	-11	0	109	110	-2	18	11	-9	254	245
-3	-9	14	1	147	154	-1	48	-51	-8	197	193
-2	13	4	2	174	177	H=	1, K=	-4	-7	436	404
-1	67	76	3	180	186	0	99	98	-6	23	26
			4	138	139	1	55	55	-5	312	291
			5	100	101	2	145	143			
			6	122	123	3	15	17			
			7	131	131	4	-10	3			
						5	62	61			
						6	40	38			
						7	28	32			
						8	37	-42			
						9	68	66			
						10	77	79			
						11	37	40			
						-11	116	124			
						-10	48	44			
						-9	71	68			
						-8	-11	-7			
						-7	41	-41			
						-6	75	-68			
						-5	72	69			
						-4	-10	-2			
						-3	17	-15			
						-2	18	11			
						-1	48	-51			
						H=	1, K=	-4			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-4	421	384	-11	177	178	-11	-11	2	-5	62	64
-3	1149	1097	-10	-12	8	-10	60	61	-4	137	132
-2	1301	1250	-9	42	44	-9	170	173	-3	209	215
-1	189	167	-8	48	-42	-8	342	349	-2	145	143
H=	1, K=	-1	-7	97	102	-7	344	349	-1	83	83
0	874	852	-6	87	-85	-6	263	260	H=	2, K=	-9
1	67	-60	-5	24	-14	-5	294	291	0	22	16
2	120	110	-4	56	52	-4	179	180	1	-11	4
3	112	112	-3	395	384	-3	216	224	2	26	-26
4	85	-71	-2	96	88	-2	90	87	-3	33	31
5	406	383	-1	94	-84	-1	171	175	-2	38	33
6	19	23	H=	2, K=	2	H=	2, K=	5	-1	17	16
7	130	135	0	441	445	0	35	35	H=	2, K=	-8
8	-10	20	1	172	181	1	64	62	0	79	81
9	225	222	2	282	275	2	98	102	1	79	83
10	46	45	3	244	238	3	112	108	2	98	100
11	105	104	4	107	-100	4	149	156	3	114	113
12	87	92	5	147	-153	5	212	210	4	101	103
-13	43	40	6	180	-177	6	150	150	5	115	113
-12	18	-6	7	271	266	7	43	38	6	130	132
-11	62	61	8	187	189	8	73	69	-7	102	105
-10	19	24	9	164	159	-11	23	23	-6	120	120
-9	359	350	10	80	85	-10	-11	6	-5	82	83
-8	186	176	-13	98	105	-9	27	32	-4	69	72
-7	316	302	-12	76	82	-8	32	29	-3	85	85
-6	88	-88	-11	163	167	-7	117	121	-2	98	102
-5	45	-38	-10	77	80	-6	104	102	-1	106	108
-4	47	-52	-9	265	269	-5	63	65	H=	2, K=	-7
-3	18	3	-8	141	147	-4	49	45	0	37	35
-2	734	686	-7	184	178	-3	-10	-6	1	46	51
-1	166	-177	-6	176	182	-2	24	-26	2	57	62
H=	2, K=	0	-5	88	95	-1	79	-80	3	79	80
0	264	232	-4	679	670	H=	2, K=	6	4	51	52
1	495	467	-3	581	564	0	164	169	5	26	26
2	301	285	-2	672	646	1	176	178	6	32	32
3	196	184	-1	319	301	2	177	182	7	44	45
4	423	413	H=	2, K=	3	3	195	203	-9	26	28
5	119	120	0	108	-108	4	139	141	-8	47	45
6	438	444	1	71	72	5	160	167	-7	61	66
7	93	97	2	103	100	6	49	47	-6	-11	-5
8	121	121	3	156	152	7	85	89	-5	16	-20
9	108	-110	4	43	-38	-10	113	110	-4	-11	-15
10	-11	-6	5	120	-123	-9	93	96	-3	28	-25
11	85	92	6	32	36	-8	44	47	-2	-11	-1
-13	48	48	7	221	217	-7	64	64	-1	19	7
-12	79	84	8	165	186	-6	99	99	H=	2, K=	-6
-11	119	122	9	47	47	-5	95	94	0	407	415
-10	329	329	10	152	156	-4	43	46	1	316	313
-9	35	33	-12	-12	6	-3	35	28	2	165	162
-8	193	195	-11	47	-49	-2	179	189	3	119	122
-7	18	-4	-10	82	78	-1	181	182	4	152	155
-6	22	13	-9	199	197	H=	2, K=	7	5	158	165
-5	272	256	-8	304	310	0	38	34	6	73	71
-4	94	-85	-7	108	109	1	59	63	7	48	42
-3	368	350	-6	56	64	2	116	115	8	-11	7
-2	66	58	-5	63	65	3	124	129	9	22	29
-1	534	524	-4	203	201	4	38	39	-10	92	95
H=	2, K=	1	-3	192	192	5	57	-54	-9	103	106
0	648	637	-2	269	266	-8	-11	6	-8	155	157
1	188	176	-1	385	374	-7	-11	-6	-7	167	165
2	201	194	H=	2, K=	4	-6	-11	-4	-6	89	90
3	170	-150	0	92	96	-5	-11	-8	-5	117	113
4	24	-18	1	258	254	-4	55	-50	-4	100	97
5	101	-98	2	308	306	-3	21	15	-3	117	115
6	22	-21	3	231	237	-2	66	68	-2	126	124
7	82	83	4	283	282	-1	43	45	-1	176	175
8	48	46	5	48	47	H=	2, K=	8	H=	2, K=	-5
9	78	82	6	340	332	0	74	76	0	364	370
10	116	-117	7	168	169	1	75	77			
11	56	56	8	142	146	2	109	109			
-13	-12	-9	9	169	173						
-12	40	43	-12	62	62						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
1	235	230	1	383	368	-1	126	119	H=	3, K=	4
2	126	124	2	326	318						
3	20	14	3	296	283	H=	3, K=	1	0	255	257
4	25	11	4	121	115				1	152	155
5	69	69	5	459	439	0	393	376	2	152	156
6	30	-14	6	243	250	1	67	65	3	111	111
7	42	-42	7	280	282	2	148	-139	4	120	118
8	36	-79	8	179	181	3	89	96	5	198	204
9	27	21	9	243	245	4	-10	9	6	233	233
10	66	69	10	103	98	5	372	374	7	174	179
-11	69	69	11	100	105	6	48	-47	8	38	41
-10	35	34	-13	65	73	7	121	122	-11	42	42
-9	39	35	-12	58	55	8	95	93	-10	-11	-6
-8	60	64	-11	124	126	9	-11	12	-9	103	105
-7	45	45	-10	123	123	-13	66	67	-8	80	83
-6	239	235	-9	360	362	-12	115	117	-7	100	99
-5	199	199	-8	152	143	-11	290	290	-6	74	74
-4	85	84	-7	241	235	-10	135	147	-5	161	163
-3	43	-38	-6	148	149	-9	114	106	-4	310	314
-2	96	-100	-5	170	163	-8	22	22	-3	172	172
-1	220	220	-4	440	406	-7	64	63	-2	152	150
			-3	283	259	-6	173	176	-1	171	173
H=	2, K=	-4	-2	402	381	-5	17	12			
			-1	349	-341	-4	324	319	H=	3, K=	5
0	128	121				-3	57	52			
1	234	229	H=	2, K=	-1	-2	137	124	0	143	147
2	329	323				-1	97	99	1	132	133
3	233	220	0	319	-310				2	39	-40
4	190	193	1	246	232	H=	3, K=	2	3	25	-24
5	65	63	2	173	161				4	45	-47
6	203	195	3	318	314	0	296	297	5	72	73
7	146	148	4	116	113	1	373	379	6	45	41
8	104	103	5	417	409	2	181	175	-10	33	27
9	91	87	6	202	194	3	181	178	-9	32	34
10	153	154	7	51	51	4	232	237	-8	-11	17
-12	145	152	8	59	59	5	180	178	-7	27	27
-11	108	109	9	69	-70	6	160	166	-6	21	21
-10	128	129	10	64	64	7	225	222	-5	64	58
-9	40	35	11	31	33	8	241	248	-4	91	96
-8	68	63	-13	100	101	9	34	33	-3	77	-74
-7	119	119	-12	-11	-11	-13	49	50	-2	22	22
-6	473	455	-11	22	-21	-12	92	96	-1	93	99
-5	579	574	-10	223	225	-11	192	189			
-4	512	498	-9	109	107	-10	301	303	H=	3, K=	6
-3	280	267	-8	94	92	-9	177	179			
-2	187	176	-7	142	-145	-8	222	225	0	139	136
-1	548	549	-6	79	79	-7	121	121	1	196	199
			-5	24	-10	-6	151	156	2	171	169
H=	2, K=	-3	-4	17	15	-5	75	80	3	108	112
			-3	234	-220	-4	147	141	4	24	18
0	138	-133	-2	222	-206	-3	281	283	5	-12	-5
1	-9	4	-1	205	-203	-2	225	217	-9	107	102
2	73	70				-1	495	481	-8	90	89
3	36	31	H=	3, K=	0				-7	121	115
4	85	87				H=	3, K=	3	-6	127	126
5	30	-24	0	479	465				-5	211	208
6	241	241	1	97	99	0	73	77	-4	58	56
7	233	221	2	89	105	1	145	146	-3	45	44
8	119	122	3	23	23	2	259	260	-2	106	102
9	138	136	4	149	151	3	55	59	-1	99	101
10	77	75	5	308	308	4	175	172			
11	106	102	6	240	245	5	38	-35	H=	3, K=	7
-12	104	100	7	81	77	6	264	260			
-11	106	110	8	38	-39	7	147	153	0	-11	-7
-10	61	57	9	111	114	8	52	50	1	44	42
-9	80	75	10	46	43	-12	-12	12	2	127	130
-8	33	-36	-13	89	89	-11	-11	-12	-7	34	34
-7	97	97	-12	122	121	-10	33	29	-6	57	56
-6	41	41	-11	232	244	-9	58	62	-5	52	59
-5	345	330	-10	142	138	-8	64	66	-4	30	26
-4	408	391	-9	196	194	-7	42	38	-3	66	69
-3	349	338	-8	107	114	-6	-10	15	-2	28	19
-2	333	312	-7	321	324	-5	88	87	-1	26	-27
-1	20	-2	-6	445	422	-4	33	-31			
			-5	502	483	-3	129	130	H=	3, K=	-8
H=	2, K=	-2	-4	204	207	-2	-9	2			
			-3	192	185	-1	117	115	0	38	35
0	316	309	-2	330	328				1	77	81

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
2	110	113	4	216	220	4	211	215	7	46	47
3	87	88	5	129	126	5	85	89	-12	56	56
4	46	42	6	178	182	6	238	239	-11	92	99
-6	87	91	7	176	174	7	100	-105	-10	82	79
-5	93	94	8	121	126	8	65	-63	-9	28	35
-4	134	138	9	170	173	9	-11	-8	-8	83	81
-3	191	197	-12	155	155	10	23	25	-7	169	172
-2	219	227	-11	178	186	-13	39	40	-6	136	143
-1	118	117	-10	61	55	-12	-12	15	-5	134	123
H=	3, K=	-7	-9	57	57	-11	47	-48	-4	63	60
0	35	32	-8	49	39	-10	169	161	-3	365	378
1	27	28	-7	122	127	-9	-11	2	-2	247	251
2	33	37	-6	152	148	-8	66	65	-1	208	204
3	46	45	-5	157	154	-7	104	102	H=	4, K=	3
4	-11	1	-4	83	80	-6	196	188	0	-10	-6
5	-11	8	-3	109	105	-5	376	365	1	107	-100
6	26	27	-2	343	338	-4	112	-114	2	27	-26
-8	157	166	-1	378	383	-3	156	155	3	17	-14
-7	115	125	H=	3, K=	-3	-2	168	165	4	25	19
-6	17	14	0	197	202	-1	150	153	5	91	90
-5	-13	0	1	97	94	H=	4, K=	0	6	-11	14
-4	41	40	2	142	148	0	219	212	-11	32	32
-3	125	128	3	263	254	1	231	234	-10	36	-41
-2	132	135	4	28	29	2	200	200	-9	33	30
-1	29	22	5	25	21	3	402	398	-8	19	-9
H=	3, K=	-6	6	36	-38	4	205	205	-7	39	37
0	283	285	7	62	62	5	411	425	-6	-11	24
1	189	189	8	62	62	6	124	126	-5	63	-62
2	144	145	9	136	143	7	49	60	-4	153	165
3	173	171	10	124	119	8	107	108	-3	228	231
4	199	196	-12	103	99	-12	150	156	-2	212	214
5	156	157	-11	46	49	-11	180	178	-1	61	61
6	70	68	-10	133	-125	-10	138	144	H=	4, K=	4
7	90	87	-9	23	14	-9	165	159	0	122	123
-10	97	104	-8	19	-15	-8	122	129	1	45	48
-9	187	189	-7	-10	19	-7	110	105	2	109	-115
-8	300	304	-6	32	-24	-6	247	238	3	17	13
-7	277	281	-5	71	-72	-5	143	141	4	43	38
-6	215	217	-4	108	114	-4	262	262	5	113	117
-5	138	139	-3	32	-29	-3	159	158	-10	56	55
-4	133	128	-2	145	132	-2	322	317	-9	137	139
-3	141	146	-1	103	102	-1	204	199	-8	177	176
-2	64	67	H=	3, K=	-2	H=	4, K=	1	-7	147	146
-1	165	161	0	36	39	0	181	178	-6	102	94
H=	3, K=	-5	1	206	202	1	183	186	-5	102	96
0	96	98	2	152	143	2	142	144	-4	228	226
1	74	75	3	292	307	3	220	221	-3	65	84
2	86	88	4	276	273	4	264	265	-2	190	189
3	104	104	5	196	201	5	100	100	-1	256	259
4	217	220	6	55	44	6	-11	5	H=	4, K=	5
5	130	131	7	30	-23	7	-11	0	0	85	89
6	60	58	8	82	76	8	110	114	1	-11	17
7	53	50	9	62	63	-12	63	68	2	57	-62
8	84	81	10	120	122	-11	79	74	3	22	19
-11	64	65	-13	117	117	-10	126	130	4	62	61
-10	68	67	-12	93	98	-9	-11	3	-9	47	45
-9	-11	10	-11	31	-33	-8	90	90	-8	87	86
-8	77	73	-10	86	91	-7	-10	4	-7	109	113
-7	131	132	-9	45	44	-6	-10	-2	-6	91	91
-6	190	188	-8	143	138	-5	-10	4	-5	118	115
-5	104	104	-7	136	131	-4	70	-72	-4	-11	-17
-4	-10	0	-6	212	221	-3	91	94	-3	78	-81
-3	32	-23	-5	242	233	-2	107	105	-2	-11	-7
-2	42	-36	-4	362	354	-1	312	315	-1	84	85
-1	175	171	-3	270	268	H=	4, K=	2	H=	4, K=	6
H=	3, K=	-4	-2	218	214	0	196	201	0	145	146
0	266	256	-1	290	275	1	137	135	1	111	109
1	214	210	H=	3, K=	-1	2	290	293	2	146	148
2	264	271	0	192	-186	3	165	167	-7	149	151
3	253	250	1	47	-33	4	293	296	-6	175	177
			2	47	-50	5	-11	10			
			3	123	-118	6	47	46			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-5	127	133	5	-11	-14	-8	92	91	-7	-11	-6
-4	-12	15	6	-11	3	-7	191	184	-6	48	-58
-3	51	47	7	82	86	-6	195	196	-5	100	-99
-2	89	84	-11	119	119	-5	166	163	-4	133	129
-1	116	111	-10	37	39	-4	104	102	-3	131	134
H=	4, K=	-8	-9	103	101	-3	121	119	-2	85	84
0	82	80	-8	97	98	-2	185	182	-1	39	35
1	121	121	-7	129	127	-1	186	-189	H=	5, K=	4
-5	89	91	-6	149	148	H=	5, K=	0	0	125	132
-4	119	121	-5	68	71	0	174	173	1	120	119
-3	175	179	-4	149	149	1	223	227	2	94	95
-2	179	182	-3	140	140	2	176	174	-8	108	111
-1	86	88	-2	171	170	3	83	84	-7	62	69
H=	4, K=	-7	-1	169	181	4	98	93	-6	34	29
0	49	49	H=	4, K=	-3	5	94	102	-5	123	124
1	88	89	0	70	-65	6	125	126	-4	152	149
2	112	114	1	17	12	-11	-12	14	-3	165	163
3	80	78	2	-122	123	-10	146	147	-2	165	167
4	56	53	3	117	122	-9	111	118	-1	163	164
-7	59	66	4	-11	-20	-8	144	144	H=	5, K=	5
-6	30	29	5	151	-146	-7	119	124	-6	23	30
-5	42	40	6	68	-76	-6	200	191	-5	54	56
-4	59	61	7	49	53	-5	319	321	-4	61	62
-3	76	77	8	99	100	-4	123	120	-3	89	89
-2	26	20	-12	85	87	-3	87	87	-2	95	96
-1	-11	-3	-11	25	-25	-2	95	92	-1	107	105
H=	4, K=	-6	-10	17	19	-1	183	184	H=	5, K=	-7
0	187	188	-9	69	66	H=	5, K=	1	0	24	-20
1	170	171	-8	125	127	0	22	11	1	28	-22
2	152	154	-7	57	59	1	-11	-3	-5	82	83
3	153	154	-6	-11	5	2	180	185	-4	96	97
4	200	193	-5	101	102	3	81	79	-3	106	105
5	173	175	-4	220	224	4	90	94	-2	89	90
6	149	152	-3	106	103	5	-11	-8	-1	44	42
-9	103	109	-2	26	-20	-11	38	48	H=	5, K=	-6
-8	125	125	-1	71	71	-10	55	54	0	111	112
-7	101	104	H=	4, K=	-2	-9	32	34	1	33	33
-6	104	105	0	78	-71	-8	27	27	2	25	-20
-5	144	147	1	49	53	-7	59	60	3	-12	15
-4	171	168	2	203	202	-6	123	135	-7	93	92
-3	147	145	3	172	174	-5	221	215	-6	115	117
-2	84	87	4	210	208	-4	29	-17	-5	115	115
-1	155	156	5	38	-46	-3	29	23	-4	91	90
H=	4, K=	-5	6	124	127	-2	73	-68	-3	107	108
0	185	186	7	144	142	-1	100	-106	-2	146	151
1	163	165	8	135	142	H=	5, K=	2	-1	147	150
2	57	59	-12	84	83	0	-11	2	H=	5, K=	-5
3	-11	4	-11	-11	11	1	60	62	0	136	138
4	35	33	-10	141	140	2	151	154	1	70	67
5	48	44	-9	179	180	3	122	128	2	45	-48
6	66	64	-8	286	284	4	72	77	3	45	-46
7	93	88	-7	262	267	5	131	128	4	23	19
-10	44	43	-6	143	146	-10	116	117	-9	52	53
-9	-12	6	-5	335	325	-9	117	116	-8	59	57
-8	-11	-4	-4	282	270	-8	70	72	-7	107	106
-7	20	18	-3	332	324	-7	90	82	-6	106	106
-6	20	21	-2	199	190	-6	113	117	-5	-11	-16
-5	26	-23	-1	89	93	-5	25	22	-4	43	-50
-4	21	-18	H=	4, K=	-1	-4	203	211	-3	45	-44
-3	43	43	0	73	-65	-3	246	247	-2	33	-33
-2	87	87	1	23	22	-2	107	106	-1	41	39
-1	116	113	2	156	163	-1	51	-47	H=	5, K=	-4
H=	4, K=	-4	3	143	174	H=	5, K=	3	0	210	214
0	267	268	4	99	110	0	31	-35	1	189	188
1	271	278	5	176	170	1	110	111	2	129	126
2	227	234	6	140	149	2	26	20	3	57	62
3	132	127	7	63	63	3	51	45	H=	5, K=	-4
4	45	-40	8	37	42	4	36	34	0	210	214
			-12	46	45	5	55	54	1	189	188
			-11	47	52	-8	64	61	2	129	126
			-10	21	19				3	57	62
			-9	121	128						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
4	115	112	-5	218	221	-7	23	25	-1	210	215
5	119	122	-4	307	308	-6	146	153			
-10	167	169	-3	223	225	-5	70	67	H=	6, K=	-3
-9	129	134	-2	218	219	-4	17	1			
-8	127	129	-1	165	165	-3	23	-27	0	80	83
-7	163	164				-2	-11	6	1	67	65
-6	148	149	H=	5, K=	-1	-1	35	33	2	74	78
-5	95	97							3	97	96
-4	64	62	0	128	132	H=	6, K=	2	-9	32	29
-3	36	31	1	215	213				-8	42	47
-2	27	27	2	73	71	0	127	127	-7	70	71
-1	172	169	3	75	77	1	216	219	-6	88	91
H=	5, K=	-3	4	21	-30	-7	80	85	-5	40	43
0	141	139	5	140	145	-6	120	116	-4	82	83
1	136	139	6	104	102	-5	73	76	-3	130	130
2	158	160	-11	-12	5	-4	149	148	-2	176	176
3	83	81	-10	20	17	-3	127	131	-1	147	147
4	71	72	-9	25	25	-2	104	102			
5	29	-31	-8	-11	15	-1	148	149	H=	6, K=	-2
6	82	83	-7	25	18						
-11	45	48	-6	91	92	H=	6, K=	3	0	126	130
-10	79	75	-5	114	116				1	93	92
-9	83	84	-4	257	254	-5	84	85	2	31	29
-8	86	87	-3	139	140	-4	100	100	3	78	79
-7	58	61	-2	127	127	-3	142	137	-9	98	97
-6	30	23	-1	84	85	-2	94	95	-8	135	135
-5	110	110	H=	6, K=	0	H=	6, K=	-5	-7	116	122
-4	44	45							-6	61	61
-3	16	3	0	111	116	0	98	100	-5	49	55
-2	43	38	1	35	36	-6	44	46	-4	206	203
-1	155	157	2	105	108	-5	-11	8	-3	183	184
H=	5, K=	-2	3	95	94	-4	26	20	-2	189	194
0	246	248	-9	64	63	-3	54	52	-1	201	204
1	270	265	-8	80	82	-2	57	57	H=	6, K=	-1
2	224	233	-7	151	147	-1	55	94			
3	202	197	-6	216	222				0	94	92
4	60	66	-5	238	235	H=	6, K=	-4	1	39	39
5	54	52	-4	33	-33				2	28	-32
6	136	144	-3	52	-55	0	185	186	3	17	-16
-11	71	75	-2	20	19	1	139	139	-9	50	51
-10	-12	25	-1	44	43	2	115	117	-8	115	113
-9	98	98	H=	6, K=	1	-8	126	126	-7	111	114
-8	111	110				-7	160	165	-6	20	17
-7	134	134	0	40	37	-6	140	147	-5	65	66
-6	157	160	1	29	30	-5	101	104	-4	-11	-11
			2	86	92	-4	69	72	-3	45	-49
			-8	-11	-9	-3	133	134	-2	15	2
						-2	182	185			

Table B-3
Observed and Calculated Structure Factors for $\text{H}_2\text{dhphpy}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
7	-22	-34	6	133	-123	H=	C, K=	2	0	-22	3
8	-23	29	7	31	-26				1	37	-31
9	39	-34	8	99	-93	0	181	183	2	-23	16
H= -15, K=	1		9	32	9	1	-15	-1	H= -20, K=	2	
1	-19	-17	10	49	-47	2	69	-66			
2	-19	20	11	52	-45	3	61	-55	1	49	45
3	149	-146	H= -3, K=	1		4	65	59	2	46	45
4	40	-29				5	152	-154	3	-22	-18
5	52	-58	1	125	141	6	64	-59	4	37	-11
6	56	-60	2	202	-206	7	-20	-18	5	73	-70
7	33	32	3	181	-161	8	-20	24	6	-23	20
8	-21	12	4	45	-51	9	-21	21	H= -18, K=	2	
9	36	52	5	106	-119	H=	E, K=	2			
H= -13, K=	1		6	80	-71	0	163	164	1	34	-42
1	295	284	7	-18	-18	1	167	-181	2	-21	8
2	218	-214	8	-19	-5	2	-16	2	3	62	52
3	232	-236	9	87	86	3	104	-117	4	31	-36
4	55	-58	10	-20	0	4	-17	3	5	93	87
5	-20	-4	11	-22	2	5	58	63	6	46	-55
6	83	-90	H= -1, K=	1		6	53	55	7	-22	7
7	34	-12				7	-21	37	8	-23	-3
8	-21	-22	1	397	-422	8	-20	9	H= -16, K=	2	
9	58	71	2	413	-414	9	-22	30			
10	42	-41	3	115	111	H=	10, K=	2	1	119	-108
H= -11, K=	1		4	149	-148	0	114	112	2	-20	-24
1	128	133	5	348	-345	1	79	86	3	69	-74
2	27	27	6	51	60	2	-17	-9	4	110	-107
3	91	-67	7	284	-283	3	29	-20	5	37	15
4	43	-35	8	145	145	4	106	108	6	40	26
5	71	68	9	-21	32	5	30	14	7	112	110
6	79	88	10	46	47	6	-21	19	8	-22	-14
7	42	40	11	-22	16	7	-21	13	9	39	38
8	56	51	H=	0, K=	2	8	31	30	H= -14, K=	2	
9	-21	3	0	431	-441	H=	12, K=	2			
10	-21	0	1	510	498	0	140	133	1	53	-61
11	-22	-10	2	93	94	1	-18	8	2	52	52
H= -9, K=	1		3	322	325	2	128	-134	3	69	66
1	334	-330	4	262	291	3	81	80	4	101	-102
2	129	122	5	149	147	4	-20	-24	5	70	-72
3	306	-301	6	63	-59	5	96	100	6	-21	35
4	115	107	7	-18	-22	6	29	2	7	80	-86
5	187	176	8	51	-43	7	-21	-26	8	91	93
6	38	37	9	104	-105	H=	14, K=	2	9	32	19
7	71	-71	10	38	-38	0	65	-62	10	-23	9
8	73	74	11	43	-43	1	55	56	H= -12, K=	2	
9	-21	24	H=	2, K=	2	2	58	-56			
10	-21	26				3	-20	10	1	66	58
11	-23	-43	0	178	153	4	66	-56	2	175	176
H= -7, K=	1		1	720	-715	5	45	46	3	154	155
1	81	-54	2	313	-311	6	47	-39	4	-18	12
2	86	-82	3	226	231	H=	16, K=	2	5	103	100
3	96	101	4	33	-44	0	40	-51	6	109	109
4	162	154	5	117	133	1	-20	-24	7	-20	-2
5	275	268	6	80	-81	2	38	-28	8	-21	-26
6	-17	12	7	50	-55	3	36	-18	9	80	-81
7	88	-89	8	-20	-6	4	54	46	10	-22	36
8	-20	-34	9	-20	-14	5	52	-47	H= -10, K=	2	
9	51	-40	10	-20	2	H=	18, K=	2			
10	36	-31	H=	4, K=	2	0	-21	-24	1	150	151
11	-22	-24				1	-21	-3	2	159	162
H= -5, K=	1		0	127	126	2	31	31	3	73	70
1	332	-332	1	404	394	3	-22	-5	4	39	-43
2	315	314	2	128	131	4	-23	16	5	224	-225
3	264	250	3	159	-162	H=	20, K=	2	6	125	134
4	64	-49	4	186	-181	0	-21	-24	7	71	75
5	323	314	5	45	-56	1	-21	-3	8	91	-95
			6	85	-86	2	31	31	9	50	56
			7	64	-58	3	-22	-5	10	83	-84
			8	74	76	4	-23	16	11	-23	8
			9	34	-27						
			10	-21	24						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= -8, K= 2			5	37	39	H= 17, K= 3			9	-21	-17
1	173	174	6	-18	-5				10	-22	19
2	313	-313	7	78	-80				H= -9, K= 3		
3	141	138	8	-20	-4	0	-21	15	1	43	33
4	121	-106	9	-21	22	1	-21	-10	2	77	-76
5	77	-77	10	-21	1	2	-21	3	3	62	-68
6	69	67	H= 5, K= 3			3	46	-43	4	136	131
7	117	-122				4	-22	-18	5	-18	-1
8	103	-105	0	107	-102	H= 19, K= 3			6	96	95
9	-21	-5	1	130	131	0	-22	-9	7	141	144
10	-21	-21	2	25	25	1	37	41	8	98	101
11	38	46	3	327	325	2	53	-44	9	-21	8
H= -6, K= 2			4	135	145	H= -21, K= 3			10	36	29
1	243	237	5	122	114				H= -7, K= 3		
2	408	-394	6	47	40	1	53	-51	1	235	236
3	360	-342	7	-20	14	2	57	-59	2	175	180
4	207	-204	8	31	-36	3	-23	28	3	41	-47
5	27	36	9	-21	6	4	-22	1	4	-16	1
6	90	90	10	35	25	H= -19, K= 3			5	94	96
7	111	114	H= 7, K= 3			1	35	-25	6	102	105
8	62	-59	0	279	-275	2	81	-76	7	84	91
9	102	-98	1	88	-93	3	56	-62	8	221	225
10	66	68	2	54	-56	4	-22	8	9	77	78
11	46	-42	3	246	248	5	-23	-14	10	-21	9
H= -4, K= 2			4	97	92	6	67	61	11	-22	3
1	710	-709	5	-18	-1	7	-23	-16	H= -5, K= 3		
2	229	-222	6	-19	5	H= -17, K= 3			1	133	127
3	467	-464	7	-20	-2	1	42	41	2	-15	-22
4	122	127	8	-20	-16	2	-21	29	3	220	-212
5	163	-166	9	-21	27	3	69	64	4	153	-156
6	-17	-9	H= 9, K= 3			4	74	75	5	72	-61
7	188	187	0	117	-122	5	32	-38	6	92	-87
8	-20	2	1	55	57	6	36	40	7	50	-49
9	102	99	2	-17	26	7	-22	-17	8	-20	5
10	95	95	3	39	38	8	-23	21	9	125	-121
11	-22	2	4	-18	11	H= -15, K= 3			10	75	-66
H= -2, K= 2			5	74	-73	1	45	58	11	-22	18
1	216	209	6	57	-61	2	-20	-7	H= -3, K= 3		
2	70	68	7	51	-52	3	43	50	1	67	-84
3	93	-87	8	45	-47	4	121	125	2	557	559
4	370	370	H= 11, K= 3			5	36	39	3	94	93
5	251	239	0	193	-199	6	-21	-3	4	157	-153
6	35	36	1	28	24	7	-22	-10	5	130	135
7	-18	-10	2	103	98	8	38	-41	6	59	-66
8	65	-68	3	59	-57	9	62	47	7	-19	-26
9	-21	8	4	32	37	H= -13, K= 3			8	84	-82
10	54	52	5	107	-114	1	46	41	9	81	-78
11	44	47	6	-20	15	2	-18	16	10	119	-116
H= 1, K= 3			7	-21	-3	3	-19	9	11	54	-48
0	150	-134	8	-22	-2	4	52	-58	H= -1, K= 3		
1	774	-775	H= 13, K= 3			5	57	-57	1	114	123
2	640	-641	0	76	75	6	110	-114	2	187	188
3	284	-278	1	89	83	7	-21	-2	3	111	-113
4	130	-131	2	43	41	8	64	-64	4	58	72
5	140	-138	3	-20	-8	9	-22	25	5	242	235
6	182	187	4	-21	-14	10	-22	-1	6	66	65
7	-16	-26	5	33	-27	H= -11, K= 3			7	26	-9
8	-19	7	6	-21	4	1	31	-24	8	43	-35
9	-20	1	7	-22	20	2	112	-111	9	-21	3
10	-20	7	H= 15, K= 3			3	26	-83	10	-21	-4
H= 3, K= 3			0	114	113	4	-18	1	11	61	54
0	678	675	1	-20	9	5	89	-90	H= 0, K= 4		
1	463	-475	2	74	77	6	233	-237	0	343	-351
2	160	-169	3	-21	23	7	53	-43	1	277	279
3	112	114	4	55	-53	8	40	-32	2	253	-241
4	133	-133	5	-22	19				3	73	-82
			6	-22	-19						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
4	407	404	4	-21	10	2	-19	10	1	112	-106
5	87	-94	5	-20	15	3	30	-40	2	165	157
6	35	36	6	-21	-8	4	132	-129	3	118	110
7	95	91	7	62	-53	5	135	142	4	52	51
8	-19	-20				6	282	294	5	208	-206
9	-20	21	H= 14, K= 4			7	225	236	6	212	-209
10	97	95	0	102	91	8	71	69	7	101	-94
H= 2, K= 4			1	61	-61	9	-21	-2	8	-20	-4
0	361	355	2	111	-107	10	43	-30	9	66	60
1	332	320	3	63	-61	H= -10, K= 4			10	-21	-1
2	156	-146	4	-21	-7	1	266	-263	H= 3, K= 5		
3	121	-117	5	-21	-2	2	153	-164	0	50	58
4	165	152	6	-22	-10	3	75	-68	1	79	-86
5	112	112	H= 16, K= 4			4	27	10	2	249	243
6	38	-30	0	-21	-3	5	80	-84	3	100	98
7	79	79	1	-21	37	6	-20	20	4	260	257
8	-20	-5	2	-21	-21	7	62	66	5	225	-226
9	-20	21	3	-21	-17	8	221	-219	6	65	68
10	46	49	4	68	71	9	-21	28	7	-19	14
H= 4, K= 4						10	-22	20	8	-20	16
0	119	112	H= 18, K= 4			H= -8, K= 4			9	-21	1
1	429	428	0	-21	11	1	37	-36	H= 5, K= 5		
2	58	67	1	-21	-4	2	107	109	0	56	47
3	140	-140	2	40	-43	3	63	-66	1	46	-63
4	76	76	3	-23	20	4	-17	-26	2	-16	6
5	34	-16	H= 20, K= 4			5	62	59	3	167	167
6	233	-240	0	-23	-11	6	165	171	4	72	-74
7	31	-23	H= -20, K= 4			7	65	-77	5	89	-89
8	51	-48				8	275	-276	6	39	29
9	38	-32				9	117	-125	7	98	97
H= 6, K= 4						10	48	-49	8	58	57
0	165	-170	1	46	23	H= -6, K= 4			9	33	44
1	79	-81	2	111	110	1	421	412	H= 7, K= 5		
2	102	-103	3	162	161	2	173	-169	0	123	125
3	81	-88	4	-23	0	3	253	249	1	40	-38
4	117	121	5	42	36	4	-16	10	2	46	-40
5	57	56	H= -18, K= 4			5	82	-90	3	53	56
6	93	-43	1	33	-40	6	-18	-3	4	41	-42
7	124	-129	2	-22	18	7	40	45	5	56	-61
8	-21	20	3	-22	17	8	56	-59	6	71	-64
9	48	-51	4	240	-240	9	-22	-28	7	97	98
H= 8, K= 4			5	-22	11	10	141	134	8	-21	-21
0	540	536	6	46	43	H= -4, K= 4			H= 9, K= 5		
1	254	-253	7	46	54	1	202	-201	0	53	44
2	-16	-5	H= -16, K= 4			2	661	-665	1	233	-235
3	122	-128	1	-21	22	3	275	277	2	169	-165
4	-18	10	2	33	39	4	36	29	3	-19	0
5	134	141	3	68	-68	5	31	-27	4	47	-47
6	58	-53	4	203	-209	6	55	58	5	71	-72
7	30	25	5	256	-261	7	93	-92	6	-21	15
8	94	99	6	63	-58	8	125	-126	7	66	62
H= 10, K= 4			7	35	-38	9	-21	25	8	-22	-11
0	145	146	8	-23	12	10	169	171	H= 11, K= 5		
1	181	174	H= -14, K= 4			H= -2, K= 4			0	160	165
2	-18	2	1	32	37	1	112	-113	1	157	-155
3	-19	-1	2	-19	7	2	-15	38	2	31	-27
4	-19	1	3	110	111	3	254	-241	3	-20	14
5	48	33	4	-20	-2	4	62	63	4	-20	-13
6	64	-69	5	-21	-17	5	44	-42	5	32	-36
7	-21	-3	6	299	304	6	-18	0	6	31	-6
8	36	30	7	42	-49	7	42	47	7	-21	26
H= 12, K= 4			8	52	-57	8	62	-59	H= 13, K= 5		
0	27	-16	9	44	-47	9	88	-90	0	-20	28
1	34	31	H= -12, K= 4			10	36	41	1	87	-86
2	171	-173	1	36	27	H= 1, K= 5			2	79	78
3	54	55				0	149	-138	3	87	91

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
4	114	115	H= -9, K= 5			H= 2, K= 6			H= 16, K= 6		
5	-21	1				0	206	195	0	-21	8
6	-21	0	1	81	-71	1	136	144	1	44	-49
H= 15, K= 5			2	65	-66	2	73	-68	2	-22	12
0	37	-44	3	67	66	3	152	148	3	-22	-9
1	-21	-5	4	93	-102	4	26	-10	H= 18, K= 6		
2	114	-107	5	168	172	5	32	29	0	39	-43
3	84	83	6	65	76	6	-19	32	1	34	-40
4	-22	19	7	219	-227	7	33	-34			
5	-22	1	8	86	90	8	39	-29			
H= 17, K= 5			9	66	71	9	-21	-15			
0	-21	0	10	90	85						
1	-22	-31	H= -7, K= 5			H= 4, K= 6			H= -18, K= 6		
2	-21	-25	1	306	-296	0	197	-191	1	73	76
3	43	52	2	179	-169	1	217	-221	2	111	-110
H= 19, K= 5			3	109	-107	2	190	-192	3	83	81
0	-23	30	4	41	-34	3	82	76	4	-22	0
1	-22	-7	5	-19	32	4	122	-115	5	47	-32
H= -19, K= 5			6	-20	-3	5	115	111	H= -16, K= 6		
1	37	-21	7	-21	-37	6	-19	-4	1	44	-46
2	131	119	8	223	-220	7	-20	8	2	-21	-3
3	183	-179	9	179	180	8	54	-42	3	58	58
4	-22	9	10	-22	0	9	-22	30	4	45	27
5	-23	28	H= -5, K= 5			H= 6, K= 6			5	70	73
H= -17, K= 5			1	365	-354	0	165	-151	6	47	-49
1	55	56	2	31	22	1	62	-56	7	80	-78
2	57	59	3	122	119	2	138	-139	H= -14, K= 6		
3	149	-145	4	245	242	3	104	-102	1	85	-89
4	101	105	5	34	-37	4	47	46	2	56	55
5	89	92	6	143	138	5	85	-82	3	146	-150
6	72	68	7	171	-169	6	52	45	4	179	176
7	-23	-9	8	75	-82	7	-20	7	5	75	-85
H= -15, K= 5			9	173	171	8	-21	0	6	-21	22
1	-21	11	10	84	-83	H= 8, K= 6			7	59	51
2	-21	6	H= -3, K= 5			0	31	24	8	-22	12
3	40	39	1	66	-59	1	237	231	H= -12, K= 6		
4	135	-135	2	220	-215	2	93	93	1	118	-116
5	263	263	3	321	320	3	32	31	2	55	-47
6	-22	-16	4	317	318	4	54	94	3	-20	18
7	-22	-18	5	150	147	5	86	-87	4	34	-14
8	38	-27	6	86	87	6	81	78	5	154	-147
H= -13, K= 5			7	62	-68	7	68	-64	6	-21	-27
1	51	-56	8	-21	24	H= 10, K= 6			7	45	-44
2	30	30	9	54	50	0	70	-59	8	61	55
3	107	-111	10	107	104	1	-19	16	9	99	95
4	89	-86	H= -1, K= 5			2	54	61	H= -10, K= 6		
5	212	217	1	196	-208	3	91	84	1	138	133
6	62	-64	2	310	-299	4	-20	23	2	-19	42
7	87	-83	3	345	327	5	61	62	3	130	132
8	82	-80	4	261	-259	6	-21	-25	4	48	-60
9	-22	-14	5	52	-47	7	-22	26	5	176	174
H= -11, K= 5			6	132	-137	H= 12, K= 6			6	196	-205
1	-18	7	7	-20	33	0	50	-42	7	57	59
2	-19	-25	8	78	-74	1	-20	5	8	-21	6
3	45	-53	9	111	114	2	-21	22	9	-22	-8
4	76	-81	10	63	49	3	66	-72	H= -8, K= 6		
5	-20	-11	H= 0, K= 6			4	-21	-34	1	50	58
6	187	191	0	263	260	5	-21	-2	2	95	86
7	253	-252	1	153	-151	6	41	-28	3	152	159
8	57	49	2	197	196	H= 14, K= 6			4	35	27
9	-22	-4	3	110	-105	0	-21	-18	5	-20	-18
			4	54	-45	1	42	25	6	44	-35
			5	60	62	2	54	50	7	106	108
			6	-19	17	3	37	-35	8	-21	7
			7	42	-36	4	-22	-24	9	-22	-11
			8	35	28	5	34	-35			
			9	-21	-2						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= -6, K= 6			1 63 58			5 55 64			0 35 28		
1 129 -136			2 79 77			6 -21 -20			1 355 369		
2 119 -117			3 45 45			7 83 -83			2 56 -62		
3 104 -100			4 -21 6			8 67 -68			3 -19 18		
4 40 -43			5 -20 14			H= -9, K= 7			4 81 -89		
5 33 -27			6 61 -58			1 49 -64			5 -20 -1		
6 39 50			7 -22 7			2 -19 21			6 -20 0		
7 118 -120			H= 9, K= 7			3 36 -54			7 41 36		
8 144 143			0 -19 -36			4 111 124			8 -21 -3		
9 73 -76			1 -19 6			5 -21 -25			H= 4, K= 8		
H= -4, K= 6			2 72 -71			6 113 109			0 125 129		
1 309 320			3 -20 9			7 51 -86			1 52 62		
2 -16 -31			4 -20 -4			8 33 -23			2 53 -50		
3 146 -149			5 33 -25			H= -7, K= 7			3 -20 -16		
4 -18 -8			6 -21 -7			1 227 -225			4 -20 -7		
5 42 -36			H= 11, K= 7			2 42 39			5 45 -34		
6 -19 5			0 50 -51			3 59 58			6 46 52		
7 34 29			1 97 -91			4 54 -40			7 -21 -19		
8 46 48			2 57 -55			5 73 82			H= 6, K= 8		
9 71 -67			3 -20 16			6 63 -64			0 39 31		
10 -22 -18			4 60 -56			7 52 -52			1 48 -51		
H= -2, K= 6			5 40 -29			8 -21 24			2 70 -72		
1 94 -96			H= 13, K= 7			9 45 40			3 211 -220		
2 71 51			0 -20 0			H= -5, K= 7			4 -21 -12		
3 -16 -7			1 72 -71			1 65 -63			5 -20 -8		
4 135 -133			2 -21 -10			2 40 57			6 -21 29		
5 -18 -21			3 -21 -14			3 82 82			7 -22 -7		
6 63 58			4 32 20			4 48 -58			H= 8, K= 8		
7 -21 3			H= 15, K= 7			5 102 107			0 67 -69		
8 -21 -30			0 -21 12			6 110 -112			1 -20 -27		
9 105 101			1 -22 -9			7 61 66			2 59 -73		
H= 1, K= 7			2 -21 24			8 65 -60			3 71 -69		
0 24 0			3 -22 19			9 84 78			4 45 42		
1 30 13			H= 17, K= 7			H= -3, K= 7			5 30 4		
2 39 -37			0 -22 17			1 80 85			6 -22 4		
3 53 51			H= -17, K= 7			2 -17 4			H= 10, K= 8		
4 43 38			1 53 -44			3 101 95			0 -21 28		
5 42 -35			2 -23 37			4 50 -100			1 -21 -29		
6 83 80			3 -23 -34			5 100 -100			2 -21 -6		
7 35 23			4 -23 -22			6 -19 -6			3 -21 12		
8 -21 1			H= -15, K= 7			7 51 -60			4 97 95		
9 -21 24			1 48 51			8 -21 31			5 134 134		
H= 3, K= 7			2 57 -61			9 49 45			H= 12, K= 8		
0 -17 -28			3 50 -51			H= -1, K= 7			0 -20 11		
1 65 -81			4 -21 -5			1 -17 -12			1 38 41		
2 37 -48			5 63 53			2 145 -148			2 -21 -16		
3 52 -52			6 77 66			3 87 85			3 -21 0		
4 93 92			H= -13, K= 7			4 -18 -8			4 38 50		
5 -19 -17			1 -21 54			5 118 -113			H= 14, K= 8		
6 37 28			2 58 -56			6 -20 14			0 -21 -19		
7 46 41			3 -21 29			7 67 -68			1 -21 -17		
8 -21 16			4 100 -94			8 41 55			2 -22 -22		
H= 5, K= 7			5 -21 29			9 44 -39			H= 16, K= 8		
0 186 196			6 -21 2			H= 0, K= 8			0 34 -33		
1 71 -66			7 40 -48			0 40 48			H= -16, K= 8		
2 -18 17			H= -11, K= 7			1 -18 20			1 55 -50		
3 -19 -6			1 -20 -3			2 60 -62			2 -22 13		
4 -19 0			2 38 33			3 47 41			3 40 -19		
5 -20 -4			3 49 -59			4 43 -44			H= -14, K= 8		
6 -21 -37			4 101 108			5 53 50			1 -22 -38		
7 55 43						6 29 -11					
8 -22 -21						7 -21 25					
H= 7, K= 7						8 54 -48					
0 41 24						H= 2, K= 8					

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
2	-22	30	6	-20	13	H=	-7, K=	9	0	-21	-7
3	-22	-23	7	-21	-26				1	95	-92
4	62	-51				1	90	96	2	98	97
5	-23	-31	H=	3, K=	9	2	-20	17	3	-22	14
6	52	-51				3	-20	-8			
H=	-12, K=	8	0	132	136	4	44	-55	H=	10, K=	10
			1	362	-371	5	82	101			
1	-20	2	2	93	-87	6	-21	42	0	-22	-35
2	82	91	3	45	-40	7	-22	35	1	-21	5
3	81	88	4	-20	-9				2	-22	-6
4	-21	2	5	69	-71	H=	-5, K=	9			
5	40	34	6	29	6				H=	12, K=	10
6	94	-83				1	52	-56			
7	-22	16	H=	5, K=	9	2	-20	1	0	-22	-21
						3	31	-48			
H=	-10, K=	8	0	40	30	4	-21	-36	H=	-12, K=	10
			1	43	23	5	77	77			
1	38	-44	2	73	-68	6	34	32	1	-22	22
2	53	55	3	317	320	7	-22	-26	2	67	-62
3	-21	50	4	110	108						
4	-21	3	5	-21	26	H=	-3, K=	9	H=	-10, K=	10
5	66	66	6	36	-18						
6	55	60				1	47	-46	1	-21	26
7	-22	23	H=	7, K=	9	2	67	-69	2	75	-83
						3	56	-52	3	-21	-6
H=	-8, K=	8	0	78	78	4	-20	-23	4	-22	-8
			1	58	-60	5	53	52			
1	49	43	2	145	-144	6	49	50	H=	-8, K=	10
2	81	-82	3	296	287	7	92	-100			
3	32	-32	4	60	53				1	31	-22
4	92	-100	5	60	60	H=	-1, K=	9	2	58	63
5	93	-86							3	41	-28
6	-21	17	H=	9, K=	9	1	-20	-4	4	48	59
7	-22	-20				2	-19	-13	5	-22	-14
8	75	69	0	-21	16	3	48	54			
			1	109	-98	4	-20	12	H=	-6, K=	10
H=	-6, K=	8	2	-21	-6	5	86	55			
			3	-21	-15	6	-21	41	1	62	58
1	28	-26	4	46	38	7	40	-46	2	58	67
2	81	-82							3	32	-29
3	79	74	H=	11, K=	9	H=	0, K=	10	4	112	111
4	60	-64							5	-21	0
5	51	-71	0	-21	-14	0	32	41	6	-22	-9
6	-20	0	1	51	45	1	28	10			
7	46	-46	2	48	-50	2	85	85	H=	-4, K=	10
8	-22	-5	3	33	33	3	58	48			
						4	-20	-1	1	103	-104
H=	-4, K=	8	H=	13, K=	9	5	-21	3	2	-20	-9
						6	38	22	3	-20	16
1	-18	-22	0	-22	-13				4	45	-50
2	120	121	1	40	36	H=	2, K=	10	5	-21	23
3	45	-45							6	-22	-31
4	29	22	H=	-13, K=	9	0	147	-143			
5	-20	6				1	-20	-20	H=	-2, K=	10
6	42	48	1	-22	34	2	146	142			
7	-21	30	2	-22	27	3	135	133	1	160	-157
8	-21	2	3	-22	-7	4	32	44	2	71	-65
			4	-22	-7	5	64	63	3	77	-72
H=	-2, K=	8	5	-22	13				4	40	-56
						H=	4, K=	10	5	31	41
1	77	-69	H=	-11, K=	9				6	67	-64
2	82	75				0	122	-136			
3	-19	16	1	51	-38	1	-20	8	H=	1, K=	11
4	72	83	2	55	56	2	-20	4			
5	58	-59	3	113	-124	3	-20	-8	0	31	9
6	-20	15	4	33	-45	4	-21	-23	1	-20	15
7	41	59	5	-21	-16	5	33	-19	2	36	-14
8	-21	-1	6	-22	30				3	-21	-16
						H=	6, K=	10	4	56	-54
H=	1, K=	9	H=	-9, K=	9						
						0	-20	24	H=	3, K=	11
0	106	104	1	42	39	1	122	-120			
1	402	-422	2	-20	20	2	115	115	0	-21	26
2	144	-143	3	92	-96	3	-22	6	1	32	-8
3	33	-34	4	55	-54	4	73	-74	2	-21	14
4	32	34	5	-21	2				3	-21	4
5	30	28	6	-22	16	H=	8, K=	10			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
			2	45	-38	H=	-5, K=	11	4	47	56
H=	5, K=	11	H=	-9, K=	11	1	-21	-22	H=	-1, K=	11
0	-21	-27				2	65	-67			
1	-21	-32	1	37	-29	3	-21	30	1	-20	2
2	-21	-13	H=	-7, K=	11	4	-21	4	2	-21	17
3	38	-35				H=	-3, K=	11	3	-21	11
H=	7, K=	11	1	63	-52				4	61	54
0	79	-72	2	51	-52	1	-21	31	H=	0, K=	12
1	54	40	3	-22	-10	2	58	61			
						3	35	35	0	107	-106

Table B-4

Observed and Calculated Structure Factors for $[\text{Ni}_2\text{Cl}(\text{H}_2\text{O})_4^-$
 $(\text{dhphpy})]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 0, K= 0			H= 6, K= 0			-4 412 -419			-28 194 -212		
2 563 -490			0 1163 -1171			-2 607 632			-27 -93 -106		
4 1938 -2036			2 3015 2987			H= 12, K= 0			-26 284 -325		
6 563 598			4 911 905			0 1691 -1722			-25 217 253		
8 135 -253			6 383 -391			2 494 -506			-24 -93 -173		
10 659 -607			8 965 -1004			4 427 434			-23 290 382		
12 314 -323			10 317 322			6 -87 152			-22 363 384		
14 -64 103			12 -79 6			8 -84 -75			-21 -96 -60		
16 130 -183			14 445 -434			-28 551 -541			-20 227 -375		
18 148 113			16 225 230			-26 211 200			-19 326 -352		
20 242 261			18 138 -93			-24 194 187			-18 -92 -25		
22 177 184			20 -84 -106			-22 142 -126			-17 -98 -422		
24 115 -142			-30 602 -576			-20 392 -399			-16 -90 412		
26 700 -691			-28 550 567			-18 177 -177			-15 -96 -68		
H= 2, K= 0			-26 747 754			-16 347 357			-14 -96 -292		
0 483 373			-24 349 -388			-14 249 256			-13 553 595		
2 2936 -2814			-22 765 -780			-12 181 -180			-12 -98 188		
4 137 -124			-20 163 185			-10 -79 38			-11 498 -522		
6 345 -303			-18 296 315			-8 -79 61			-10 190 -247		
8 1693 1682			-16 929 -921			-6 -90 -14			-9 847 -807		
10 124 -119			-14 167 197			-4 374 362			-8 445 512		
12 115 107			-12 167 119			-2 1073 1111			-7 201 -232		
14 645 649			-10 147 -99			H= 14, K= 0			-6 798 -785		
16 555 -547			-8 1553 1483			0 586 -594			-5 1418 1462		
18 255 251			-6 973 936			2 433 436			-4 827 -696		
20 348 362			-4 816 741			-24 -83 -16			-3 393 244		
22 342 -354			-2 2496 -2505			-22 346 -328			-2 857 728		
24 413 -402			H= 8, K= 0			-20 -81 66			-1 124 51		
26 311 292			0 3957 4100			-18 284 277			H= 3, K= 1		
-28 549 -541			2 411 421			-16 306 -323			0 758 -639		
-26 448 -459			4 429 -436			-14 171 -187			1 348 317		
-24 206 181			6 252 278			-12 -31 -111			2 -70 -126		
-22 426 443			8 -76 -83			-10 197 -226			3 381 -331		
-20 111 -109			10 -81 -128			-8 141 136			4 390 -408		
-18 269 -274			12 196 -195			-6 394 399			5 559 559		
-16 860 846			14 -79 57			-4 371 360			6 -67 19		
-14 568 -551			16 -81 -11			-2 378 -411			7 -67 -43		
-12 283 -322			-30 472 474			H= 16, K= 0			8 472 -485		
-10 273 332			-28 521 526			-16 322 -311			9 447 -461		
-8 2573 -2519			-26 341 -332			-14 203 -207			10 -66 -92		
-6 1888 -1866			-24 -78 18			-12 192 202			11 500 -516		
-4 329 -390			-22 -78 -24			-10 -84 5			12 -69 59		
-2 3358 3505			-20 -77 92			H= 1, K= 1			13 621 605		
H= 4, K= 0			-18 139 168			0 1935 2098			14 199 238		
0 7329 -8496			-16 448 -446			1 1346 -1410			15 301 299		
2 242 -231			-14 315 -276			2 1854 -1916			16 475 -478		
4 1140 1162			-12 126 109			3 617 -569			17 386 -382		
6 306 -285			-10 277 -252			4 1209 -1108			18 -81 51		
8 351 -306			-8 138 100			5 712 -736			19 426 -455		
10 99 120			-6 -55 46			6 347 323			20 411 398		
12 425 433			-4 1229 -1237			7 338 -273			21 -82 -59		
14 199 -227			-2 1643 -1668			8 187 -142			22 450 -430		
16 -80 86			H= 10, K= 0			9 172 193			23 273 243		
18 -80 27			0 655 660			10 256 -241			24 -84 44		
20 271 -285			2 942 -965			11 700 -693			-29 -103 -181		
22 195 -158			4 424 -438			12 1185 1242			-28 -100 -298		
-30 469 -434			6 -80 96			13 -70 46			-27 264 291		
-28 396 -389			8 529 527			14 438 437			-26 132 -171		
-26 574 573			10 257 -265			15 793 797			-25 200 249		
-24 218 209			12 140 -153			16 353 -364			-24 569 577		
-22 216 -217			-30 514 502			17 310 335			-23 406 -433		
-20 427 -417			-28 226 -223			18 -82 -57			-22 316 327		
-18 192 162			-26 539 -552			19 551 565			-21 233 -240		
-16 674 657			-24 113 129			20 551 565			-20 683 -670		
-14 134 126			-22 668 675			21 251 -253			-19 -74 -104		
-12 310 246			-20 131 -135			22 -82 -47			-18 571 573		
-10 565 542			-18 642 -619			23 336 -356			-17 392 392		
-8 659 588			-16 759 758			24 670 -656			-16 352 362		
-6 219 -147			-14 343 349			25 -91 184			-15 1384 1345		
-4 427 380			-12 -72 57			26 -85 -23			-14 643 -681		
-2 1524 1519			-10 319 325						-13 105 -108		
			-8 574 -580						-12 1674 -1524		
			-6 519 -544						-11 1778 -1789		
									-10 723 640		
									-9 -67 88		
									-8 148 -144		

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-7	281	230	12	117	38	-9	735	-721	-11	-81	-21
-6	753	-765	13	123	-155	-8	144	157	-10	-80	32
-5	697	-574	14	175	-151	-7	517	-504	-9	201	245
-4	1044	1036	15	-80	-67	-6	206	-191	-8	-82	-108
-3	459	-483	16	149	153	-5	428	431	-7	299	332
-2	1737	1655	17	-84	150	-4	385	-385	-6	-80	-10
-1	1005	-945	18	126	70	-3	203	210	-5	257	-240
H=	5, K=	1	19	251	254	-2	443	-455	-4	319	322
0	1566	-1596	-30	-84	33	-1	-73	-39	-3	225	-218
1	942	945	-29	200	223	H=	11, K=	1	-2	357	369
2	958	923	-28	486	473	0	-82	34	-1	-84	17
3	465	439	-27	312	-317	1	-82	58	H=	15, K=	1
4	1415	1442	-26	295	265	2	391	-378	-22	158	-118
5	350	372	-25	338	-339	3	-80	-44	-21	126	162
6	340	-347	-24	477	-484	4	-81	-4	-20	277	273
7	390	-379	-23	393	407	5	271	270	-19	-85	58
8	335	-338	-22	314	-331	6	221	226	-18	-84	55
9	356	-360	-21	246	208	7	-82	77	-17	-84	9
10	570	553	-20	481	477	8	234	-199	-16	297	-277
11	645	640	-19	-73	22	9	171	-137	-15	415	-415
12	452	-450	-18	450	-455	10	236	-214	-14	-85	-113
13	176	218	-17	-70	-15	11	228	-237	-13	208	-219
14	365	-342	-16	337	-328	-29	242	-240	-12	300	302
15	466	-452	-15	832	-829	-28	329	-307	-11	416	414
16	230	-205	-14	212	209	-27	205	215	-10	-85	-85
17	204	-229	-13	292	-278	-26	357	-349	-9	188	174
18	-81	124	-12	1029	1043	-25	307	300	-8	-85	-31
19	-81	-11	-11	1070	1055	-24	300	305	-7	181	-173
20	276	-275	-10	395	-403	-23	297	-295	-6	252	253
21	-84	79	-9	-70	70	-22	298	283	-5	157	-123
22	-84	3	-8	70	17	-21	316	-502	-4	-86	-14
-30	551	-545	-7	997	963	-20	632	-630	-3	-87	47
-29	245	240	-6	-70	-36	-19	155	-143	H=	0, K=	2
-28	-81	-14	-5	885	-880	-18	117	120	0	321	-349
-27	-82	152	-4	574	587	-17	-80	89	1	90	250
-26	421	415	-3	2150	-2151	-16	524	541	2	761	-703
-25	219	-236	-2	1041	1025	-15	753	770	3	238	-327
-24	319	293	H=	9, K=	1	-14	-78	13	4	402	425
-23	582	-568	0	700	712	-13	249	275	5	614	-490
-22	687	-681	1	348	-347	-12	579	-554	6	143	67
-21	-77	4	2	187	-153	-11	594	-601	7	875	821
-20	383	369	3	-77	-53	-10	143	151	8	550	537
-19	551	583	4	443	-447	-9	-77	-105	9	650	652
-18	519	488	5	213	-246	-8	-76	-23	10	376	-376
-17	690	694	6	-80	-27	-7	128	89	11	-71	-8
-16	506	-477	7	-80	43	-6	297	-287	12	715	-742
-15	123	55	8	119	83	-5	-78	-39	13	1073	-1095
-14	-64	55	9	129	150	-4	290	292	14	975	981
-13	702	-622	10	272	-286	-3	141	-144	15	-73	-38
-12	566	-560	11	243	-258	-2	895	904	16	409	426
-11	328	285	12	-81	41	-1	407	-427	17	-86	-31
-10	443	393	13	221	-199	H=	13, K=	1	18	432	-457
-9	140	148	14	162	146	0	611	-641	19	-94	-50
-8	425	408	15	256	232	1	228	254	20	264	-311
-7	319	275	-30	497	491	2	-83	-16	21	235	-230
-6	345	297	-29	196	-210	3	-84	71	22	-35	86
-5	476	-449	-28	154	177	4	379	364	23	240	-274
-4	109	110	-27	161	-140	5	149	141	24	276	-359
-3	-68	-70	-26	156	-129	-27	124	108	25	323	312
-2	505	448	-25	-30	39	-26	187	175	26	207	-255
-1	-68	93	-24	311	-305	-25	-84	-35	27	-88	65
H=	7, K=	1	-23	441	428	-24	256	259	H=	2, K=	2
0	473	456	-22	355	349	-23	320	-340	0	94	58
1	-67	-62	-21	-78	11	-22	303	-298	1	183	-122
2	812	843	-20	127	-109	-21	-79	-47	2	195	129
3	-68	65	-19	373	-349	-20	-79	-6	3	94	12
4	-69	-6	-18	474	-480	-19	213	179	4	499	510
5	428	-443	-17	545	-555	-18	303	318	5	547	589
6	-72	-86	-16	254	265	-17	227	248	6	1059	-1043
7	-73	-55	-15	-72	-5	-16	156	-112	7	300	318
8	360	379	-14	352	321	-15	116	110	8	-67	-23
9	-77	105	-13	900	887	-14	140	-124	9	875	860
10	-78	67	-12	415	427	-13	308	-326			
11	219	222	-11	-59	-97	-12	359	-356			
			-10	270	-265						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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15	1101	1109	-19	-75	-71	2	214	-243	-15	744	763
16	410	-423	-18	1108	1065	3	242	242	-14	576	587
17	146	-163	-17	382	375	4	152	163	-13	465	456
18	263	-318	-16	473	-477	5	145	-140	-12	1029	-1004
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22	173	158	-12	737	721	9	260	275	-8	264	255
23	-81	-31	-11	397	-375	10	161	-142	-7	178	166
24	159	-154	-10	614	619	11	170	155	-6	206	214
25	-66	35	-9	804	754	12	497	-496	-5	290	279
-29	-89	-37	-8	293	-263	13	455	-477	-4	433	-432
-28	158	-147	-7	550	602	14	288	298	-3	-75	137
-27	-94	32	-6	886	893	15	-84	-95	-2	-76	-131
-26	305	-321	-5	-69	-32	16	335	343	-1	-77	-94
-25	-84	-3	-4	418	-397	17	170	179			
-24	-81	28	-3	-70	-82	-30	127	-126	H=	12, K=	2
-23	-82	-142	-2	371	364	-29	153	-156			
-22	-81	-59	-1	-69	-164	-28	333	322	0	281	237
-21	-82	31				-27	-79	-50	1	-31	-60
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-19	717	-717				-25	472	-476	3	140	-142
-18	-82	143	0	542	-523	-24	387	-410	4	-82	23
-17	499	-541	1	352	355	-23	127	98	5	155	174
-16	655	660	2	238	245	-22	-79	-66	6	131	-71
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-14	-66	-120	4	495	-482	-20	261	-229	8	186	-184
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-12	2017	-1994	6	253	259	-18	738	-732	-27	-86	5
-11	1867	-1741	7	401	-436	-17	-73	-27	-26	258	-270
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-9	451	332	9	507	-501	-15	362	-343	-24	336	315
-8	797	786	10	591	598	-14	1053	1074	-23	131	-71
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-4	1370	-1344	14	253	-251	-10	853	-843	-19	-81	24
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-2	352	-380	16	-82	38	-8	132	140	-17	-83	52
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3	129	-163	-28	-30	12	-1	121	136	-10	122	115
4	401	-395	-27	-82	-82				-9	245	227
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6	290	-286	-25	-81	18				-7	457	466
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12	1036	1023	-19	662	653	5	-79	74	-1	-83	-114
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15	-80	100	-16	746	-737	8	180	-181			
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17	163	-224	-14	561	-546	10	483	-501	1	151	65
18	234	227	-13	-56	3	11	291	-305	2	-86	24
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20	164	152	-11	936	952	13	152	-137	-24	-84	93
21	197	168	-10	115	84	-30	303	291	-23	-33	42
22	-85	-105	-9	315	-331	-29	151	-113	-22	-82	19
23	231	217	-8	-68	-58	-28	121	120	-21	121	-107
-30	-86	44	-7	341	-327	-27	-80	71	-20	-81	92
-29	-87	140	-6	422	-444	-26	302	-340	-19	-83	103
-28	343	-318	-5	708	-739	-25	-78	-19	-18	-83	64
-27	-82	90	-4	1155	1183	-24	-79	-89	-17	252	265
-26	-81	92	-3	167	-106	-23	-80	-42	-16	341	-359
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L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-12	402	415	-1	-64	181	17	136	-157	-9	316	-282
-11	406	410				18	436	413	-8	1335	-1311
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-9	273	272				20	154	141	-6	528	557
-8	325	-320	0	-68	-30	21	250	-235	-5	780	757
-7	-81	-66	1	-68	8	-30	-84	69	-4	807	911
-6	150	-171	2	1777	-1730	-29	137	-100	-3	531	515
-5	303	-304	3	335	418	-28	278	-297	-2	222	219
-4	378	347	4	264	-292	-27	209	-233	-1	583	-621
-3	-85	-96	5	685	674	-26	232	-226			
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-16	143	-150	10	955	928	-21	810	-799	2	204	201
-15	271	-282	11	588	-598	-20	596	572	3	-78	78
-14	307	358	12	1624	1634	-19	345	-349	4	275	297
-13	220	241	13	-77	-5	-18	263	-247	5	278	-276
-12	197	199	14	-76	-34	-17	345	352	6	212	219
-11	349	324	15	256	253	-16	943	-946	7	125	-133
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21	415	460	-16	312	-307	6	207	-203	-16	737	735
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23	210	274	-14	937	-928	8	684	711	-14	910	903
24	-90	-187	-13	903	-826	9	-79	-57	-13	161	153
25	-87	109	-12	1017	-1008	10	287	-295	-12	775	-783
26	206	211	-11	859	-871	11	221	197	-11	481	-481
-28	140	148	-10	1038	1072	12	760	-772	-10	1555	-1529
-27	127	139	-9	802	808	13	-83	68	-9	827	-817
-26	-82	81	-8	1656	1549	14	-80	-36	-8	439	435
-25	-87	-200	-7	478	391	15	130	-87	-7	303	303
-24	491	-488	-6	863	-808	16	281	277	-6	-71	-74
-23	-83	-73	-5	1071	-1007	17	133	110	-5	495	503
-22	172	204	-4	566	-606	18	361	333	-4	337	-339
-21	651	651	-3	356	-365	-30	285	-277	-3	-73	31
-20	325	-355	-2	608	-536	-29	269	-262	-2	266	275
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-16	657	662	1	758	-770	-25	-80	-97	1	-81	49
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-13	-71	-86	4	737	-793	-22	240	226	4	-79	19
-12	1523	-1529	5	892	944	-21	815	-840	5	-60	-57
-11	617	-621	6	779	-754	-20	-77	-76	6	-81	81
-10	1373	-1803	7	113	131	-19	201	211	7	239	253
-9	416	-402	8	710	693	-18	1237	-1192	8	510	-507
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-6	598	-503	11	-77	65	-15	237	-240	-29	196	188
-5	1175	1208	12	258	-240	-14	-68	105	-28	-80	30
-4	339	-356	13	376	330	-13	515	485	-27	141	-141
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			15	298	-289	-11	716	680	-25	-80	29

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
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-23	-80	133	-4	184	192	-11	-70	-33	9	692	-693
-22	292	-293				-10	146	-180	10	152	225
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-20	153	-80				-8	935	1008	12	497	-497
-19	-82	-106	0	350	316	-7	1053	1064	13	208	-189
-18	1002	1005	1	1399	1346	-6	1111	1078	14	169	-137
-17	202	-197	2	516	-539	-5	239	-216	15	-80	53
-16	117	150	3	1039	981	-4	410	-370	16	-81	3
-15	299	301	4	279	333	-3	1273	-1252	17	340	321
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-13	224	-226	6	-57	-82	-1	790	806	19	-86	47
-12	350	-359	7	1431	-1418				20	-35	-25
-11	445	-449	8	-69	-24	H=	4, K=	4	-30	142	-176
-10	-78	90	9	466	435				-29	518	-510
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-8	515	502	11	315	322	1	551	-514	-27	203	194
-7	299	269	12	226	-221	2	415	439	-26	-82	21
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-5	150	-152	14	1093	1098	4	212	-216	-24	-82	121
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-3	126	-111	16	343	365	6	190	-193	-22	-80	68
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3	187	-172	24	-85	44	14	833	-831	-14	214	-215
4	152	-153	25	160	202	15	451	-453	-13	-67	-62
5	154	168	26	-96	-145	16	312	-325	-12	843	841
-26	357	-353	27	411	-459	17	-82	-28	-11	-66	76
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-22	-82	-100	1	725	768	21	-82	21	-7	474	-461
-21	220	-213	2	563	-626	22	145	-98	-6	820	-851
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-19	290	-294	4	116	-51	-28	243	-377	-4	255	264
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-14	478	-494	9	815	802	-23	522	529	H=	8, K=	4
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-9	367	381	14	288	296	-18	521	511	4	221	232
-8	173	-178	15	257	-245	-17	503	-495	5	157	131
-7	-81	-7	16	-81	-88	-16	395	-383	6	-80	121
-6	133	-130	17	713	-713	-15	709	679	7	493	-490
-5	203	-230	18	-85	-101	-14	1312	-1319	8	-81	24
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-2	-81	63	21	554	556	-11	373	393	11	235	220
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-18	454	-433	-27	228	-228	-4	209	-103	-29	368	379
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-16	-86	-131	-25	336	-306	-2	366	370	-27	-79	115
-15	188	-190	-24	-80	-79	-1	120	-33	-26	-77	17
-14	-86	69	-23	-77	-9				-25	126	133
-13	-83	9	-22	-33	-13	H=	6, K=	4	-24	301	-324
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-8	457	-445	-17	844	-849	4	-63	-58	-18	432	-440
-7	261	-288	-16	197	266	5	726	726	-17	414	425
-6	-86	14	-15	517	-534	6	532	543	-16	-75	71
			-14	-57	15	7	130	-170	-15	452	-433
			-13	204	230						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-13	203	-188	-18	307	300	-24	204	-207	-1	502	-475
-12	-70	99	-17	350	-358	-23	457	-437			
-11	274	-270	-16	-82	-13	-22	-82	110	H=	5, K=	5
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6	169	-168	-23	271	285	-3	2335	-2282	18	-83	-34
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12	198	215	-17	-82	55	2	896	-878	-27	-82	-15
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-26	137	97	-16	-84	-111	-1	-63	49	-20	228	-235
-25	208	-189	-15	-81	27	H=	3, K=	9	-19	329	-311
-24	407	405	-14	-82	5	0	944	975	-18	239	-255
-23	-80	-82	-13	267	-271	1	112	-42	-17	237	250
-22	-77	-29	-12	-32	94	2	465	474	-16	117	-94
-21	-80	-98	-11	239	-292	3	105	109	-15	122	-113
-20	339	-357	-10	-32	-64	4	286	-297	-14	-79	-56
-19	185	185	-9	193	200	5	264	235	-13	633	642
-18	465	478	-8	209	227	6	296	-272	-12	-77	-110
-17	-80	9	-7	429	424	7	852	878	-11	290	319
-16	137	109	-6	-84	31	8	-79	-83	-10	-75	34
-15	154	-171	-5	-83	84				-9	407	401

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-6	331	-348	-11	236	-244	15	171	171	-22	243	237
-5	423	-408	-10	-81	-57	16	-81	102	-21	200	168
-4	722	-738	-9	373	-373	17	369	-373	-20	-82	108
-3	248	-243	-8	132	-120	18	182	-190	-19	590	-576
-2	200	197	-7	373	355	19	481	-430	-18	-80	59
-1	211	-222	-6	290	264	20	-83	-20	-17	650	-637
			-5	346	321	21	-84	22	-16	199	-184
H=	7, K=	9	-4	597	597	22	238	-246	-15	-80	23
0	630	-625	-3	-82	64				-14	240	244
1	-81	16	-2	-81	-14	H=	2, K=	10	-13	361	342
2	701	-582	-1	-81	97	0	-72	81	-12	334	339
3	-81	68				1	220	214	-11	471	506
4	169	189	H=	11, K=	9	2	402	410	-10	653	-672
5	-80	39	0	174	141	3	744	-751	-9	-77	-88
6	283	294	1	-84	-60	4	326	331	-8	-76	-58
7	443	-450	2	349	341	5	219	-189	-7	204	-216
8	-81	84	3	-87	-95	6	317	-322	-6	253	254
9	-80	-24	4	-87	-33	7	-79	90	-5	-75	-83
10	233	-244	-23	-84	52	8	-78	-3	-4	516	-540
11	-82	-72	-22	289	-301	9	492	472	-3	-75	79
12	-83	6	-21	461	465	10	333	321	-2	217	-230
13	256	227	-20	425	462	11	456	442	-1	539	544
14	-86	33	-19	-82	-51	12	379	-383	H=	6, K=	10
-26	129	-81	-18	-81	27	13	-82	47	0	211	188
-25	218	235	-17	-81	17	14	204	-213	1	388	-382
-24	481	499	-16	350	-344	15	473	-438	2	452	-455
-23	156	-143	-15	159	-155	16	-82	38	3	509	531
-22	231	215	-14	209	-225	17	454	-437	4	351	-328
-21	479	-458	-13	-80	-42	18	218	233	5	378	373
-20	382	-397	-12	-79	6	19	-38	103	6	386	380
-19	219	227	-11	122	-150	20	466	-452	7	-60	52
-18	128	153	-10	257	-260	-23	155	136	8	-80	10
-17	118	-52	-9	147	113	-22	341	-349	9	318	-293
-16	289	284	-8	246	225	-21	226	202	10	434	-443
-15	228	219	-7	330	317	-20	441	443	11	374	-357
-14	151	182	-6	323	333	-19	165	211	12	-86	144
-13	-80	-93	-5	236	-243	-18	158	-212	13	177	-125
-12	143	117	-4	119	-115	-17	428	-434	14	172	168
-11	224	212	-3	125	-79	-16	-81	6	-24	166	166
-10	428	437	-2	354	-358	-15	555	-606	-23	-83	-32
-9	225	-191	-1	-34	-7	-14	256	262	-22	468	456
-8	537	-544				-13	-78	-9	-21	254	-232
-7	372	-405	H=	13, K=	9	-12	490	503	-20	556	-558
-6	708	-718	-18	-85	-36	-11	484	499	-19	348	-345
-5	617	614	-17	-87	122	-10	438	-439	-18	-79	30
-4	377	383	-16	-86	-72	-9	640	639	-17	263	214
-3	184	150	-15	190	-173	-8	196	-191	-16	127	64
-2	777	780	-14	-85	-30	-7	145	146	-15	525	536
-1	-80	-17	-13	146	154	-6	561	560	-14	-80	-7
			-12	-85	20	-5	322	-349	-13	147	111
H=	9, K=	9	-11	155	97	-4	255	-258	-12	233	-243
0	666	-662	-10	-85	59	-3	753	-760	-11	213	-236
1	-80	-8	-9	246	210	-2	377	-391	-10	264	283
2	-81	111	-8	-87	120	-1	302	309	-9	367	-346
3	115	129	-7	-87	-45				-8	169	169
4	327	342	-6	-38	-94	H=	4, K=	10	-7	231	-215
5	348	-342	-5	-87	-135	0	695	719	-6	445	-449
6	-83	-68	-4	420	-405	1	461	-473	-5	-80	115
7	219	-216				2	344	343	-4	-76	-15
8	284	-274	H=	0, K=	10	3	435	-397	-3	583	590
9	235	191	0	1132	-1196	4	538	-511	-2	334	337
10	135	138	1	752	775	5	-79	52	-1	281	-253
-25	169	-127	2	-72	-1	6	261	250			
-24	-84	35	3	415	395	7	414	435	H=	8, K=	10
-23	328	-325	4	820	823	8	395	401	0	458	-470
-22	477	-493	5	155	-151	9	321	293	1	312	334
-21	233	230	6	442	-443	10	400	-402	2	233	-237
-20	-81	88	7	335	-335	11	277	-283	3	352	324
-19	328	351	8	384	-384	12	-81	-109	4	394	406
-18	130	105	9	141	-158	13	257	-250	5	-80	-18
-17	221	-253	10	528	536	14	138	158	6	151	-140
-16	-79	101	11	365	376	15	295	-276	7	201	-219
-15	-80	81	12	149	-106	16	-84	11	8	241	-254
-14	-80	6	13	232	223	17	218	200	9	159	-160
-13	362	-366	14	117	-93	-24	233	-233	10	198	165
-12	-81	26				-23	422	419			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
11	-85	115	H=	1, K=	11	-9	240	-237	-11	358	-348
-24	161	171				-8	497	-520	-10	231	267
-23	385	-373	0	156	-211	-7	175	-106	-9	-81	103
-22	179	-172	1	-76	-112	-6	311	311	-8	538	544
-21	240	-209	2	259	248	-5	-79	-137	-7	-82	-46
-20	-81	-123	3	168	139	-4	121	113	-6	338	-353
-19	358	349	4	-76	-22	-3	471	474	-5	-83	72
-18	160	-183	5	396	-386	-2	193	-208	-4	305	-305
-17	494	499	6	337	-310	-1	114	-94	-3	341	-353
-16	146	136	7	-79	-28				-2	337	311
-15	-80	102	8	253	233	H=	5, K=	11	-1	-81	-49
-14	-80	-72	9	171	-186						
-13	226	-229	10	548	558	0	229	241	H=	9, K=	11
-12	271	-277	11	306	389	1	153	110			
-11	371	-367	12	704	-690	2	-80	-71	0	136	-107
-10	590	600	13	306	269	3	296	-309	1	-82	-8
-9	-82	60	14	534	-511	4	-80	-66	2	-80	5
-8	-81	44	15	315	-305	5	267	300	3	172	156
-7	213	231	16	-82	33	6	306	319	4	-84	82
-6	396	-373	17	-84	-53	7	195	174	5	213	-197
-5	-82	99	18	418	413	8	124	-101	6	-83	-85
-4	469	482	19	-35	-121	9	241	225	-21	170	98
-3	190	-193	20	-86	-44	10	729	-738	-20	369	369
-2	351	356	-21	256	248	11	306	-278	-19	353	368
-1	460	-447	-20	410	410	12	355	300	-18	202	174
			-19	239	266	13	292	-269	-17	281	303
H=	10, K=	10	-18	-80	-68	14	491	475	-16	276	-286
0	124	-104	-17	128	167	15	196	184	-15	164	-164
1	135	164	-16	224	-222	-23	188	173	-14	526	-540
2	134	123	-15	364	-352	-22	-84	76	-13	270	-257
3	241	-225	-14	409	-413	-21	223	-225	-12	143	157
4	252	228	-13	403	-376	-20	522	-527	-11	-81	-22
5	255	-245	-12	773	489	-19	448	-402	-10	657	576
6	-87	-105	-11	-80	70	-18	-83	-122	-9	-81	58
-22	432	-432	-10	638	710	-17	255	-247	-8	194	-216
-21	242	202	-9	112	-18	-16	348	345	-7	-81	72
-20	421	413	-8	687	-727	-15	340	305	-6	531	-521
-19	391	410	-7	195	206	-14	536	565	-5	157	-180
-18	-84	62	-6	729	-759	-13	320	333	-4	140	121
-17	-83	-87	-5	282	-291	-12	230	-214	-3	-81	-119
-16	170	-152	-4	331	357	-11	-81	-46	-2	143	151
-15	499	-500	-3	204	-242	-10	680	-705	-1	292	304
-14	196	-159	-2	-76	-32	-9	-81	55			
-13	163	-184	-1	393	415	-8	276	275	H=	11, K=	11
-12	247	226				-7	172	-150			
-11	183	169	H=	3, K=	11	-6	524	551	0	140	-141
-10	-82	-86	0	126	115	-5	120	81	-18	308	-312
-9	270	264	1	255	255	-4	240	-239	-17	-87	-68
-8	146	-183	2	162	175	-3	198	174	-16	375	-374
-7	129	149	3	211	-186	-2	165	-136	-15	323	-318
-6	138	135	4	154	-173	-1	196	-195	-14	-85	38
-5	145	-86	5	297	-304				-13	124	-43
-4	124	-84	6	536	556	H=	7, K=	11	-12	644	645
-3	315	-285	7	125	115	0	-81	59	-11	215	225
-2	-82	-84	8	622	600	1	157	-145	-10	-85	0
-1	-83	106	9	-82	56	2	-82	-155	-9	141	-119
			10	447	-440	3	167	213	-8	353	-353
H=	12, K=	10	11	197	229	4	253	273	-7	-84	7
-18	-86	70	12	547	-546	5	191	167	-6	-86	130
-17	360	-328	13	332	-280	6	324	-293	-5	-86	28
-16	172	-184	14	277	292	7	164	-153	-4	190	189
-15	184	-188	15	432	-398	8	467	-456	-3	179	184
-14	-87	15	16	239	287	9	-85	-19	-2	187	-192
-13	-86	79	17	-86	85	10	-87	122	-1	-88	38
-12	318	295	-22	126	-14	11	-88	-132			
-11	199	192	-21	231	298	-23	214	-210	H=	0, K=	12
-10	222	-238	-20	-82	73	-22	-84	23	0	370	-384
-9	-85	-15	-19	-81	-33	-21	289	-285	1	327	-331
-8	-85	-84	-18	532	-539	-20	132	-102	2	132	129
-7	-86	-31	-17	-30	-105	-19	-83	12	3	661	-656
-6	237	227	-16	220	-236	-18	400	409	4	140	-125
-5	-87	-29	-15	519	-476	-17	-80	59	5	-80	-108
-4	258	-226	-14	532	609	-16	295	295	6	169	-204
-3	129	60	-13	252	241	-15	431	413	7	291	298
-2	320	-332	-12	1005	1038	-14	162	-174	8	-80	-62
			-11	564	545	-13	117	-1	9	125	-150
			-10	591	-500	-12	832	-839	10	651	560

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
-3	-80	49	-6	165	183	-12	-83	-36	0	501	496
-2	512	516	-5	411	410	-11	-85	-115	1	353	346
-1	582	562	-4	201	-203	-10	-84	-29	2	-86	33
H=	9, K=	13	-3	130	104	-9	202	202	3	242	-250
0	264	-235	-2	542	-575	-8	313	-325	4	361	-362
-15	289	270	-1	178	-189	-7	146	-157	-13	466	474
-14	315	-295	H=	4, K=	14	-6	204	216	-12	191	147
-13	-84	0	0	565	555	-5	263	-270	-11	152	-167
-12	170	183	1	-83	-112	-4	130	145	-10	-84	11
-11	-85	64	2	133	133	-3	239	224	-9	237	-253
-10	149	139	3	475	438	-2	206	210	-8	161	-146
-9	-83	-26	4	-33	4	-1	-84	62	-7	-84	36
-8	434	-425	5	117	-59	H=	1, K=	15	-6	379	-389
-7	278	-280	6	357	-369	0	422	-428	-5	372	377
-6	193	187	7	313	-298	1	455	-429	-4	263	-245
-5	270	254	8	-85	83	2	135	115	-3	230	-209
-4	240	256	9	225	214	3	421	404	-2	178	184
-3	189	154	10	142	113	4	491	460	-1	172	-132
-2	-83	-23	-17	213	-162	5	-82	97	H=	7, K=	15
-1	-83	73	-15	211	-209	6	147	-119	-8	274	-287
H=	0, K=	14	-15	-84	-86	7	198	-166	-7	230	229
0	746	-779	-14	186	205	8	280	-242	-6	170	-171
1	-81	-50	-13	-83	86	9	-85	-114	-5	-86	28
2	-80	-41	-12	126	-73	10	-84	55	-4	390	386
3	502	-479	-11	210	220	11	245	221	-3	328	-334
4	-80	62	-10	142	80	-13	440	-445	H=	0, K=	16
5	313	315	-9	148	-150	-12	130	-47	0	237	-274
6	411	409	-8	270	281	-11	375	377	1	-85	-93
7	407	399	-7	251	270	-10	-82	-6	2	153	113
8	117	-125	-6	314	-346	-9	265	279	3	140	91
9	281	-271	-5	208	240	-8	191	153	4	-84	79
10	-81	-54	-4	-81	-47	-7	199	-158	5	273	253
11	-82	65	-3	328	-320	-6	433	436	6	-84	-58
12	146	120	-2	-81	-116	-5	402	-438	7	199	-163
13	157	112	-1	-79	-16	-4	-83	93	8	132	146
14	191	-200	H=	6, K=	14	-3	300	294	H=	2, K=	16
15	-84	46	0	339	332	-2	371	-402	0	-85	46
H=	2, K=	14	1	275	233	-1	-82	15	1	-84	-77
0	128	-140	2	351	-378	H=	3, K=	15	2	-85	123
1	123	-164	3	-83	-6	0	302	310	3	-85	133
2	465	463	4	283	-271	1	-83	-38	4	185	132
3	-81	41	5	365	-355	2	360	346	5	-86	-72
4	277	252	6	-86	30	3	258	288	-9	351	354
5	344	358	-16	128	114	4	-85	86	-8	157	155
6	-80	-32	-15	-86	-67	5	249	-257	-7	404	-410
7	355	-335	-14	-84	92	6	326	-307	-6	285	-242
8	132	-110	-13	234	225	7	127	-100	-5	174	-191
9	161	-134	-12	154	-179	8	260	-185	-4	241	-255
10	199	182	-11	-82	-41	-13	207	202	-3	167	196
11	-85	25	-10	-84	51	-12	196	149	-2	146	-125
12	-87	-144	-9	-83	34	-11	427	398	-1	-85	17
13	238	-205	-8	188	-163	-10	-85	30	H=	4, K=	16
-16	194	-182	-7	447	418	-9	-82	-18	0	264	249
-15	-82	4	-6	181	-151	-8	298	310	1	-86	109
-14	-84	-64	-5	300	-324	-7	229	-210	-7	253	-249
-13	204	-182	-4	-81	58	-6	-84	57	-6	-85	-53
-12	170	220	-3	320	-294	-5	-85	-23	-5	230	217
-11	-81	106	-2	422	442	-4	537	-525	-4	-86	-103
-10	-81	-122	-1	-83	50	-3	346	347	-3	129	134
-9	-80	-104	H=	8, K=	14	-2	173	-120	-2	140	-122
-8	224	201	0	382	-377	-1	339	-321	H=	5, K=	15
-7	462	-451	-13	-84	-53						

Table B-5
Observed and Calculated Structure Factors for $C_4(fph)_4Rh(cp)(tpp)$

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 0, K= 0			-18	177	173	-14	323	336	-7	461	-489
1	-21	1092	-17	-65	22	-13	374	348	-6	526	-544
2	1897	-1630	-16	190	-191	-12	410	-402	-5	-56	49
3	871	-822	-15	187	183	-11	496	-515	-4	-56	-6
4	213	-164	-14	172	157	-10	176	180	-3	567	-560
5	908	850	-13	-61	-60	-9	409	431	-2	90	6
6	334	-311	-12	617	-621	-8	217	208	-1	470	-415
7	1247	-1240	-11	541	-504	-7	238	-262			
8	631	-596	-10	465	453	-6	160	-225	H= 0, K= 7		
9	719	733	-9	313	299	-5	1102	1068	0	590	-603
10	361	344	-8	522	-537	-4	838	897	1	105	-107
11	-50	39	-7	1485	-1493	-3	550	-509	2	406	415
12	392	-395	-6	-54	-53	-2	682	-613	3	-66	-8
13	144	-172	-5	1687	1629	-1	-57	25	4	-67	1
14	539	536	-4	353	429	H= 0, K= 5			5	252	-241
15	214	234	-3	-45	189	0	353	347	6	173	-164
16	325	-322	-2	920	-548	1	337	-371	7	244	249
17	138	-173	-1	106	154	2	648	646	8	113	132
H= 0, K= 1			H= 0, K= 3			3	593	586	9	205	-188
0	1644	-2458	0	1047	699	4	301	-269	-21	242	237
1	155	-81	1	307	-260	5	460	-475	-20	-67	81
2	301	-154	2	589	525	6	167	165	-19	98	-86
3	1179	1084	3	464	442	7	235	223	-18	-64	-71
4	332	-259	4	149	186	8	165	151	-17	-65	-41
5	1289	-1263	5	274	218	9	143	-156	-16	452	449
6	128	-108	6	-55	-12	10	305	-305	-15	217	216
7	537	519	7	257	279	11	135	164	-14	395	-389
8	389	423	8	-62	104	12	238	252	-13	180	-186
9	254	-248	9	211	-197	-20	-68	56	-12	300	309
10	410	-423	10	330	-338	-19	315	-307	-11	441	415
11	-63	-6	11	-69	85	-18	-55	-52	-10	145	-149
12	427	403	12	293	296	-17	423	422	-9	438	-458
13	120	134	13	-69	-64	-16	218	237	-8	378	-381
14	282	-283	14	130	-128	-15	184	175	-7	176	199
15	-68	1	-19	244	-243	-14	222	-225	-6	102	41
16	225	237	-18	311	-310	-13	108	96	-5	330	-337
-18	-67	-9	-17	357	368	-12	852	852	-4	-54	-20
-17	158	174	-16	-66	94	-11	720	741	-3	134	128
-16	192	187	-15	239	-232	-10	54	122	-2	326	367
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-9	331	-304	-8	220	201	-3	1195	1156	4	140	-118
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-5	999	-915	-4	254	-223	0	1116	1108	8	108	-72
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-3	508	553	-2	116	253	2	188	-178	-20	-68	-103
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3	1243	-1280	4	324	328	9	132	147	-13	247	232
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9	243	252	10	165	153	-17	183	-191	-7	541	-546
10	329	334	11	260	-261	-16	627	-638	-6	300	-295
11	-66	-30	12	358	-352	-15	-65	-124	-5	573	557
12	323	-317	13	104	-125	-14	279	283	-4	390	392
13	-67	36	-20	150	-135	-13	138	-146	-3	-60	-22
14	301	301	-19	390	384	-12	330	-344	-2	799	-823
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			-16	-64	-18	-9	596	589	0	444	-449
			-15	-63	71	-8	209	211			

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11	406	-390	9	445	-455	-8	190	163	-2	364	363
12	155	-163	10	224	207	-7	308	325	-1	145	146
13	202	217	11	305	297	-6	310	-296	H= 1, K= -4		
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15	92	-61	13	-62	-4	-4	125	-110	1	490	425
16	-64	-42	14	197	-202	-3	421	358	2	743	-923
17	-68	-40	15	-66	18	-2	598	590	3	244	-312
18	309	296	16	397	402	-1	186	-182	4	1010	1004
19	-67	0	17	-63	-37	H= 1, K= -6			5	-54	92
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3	110	-95	-5	174	-188	5	429	471	11	358	-374
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6	210	208	-2	-67	83	8	-50	36	14	191	185
7	190	159	-1	139	-153	9	305	295	15	-64	-42
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11	553	535	2	268	-246	13	105	108	19	170	175
12	222	231	3	84	83	14	357	358	-14	-68	62
13	187	-182	4	619	577	15	256	-235	-13	-65	33
14	96	124	5	348	338	16	-66	-59	-12	434	-447
15	-66	-126	6	268	-270	17	121	142	-11	133	-141
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17	211	192	8	254	285	19	224	205	-9	-62	-31
18	252	-260	9	345	378	20	-68	-35	-8	360	-376
19	-67	-13	10	-58	-87	-12	203	-220	-7	-56	37
-3	274	271	11	328	-320	-11	127	-117	-6	-54	74
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4	303	286	19	148	160	-3	287	-383	1	854	563
5	180	197	20	190	-190	-2	426	-414	2	1744	1547
6	571	-578	-9	138	106	-1	592	617	3	283	163
7	593	-601	-8	165	-182	H= 1, K= -5			4	820	-778
8	320	312	-7	278	-275	0	845	-887	5	267	-253
9	431	424	-6	175	180	1	1124	-1087	6	156	-123
10	140	-105	-5	258	275	2	1322	1200	7	265	250
11	693	-714	-4	-65	-40	3	209	-233	8	-53	-30
12	-65	-46	-3	-63	0	4	944	-929	9	554	-558
13	519	527	-2	391	-336	5	377	-320	10	294	-276
14	364	347	-1	163	151	6	112	-79	11	352	354
15	207	-194	H= 1, K= -7			7	-54	119	12	386	390
16	589	-613	0	146	-166	8	146	-161	13	170	-208
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18	108	109	2	92	-66	10	361	-350	15	271	-299
19	-66	16	3	140	130	11	851	870	16	325	324
20	177	-164	4	626	542	12	582	574	17	-66	53
-6	110	104	5	637	-556	13	158	-189	18	248	-256
-5	298	286	6	-53	-1	14	-61	31	-15	-69	-5
-4	-68	-72	7	393	417	15	211	195	-14	239	-237
-3	268	-289	8	-53	37	16	354	355	-13	-64	34
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2	-60	54	14	462	-445	-11	-66	-19	-7	553	555
			15	183	176	-10	353	-361	-6	361	390
			16	126	130	-9	-67	-106	-5	538	-532

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-2	479	-602				0	145	-68	4	421	408
-1	1237	-870	H=	2, K=	0	1	310	196	5	298	290
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1	502	234	2	371	-360	4	332	306	8	-67	-4
2	689	-828	3	694	585	5	607	593	9	496	480
3	292	-284	4	132	-145	6	242	-291	10	-68	-48
4	793	823	5	261	247	7	254	-230	11	160	-173
5	858	751	6	862	-632	8	344	341	-21	243	-231
6	599	-540	7	599	-573	9	348	339	-20	156	164
7	745	-393	8	286	289	10	131	234	-19	418	414
8	190	151	9	195	184	11	259	-264	-18	-64	-13
9	586	568	10	-63	89	12	122	-107	-17	218	-206
10	201	207	11	286	-273	13	-69	123	-16	118	-193
11	699	-701	12	269	-268	14	-73	124	-15	211	181
12	297	-259	13	561	581	-20	-68	63	-14	595	585
13	146	-132	14	287	314	-19	412	403	-13	313	-318
14	202	209	15	-68	-85	-18	130	138	-12	318	-348
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17	-68	-49	18	-65	9	-15	270	200	-9	588	603
18	-71	120	19	630	619	-14	377	381	-8	-54	-78
-16	165	-135	-14	294	280	-13	-57	-38	-7	1205	-1232
-15	134	186	-13	-61	25	-12	381	-295	-6	363	317
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3	87	-176	4	734	-781	6	302	375	-20	188	-186
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5	970	-904	6	1024	1029	8	105	-134	-18	-63	2
6	1006	974	7	203	236	9	363	-358	-17	151	111
7	1558	1455	8	407	-412	10	217	-245	-16	243	270
8	76	65	9	276	-267	11	252	301	-15	-60	-15
9	540	-500	10	153	-134	12	-68	42	-14	293	-301
10	-56	-51	11	262	261	-20	103	-110	-13	-57	87
11	360	378	12	191	184	-19	490	-480	-12	785	801
12	200	223	13	384	-306	-18	107	-99	-11	-53	19
13	118	-102	14	189	-109	-17	306	311	-10	315	-308
14	460	-458	15	196	-159	-16	-63	64	-9	191	-196
15	-69	39	-19	196	-159	-15	229	-219	-8	179	198
16	248	230	-18	194	-171	-14	535	-505	-7	407	431
17	143	166	-17	437	440	-13	224	-210	-6	108	-149
-17	275	264	-16	167	176	-12	286	307	-5	1211	-1229
-16	159	163	-15	377	-370	-11	262	272	-4	-58	-125
-15	274	-255	-14	254	-255	-10	223	-189	-3	1007	1030
-14	117	-125	-13	-59	-85	-9	350	-390	-2	520	516
-13	221	214	-12	386	375	-8	80	72	-1	77	80
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-8	121	-93	-7	609	-640	-3	510	624	3	94	-108
-7	319	257	-6	132	93	-2	397	-409	4	-68	60
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			-1	1746	1546						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-21	195	-198	-5	108	127	-6	-68	-42	3	265	259
-20	103	85	-4	582	590	-5	432	-442	4	300	248
-19	150	180	-3	334	-362	-4	162	-103	5	210	-193
-18	150	141	-2	463	-462	-3	220	208	6	382	-385
-17	172	-194	-1	135	130	-2	104	125	7	98	-71
-16	352	-353				-1	-71	-6	8	200	210
-15	268	284	H=	2, K=	9				9	259	260
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-10	223	245	3	104	113	-16	129	-109	14	123	118
-9	555	564	4	188	-167	-15	-66	42	15	154	156
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-20	-66	-31	-2	144	-152	-11	-71	22	12	59	-67
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-9	222	-202	-17	292	-295	8	198	194	-1	-67	0
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2	128	-138	-4	106	96	2	162	165	10	260	-262
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4	154	139	-2	374	-368	4	195	-196	12	215	212
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-18	-64	48	-20	-69	-5	9	169	-201	17	136	119
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-16	237	-242	-18	130	-144	11	311	305	19	-67	-30
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-12	306	-315	-14	237	-242	15	-70	129	-3	137	-161
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-10	453	447	-12	449	472	17	-67	16	-1	404	403
-9	131	174	-11	-66	30						
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			-8	134	144						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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0	737	-732	12	410	411	-14	-69	-102	-11	-62	36
1	160	144	13	526	-548	-13	-69	107	-10	425	-403
2	265	277	14	-63	4	-12	231	236	-9	-57	-78
3	124	112	15	206	207	-11	-65	-61	-8	100	115
4	295	-294	16	274	268	-10	286	-270	-7	404	403
5	110	-139	17	-65	100	-9	-63	-64	-6	-56	-13
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15	237	-232	-9	-66	-65	-5	1337	1306	-3	1459	-1084
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7	227	213	13	126	-87	17	-66	-9	-16	-67	113
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			18	257	-232	-13	158	174	-11	-56	-16

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-9	539	531	-3	412	-409	3	134	58	-8	-64	-63
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-3	503	-511	-17	180	-198	-2	108	127	17	287	-262
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2	143	178	-11	137	-146	2	176	199	-5	334	-334
-21	-67	63	-10	167	181	3	409	-410	-4	119	108
-20	111	133	-9	165	176	4	171	-163	-3	191	177
-19	-66	-73	-8	-72	-98	5	169	165	-2	-64	-46
-18	-65	-35	-7	213	-210	6	166	182	-1	334	-330
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						14	-64	-16	-5	328	-331
									-4	-59	-1
									-3	497	522

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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13	393	-415	16	312	294	-15	181	-194	-9	784	705
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15	287	283	-17	131	104	-13	312	304	-7	422	287
16	227	247	-16	-67	70	-12	110	107	-6	776	-500
17	-67	-20	-15	340	-341	-11	135	90	-5	1192	-1016
18	302	-287	-14	138	-147	-10	278	-281	-4	430	394
-14	167	-155	-13	292	285	-9	-52	-24	-3	397	425
-13	231	238	-12	106	111	-8	176	169	-2	340	-245
-12	160	168	-11	400	-486	-7	402	428	-1	819	-789
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-10	355	-383	-9	138	-122	-5	-14	-7	0	344	346
-9	105	-142	-8	327	335	-4	1890	1267	1	576	-520
-8	173	180	-7	239	211	-3	303	62	2	765	-761
-7	336	337	-6	467	-488	-2	779	-475	3	90	68
-6	404	-443	-5	954	-939	-1	101	-175	4	361	366
-5	525	-511	-4	418	224	H=	4, K=	0	5	117	104
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-3	531	613	-2	511	-214	1	489	-406	7	194	-190
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-1	619	526	H=	3, K=	-2	3	254	-210	9	325	345
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1	364	-403	2	-54	9	6	312	-324	-21	126	-109
			3	460	409	7	143	-173	-20	264	251
			4	396	419	8	96	133	-19	333	324

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
-18	-65	-90	-9	419	436	2	224	230	-20	103	109
-17	232	-210	-8	404	-389	3	-70	-46	-19	151	163
-16	191	189	-7	101	-140	4	269	-271	-18	-68	-78
-15	428	429	-6	1356	1284	-21	-67	69	-17	316	-347
-14	159	154	-5	625	635	-20	113	-87	-16	-66	-93
-13	377	-420	-4	101	-102	-19	150	-142	-15	234	241
-12	441	-406	-3	353	-352	-18	-65	-25	-14	239	252
-11	865	849	-2	515	-537	-17	387	389	-13	-66	-59
-10	676	652	-1	114	119	-16	325	323	-12	210	-210
-9	-51	4				-15	214	-226	-11	-66	9
-8	559	-535	H=	4, K=	5	-14	-66	101	-10	-67	95
-7	524	-489				-13	-63	-39	-9	-67	63
-6	833	694	0	384	-375	-12	266	263	-8	106	-129
-5	1307	1266	1	378	380	-11	-63	49	-7	212	-225
-4	635	-605	2	160	105	-10	513	-514	-6	118	146
-3	629	-607	3	-68	-7	-9	-62	-7	-5	370	393
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			6	358	350	-6	-65	34	-2	-71	-14
H=	4, K=	3	7	215	249	-5	-65	27			
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1	-57	42	-20	255	-242	-3	627	624	-18	-68	0
2	459	452	-19	148	-144	-2	-71	54	-17	149	164
3	144	175	-18	-65	64	-1	456	-469	-16	-68	71
4	253	-262	-17	320	307	H=	4, K=	8	-15	193	-222
5	-65	-21	-16	-64	23				-14	191	-183
6	312	304	-15	275	-297	0	-69	57	-13	165	170
7	276	279	-14	93	41	1	129	-100	-12	169	152
8	171	-151	-13	482	477	2	240	-275	-11	-68	-40
9	179	-185	-12	276	270	-21	208	-184	-10	154	-175
10	-69	48	-11	-57	25	-20	137	134	-9	-69	-52
-21	151	133	-10	472	-476	-19	235	239	-8	142	136
-20	261	-254	-9	124	-128	-18	-66	34	-7	160	184
-19	151	-133	-8	533	550	-17	323	-333	-6	-73	-125
-18	-65	79	-7	-50	91	-16	450	-439	-5	205	-207
-17	103	126	-6	687	-688	-15	100	-60			
-16	202	-230	-5	324	-329	-14	221	226	H=	4, K=	12
-15	420	-425	-4	354	-363	-13	-68	118	-16	-69	-32
-14	-60	-20	-3	187	192	-12	374	-372	-15	258	267
-13	439	444	-2	261	242	-11	146	162	-14	-73	117
-12	412	430	-1	486	-484	-10	508	529	-13	178	-145
-11	436	-400	H=	4, K=	6	-9	103	74	-12	167	-200
-10	610	-612				-8	-67	-55	-11	112	-25
-9	387	429	0	240	219	-7	-66	-43	-10	158	176
-8	647	636	1	366	-364	-6	115	121	H=	4, K=	-15
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-6	673	-936	3	-67	68	-4	236	-257	8	152	-145
-5	905	-868	4	253	267	-3	-69	-74	9	123	-126
-4	149	129	5	-69	34	-2	-68	27	10	139	125
-3	590	557	6	273	-253	-1	-68	36	H=	4, K=	-14
-2	370	-335	-22	225	-223	H=	4, K=	9	2	-70	-104
-1	809	-851	-21	-68	-63				3	176	198
			-20	188	190	0	102	-79	4	173	165
H=	4, K=	4	-19	180	195	-21	379	360	5	146	-157
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1	338	-355	-17	227	-234	-19	267	-244	7	103	-92
2	290	-270	-16	212	-228	-18	-66	65	8	103	113
3	275	292	-15	225	229	-17	234	227	9	175	160
4	269	268	-14	-63	34	-16	-65	-33	10	168	-163
5	189	200	-13	314	-304	-15	-68	-102	11	171	-175
6	148	-142	-12	152	-167	-14	154	-128	12	203	183
7	287	-306	-11	96	72	-13	116	-119	13	129	139
8	191	195	-10	553	553	-12	295	298	14	-68	-43
9	126	141	-9	-59	76	-11	98	-80	H=	4, K=	-13
-21	-68	-29	-8	497	-463	-10	251	-257	0	141	131
-20	163	173	-7	277	-288	-9	168	175	1	275	307
-19	97	-82	-6	209	-230	-8	-67	62	2	-66	-43
-18	-62	6	-5	-61	-9	-7	330	321	3	253	-244
-17	231	-236	-4	91	-80	-6	-69	16	4	-66	-22
-16	143	-146	-3	277	-264	-5	304	-313			
-15	490	483	-2	-65	-100	-4	-68	-66			
-14	-60	26	-1	490	473	-3	227	219			
-13	627	-656	H=	4, K=	7	-2	-70	-79			
-12	243	-246				-1	257	-226			
-11	155	156	0	176	-177	H=	4, K=	10			
-10	465	488	1	-68	108						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
5	151	167	10	-63	26	-1	500	498	6	103	96
6	-64	-1	11	157	-136				7	108	122
7	-65	-45	12	105	47	H=	4, K= -7		8	615	-610
8	107	-118	13	465	467				9	387	-389
9	-66	93	14	103	107	0	771	777	10	482	488
10	221	214	15	340	-353	1	545	570	11	114	103
11	-66	67	16	135	-152	2	445	424	12	-63	-46
12	96	-102	17	211	217	3	89	23	13	196	-172
13	161	-179	-8	231	-222	4	645	-657	14	144	146
14	104	106	-7	116	-119	5	329	287	15	197	209
15	238	226	-6	-67	42	6	463	458	16	209	262
16	-68	-26	-5	140	162	7	-54	46	17	133	-114
-1	-68	0	-4	144	-114	8	477	-490	-15	146	-165
			-3	-64	-53	9	529	-514	-14	-68	23
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0	103	92	-1	194	176	11	426	402	-12	119	-160
1	212	-167	H=	4, K= -9		12	334	-347	-11	294	-264
2	-66	-73				13	438	-440	-10	283	-285
3	301	297	0	106	-11	14	242	261	-9	-62	33
4	-66	63	1	291	332	15	421	445	-8	426	439
5	-65	-64	2	87	-65	16	239	239	-7	187	-156
6	161	-133	3	208	-200	17	-67	-3	-6	647	-642
7	-66	-17	4	-57	-17	-12	114	156	-5	101	-15
8	352	359	5	246	230	-11	191	-172	-4	782	736
9	152	-151	6	501	511	-10	153	-171	-3	691	612
10	366	-392	7	550	-549	-9	292	298	-2	117	77
11	310	-308	8	489	-459	-8	-65	29	-1	870	-796
12	108	149	9	203	-217	-7	207	-199			
13	315	320	10	-64	89	-6	302	-306	H=	4, K= -4	
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15	216	-198	12	102	-115	-4	-60	65	0	439	447
16	116	-88	13	487	-516	-3	481	461	1	940	-861
17	253	273	14	163	-169	-2	848	-793	2	1176	-1074
-4	108	-131	15	263	255	-1	349	-364	3	829	779
-3	-67	-12	16	-65	21				4	254	262
-2	-66	53	17	-66	-75	H=	4, K= -6		5	216	-216
-1	-68	74	-10	208	-209				6	641	-636
			-9	-68	12	0	150	170	7	152	-163
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1	215	215	-6	261	-249	3	540	532	10	233	-226
2	154	-153	-5	-67	-60	4	773	726	11	178	-198
3	401	-403	-4	283	289	5	-52	72	12	-64	-60
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5	95	18	-2	147	-121	7	263	-242	14	120	106
6	203	190	-1	405	-409	8	402	385	15	258	-286
7	-65	-74				9	348	365	16	283	-245
8	362	-344	H=	4, K= -8		10	261	-247	-16	-66	0
9	198	214				11	291	-365	-15	196	189
10	451	435	0	112	103	12	225	233	-14	-65	10
11	257	-254	1	473	-434	13	344	345	-13	309	-384
12	192	-200	2	150	-158	14	223	-248	-12	-65	-35
13	98	-83	3	599	576	15	249	-252	-11	359	352
14	-65	-26	4	807	750	16	202	-194	-10	365	370
15	242	223	5	297	-303	17	-68	55	-9	-60	-55
16	206	200	6	638	-589	-14	-69	62	-8	700	-731
17	281	-276	7	117	-84	-13	188	-202	-7	428	-385
-6	212	-209	8	402	412	-12	-68	-40	-6	234	241
-5	-68	35	9	406	379	-11	277	284	-5	466	572
-4	-67	85	10	261	-267	-10	118	-69	-4	837	-834
-3	-64	-3	11	424	-442	-9	409	-421	-3	968	-1107
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			14	-64	55	-6	180	189			
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2	207	-211	-11	196	204	-2	1010	962	1	1215	1101
3	150	159	-10	229	239	-1	425	425	2	388	393
4	166	133	-9	-66	-69				3	349	-327
5	100	-30	-8	170	-169	H=	4, K= -5		4	-55	-52
6	573	-566	-7	209	197				5	74	10
7	-63	38	-6	126	151	0	291	-175	6	758	725
8	475	491	-5	147	162	1	711	713	7	262	284
9	132	116	-4	209	-224	2	145	-161	8	399	-415
			-3	542	-525	3	874	-828	9	164	-160
			-2	98	134	4	520	-496	10	236	233
						5	252	-250	11	345	332

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
12	340	341	-17	182	188	-10	299	258			
13	432	-455	-16	-64	-80	-9	716	716	H=	5, K=	4
14	448	-458	-15	134	-136	-8	109	-5			
15	333	336	-14	103	81	-7	89	-80	0	177	-164
-17	168	163	-13	221	230	-6	769	-736	1	495	-482
-16	-65	-15	-12	420	441	-5	301	-285	2	-66	-20
-15	256	-258	-11	-56	-33	-4	759	689	3	-68	-15
-14	142	116	-10	461	-497	-3	426	374	4	299	296
-13	317	316	-9	409	418	-2	187	-165	5	141	153
-12	-64	97	-8	459	417	-1	511	-478	6	330	-323
-11	138	-172	-7	173	-199				7	-72	-108
-10	240	-245	-6	264	-290	H=	5, K=	2	-21	-68	21
-9	121	112	-5	337	471				-20	132	102
-8	731	717	-4	672	-587	0	336	329	-19	-84	69
-7	224	236	-3	445	-534	1	777	-754	-18	-66	-98
-6	150	-217	-2	751	-583	2	582	-575	-17	625	-605
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-4	449	462				4	359	367	-15	315	314
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-2	177	162				6	222	-190	-13	269	-286
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			1	370	-348	8	121	152	-11	361	357
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			3	109	118	10	-69	13	-9	198	165
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1	287	-277	5	141	137	-20	301	276	-7	129	114
2	327	-359	6	444	-431	-19	-65	-9	-6	-57	121
3	1049	939	7	185	-190	-18	247	-249	-5	166	-128
4	1140	1160	8	275	272	-17	96	-86	-4	296	-311
5	445	411	9	243	228	-16	-64	27	-3	566	-548
6	499	-477	10	169	-179	-15	-64	89	-2	199	-204
7	703	-697	11	393	-374	-14	203	-183	-1	425	435
8	266	285	12	-71	-7	-13	647	-649			
9	102	-70	-20	133	130	-12	232	-341	H=	5, K=	5
10	223	-233	-19	101	116	-11	285	283			
11	474	-461	-18	205	-205	-10	575	549	0	-67	41
12	189	-189	-17	-65	-12	-9	-54	-80	1	263	238
13	217	235	-16	386	368	-8	-52	-107	2	205	195
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15	169	-164	-14	-62	40	-6	739	716	4	348	-344
-18	-67	-69	-13	167	-192	-5	114	132	5	-70	9
-17	234	-222	-12	378	-407	-4	787	-788	6	276	286
-16	-65	-10	-11	470	473	-3	332	-374	-21	-67	-34
-15	232	239	-10	793	778	-2	-54	75	-20	150	-175
-14	173	185	-9	1019	-952	-1	573	556	-19	-64	-76
-13	210	-232	-8	575	-565				-18	341	334
-12	230	-216	-7	472	492	H=	5, K=	3	-17	573	566
-11	158	134	-6	1111	1044				-16	176	165
-10	619	632	-5	1033	941	0	258	-264	-15	365	-324
-9	164	104	-4	680	-624	1	625	598	-14	-63	20
-8	692	-695	-3	216	131	2	379	382	-13	535	538
-7	-55	11	-2	514	502	3	212	-190	-12	-60	-29
-6	884	822	-1	560	606	4	236	-241	-11	444	-421
-5	519	-231				5	133	130	-10	529	-540
-4	941	-925	H=	5, K=	1	6	144	173	-9	-60	-79
-3	68	-234				7	232	211	-8	795	776
-2	797	-754	0	589	-603	8	-71	-89	-7	-59	-5
-1	-54	113	1	769	749	-21	-68	-33	-6	485	-490
			2	901	857	-20	221	-229	-5	426	-433
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			4	352	-346	-18	-64	49	-3	430	417
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1	804	710	6	290	318	-16	-65	-84	-1	476	-455
2	392	389	7	-67	71	-15	180	-173			
3	230	-255	8	225	-228	-14	-62	-24	H=	5, K=	6
4	1059	-980	9	269	-272	-13	262	262			
5	-54	-54	10	-68	33	-12	294	304	0	-70	-95
6	558	543	11	259	258	-11	279	-277	1	137	-159
7	331	316	-20	204	-202	-10	293	-319	2	178	-167
8	91	-81	-19	-66	-27	-9	133	90	3	-70	60
9	119	-118	-18	301	298	-8	353	361	4	183	198
10	-65	13	-17	-65	44	-7	334	343	-21	98	-85
11	195	186	-16	160	-125	-6	450	-422	-20	124	151
12	177	164	-15	93	-92	-5	144	-176	-19	118	123
13	127	-152	-14	88	59	-4	150	185	-18	281	-288
14	-68	-75	-13	431	432	-3	298	285	-17	451	-447
-19	-68	-80	-12	425	464	-2	159	-148	-16	125	108
-18	-68	81	-11	573	-544	-1	327	-327	-15	648	659

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-14	109	-86	-11	128	-145	13	225	-250	-3	100	-84
-13	135	-135	-10	288	-280	14	-68	54	-2	396	383
-12	-62	11	-9	170	-159	-2	-68	-44	-1	430	422
-11	120	-90	-8	199	224	-1	-70	-123	H= 5, K= -9		
-10	585	585	-7	329	330	H= 5, K= -12			0	109	106
-9	-62	-41	-6	231	-246	0	-65	28	1	286	287
-8	452	-466	-5	251	-253	1	322	-335	2	-59	25
-7	-63	-38	-4	113	98	2	-66	-62	3	-59	-35
-6	221	202	-3	112	117	3	293	296	4	310	-290
-5	511	511	-2	-72	-34	4	132	114	5	436	444
-4	-65	35	H= 5, K= 10			5	155	137	6	333	316
-3	358	-238	-19	178	168	6	279	-286	7	286	-284
-2	-70	105	-18	-68	-28	7	-64	-36	8	422	-426
-1	464	472	-17	128	-159	8	107	103	9	-63	-32
H= 5, K= 7			-16	-66	2	9	179	-207	10	173	162
0	204	-196	-15	217	217	10	303	-302	11	181	194
1	107	96	-14	168	183	11	144	-120	12	140	-163
2	165	176	-13	146	-131	12	-67	106	13	278	-293
-21	127	102	-12	229	-243	13	405	381	14	212	225
-20	131	-127	-11	-69	54	14	124	118	15	269	278
-19	159	-164	-10	204	217	15	250	-232	16	-66	50
-18	245	250	-9	-69	-24	-4	194	-180	-10	-71	47
-17	332	319	-8	134	-153	-3	191	-202	-9	348	356
-16	221	-208	-7	-70	-43	-2	-69	121	-8	191	204
-15	628	-643	-6	118	145	-1	368	378	-7	229	-231
-14	223	-203	-5	235	240	H= 5, K= -11			-6	196	-184
-13	107	118	H= 5, K= 11			0	-65	8	-5	-65	-12
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-11	-65	10	-16	111	124	2	129	-115	-3	237	212
-10	561	-558	-15	273	-274	3	271	-261	-2	283	-291
-9	141	116	-14	110	-111	4	-66	13	-1	160	-148
-8	307	309	-13	276	261	5	174	-173	H= 5, K= -8		
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-6	-66	30	-11	-71	-121	7	99	82	1	545	-544
-5	278	-265	-10	-73	-115	8	127	-123	2	335	-309
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-3	438	426	H= 5, K= -15			10	-66	43	4	363	379
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H= 5, K= 8			9	116	92	13	123	-124	7	133	125
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-19	175	156	3	319	312	-6	121	-110	11	269	-220
-18	-66	-86	4	121	103	-5	-68	4	12	103	129
-17	98	-95	5	253	-245	-4	-65	90	13	224	235
-16	-65	-91	6	183	-168	-3	126	112	14	126	-99
-15	269	293	7	-63	81	-2	96	-73	15	299	-301
-14	189	214	8	346	352	-1	185	-207	16	220	-203
-13	235	-230	9	141	129	H= 5, K= -10			-11	138	166
-12	293	-307	10	283	-261	0	-65	-3	-10	136	110
-11	-68	119	11	-67	-83	1	404	-447	-9	378	-381
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-5	218	188	2	-66	6	7	165	155	-3	225	-238
-4	-65	-33	3	165	-166	8	611	608	-2	413	423
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H= 5, K= 9			7	-67	100	12	277	271	1	414	378
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-19	122	-136	9	-65	-68	14	329	-341	3	525	-509
-18	-67	22	10	190	190	15	327	-351	4	242	-229
-17	-66	-84	11	121	112	16	-66	66	5	653	632
-16	-67	-98	12	213	-215	-8	239	-240	6	-56	18
-15	253	-247				-7	119	105	7	117	-120
-14	210	-219				-6	234	243	8	222	-207
-13	177	178				-5	-64	-11	9	357	-336
-12	354	337				-4	125	-141	10	198	215

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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15	160	167	-5	280	254	0	-55	6	7	-66	76
16	256	253	-4	117	203	1	576	-555	8	252	267
-13	109	148	-3	106	145	2	320	289	9	168	149
-12	174	174	-2	553	-516	3	285	292	10	186	-196
-11	362	-351	-1	193	-232	4	406	405	-20	178	180
-10	225	-221				5	104	-120	-19	-66	4
-9	120	106	H=	5, K=	-4	6	659	-663	-18	294	-286
-8	-66	65				7	54	-46	-17	155	-156
-7	-54	-14	0	228	250	8	200	176	-16	148	144
-6	349	-354	1	581	-586	9	118	-101	-15	156	150
-5	191	-164	2	594	580	10	-66	-99	-14	145	170
-4	533	560	3	1101	1020	11	108	-67	-13	345	-350
-3	-59	-18	4	448	455	12	-67	-42	-12	166	-191
-2	669	-631	5	-54	21	13	356	352	-11	831	855
-1	108	-73	6	513	-526	-18	-67	-89	-10	-57	62
			7	197	-199	-17	300	-296	-9	431	-442
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2	538	-540	11	341	-330	-13	320	-349	-5	551	527
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6	577	-520	15	319	-321	-9	94	-91	-1	260	279
7	-56	18	-16	-68	42	-8	490	-514			
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10	584	-563	-13	301	-314	-5	360	309	1	501	505
11	421	-414	-12	170	181	-4	568	-467	2	-62	-85
12	-65	-18	-11	286	301	-3	1213	-1184	3	296	-311
13	175	181	-10	173	184	-2	-55	-51	4	123	-101
14	125	117	-9	-62	-139	-1	1228	1209	5	190	173
15	170	-201	-8	544	-578				6	199	177
16	207	-187	-7	-56	64	H=	5, K=	-1	7	-66	47
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-13	225	-248	-5	128	-169	1	444	404	9	172	-153
-12	120	-128	-4	509	-454	2	601	595	-20	206	-191
-11	150	156	-3	462	-415	3	369	-350	-19	-67	36
-10	103	88	-2	818	774	4	500	-512	-18	224	245
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-6	392	-381	0	323	312	8	146	-143	-14	175	-168
-5	109	99	1	910	925	9	310	-338	-13	542	-569
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-3	139	-115	3	242	-234	11	243	236	-11	305	-264
-2	-54	103	4	374	-380	12	-67	-47	-10	98	-70
-1	345	334	5	98	96	13	297	-296	-9	216	-196
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0	90	127	8	576	-588	-17	133	160	-6	644	-666
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2	471	428	10	450	456	-15	117	-102	-4	737	720
3	1008	-998	11	170	197	-14	-64	89	-3	-53	73
4	1005	-935	12	-65	-52	-13	292	279	-2	334	-331
5	132	117	13	511	-507	-12	112	95	-1	427	-422
6	766	754	14	134	-124	-11	461	-422			
7	-58	79	-17	143	167	-10	395	-413	H=	6, K=	2
8	592	-571	-16	212	-199	-9	140	-81	0	-61	-11
9	97	-90	-15	259	-259	-8	470	453	1	634	-617
10	596	573	-14	147	160	-7	166	-84	2	206	-190
11	469	455	-13	227	271	-6	398	-452	3	324	314
12	-65	-122	-12	-64	11	-5	1193	-1195	4	118	137
13	241	-251	-11	50	-110	-4	-54	7	5	-64	-44
14	111	-126	-10	222	-235	-3	419	-447	6	149	-144
15	276	284	-9	-55	54	-2	818	-775	7	-69	-36
-15	-69	-111	-8	396	357	-1	440	-415	8	376	371
-14	135	128	-7	250	-225				-21	-66	23
-13	304	297	-6	311	-395	H=	6, K=	0	-20	165	162
-12	119	95	-5	130	-212	0	-56	102	-19	136	-95
-11	221	-221	-4	362	450	1	444	-450	-18	326	-319
-10	-65	94	-3	1023	1016	2	330	-323	-17	183	-194
			-2	740	-742						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-14	-63	-67				-1	246	-250	7	297	-290
-13	625	-625	0	-68	89				8	380	-362
-12	-59	1	1	137	158	H=	6, K=	8	9	196	170
-11	292	320	2	-69	95	-20	277	265	10	272	272
-10	251	253	3	128	-115	-19	126	105	11	-67	-19
-9	216	-207	4	163	-172	-18	143	-152	12	-68	-98
-8	402	-406	-21	171	-166	-17	173	-195	13	103	-90
-7	-53	-33	-20	231	-219	-16	125	-64	-2	161	-154
-6	572	567	-19	116	-80	-15	381	356	-1	-69	-23
-5	207	183	-18	-66	84	-14	-67	79	H=	6, K=	-12
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-3	109	71	-16	239	-223	-12	163	-180	1	369	-357
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3	252	-246	-9	245	219	-5	397	398	8	209	231
4	220	-205	-8	556	566	-4	112	-105	9	117	-105
5	-67	-22	-7	234	-274	-3	236	-231	10	155	-132
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-16	306	-309	0	-68	56	-14	-68	-72	-2	383	370
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-14	-63	-47	2	154	-146	-12	201	200	H=	6, K=	-11
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-8	495	475	-16	192	184	-6	159	-166	5	101	88
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-1	462	-475	-9	274	-259	-13	233	-222	12	131	103
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2	103	-95	-5	135	142	-9	-72	63	-7	-73	-151
3	213	210	-4	202	-194	-8	122	-76	-6	148	-126
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5	-71	-77	-2	250	218	1	110	-120	-4	150	153
-21	183	159	-1	130	126	2	179	152	-3	159	143
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-16	295	295	-19	199	-187	7	-67	54	1	308	-326
-15	510	512	-18	270	251	8	221	220	2	-65	-44
-14	90	-73	-17	255	257	9	-69	-73	3	173	150
-13	150	-131	-16	271	-268	10	205	-203	4	486	460
-12	132	-138	-15	335	-336	11	-70	58	5	179	-155
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-8	123	-120	-11	272	-297	2	-66	15	9	93	-53
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-6	229	239	-9	299	305	4	-66	-46	11	336	-344
-5	-62	-40	-8	211	224	H=	6, K=	-12	12	-64	-30
-4	335	-237	-7	102	-62	0	221	205	13	238	250
-3	320	-345	-6	104	-115	1	215	214	14	-67	-36
-2	-66	50	-5	395	-376	2	-66	15			
-1	298	293	-4	307	277	3	217	-220			
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L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-9	318	-306	6	90	94	-10	481	-501	H=	6, K=	-2
-8	122	-88	7	-61	-79	-9	-65	-103	0	161	161
-7	208	199	8	603	-604	-8	295	283	1	555	-541
-6	136	129	9	174	-162	-7	712	-642	2	544	-513
-5	-66	-43	10	541	528	-6	685	-689	3	342	342
-4	251	-235	11	-64	-6	-5	338	301	4	550	546
-3	-65	15	12	382	-386	-4	569	520	5	212	-214
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3	277	-310	-10	250	245	2	-54	-88	12	-69	18
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7	129	-151	-6	354	-397	6	408	-457	-15	380	371
8	104	-104	-5	212	-226	7	92	46	-14	291	-269
9	-64	-14	-4	133	131	8	506	507	-13	-64	-8
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11	309	321	-2	330	-312	10	406	-407	-11	432	447
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13	315	-306	H=	6, K=	-6	12	-67	78	-9	-55	-32
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15	138	154	1	96	-155	-17	-70	-98	-7	-53	106
-10	-69	57	2	-55	-34	-16	118	126	-6	-52	-10
-9	155	149	3	403	414	-15	105	86	-5	257	-268
-8	-66	-34	4	95	75	-14	215	-211	-4	738	-695
-7	135	-127	5	424	-412	-13	246	-237	-3	1030	-966
-6	209	-208	6	-59	0	-12	159	-171	-2	-51	-11
-5	-65	-25	7	-60	-2	-11	-64	39	-1	385	374
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-2	460	-479	10	410	-403	-8	285	-317	1	1014	976
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3	731	726	-13	272	-272	-2	-52	81	7	-65	25
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5	429	-402	-11	483	510	H=	6, K=	-3	9	177	-184
6	194	-182	-10	106	119	0	244	270	10	122	117
7	-60	21	-9	106	-103	1	445	436	11	-71	108
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9	132	130	-7	95	-67	3	456	-454	-18	102	126
10	545	-571	-6	541	550	4	775	-757	-17	245	242
11	-64	28	-5	-58	26	5	216	212	-16	105	-107
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13	144	136	-3	141	-153	7	349	-354	-14	145	169
14	159	-187	-2	640	642	8	227	-204	-13	158	186
15	167	-196	-1	517	440	9	287	273	-12	305	301
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-10	-69	-94	1	389	400	12	134	-95	-9	493	470
-9	269	-273	2	177	-183	13	424	-403	-8	913	864
-8	-65	-48	3	683	-669	-17	111	112	-7	-53	18
-7	-65	63	4	280	256	-16	219	-216	-6	418	-416
-6	267	264	5	549	531	-15	251	-259	-5	-52	-40
-5	113	-164	6	286	301	-14	172	204	-4	467	521
-4	449	-460	7	-61	8	-13	130	166	-3	331	356
-3	141	-146	8	385	-377	-12	221	203	-2	402	-411
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1	657	686	13	170	-179	-7	614	-530	2	201	-205
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3	481	-512	-15	124	-133	-5	114	18	4	-65	-60
4	126	93	-14	172	185	-4	310	238	5	196	-195
			-13	350	363	-3	220	235			
			-12	121	-123	-2	705	-683			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
6	-66	-59	-5	-61	36	-12	118	106	-17	-67	13
7	190	170	-4	-62	-69	-11	278	-280	-16	-70	-75
8	273	280	-3	180	-158	-10	140	-105	-15	319	-322
-19	159	-155	-2	-64	-53	-9	280	285	-14	-69	36
-18	164	-156	-1	230	219	-8	216	219	-13	258	248
-17	128	173				-7	199	-193	-12	-71	-35
-16	404	404	H=	7, K=	3	-6	152	-141	-11	-69	-79
-15	247	247				-5	-67	-71	-10	-71	-44
-14	-65	47	0	-67	53	-4	424	419	-9	232	249
-13	425	-407	1	273	269	-3	428	433			
-12	-62	-21	2	-65	-40	-2	344	-348			
-11	145	145	3	246	-237	-1	204	-211	H=	7, K=	-14
-10	-59	-66	4	274	-218						
-9	159	156	5	-70	65	H=	7, K=	6	2	-71	110
-8	421	-382	-21	-69	-84				3	216	198
-7	197	191	-22	227	-249	0	-71	-11	4	-70	-71
-6	390	416	-19	110	-83	-20	205	177	5	-70	-131
-5	-56	-112	-18	115	118	-19	-67	74	6	114	-120
-4	708	-700	-17	143	161	-18	220	-223	7	140	125
-3	128	-111	-16	-66	-66	-17	-67	-60	8	258	248
-2	203	180	-15	316	-320	-16	226	223	9	155	-156
-1	150	143	-14	225	234	-15	-66	66			
			-13	414	410	-14	95	42	H=	7, K=	-13
H=	7, K=	1	-12	-63	34	-13	323	-330			
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1	286	272	-10	-62	-4	-11	231	242	1	191	187
2	-69	-152	-9	444	435	-10	106	133	2	177	-171
3	235	-224	-8	330	328	-9	-68	-103	3	229	-239
4	120	140	-7	164	146	-8	242	-246	4	-65	-22
5	-64	81	-6	439	-439	-7	103	120	5	122	134
6	161	172	-5	155	-148	-6	115	88	6	-67	68
7	-70	-95	-4	364	354	-5	-68	84	7	142	-158
-20	183	-173	-3	157	217	-4	402	-394	8	178	-159
-19	104	84	-2	-66	-7	-3	193	-196	9	191	187
-18	144	135	-1	224	-215	-2	385	366	10	349	355
-17	144	-157				-1	211	180	11	-69	50
-16	171	-155	H=	7, K=	4				-2	194	-169
-15	370	-370	0	153	-142	H=	7, K=	7	-1	-69	-19
-14	185	169	1	178	-159	-20	218	-202			
-13	309	307	2	-69	10	-19	-68	-10	H=	7, K=	-12
-12	-63	-62	3	130	147	-18	426	421	0	276	-297
-11	140	-146	-21	-68	45	-17	-68	-22	1	129	-134
-10	476	-498	-20	104	98	-16	187	-181	2	201	224
-9	168	188	-19	-65	40	-15	194	-199	3	260	265
-8	452	469	-18	200	-207	-14	-66	78	4	-65	75
-7	383	-365	-17	391	-404	-13	297	309	5	116	-119
-6	379	-397	-16	177	189	-12	-67	-24	6	-66	-84
-5	391	378	-15	126	126	-11	279	-275	7	-64	28
-4	478	482	-14	276	-275	-10	172	-169	8	230	238
-3	166	-134	-13	247	-236	-9	107	122	9	101	-55
-2	198	-191	-12	105	-73	-8	190	183	10	275	-285
-1	203	-211	-11	107	128	-7	-66	29	11	174	-170
			-10	147	111	-6	143	-176	12	305	295
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0	114	-93	-8	245	-252	-4	375	368	-4	203	-180
1	328	-338	-7	174	170	-3	122	155	-3	-69	49
2	130	131	-6	133	109	-2	235	-241	-2	261	247
3	183	190	-5	-66	-90				-1	132	136
4	-65	47	-4	234	-216	H=	7, K=	8			
5	-66	-2	-3	528	-524	-19	-67	24	H=	7, K=	-11
6	207	-209	-2	125	136	-18	156	-148	0	320	309
-20	260	234	-1	395	412	-17	105	-109	1	166	169
-19	-64	25				-16	-68	-69	2	315	-289
-18	-66	-40	H=	7, K=	5	-15	277	265	3	169	-195
-17	-65	-53	0	-68	-30	-14	-68	-38	4	152	174
-16	-65	8	1	-68	49	-13	301	-293	5	611	610
-15	363	355	2	136	118	-12	-67	34	6	265	249
-14	340	-347	-21	-69	-82	-11	197	174	7	-526	-537
-13	301	-272	-20	176	-187	-10	190	176	8	266	-268
-12	-62	47	-19	-64	-27	-9	185	-182	9	-67	114
-11	356	370	-18	179	207	-8	346	-322	10	-65	112
-10	436	404	-17	238	236	-7	151	171	11	-64	2
-9	114	-97	-16	237	-236	-6	232	261	12	205	-202
-8	393	-375	-15	-64	-50	-5	119	113	13	237	-243
-7	231	210	-14	-65	-5				-7	218	-170
-6	423	411	-13	257	225	H=	7, K=	9	-6	-70	-50

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-5	-66	0	-9	100	-144	5	323	323	-11	430	-408
-4	109	88	-8	-65	-63	6	234	246	-10	185	-207
-3	-68	75	-7	232	239	7	280	-298	-9	593	627
-2	297	-309	-6	238	273	8	339	-331	-8	207	204
-1	146	-142	-5	217	-241	9	-66	100	-7	-57	-110
H=	7, K= -10		-4	235	-219	10	313	318	-6	540	-506
0	210	-237	-3	243	241	11	-64	-32	-5	184	-183
1	110	-86	-2	233	237	12	-69	-110	-4	719	646
2	-64	47	-1	162	150	-16	127	-125	-3	381	361
3	219	215	H=	7, K= -7		-15	121	-120	-2	1056	-1004
4	142	-138	0	171	186	-14	194	194	-1	198	-186
5	765	-782	1	554	556	-13	-65	27	H=	7, K= -2	
6	151	-120	2	257	256	-12	229	-235	0	119	-91
7	320	344	3	259	-255	-11	261	-275	1	143	-150
8	127	131	4	-62	74	-10	168	-166	2	142	-147
9	-62	-58	5	263	277	-9	299	318	3	440	469
10	201	-193	6	-63	30	-8	-62	-20	4	427	422
11	-64	-27	7	200	-209	-7	294	-323	5	292	-292
12	325	331	8	404	-401	-6	99	73	6	138	-156
13	222	227	9	-63	64	-5	173	176	7	-66	85
-9	190	-170	10	237	235	-4	488	503	8	407	429
-8	-69	11	11	-63	18	-3	347	340	9	125	110
-7	137	138	12	143	-137	-2	421	-357	10	207	-217
-6	130	89	13	98	-28	-1	372	-357	-18	340	-341
-5	-66	-87	-13	309	311	H=	7, K= -4		-17	164	-190
-4	267	-268	-12	117	-137	0	434	-407	-16	486	495
-3	-65	51	-11	94	-116	1	294	-273	-15	355	338
-2	343	349	-10	-65	46	2	-57	-34	-14	-65	-40
-1	149	137	-9	-64	69	3	103	123	-13	166	-173
H=	7, K= -9		-8	103	75	4	51	64	-12	179	-172
0	141	119	-7	170	-149	5	130	-118	-11	461	457
1	-64	92	-6	514	-513	6	220	-222	-10	355	353
2	-64	70	-5	163	176	7	128	155	-9	626	-598
3	342	-359	-4	518	520	8	269	266	-8	641	-594
4	-64	-2	-3	-62	-95	9	122	-84	-7	-57	29
5	400	399	-2	169	-164	10	254	-263	-6	493	471
6	204	216	-1	-61	-81	11	-67	-78	-5	532	500
7	141	-139	H=	7, K= -6		12	145	163	-4	228	-254
8	116	-106	0	285	-286	-17	133	-117	-3	565	-567
9	-63	92	1	607	-626	-16	116	85	-2	357	374
10	343	356	2	138	129	-15	201	190	-1	593	595
11	-65	-37	3	485	477	-14	241	-251	H=	7, K= -1	
12	385	-402	4	-60	-46	-13	121	-119	0	116	-119
13	132	-145	5	251	-248	-12	128	128	1	455	459
-10	-67	10	6	-63	-55	-11	591	600	2	334	315
-9	145	167	7	144	122	-10	347	252	3	520	-533
-8	-64	13	8	313	315	-9	293	-247	4	129	-104
-7	228	-223	9	140	-153	-8	113	-119	5	390	397
-6	290	-208	10	280	-277	-7	172	125	6	152	145
-5	108	123	11	-64	67	-6	318	317	7	316	-327
-4	272	272	12	194	180	-5	152	-122	8	358	-377
-3	99	-96	13	-68	92	-4	518	-535	9	-67	-21
-2	408	-402	-14	204	-207	-3	377	-394	-19	-67	42
-1	-63	-27	-13	212	-200	-2	86	128	-18	208	219
H=	7, K= -8		-12	188	170	-1	251	266	-17	-66	-15
0	108	-101	-11	-64	-9	H=	7, K= -3		-16	456	-441
1	216	-235	-10	-57	-73	0	668	678	-15	263	-275
2	106	-78	-9	-67	-70	1	161	205	-14	-65	-63
3	193	187	-8	245	-251	2	-57	-10	-13	259	274
4	116	116	-7	240	217	3	346	-337	-12	-63	-58
5	123	-84	-6	278	272	4	274	-264	-11	661	-641
6	138	-141	-5	356	-336	5	192	179	-10	-60	6
7	94	87	-4	443	-423	6	133	116	-9	802	808
8	347	379	-3	303	-314	7	139	-113	-8	227	234
9	-65	-138	-2	159	-121	8	-64	-5	-7	174	-158
10	236	-243	-1	246	250	9	110	-113	-6	315	-328
11	-63	42	H=	7, K= -5		10	270	264	-5	171	-170
12	-66	95	0	314	343	11	222	213	-4	325	286
13	-66	69	1	433	424	-17	134	101	-3	107	103
-12	-70	90	2	322	-333	-16	362	-350	-2	454	-468
-11	273	288	3	238	-231	-15	264	-276	-1	221	-216
-10	-66	-23	4	155	136	-14	374	374			
						-13	307	337			
						-12	253	262			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	8, K=	0	-7	470	467	-4	-67	91	7	218	230
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1	229	-237	-5	156	-163	-2	118	-100	9	-172	-148
2	-66	90	-4	396	-408	-1	-67	-16	10	150	-126
3	291	299	-3	-67	-61	H=	8, K=	6	11	-68	78
4	-64	5	-2	359	349	-19	-68	-29	-4	205	-212
5	178	-186	-1	383	370	-18	253	-266	-3	-70	28
6	260	-251	H=	8, K=	3	-17	156	155	-2	327	321
-19	119	-115	0	203	211	-16	156	165	-1	122	86
-18	170	-147	1	137	139	-15	123	152	H=	8, K=	-11
-17	-64	-11	2	-69	-65	-14	-64	16	0	188	186
-16	118	117	3	-70	-119	-13	270	-279	1	-64	-33
-15	367	371	-20	203	-205	-12	-65	-58	2	158	-155
-14	-66	-46	-19	-67	6	-11	196	167	3	152	-192
-13	432	-415	-18	208	187	-10	-66	0	4	139	125
-12	-65	-67	-17	-66	58	-9	136	-138	5	308	309
-11	151	138	-16	196	-185	-8	99	-89	6	-64	-48
-10	108	-63	-15	-66	-103	-7	-65	60	7	272	-263
-9	329	-352	-14	192	185	-6	220	236	8	132	-120
-8	286	-302	-13	174	162	-5	120	138	9	113	92
-7	-62	63	-12	-66	-82	-4	177	-177	10	124	118
-6	363	355	-11	295	-271	-3	-69	1	11	-68	-49
-5	-60	29	-10	217	-201	H=	8, K=	7	-7	151	-166
-4	461	-482	-9	284	287	-18	199	204	-6	-69	-29
-3	111	-127	-8	270	249	-17	-69	-43	-5	-68	81
-2	261	256	-7	398	-409	-16	241	-212	-4	235	232
-1	336	342	-6	322	-328	-15	271	-272	-3	-67	59
H=	8, K=	1	-5	284	282	-14	-66	12	-2	-68	-147
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1	290	286	-3	-66	38	-12	-67	10	H=	8, K=	-10
2	199	-196	-2	371	-370	-11	241	-222	0	216	-228
3	251	-262	-1	327	-323	-10	-67	-66	1	137	-111
4	-68	-76	H=	8, K=	4	-9	-67	59	2	232	-229
5	209	203	0	-63	-78	-8	210	222	3	170	192
-19	133	132	1	-69	-1	-7	-70	-64	4	108	-116
-18	168	146	-20	212	197	-6	259	-253	5	113	-113
-17	219	205	-19	-67	48	H=	8, K=	8	6	151	142
-16	163	-199	-18	271	-262	-15	217	240	7	210	228
-15	345	-342	-17	-65	-55	-14	131	-140	8	133	126
-14	364	344	-16	113	76	-13	262	-264	9	108	-95
-13	197	187	-15	-65	-4	-12	168	141	10	186	-185
-12	124	-123	-14	-64	-72	-11	142	122	11	-68	43
-11	-63	-16	-13	134	-139	-10	-70	21	12	374	386
-10	88	24	-12	-65	9	H=	8, K=	-14	-8	-69	73
-9	218	222	-11	342	346	4	121	-101	-7	-67	87
-8	268	256	-10	-66	90	5	159	-157	-6	-65	41
-7	128	-141	-9	269	-239	H=	8, K=	-13	-5	-64	-3
-6	96	-98	-8	-64	-46	0	280	264	-4	160	-164
-5	311	281	-7	234	228	1	-69	23	-3	-63	27
-4	436	423	-6	-65	64	2	154	-177	-2	220	227
-3	267	241	-5	-66	-59	3	-65	8	-1	129	-121
-2	189	-197	-4	132	-120	4	-67	72	H=	8, K=	-9
-1	423	-427	-3	129	-134	5	237	230	0	-67	130
H=	8, K=	2	-2	368	364	6	226	-216	1	263	272
0	306	-297	-1	-67	11	7	-70	-80	2	211	-218
1	317	-328	H=	8, K=	5	8	296	273	3	-67	-60
2	-66	80	-20	174	-184	-1	-69	59	4	484	471
3	201	188	-19	-65	-19	H=	8, K=	-12	5	374	363
4	101	90	-18	273	272	0	134	-138	6	114	-127
-20	-71	124	-17	-65	74	1	-66	-10	7	202	-192
-19	-66	-63	-16	-65	-49	2	-65	31	8	-62	-51
-18	228	-231	-15	185	-179	3	271	251	9	-66	95
-17	255	-252	-14	-64	30	4	-67	13	10	174	168
-16	225	243	-13	151	153	5	395	-397	11	125	-134
-15	-63	17	-12	-64	22	6	213	-187	12	320	-325
-14	284	-271	-11	213	-232	H=	8, K=	-11	-10	-68	52
-13	271	-257	-10	-64	18	0	134	-138	-9	144	143
-12	-65	88	-9	266	255	1	-66	-10	-8	-66	-5
-11	109	53	-8	116	140	2	-65	31	-7	-66	-20
-10	218	223	-7	155	-170	3	271	251	-6	-64	-2
-9	167	-185	-6	172	-187	4	-67	-13	-5	122	132
-8	262	-251	-5	-67	-72	5	395	-397	-4	257	263

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-3	209	-211	-10	-63	52	5	444	439	-5	-59	-40
-2	278	-268	-9	256	-253	6	-66	77	-4	244	223
-1	-66	67	-8	225	-193	7	131	-124	-3	-60	0
H=	8, K=	-8	-7	363	350	8	141	-144	-2	305	-294
0	309	-314	-6	134	134	9	-68	104	-1	192	-186
1	277	-278	-5	215	-243	-17	312	-303	H=	9, K=	0
2	570	578	-4	259	-229	-16	294	-297	0	172	-185
3	274	264	-3	-63	-71	-15	-66	79	1	199	-198
4	216	-244	-2	239	209	-14	242	236	2	102	105
5	357	-348	-1	89	133	-13	-64	28	3	299	315
6	-64	-26	H=	8, K=	-5	-12	312	-302	4	-68	-18
7	277	280	0	140	172	-11	428	-409	-18	-67	-33
8	238	247	1	-61	25	-10	-64	-73	-17	-66	-6
9	-65	-77	2	96	-95	-9	563	549	-16	169	155
10	277	-276	3	403	-407	-8	-61	43	-15	-66	133
11	-67	15	4	-65	-139	-7	253	-268	-14	413	-412
12	220	209	5	324	336	-6	114	-121	-13	368	-343
-12	155	167	6	-64	28	-5	178	196	-12	254	221
-11	155	168	7	333	-338	-4	737	719	-11	227	220
-10	-65	0	8	247	-238	-3	255	-262	-10	96	-113
-9	-68	-122	9	177	190	-2	875	-887	-9	214	-201
-8	-64	-62	10	-67	89	-1	-60	20	-8	-65	-53
-7	-63	30	11	99	17	H=	3, K=	-2	-7	458	463
-6	-66	101	-15	119	-91	0	-63	73	-6	303	295
-5	151	-161	-14	212	201	1	170	-186	-5	373	-364
-4	313	-321	-13	146	128	2	95	-34	-4	-66	57
-3	-64	-33	-12	-64	-19	3	510	507	-3	349	334
-2	184	180	-11	-65	-19	4	180	-178	-2	296	293
-1	146	139	-10	-66	59	5	413	-413	-1	-66	29
H=	8, K=	-7	-9	340	338	6	108	-51	H=	9, K=	1
0	434	449	-8	-64	11	7	184	180	0	246	247
1	478	485	-7	487	-464	8	210	203	1	225	189
2	514	-511	-6	191	-203	-18	224	-203	2	179	-176
3	294	-282	-5	376	392	-17	-69	79	3	257	-254
4	137	-125	-4	476	494	-16	158	156	-19	-68	34
5	-66	102	-3	118	99	-15	-64	-29	-18	138	134
6	126	136	-2	-60	7	-14	402	-412	-17	-67	34
7	271	-292	-1	279	-271	-13	268	-302	-16	418	-442
8	444	-440	H=	8, K=	-4	-12	274	249	-15	-64	-24
9	-66	53	0	398	-402	-11	642	658	-14	172	187
10	423	429	1	222	-217	-10	-63	9	-13	-64	-43
11	-67	-12	2	-62	6	-9	692	-704	-12	201	-194
-13	111	111	3	505	505	-8	-60	-34	-11	154	-165
-12	154	-151	4	-65	68	-7	116	123	-10	103	37
-11	171	-167	5	261	-267	-6	343	323	-9	367	364
-10	-63	36	6	-65	24	-5	-59	-54	-8	269	266
-9	170	182	7	314	315	-4	626	-614	-7	412	-438
-8	192	185	8	156	134	-3	191	-232	-6	186	-175
-7	347	-363	9	216	-216	-2	569	594	-5	-67	32
-6	467	-467	10	-68	-97	-1	-61	0	-4	-68	-81
-5	212	224	-16	288	292	H=	8, K=	-1	-3	-66	61
-4	-64	59	-15	-66	31	0	-63	-18	-2	275	-280
-3	204	-195	-14	-64	-81	1	382	397	-1	-65	6
-2	145	-149	-13	-64	-25	2	269	-279	H=	9, K=	2
-1	160	-165	-12	117	100	3	263	-276	0	360	-361
H=	8, K=	-6	-11	144	114	4	158	180	1	232	-226
0	360	-360	-10	-64	44	5	140	157	-19	104	-4
1	-62	-67	-9	461	-447	6	-68	121	-18	274	-294
2	173	153	-8	-65	-35	7	140	-114	-17	-66	26
3	297	301	-7	545	553	8	254	-254	-16	264	241
4	268	288	-6	411	396	-19	-71	77	-15	104	91
5	132	-139	-5	-59	-44	-18	126	143	-14	166	-164
6	198	-184	-4	359	-352	-17	-64	2	-13	150	-131
7	289	276	-3	161	-148	-16	136	-126	-12	114	124
8	284	281	-2	317	313	-15	167	-134	-11	168	159
9	-67	-91	-1	174	150	-14	437	439	-10	-66	67
10	242	-238	H=	8, K=	-3	-13	253	254	-9	459	-455
11	-66	2	0	240	238	-12	117	-115	-8	-66	-85
-14	195	-208	1	156	138	-11	323	-319	-7	452	459
-13	-69	-106	2	-63	39	-10	434	447	-6	226	227
-12	109	106	3	325	-325	-9	604	607	-5	-66	25
-11	152	163	4	172	-145	-8	238	230	-4	-66	-89
						-7	174	-180			
						-6	494	-454			

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-3	244	-257	-7	-71	84	8	145	-148	-13	-67	-34
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-1	-68	33	H=	9, K=	-13	10	205	214	-11	-64	61
H=	9, K=	3				-10	112	111	-10	-64	0
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-19	-69	52	1	-69	-51	-8	-67	-20	-8	-65	-20
-18	248	252	2	-68	-21	-7	175	-173	-7	382	412
-17	-66	-42	3	203	-176	-6	219	-231	-6	117	76
-16	169	-187	4	156	129	-5	-66	127	-5	-66	-161
-15	150	-146	5	191	152	-4	145	162	-4	145	-173
-14	230	213	6	-68	-18	-3	222	-227	-3	-64	-37
-13	248	266	H=	9, K=	-12	-2	-64	50	-2	315	320
-12	-64	-83				-1	-64	-31	-1	-65	-68
-11	233	-224	0	156	-159	H=	9, K=	-8	H=	9, K=	-5
-10	102	-69	1	-65	-14						
-9	162	236	2	317	301	0	370	-384	0	372	381
-8	-65	52	3	185	169	1	-65	-76	1	251	249
-7	203	-224	4	314	-294	2	165	158	2	324	-317
-6	254	-258	5	205	-231	3	-65	7	3	345	-326
-5	109	-89	6	103	81	4	160	-142	4	-64	-34
-4	352	363	7	164	161	5	184	-175	5	221	218
-3	219	224	8	-67	18	6	-62	-17	6	91	87
-2	277	-235	-3	140	155	7	376	400	7	209	-201
-1	100	-75	-2	245	245	8	202	203	8	144	-122
H=	9, K=	4	-1	-68	-106	9	215	-219	9	122	126
			H=	9, K=	-11	10	158	-186	-15	-67	73
-19	-68	-43				-11	145	126	-14	121	133
-18	264	-273	0	126	126	-10	-67	-78	-13	-65	60
-17	-68	7	1	159	-131	-9	185	-217	-12	190	-168
-16	177	165	2	214	-214	-8	-65	-24	-11	138	-141
-15	152	140	3	-63	-15	-7	226	232	-10	136	169
-14	249	-245	4	220	207	-6	165	177	-9	392	373
-13	242	-262	5	242	222	-5	181	-289	-8	-66	-9
-12	-64	85	6	-68	-109	-4	-65	-111	-7	334	-350
-11	229	246	7	220	-210	-3	126	128	-6	141	155
-10	192	175	8	-66	-54	-2	139	123	-5	117	65
-9	-68	-121	9	115	120	-1	113	79	-1	195	196
-8	-65	-8	-6	-67	-12	H=	9, K=	-7	-3	237	256
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-6	196	200	-4	197	189	0	520	516	-1	122	-119
-5	-66	16	-3	114	-148	1	202	-201	H=	9, K=	-4
-4	383	-395	-2	239	-261	2	312	-306			
-3	102	-68	-1	144	124	3	124	-120	0	221	-209
-2	171	172	H=	9, K=	-10	4	170	174	1	305	-303
H=	9, K=	5				5	285	319	2	214	225
-18	276	280	0	130	66	6	-64	12	3	267	265
-17	-68	27	1	274	-273	7	319	-308	4	-66	117
-16	165	-155	2	214	203	8	113	-126	5	308	-296
-15	118	-91	3	424	420	9	254	239	6	161	-171
-14	162	157	4	-64	18	-13	-68	52	7	270	234
-13	278	288	5	274	-267	-12	153	-146	8	101	138
-12	-67	-60	6	-68	66	-11	-65	-82	-16	-63	-8
-11	375	-373	7	252	251	-10	102	118	-15	-69	-35
-10	-66	-4	8	-64	45	-9	184	174	-14	184	-186
-9	215	214	9	127	-136	-8	-64	-19	-13	214	-210
-8	-68	62	10	209	-191	-7	407	-405	-12	188	209
-7	137	-123	-8	-68	-3	-6	-66	-81	-11	-65	67
-6	251	-249	-7	-67	90	-5	338	334	-10	185	-205
-5	-69	28	-6	145	143	-4	139	150	-9	458	-476
-4	315	301	-5	159	-138	-3	-65	-69	-8	-66	43
H=	9, K=	6	-4	323	-339	-2	292	-280	-7	375	369
			-3	181	170	-1	-64	-46	-6	101	-122
-17	-70	84	-2	185	194	H=	9, K=	-6	-5	-63	-78
-16	-68	18	-1	-66	-133				-4	356	-358
-15	-67	49				0	376	-380	-3	-64	-56
-14	160	-152	H=	9, K=	-9	1	-65	63	-2	420	411
-13	232	-247				2	477	489	-1	201	-199
-12	113	111	0	101	92	3	344	354	H=	9, K=	-3
-11	248	253	1	233	235	4	-66	-90			
-10	107	-81	2	180	-201	5	213	-230	0	100	135
-9	178	-148	3	263	-278	6	-64	-10	1	219	204
-8	186	-165	4	-64	-20	7	144	119	2	158	-143
			5	199	181	8	-68	66	3	560	-550
			6	-62	-22	9	194	-195	4	162	183
			7	205	-195	-14	227	-221	5	563	560

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
3	110	-139	-14	-67	-67	-10	189	-188	-2	103	-97
4	170	149	-13	-65	-50	-9	140	-119	-1	235	256
5	304	313	-12	172	102	-8	104	109			
6	-67	-70	-11	-63	17	-7	202	198	H=	11, K=	-6
-14	101	79	-10	161	-205	-6	-69	61			
-13	-66	55	-9	-64	-64				0	396	-408
-12	208	-201	-3	95	85	I=	11, K=	3	1	-66	-59
-11	144	-160	-7	227	230				2	137	121
-10	-65	89	-6	134	141	-13	175	169	3	272	236
-9	138	159	-5	120	-131	-12	192	-215	4	-70	-100
-8	-65	-104	-4	105	-123	-11	233	-216	-12	131	140
-7	320	-323	-3	111	108	-10	152	153	-11	154	178
-6	-64	41	-2	97	106	-9	177	158	-10	262	-240
-5	249	262	-1	-64	-48				-9	104	-146
-4	273	262				H=	11, K=	-11	-8	165	160
-3	371	-290							-7	198	212
-2	556	-586	H=	10, K=	-1	0	168	184	-6	127	138
-1	186	175				H=	11, K=	-10	-5	-65	-91
			0	325	337				-4	135	-122
			1	245	242				-3	-67	90
H=	10, K=	-4	2	259	-266	0	267	-269	-2	134	146
			3	247	-249	1	-67	-31	-1	245	-244
0	336	-324	-17	-68	-16	2	320	332			
1	-64	53	-16	221	-208	3	-69	70	H=	11, K=	-5
2	195	196	-15	267	-282	-5	293	-263			
3	293	298	-14	187	176	-4	-71	-2	0	284	276
4	171	-165	-13	148	164	-3	340	311	1	134	135
5	358	-374	-12	295	-266	-2	148	147	2	-69	-84
6	152	146	-11	-63	-64	-1	124	-141	3	195	-183
-15	-68	-30	-10	146	140				-13	-67	22
-14	-67	-123	-9	128	111	H=	11, K=	-9	-12	193	-202
-13	-66	-12	-8	-64	-26				-11	125	-115
-12	281	286	-7	325	-326	0	263	250	-10	249	250
-11	133	124	-6	297	-301	1	-66	30	-9	141	143
-10	94	-92	-5	233	220	2	268	-304	-8	-62	-20
-9	216	-235	-4	105	110	3	-66	25	-7	225	-221
-8	156	130	-3	109	121	4	220	208	-6	-64	-28
-7	260	248	-2	281	-267	-7	255	-244	-5	98	116
-6	147	-114	-1	91	-4	-6	-69	106	-4	193	212
-5	109	20				-5	199	192	-3	-64	-23
-4	-66	65	H=	11, K=	0	-4	147	-116	-2	338	-345
-3	509	517				-3	254	-255	-1	123	97
-2	-66	69	-15	104	-86	-2	182	-193			
-1	320	-310	-14	208	-185	-1	140	143	H=	11, K=	-4
			-13	-66	54						
H=	10, K=	-3	-12	169	175	H=	11, K=	-8	0	-65	-49
			-11	149	147				1	-67	9
0	274	273	-10	117	-127	0	287	-287	2	159	162
1	116	114	-9	255	-276	1	-68	102	3	155	126
2	309	-315	-8	-65	17	2	203	213	-14	154	-171
3	279	-273	-7	277	275	3	-65	-35	-13	-69	-60
4	360	374	-6	-66	94	4	161	-152	-12	243	241
5	253	274	-5	127	-112	-9	144	-133	-11	188	179
-16	-66	-35	-4	100	-140	-8	171	190	-10	136	-119
-15	-66	35	-3	130	129	-7	123	116	-9	-63	-55
-14	178	187	-2	131	150	-6	156	-194	-8	-64	3
-13	-65	44				-5	152	-147	-7	111	161
-12	345	-330	H=	11, K=	1	-4	119	117	-6	115	54
-11	-65	-84				-3	307	302	-5	140	-141
-10	257	246	-15	-66	28	-2	101	117	-4	205	-206
-9	198	194	-14	-67	74	-1	214	-204	-3	-65	-44
-8	-64	14	-13	-66	-29				-2	270	264
-7	-65	-70	-12	115	-152	H=	11, K=	-7	-1	111	-62
-6	-64	41	-11	263	-254						
-5	238	213	-10	220	220	0	353	350	H=	11, K=	-3
-4	-66	-44	-9	297	239	1	148	-147			
-3	502	-485	-8	-67	-85	2	222	-233	0	-68	-81
-2	110	-125	-7	151	-182	3	159	-127	1	-67	-31
-1	212	192	-6	-67	-56	4	-70	81	2	185	-199
			-5	132	146	-11	-69	-91	-14	-175	187
H=	10, K=	-2	-4	112	144	-10	143	138	-13	-68	61
						-9	216	203	-12	302	-307
0	186	-201	H=	11, K=	2	-8	266	-273	-11	105	-100
1	133	-101				-7	216	-216	-10	-66	66
2	262	285	-15	134	-136	-6	121	90	-9	-66	115
3	-69	83	-14	100	-114	-5	126	124	-8	-64	68
4	187	-205	-13	110	-113	-4	-65	-11	-7	289	-305
-16	142	112	-12	169	148	-3	119	-143	-6	100	78
-15	-66	94	-11	243	222						

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-5	430	435	-6	-66	66	0	118	-88			
-4	124	155	-5	167	170	-9	-69	-80	H=	12, K=	-3
-3	252	-246	-4	-67	99	-8	107	103			
-2	111	-121	-3	-68	-119	-7	-68	88	-12	255	-249
-1	210	181	-2	222	-204	-6	203	-205	-11	-67	42
			-1	-68	53	-5	346	-371	-10	141	120
H=	11, K=	-2				-4	-67	65	-9	138	150
0	160	-174	H=	12, K=	0	-3	305	309	-8	-67	-34
1	-69	-65	-11	114	114	-2	150	145	-7	222	-249
-15	-68	-40	-10	207	-213	-1	197	-216	-6	110	84
-14	233	-248	-9	236	-208	H=	12, K=	-5	-5	223	225
-13	-67	-22	-8	101	102				-4	-67	23
-12	285	303				-11	-67	-38	-3	123	-151
-11	-66	-9	H=	12, K=	-8	-10	211	218	-2	167	-148
-10	-64	-32				-9	-66	15	H=	12, K=	-2
-9	259	-254	0	172	-199	-8	142	-137			
-8	-65	-78	-6	-68	-25	-7	106	-66	-12	-70	132
-7	271	274	-5	149	-155	-6	142	120	-11	-66	60
-6	-67	-55	-4	120	-138	-5	293	287	-10	114	-82
-5	402	-409	-3	-68	98	-4	-69	60	-9	183	-201
-4	-66	-62	-2	160	143	-3	208	-233	-8	103	116
-3	199	194	-1	194	-181	-2	117	-157	-7	270	302
-2	-66	35				-1	217	229	-6	126	-81
-1	-66	7	H=	12, K=	-7				-5	210	-219
						H=	12, K=	-4	-4	116	-101
H=	11, K=	-1	0	146	122				H=	12, K=	-1
			-8	155	-143	-11	-69	-25			
0	355	352	-7	130	-134	-10	226	-235			
-15	152	136	-6	-69	60	-9	-66	-75	-12	165	-152
-14	377	375	-5	264	279	-8	-65	26	-11	97	-103
-13	-70	-115	-4	119	101	-7	150	176	-10	193	185
-12	287	-288	-3	210	-236	-6	-67	42	-9	201	220
-11	-66	-68	-2	132	-119	-5	153	-158	-8	127	-129
-10	-66	94	-1	177	191	-4	103	-65	-7	213	-214
-9	298	301				-3	177	147	-6	-67	46
-8	-64	-14	H=	12, K=	-6	-2	111	141			
-7	301	-288				-1	150	-144			

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Douglas Allen Sullivan was born November 9, 1945, in Huntington, West Virginia. In May, 1963, he was graduated from Vinson High School, Huntington, West Virginia. He received the degree of Bachelor of Science in Chemistry from Marshall University in May, 1967. After studying at the University of Florida from September, 1967, to August, 1968, Mr. Sullivan taught chemistry, physics, physical science, and mathematics for the Wayne County (West Virginia) Board of Education. He then returned to the University of Florida in September, 1972, and received a Master of Science in Teaching degree majoring in chemistry in December, 1974. He is a member of the American Chemical Society. Mr. Sullivan is married to the former Jeanie Delaine Puckett of Titusville, Florida. They have a three-year-old son, David O'Donald Sullivan.

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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