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STRUCTURAL STUDIES OF A TEMPLATE CONDENSATION AND OTHER COORDINATION COMPOUNDS

by

Alan R. Davis

B.Sc.(Hons.), University College, London, 1972

M.Sc., Simon Fraser University, 1975

A THESIS SUBMITTED IN PARTIAL FULFILLMENT

OF THE REQUIREMENTS FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

in the Department

of

Chemistry

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September 1979

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"Structural Studies of a Template Condensation and Other Coordination Compounds"

Author: _____
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APPROVAL

Name: Alan R. Davis

Degree: Doctor of Philosophy

Title of thesis: Structural Studies of a Template Condensation and other Coordination Compounds

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Date Approved: September 14, 1979

ABSTRACT

This thesis describes studies made in various areas of coordination chemistry. In each instance, this involved a complete, single crystal, X-ray diffraction investigation, commencing with a preliminary photographic study using Cu radiation (λ=1.5418 Å), followed by intensity data collection using a computer-controlled, four-circle diffractometer, and graphite-monochromatised radiation (λ=0.70926 Å). Structures were solved using heavy atom or direct methods, and the final results were obtained from full-matrix, least squares refinement of the determined models.

The major portion of the thesis concerns the condensation reaction of 2,3-butanedione with the Ni(II) complex of the tetradentate ligand 3,5,5,10,10,12-hexamethyl-1,2,6,9,13,14-hexaazatetradeca-2,12,diene, (L0). The reaction proceeds via three isolatable complexes ($Ni(L1)^{2+}$, $Ni(L2)^{2+}$, and $Ni(L3)^{2+}$) to give a complex of the 16 macrocycle 3,4,7,9,9,14,14,16-octamethyl-1,2,5,6,10,13-hexaazacyclo-hexadeca-2,4,6,16-tetraene, (L4). A structural investigation of the following complexes was undertaken: $Ni(L0)(NCS)_2 \cdot H_2O$, $Ni(L0)(NO_2)ClO_4$, $Ni(L2)H_2O(ClO_4)_2 \cdot 3H_2O$, $Ni(L3)(NO_2)ClO_4 \cdot \frac{1}{2}H_2O$, and $Ni(L4)(ClO_4)_2$. The results establish L4 as the fully-condensed, 16 macrocycle; L2 as the cyclic ligand 4-hydroxy-3,4,7,9,9,14,14,16-octamethyl-1,2,5,6,10,13-hexaazacyclo-hexadeca-2,6,16-triene, stabilised in the aqueo Ni(II) complex by coordination of the pendant hydroxy group to the metal ion; and

L3 as the non-cyclic ligand 1,2,5,7,7,12,12,14-octamethyl-3,4,8,11,15-hexaazahexadeca-2,4,14-triene-1-one, which is tautomeric with L2. These results are discussed in terms of a proposed scheme for the sequence of steps comprising the condensation reaction, and in terms of the various conformations and configurations of the cyclic and non-cyclic ligands involved.

μ-carbonatabis(2,4,4,9-tetramethyl-1,5,9-triazacyclododec-1-ene)-dicopper(II) perchlorate exhibits complete diamagnetism in the range 100 to 300 deg K. A structural investigation was undertaken on the dimethylformamide solvate of this compound in order to determine the precise geometry which gives rise to this magnetic behavior. The results show a dimeric cation which exhibits a novel mode of carbon bridging, with the carbonate acting as a symmetrical, bidentate ligand to both metal ions. Both halves of the dimer are related by a crystallographic two-fold axis of symmetry which passes through the carbon and one oxygen atom of the bridging ligand, with the CuOCu angle = 176.6(2) deg. The geometry about each metal most closely resembles a square pyramid, with the carbonate oxygen atoms and two nitrogen atoms of the macrocycle forming the basal plane, and the third nitrogen donor apical. The relationship of this geometry and that of the dimer to the unusual magnetic behavior is discussed.

Tetrakis(tropolonato)zirconium(IV), which crystallizes as a chloroform solvate, was subject to a structural analysis in order to obtain more information on the factors which affect the shapes of high coordinate species.

The resulting structure shows the geometry about the Zr ion to be very nearly dodecahedral. The two shortest O...O inter-ligand contacts in the 'ZrO_8' polyhedron occur between adjacent ligands which are approximately coplanar, providing a further example of what appears to be a trend among high coordinate chelate complexes, and it is proposed that this should be taken into account in any theory of high coordinate structure.

$\{Ru(DMSO)_6\}\{BF_4\}_2$, DMSO = dimethylsulphoxide), catalyses in solution the hydrogenation of acrylamide to propionamide. A structural investigation was undertaken in order to determine which of the many possible linkage and geometric isomers of the $Ru(DMSO)_6^{2+}$ ion was responsible for this catalytic activity. The resulting structure shows two crystallographically-distinct cations in the asymmetric unit which are chemically identical. The ruthenium ion is coordinated to three DMSO ligands via the oxygen atoms, and to three DMSO ligands via the sulphur atoms, to give the facial isomer of irregular octahedral geometry. Detailed analysis of the structural parameters show this isomer to be electronically rather than sterically determined. The catalytic behavior of the cation is discussed in terms of the structure and available infra-red and nuclear magnetic resonance data.

DEDICATION

Unworthy as it is, this thesis
is dedicated to the memory of
my father
Ross Arthur Davis
1916 06 20 - 1971 04 23,

and to my mother

ACKNOWLEDGMENTS

The inadequacies in this thesis originate with the author; anything worthwhile has been achieved only with the help of the following, whom I wish to thank.

My friends and collegues in the Deparment of Chemistry, SFU, for their help in various ways, in particular, Drs. Rodger Cobbledick and Tony Willis.

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Finally, four ladies: Kathy, Caitlin, Hilary and Alexis, without whom this work would not have been accomplished, nor would it have been worthwhile.

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Chapter 1

Metal Template Condensation Reactions

1i. Introduction

A ligand bonded to a metal ion by more than one atom forms a heterocyclic ring called a chelate ring, and the resulting complex is termed a metal chelate. The properties of the metal ion and the ligand are influenced by each other, and though the range of metal ions forming such complexes is wide, the variation in suitable ligands is limited only by the immense scope of organic synthetic chemistry.

Many studies[1,2] have confirmed that metal chelates are thermodynamically and kinetically more stable than those of unidentate ligands, and for two similar metal chelates, the one with the more chelate rings is generally more stable. These enhanced stabilities of multidentate ligands are grouped under the general title of the 'chelate effect'. Chelates which contain three or more donor atoms, and are cyclic, are called macrocycles, and of these, complexes of quadridentate systems containing N, O, and S donors with transition metal ions have been the most studied. Such complexes have been known for more than 60 years, originating with examples of natural products (e.g., complexes of porphyrins and corrins), and the phthalocyanine complexes. Since about 1960, however, the synthesis of new macrocyclic ligands as their metal complexes has increased rapidly, with a recognition of the 'metal template effects', whereby the yield of cyclic macrocycle over linear

polymers is dramatically improved by the presence of the metal ion. In many cases, however, the underlying principles of the synthetic procedures are not yet understood, and, as has been clearly stated in one review, "the elucidation of the mechanisms of the formation of macrocyclic complexes will undoubtedly be of great benefit in the design of new syntheses"[1].

The relationship of synthetic macrocycles to biological systems has been recognised from the outset[3], and the understanding of its significance is bound to increase.

lii. Ligand Shape and Conformation

The factors which govern the shapes and conformations of chelate rings are essentially those which apply to organic ring systems[4,5]. For instance, it is possible to successfully predict the shapes of the saturated chelate rings in the tris(1,2-diaminoethane)cobalt(III) ion from a conformational analysis of cyclopentane.

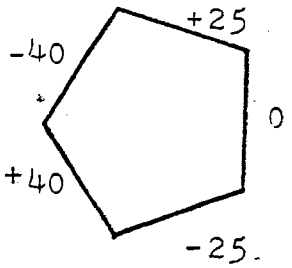
The most convenient parameters for defining the spatial arrangement of the atoms in a molecule are the bond lengths, the bond angles, and the torsion angles. In particular, the use of torsion angels to provide a useful and convenient description of steric relationships across single bonds is well established, and the applications of this concept to the conformation analysis of saturated and unsaturated cyclic systems have been recently reviewed[5].

The description of the geometry of a ring is given by the sequence of the values of its torsion angles; in a planar representation these values are written along each central bond. The information contained in such a sequence is both qualitative and quantitative: the simple sequence of the signs of the torsion angles indicates the type of conformation; the absolute values allow the deformation with respect to a reference conformation to be estimated. The sum of the torsion angles of a ring may be taken as a relative measure of the puckering or flattening of a deformed conformation. Some conformations of regular alicyclic five-, six-, and seven-membered rings pertinent to this work are shown in figure 1.1 in terms of their torsion angles.

Further comment at this stage is not felt necessary, save to point out that proofs have been established which show that the criteria which apply to "regular" rings (equal bond lengths and regular tetrahedral or trigonal angles) are quite applicable to rings with non-equal bond-lengths and angles[6]. However, certain constraints are placed on a ring system which includes a metal ion, and this limits the number of possible conformations of the chelate rings, and the location of its donor atoms among the available coordination sites of the metal ion.

Firstly, there are the stereochemical preferences of the metal ion, and some ligands are better able to conform to the preferred environment than others. Secondly, there are the

Figure 1.1



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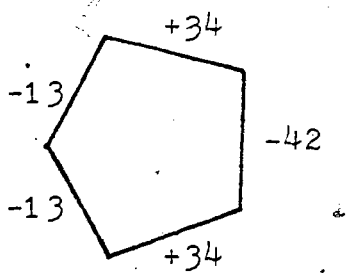

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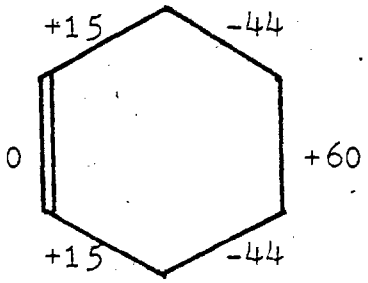

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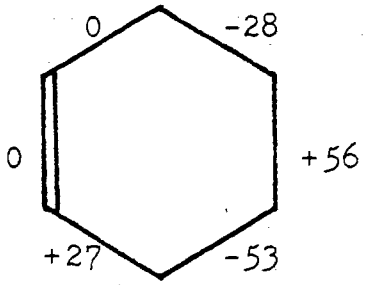
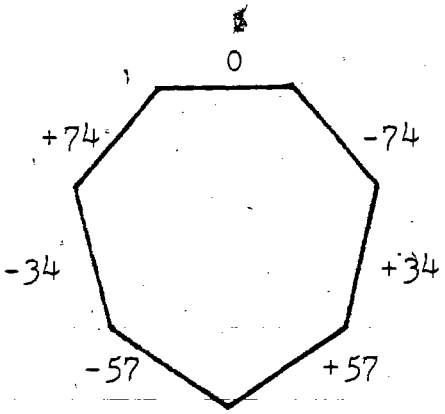
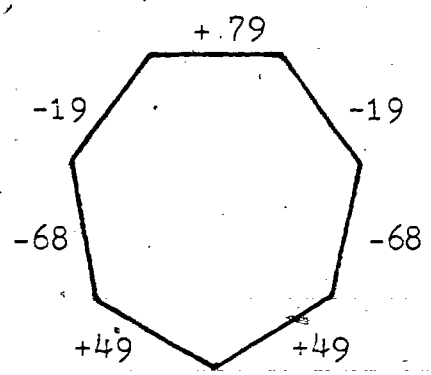


1,2-planar (sofa)



boat



twist-boat

Selected Conformations of Alicyclic Rings as Described by their Torsion Angles [5] (deg)

various geometrical constraints of the donor atoms. For example, nitrogen can act as a donor while present in a number of functional groups on the ligand: primary, secondary, and tertiary amine; imine, azo, and oxime. The bond distribution about the donor atom influences the geometry of the ligand in the complex, and consequently the configuration of the complex itself.

For quadridentate chelating agents, there are a number of possible arrangements of the donor atoms. One of the most common is a simple linear (non-cyclic) arrangement, which is relevant to the present work and serves as a useful example for this discussion. Goodwin[7] has subdivided these ligands into three stereochemical types: planar (only able to coordinate the metal ion to give a square planar complex; this is usually the result of unsaturation, commonly provided by imine groups in the ligand), tetrahedral (donor atoms cannot lie in a plane, often as a result of steric interactions among bulky substituents in the ligand chain, but may be arranged tetrahedrally about the metal ion), and facultative (flexible, so that the ligand can bind in a planar or non-planar arrangement, and this is usually the case with ligands having little unsaturation or no bulky substituents).

For the majority of macrocyclic quadridentate systems bonded to first row transtion metal ions, ring sizes of 13 to 16 members are most common, with donor atoms so positioned that they are able to form five- or six-membered chelate rings upon

coordination. Other ring sizes may be suitable in complexes of metals having different ionic radii[8].

The conflict between the stereochemical preferences of the metal ion and the geometrical constraints of the ligand and its donor atoms is important in ligand design. In order to produce a highly stable metal chelate, then the ligand should be designed so as to be flexible enough to satisfy one of the preferrred metal geometries; on the other hand, if new and unusual metal complex properties are being investigated, a rigid ligand may force a metal ion into a non-ideal geometry.

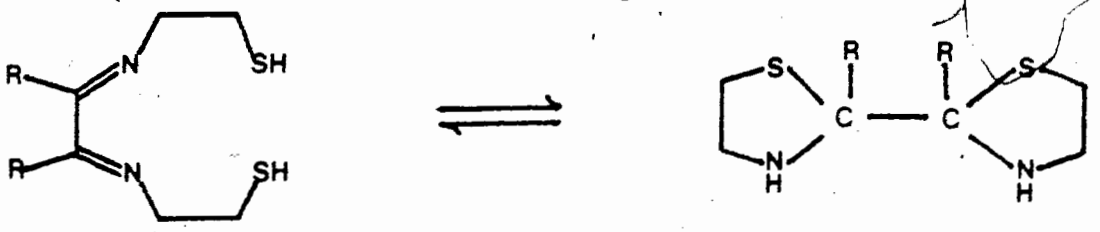
One further aspect of metal chelate stereochemistry which deserves mention is the possibility of chirality to be introduced by ligands that are unsymmetrical, which confer chirality as a result of their conformation, which coordinate via a donor atom which is asymmetric, or by the distribution of the ligands about the metal ion. Excellent accounts of these possibilities are available[5,9], and further detailed reference will be made where necessary.

liii. <u>The Coordination Template Effects</u>[1,10]

The synthesis of organic macrocyclic ligands in the absence of a metal ion is very often a low-yield reaction since it is dominated by the competing linear polymerization. Often, however, the yield of the cyclic product as its metal complex is dramatically increased upon addition of the metal ion during or before the cyclization step. The improvement in yield is a

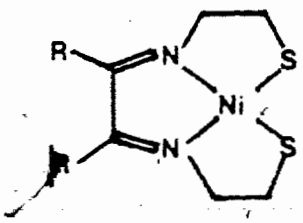
result of one or more metal ion effects known collectively as the coordination template effects.

If the metal ion perturbs an existing equilibrium in the organic system by stabilizing one of its components, the process is referred to as the thermodynamic template effect. An early example of this was reported by Busch[11] who wished to synthesize the macrocycle I by condensation of an α-diketone with 2-aminoethanethiol. The major product of the direct reaction was, however, the thiazoline II, although it was determined that I and II were in equilibrium:



I II

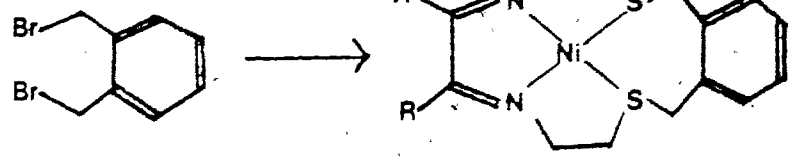
When the same reaction took place in the presence of nickel(II) acetate, the Ni complex of the desired product (III) was obtained in 70% yield.



III

In this case, the Ni(II) ion stabilizes the dianion of I by chelation, removing it from the equilibrium as it is produced.

If the influence of the metal ion is to control the steric course of a stepwise reaction, the process is called the kinetic template effect. Using the same example as above, in order to use I as the core of a macrocyclic ligand, it was found[12] that the reaction of the metal complex III with an organic dihalide gave complexes of the type shown by IV in good yield: here the metal ion has been used to hold reactive groups so that a stereochemically selective multistep reaction may occur.

III + 

IV

There are other ways in which metal ions can substantially improve the yield of products. For example, when chelation of the metal ion to one of the products facilitates its separation without affecting the kinetics or thermodynamics of the formation reaction. This would amount to an inversion of the usual function of a metal ion and ligand in sequestration[2].

liv. Coordination Chemistry of Nickel(II)

The first three chapters of this thesis deal with various macrocyclic complexes of Ni(II), and it is therefore pertinent to review some of the essential details of Ni(II)

magnetism, spectra, and structural behavior. Anticipating the results somewhat, and recognizing the broad range of Ni(II) chemistry, attention is restricted to octahedral and square planar complexes of O- and N- donor atoms[13, 14].

Russell-Saunders terms, in order of increasing energy, for the free Ni^{2+} ion, are ^3F, ^1D, ^3P, ^1G, and ^1S, with the triplet term $^3F_4$ representing the electronic ground state. Ni(II) complexes are found with six-coordinate octahedral, five-coordinate trigonal bipyramidal or square pyramidal, and four-coordinate square planar or tetrahedral stereochemistries. Often these only approximate the regular polyhedra, and it is a peculiarity of Ni(II) chemistry that complexes can often be easily converted from one configuration to another, and many cases of structural isomerism are known.

Ni^{2+} is on the borderline of the "class a/class b"[15] (or the related "hard/soft"[16]) classification of metal ions. Since, for instance, it forms stronger complexes with the lighter halogens, and bonds to nitrogen rather than sulphur in monomeric thiocyanate complexes, it appears to act in its classical complexes as a "class a" type, "hard" acceptor, with a limited tendency for metal - ligand π-bonding.

Octahedral Complexes. In almost all cases, nickel complexes of coordination number six are octahedral (distorted or regular) and have high-spin (S=1) electron configurations. They have a characteristic electronic spectrum comprising three moderately intense bands which are simply interpreted by

application of an O_h crystal field to the ^3F and ^3P terms of the free ion as:

$$^3A_g(F) \text{ —— } ^3T_{2g}(F)$$
$$\text{"} \text{ —— } ^3T_{1g}(F)$$
$$\text{"} \text{ —— } ^3T_{1g}(P)$$

The values of Dq found in octahedral complexes vary from 640 cm^{-1} to 1270 cm^{-1}, depending on the position of the ligand in the spectrochemical series, and the value of β, the ratio of the Racah parameter B for the complex to that for the free ion, is 0.7 to 0.9, the lower the value of β being related to increased covalent character in the metal - ligand bond. Examples for O_6 and N_6 complexes are $\{Ni(MeOH)_6\}(Cl)_4)_2$, D_q = 843 cm^{-1} and β = 0.88, and $\{Ni(CH_3NH_2)_6\}(ClO_4)_2$, D_q = 993 cm^{-1} and β = 0.84[13].

Geometric distortions and/or non-identical donor atoms cause departures from O_h symmetry, and the effects on d electron energy levels are well documented[13]. For the substitution of two weaker ligands, a <u>trans</u> arrangement leads to larger splittings in the triplets $^3T_{1g}$ and $^3T_{2g}$, as for example in $Ni(pyridine)_4Cl_2$[17].

Since the ground state of a regular octahedral complex is always $^3A_{2g}$, and no singlet level can cross it no matter what ligand field strength is applied, regular octahedral complexes are always paramagnetic with S = 1. In fact, values of the magnetic moment are usually found between 2.9 and 3.3 B.M., near the spin-only value of 2.83 B.M.[18] Reduced

paramagnetism and diamagnetism can result from large trigonal distortion or large tetragonal distortion[19].

Structurally, octahedral Ni(II) complexes are the most extensively studied[13]. Since no Jahn-Teller-type distortion is predicted, any distortions from regularity must be attributed to steric or crystal packing effects. Ni(II)-N and Ni(II)-O bond lengths in monomeric complexes are usually in the range 2.0 to 2.2 Å[13].

Square Planar Complexes. Energetically, the tetrahedral geometry is favoured with respect to a square planar geometry if the four bonds have a purely ionic character. In accordance with this, complexes of the type $Ni(halide)_4^{2-}$, where the bonding is largely ionic, are tetrahedral. On the other hand, any strong covalent Ni - ligand interaction can stabilize the planar configurations by σ and/or π effects, leading to appreciably shorter nickel - ligand bond lengths.

In the D_{4h} crystal field, the five degenerate d orbitals are split as:

$d_{x^2-y^2}$	b_{1g}
d_{xy}	b_{2g}
d_{z^2}	a_{1g}
d_{xy}, x_{yz}	e_{1g}

The ground state may therefore be either $(e_g)^4(a_{1g})^2(b_{2g})^2$ - a spin-singlet term $^1A_{1g}$, or $(e_g)^4(a_{1g})^2(b_{2g})^1(b_{1g})^1$ - a spin-triplet term, $^3A_{2g}$. The relative stabilities of the low and high spin states are determined by the energy separation

(Δ) of the d_{xy} and $d_{x^2-y^2}$ orbitals. Calculations show that the low spin state is stable if Δ is greater than $\sim$ 10 000 cm^{-1}. As the ligand field strength is increased, the possible ground states do not mix via spin - orbit coupling, and therefore a crossover point between high spin (weak field) and low spin (strong field) systems is possible. To date, there is no evidence for any square planar nickel(II) complex which is not diamagnetic.

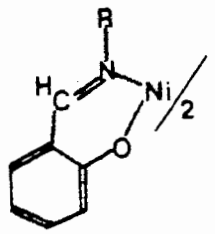
If a square planar complex is approached by one or two ligands along the four-fold axis, the separation between d_{xy} and $d_{x^2-y^2}$ orbitals can be decreased, and the triplet spin state becomes fundamental. Cases of conversion from singlet to triplet states by the formation of bis - adducts with solvents such as pyridine, water, etc., are numerous[20].

Certain systems are explicable on the basis of equilibria between co-existing singlet and triplet states whose energy states differ by amounts comparable with thermal energies. For such an equilibrium between spin isomers, the distribution between the two states can be described by Maxwell-Boltzmann statistics. One group of Ni(II) compounds which shows this is found among some tetragonal complexes containing planar, quadridentate macrocyclic ligands[21].

There are a few square planar complexes in which no bis - adduct formation is sufficiently powerful to stabilize the triplet ground state. These include the porphyrin and phthalocyanine complexes, where considerable stabilization of

the square planar structure occurs via extensive delocalization[13].

Lastly, it has been found that many α-branched alkylsalicylaldimino complexes of Ni(II) exhibit configurational isomerism in solution, with equilibria between square planar diamagnetic and tetrahedral paramagnetic allogons, leading to some unusual magnetic behavior. The extent of this effect is related to the size of the N-alkyl derivative, R in V:[22]



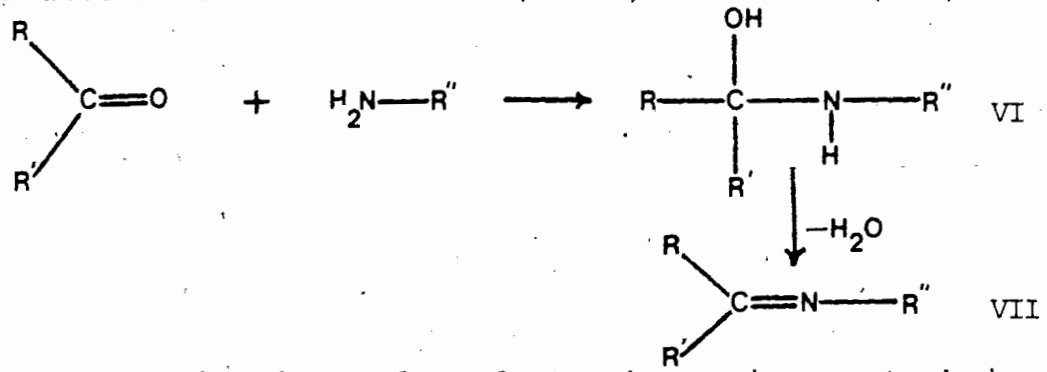
V

lv. Schiff Base Condensation Syntheses[1,23,24]

Condensation reactions between carbonyl compounds and primary amines are responsible for the majority of macrocyclic ligand formation processes, and the use of the Schiff base reaction plays a central role. The syntheses and properties of Schiff base complexes are very often intimately related to the associated metal ion. Furthermore, there are aspects of the synthetic chemistry involved which are relevant to the large number of biochemical processes[25] involving Schiff-base complexes (e.g., in the function of aldoses, aminotransferases, and thiolases).

In the absence of metal ion, the reaction is known to proceed via addition of an amino group to a carbonyl group as a

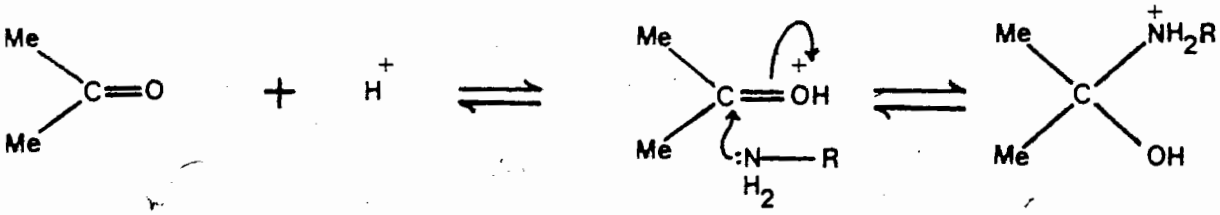
result of nucleophilic attack by the lone pair of electrons on the nitrogen at the carbonyl carbon atom, leading to the formation of a carbinolamine intermediate (IV). Elimination of water results in the Schiff base (imine) formation (VII):



VI

VII

The rate of reaction is pH dependent, the maximum rate being achieved where there is most protonation of the carbonyl oxygen (thus enhancing the reactivity) relative to protonation of the amine (which blocks its use as a nucleophile). For example,

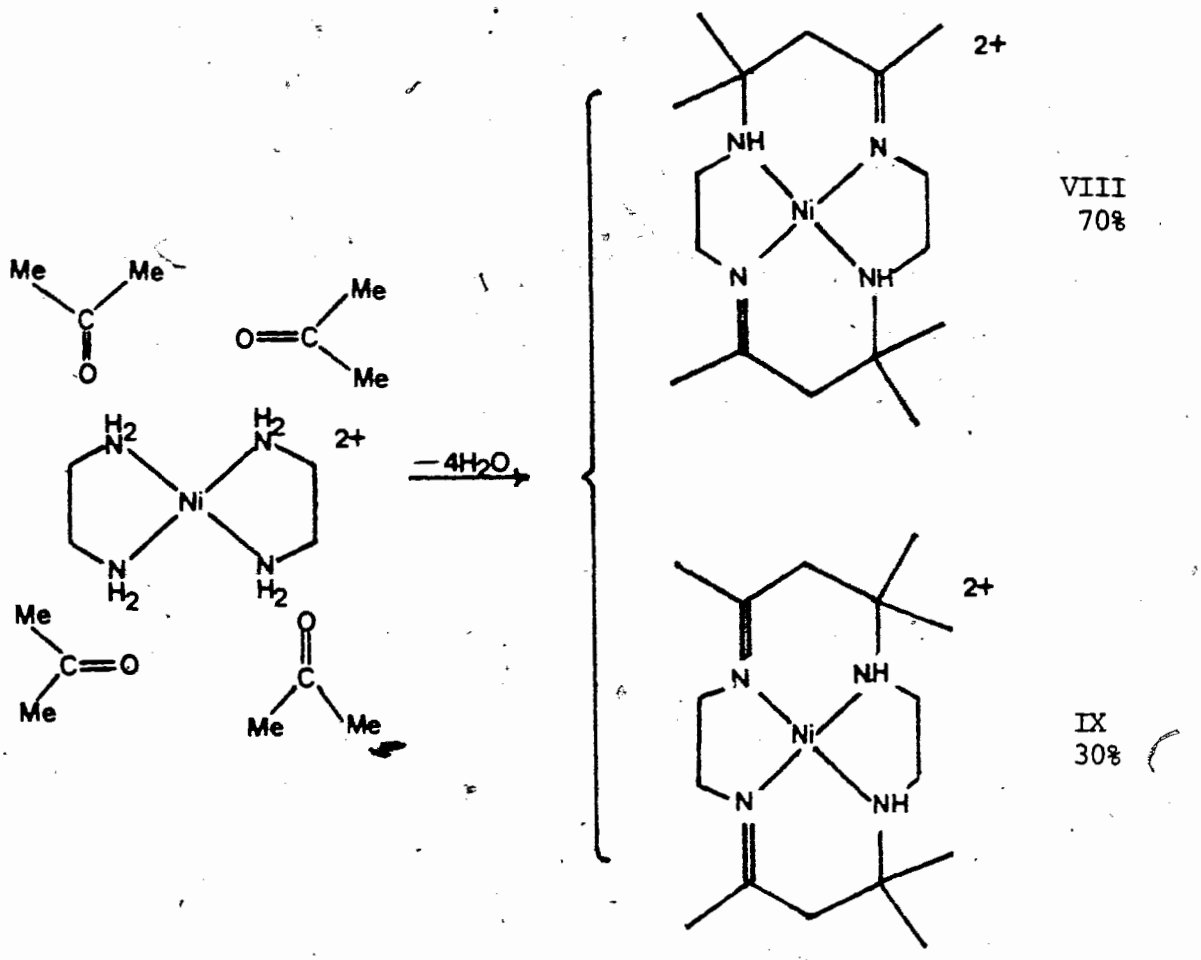


Reactions which take place in the presence of metal ions involve initial coordination of either the carbonyl oxygen or amino nitrogen. Coordination of the oxygen favours the reaction by making the carbonyl carbon more susceptible to nucleophilic attack. However, carbonyl oxygen is a relatively poor donor atom and is generally readily displaced in solution by solvent molecules. Coordination is assisted, however, by formation of a chelate ring with another donor atom in the same

moiety. Thus, for instance, condensations with coordinated salicylaldehyde have been successful in the preparation of a wide variety of salicylaldimino complexes[26].

Coordination of the amine group, on the other hand, decreases its nucleophilic character, thereby hindering formation of the Schiff base. For reactions where a co-ordinated amine is used, there is little evidence that the amine remains coordinated during the condensation. One of the most intensively studied examples of this is the Ni(II) - amine complex condensations with aliphatic carbonyl compounds, leading to macrocyclic ligand formation, first reported by Curtis in 1960[23], and which have been thoroughly reviewed. In these syntheses, reaction is considered to occur with transient species which have one amino group of the diamine detached from the metal ion, the imino group then re-coordinating after condensation.

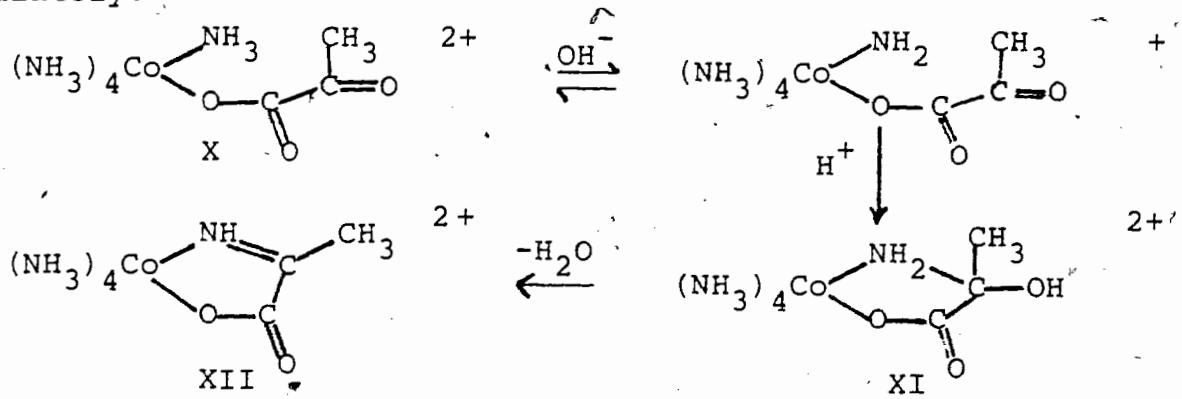
Reaction of the violet tris(ethylenediamine)nickel(II) perchlorate with acetone at room temperature gives a brown-coloured solution almost immediately from which a yellow crystalline product is isolated. Approximately 70% of the product is isolated as the trans-hexamethyltetraazadecadiene complex VIII and 30% as the cis-isomer IX:



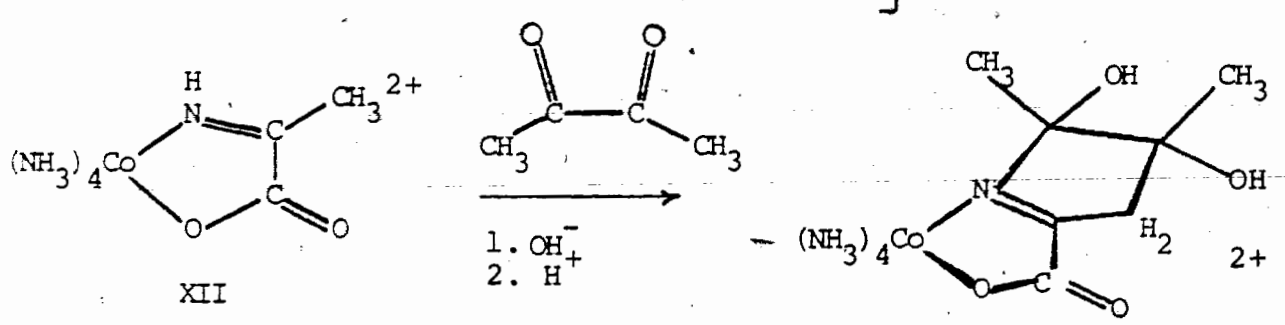
Only amine complexes of Ni(II) and Cu(II) are known to react thusly; complexes which are stable with respect to ligand dissociation (e.g., complexes of Co(III)) do not react in a way consistent with a mechanism requiring a temporarily dissociated $-NH_2$ group. One interesting point about this reaction is that the trans-isomer VIII can be formed in the absence of the metal ion, but the cis-isomer formation requires the metal ion, and its synthesis is properly classified as a kinetic template reaction[23].

A reaction recently reported where cis-coordinated

ammonia and C=O containing ligands condense is the first proof that such reactions can occur with the reactants fully co-ordinated. In basic solution, pyruvatopentamine cobalt(III) (X) yields a pyruvilidene-imine structure XII[27]. The reaction is considered to proceed via deprotonation of an ammonia group and nucleophilic attack by the subsequent amide on the carbonyl centre of the keto-form of the coordinated pyruvate to give the carbinolamine intermediate XI which eliminates water immediately:

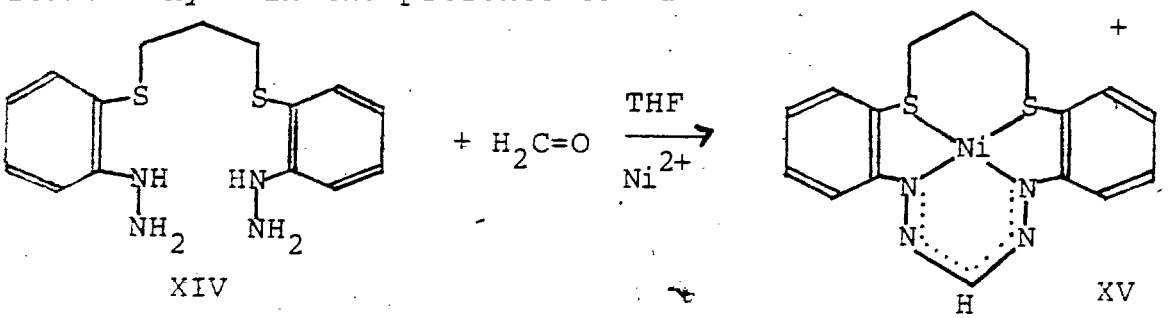


Recognizing the fact that further condensations with coordinated ammonia groups were possible, and that the nitrogen of the iminonium species was highly acidic, the same researchers reacted the complex XII with 2,3-butanedione, to give a complex of the novel chelating ligand XIII:



Clearly, reactions of this type expand the processes available in metal template, multidentate ligand syntheses. The kinetics of these reactions have also been investigated, and, along with other aspects, have some bearing on the present work, and will be considered again where pertinent.

One method of overcoming the masking of nucleophilic character of amines by coordination to a metal, while at the same time utilizing the steric benefits of template syntheses is the use of dihydrazine or dihydrazone moieties[28,29]. A typical preparation is shown below. Salts of XV have been isolated from the reaction of the linear dihydrazine XIV with formaldehyde in the presence of Ni^{2+} ions:



XIV XV

Reaction of a coordinated dihydrazone ligand with an α-diketone is the subject of this investigation, and the details of the reaction are given in the following section.

Condensations involving metal ions generally proceed without the isolation of the metal-free Schiff base, although the latter can sometimes be obtained by ligand exchange with cyanide. However, this may not be possible because of the frequent instability of the Schiff base towards hydrolysis in the absence of the metal ion. However, when the ligand is coordinated, any drain of electron density from the -C=N-

linkage towards a metal ion will make the imine carbon more susceptible to nucleophilic attack, and thus aid hyrolytic cleavage. Cases are known, in fact, where the ligand is more unstable with respect to hydrolysis when coordinated[31].

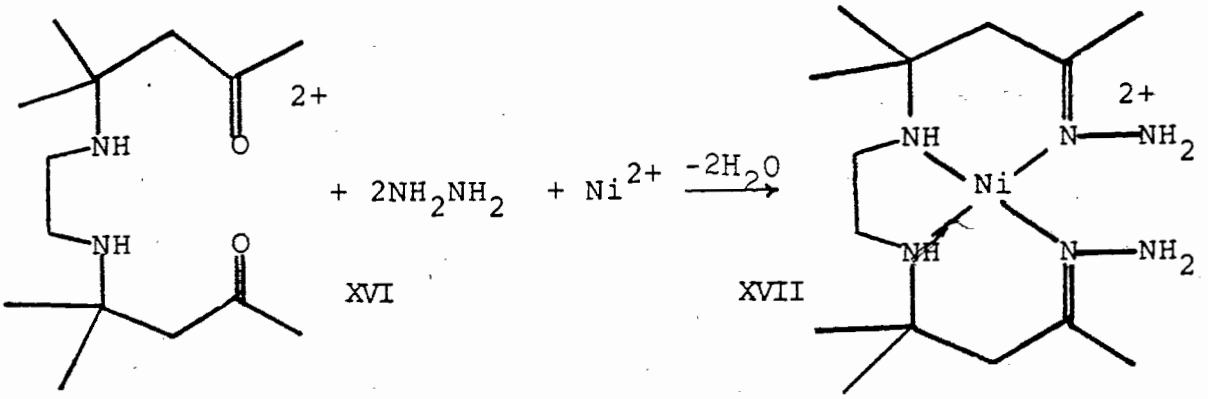
Other important effects on the reactivity of the coordinated amine linkage have been noted[24]. For instance, back donation of metal electrons into π-acceptor orbitals on the imine reduces the effective positive charge on the imine carbon. In some cases, the simple increase of thermodynamic stability of the chelate effect is recognized as being sufficient to counteract the effect of electron withdrawal from the imine linkage[32]. Finally, steric strain in the cyclic ligand can distort imine linkages, making C-N π overlap less effective, and therefore more susceptible to hydrolytic cleavage[24].

1vi. The Condensation of a Coordinated Quadridentate Diamine Dihydrazone with 2,3-Butanedione: An Outline of the Reaction Sequence

The syntheses described in this section were carried out at the Victoria University of Wellington, New Zealand, in the laboratory of Professor N. F. Curtis. Details of these syntheses, together with spectral and analytical data have been kindly supplied by Professor Curtis, and are given in the Appendix of this thesis. Reference will be made to this data where necessary to complement the crystallographic results presented in Chapter 3.

The purpose of this section is to provide an outline of the reaction under consideration, and to review the available spectral and analytical information from which a tentative proposal for the sequence of steps involved in the reaction was made prior to the crystallographic investigation.

Complexes of the linear, quadridentate ligand XVII are prepared by the reaction of metal (Ni(II) or Cu(II)) perchlorate, hydrazine, and the perchlorate salt of 4,4,9,9-tetramethyl-5,8-diazadodecane-2,11-dione (XVl).



The orange perchlorate salt of XVII (hereon designated as $Ni(LO)^{2+}$) dissolves in water to give an orange solution. Upon addition of 2,3-butanedione, a blue-violet solution is formed, from which a poorly crystalline, blue-violet compound, $Ni(Ll)(ClO_4)_2$, is deposited. The designation Ll is used to imply that incorporation of the diketone into the complex in some way has taken place, as suggested by the spectral and analytical data (Appendix, section Ai), although any firm structural details are difficult to infer.

Dissolution of $Ni(Ll)(ClO_4)_2$ in water gives, over a period of hours, a dark blue solution which deposits dark blue crystals of the hydrated complex, $Ni(L2)H_2O(ClO_4)_2 \cdot 3H_2O$. Again, the change in ligand designation and the presence of

water in the coordination sphere to give an NiO_2N_4 chromophore is made on the basis of the i.r. and reflectance spectral data (section Aiv). On the other hand, in non-aqueous solvent, e.g., methanol, $Ni(L1)^{2+}$ is converted in hours to an orange solution, from which orange crystals of $Ni(L3)(ClO_4)_2$ are obtained, containing yet another ligand type, characterized in particular by the presence of a strong, sharp band in the i.r. at 1717 cm^{-1}, assigned to ν (C=O) (see figure A.6, Appendix). $Ni(L2)H_2O^{2+}$ or $Ni(L3)^{2+}$ in water or methanol are eventually converted in hours to a red solution of $Ni(L4)^{2+}$, which can also be isolated in crystalline form. Spectral and analytical data for this product (section Avii) are consistent with $Ni(L4)^{2+}$ being a complex of a [16] macrocycle, incorporating (it was proposed) a novel, seven-membered di-imine chelate.

The objects of the ensuing structural investigation are clear: to confirm the proposed structure of the fully-condensed product $Ni(L4)^{2+}$; to determine the identities of the ligands L1, L2, and L3, which are assumed to incorporate the diketone in various ways, although the available spectral and analytical data do not permit any definite structural proposals. It was considered that if these structures could be established, some understanding of the sequence of steps involved in the condensation reaction would be possible.

The problems associated with such an approach, however, include the availability of suitable crystals, the assumption that the nature of the crystalline products represent species which are formed in solution, and the

difficulties of interpreting the structures of isolatable intermediates (a thermodynamic feature of the reaction) in terms of the reaction mechanism. The latter problem can be reserved for consideration in the discussion of of the determined structures in Chapter 3. Concurrence of solution and solid state spectra was indicated by Professor Curtis, and the assumption was made, therefore, that the crystalline structures would represent solution species. The availability of crystals containing each ligand type was the most immediate problem. For $Ni(L2)H_2O(ClO_4)\cdot 3H_2O$ and $Ni(L4)(ClO_4)_2$, crystals of the simple salts were adequate. For $Ni(L1)(ClO_4)_2$ and $Ni(L3)(ClO_4)_2$, however, this was not the case, but derivatives of each were available which could also be considered.

$Ni(L1)(ClO_4)_2$ reacts with NaNCS and $NaNO_2$ to give the adducts $Ni(L1)(NCS)_2$ and $Ni(L1)NO_2(ClO_4)$ (sections Aii and Aiii). The assignment of the ligand as L1 was made on the basis of analytical and spectral data. Unfortunately, however, as will be apparent from the structural investigations to follow, both these derivatives contain the starting diamine dihydrazone species L0. A discussion of the incorrect assignment, and the implications of this on the nature of L1, is given in Chapter 3.

$Ni(L3)(ClO_4)_2$ reacts with $NaNO_2$ in methanol (section Avi) to give an immediate lavender solution from which lavender crystals of $Ni(L3)NO_2(ClO_4)$ are obtained. Over a period of hours, however, a solution of the lavender product (referred to hereon as α-$Ni(L3)NO_2(ClO_4)$), in methanol, yields a navy

blue solution, from which navy blue crystals of a second derivative, β-Ni(L3)$NO_2(ClO_4)$.$\frac{1}{2}H_2O$ are obtained (section Avii).

A comparison of the i.r. and u.v./visible spectral data for Ni(L3)$(ClO_4)_2$ (figure A.6, section Av), α-Ni(L3)NO_2-(ClO_4) (figure A.7, section Avi), and β-Ni(L3)$NO_2(ClO_4)$.$\frac{1}{2}H_2O$ (figure A.8, section Avii), show that the assignment of the ligand as L3 in the β-derivative is reasonable, but that the α-derivative exhibits some kind of tautomeric or configurational difference to L3 in Ni(L3)$(ClO_4)_2$. This conclusion is considered in more detail in section 3vii.

On the assumption that β-Ni(L3)$NO_2(ClO_4)$ ·$\frac{1}{2}H_2O$ does indeed contain L3, and because the crystals obtained were of sufficiently good quality for the x-ray diffraction method, this derivative was selected for investigation. The occurrence and possible identity of the α-Ni(L3)$NO_2(ClO_4)$ derivative will be considered in Chapter 3.

To summarize, therefore, the x-ray crystal structures of the following compounds were determined in order to gain some understanding of the sequence of steps involved in the condensation reaction of $Ni(L0)^{2+}$ with 2,3-butanedione: Ni(L0)$(NCS)_2$.H_2O; Ni(L0)$NO_2(ClO_4)$; Ni(L2)$H_2O(ClO_4)_2$.$3H_2O$; Ni(L3)$NO_2(ClO_4)$.$\frac{1}{2}H_2O$; Ni(L4)$(ClO_4)_2$.

Chapter 2

The Ni(II)-Dihydrazone/2,3-Butanedione Condensation: Experimental Procedures and Structural Determinations

2i Organisation

For each of the five structural determinations comprising this investigation (as listed on page 23), the experimental conditions under which the diffraction data were collected are very similar, and it is therefore useful to describe these conditions in general terms (section 2ii and 2iii), and to tabulate specific particulars (tables 2.1 and 2.2).

The actual crystalline samples used in the investigation were those received from Professor Curtis. Details of the conditions under which each of the crystalline samples were obtained are therefore included with the preparative procedures in the Appendix to this thesis.

The calculations used in the solution of each structure are described separately (sections 2v through 2ix). Computer programs used in the determinations have been listed previously[34].

2ii Preliminary Investigation

Crystals selected for the investigations were mounted using shellac on a thin glass fibre. No special crystal environments were required, and in no case was any deterioration

of crystalline character apparent. Copper radiation (Cu-K_α, λ= 1.5418Å) was used to obtain oscillation, Weissenberg and precession photographs as listed in table 2.1. The space group assignments made on the basis of the photographic investigation were confirmed in later calculations. A special note should be made, however, concerning the space group of crystalline $Ni(L0)(NO_2)ClO_4$. An initial study suggested a triclinic lattice with the crystal mounted approximately about c^*. However, one of the cell angles (γ) was found to be very close to 90 deg, and the possibility that the crystal was in fact mounted about some diagonal of a cell of higher symmetry, was investigated by performing a Delauney reduction on the triclinic cell (Dr. R.E. Cobbledick's close involvement in this step is gratefully acknowledged). These calculations indicated a C-centered monoclinic cell, and this was confirmed by re-mounting the crystal and taking a new set of photographs which revealed the reduced cell, and its translational symmetry, with a^* of the new cell now approximately coincident with the spindle axes of the cameras.

In each case, the same crystals used in the photographic investigations were mounted on a Picker FACS-1, computer-controlled, four circle diffractometer and optically centered with respect to the four circle geometry. A rough orientation of each crystal was found by manually locating two strong reflections with χ angles close to 0 deg, and seperated in ϕ by approximately 90 deg, and indexing them using the the photographic information. Twelve of the strongest reflec-

tions having 2θ values greater than 25 deg, sampled from all areas of the unique set of reflections, were automatically centered using Mo-K_α radiation (λ=0.70926 A). The observations thus generated were used in a least-squares refinement of the cell and orientation parameters. Typically, 2 cycles of refinement gave parameters suitable for data collection, and the cell dimensions calculated were used in all subsequent computations.

Density measurements on each crystalline sample were made by flotation in halomethane solvent mixtures. Absorbtion coefficients were calculated and deemed not to necessitate any absorbtion correction to subsequent reflection intensity data (table 2.1).

2iii Data Collection

Reflections for the unique set of data were collected for each compound using graphite-monochromatised Mo-K_α radiation (λ=0.70926 Å) and a scintillation detector with pulse height analysis. A symmetrical θ-2θ scanning mode was employed with a scan speed of 2 deg min^{-1}. The selected scan widths (chosen in each instance to take account of the size and shape of the diffracted rays), were increased to allow for dispersion, and background counts were measured at both scan limits. Specific details of the data collection for each crystal are given in table 2.2.

The reflection intensities were measured in two sets based on 2θ values. Typically, for the inner set of data (2θ<20 or 30 deg), larger scan widths were used than in the outer set (2θ<45 deg). After every 100 reflection data measured,

two standard reflections were monitored in order to check instrumental stability and the crystal position with respect to the geometry of the diffractometer. Measured intensities were corrected for Lorentz and polarisation effects, and were classed as observed if $I>2.3\sigma_I$, where $\sigma_I=\{T+(t_b/t_s)^2(B_1+B_2) + (kI)^2\}$; T is the total count, B_1 and B_2 are the background counts, t_s is the scan time, t_b is the total background time, k is a constant set to 0.03, and I is the net count.

Table 2.1

Crystal Data for the Ni(II) Hexaazamacrocycles

	(L0)$(NCS)_2$	(L0)(NO_2)	(L2)(H_2O)	(L3)(NO_2)	(L4)
Colour	royal blue	violet	dark blue	navy blue	salmon red
Habit	cubic	rhombohedral	rhombohedral	elongated plates	needles
Crystal Size (mm)	.7x.7x.7	.3x.4x.6	.3x.3x.2	.5x.2x.1	.5x.1x.1
Photographs Weissenberg Precession	hk0,hkl $h\bar{0}1$,$h\bar{1}1$, $0k\bar{1}$,$1k\bar{1}$	0kl,1kl $h0\bar{1}$,$h1\bar{1}$, $hk\bar{0}$	hko,hkl $h\bar{0}1$,$h\bar{1}1$, $0k\bar{1}$,$1k\bar{1}$	hk0,hkl $h\bar{0}1$,$h\bar{1}1$, $0k\bar{1}$,$1k\bar{1}$	hk0,hkl $h\bar{0}1$,$0k\bar{1}$
Laue Symmetry	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
Systematic Absences	h0l,h+l=2n+1 0k0,k=2n+1	h0l,l=2n+1 hkl,h+k=2n+1	h0l,h+l=2n+1 0k0,k=2n+1	h0l,l=2n+1 hkl,h+k=2n+1	none
Space Group(s)	$P2_1/n$	C2/c,Cc	$P2_1/n$	C2/c,Cc	$P\bar{1}$,P1
Formula Weight	$NiS_2ON_8C_{16}H_{34}$ 477.3	$NiClO_6N_7C_{14}H_{32}$ 487.6	$NiCl_2O_{13}N_6C_{18}H_{44}$ 682.2	$NiClO_{7.5}N_7C_{18}H_{37}$ 565.7	$NiCl_2O_8N_6C_{18}H_{34}$ 592.1
Cell Parameters					
a (Å)	11.23(1)	31.14(1)	9.69(1)	27.02(2)	13.415(6)
b (Å)	12.09(1)	11.278(2)	19.22(1)	14.23(1)	10.609(6)
c (Å)	16.89(1)	14.920(4)	16.65(1)	15.54(1)	11.764(6)
α (deg)					118.41(1)
β (deg)	99.39(4)	123.37(1)	94.88(1)	118.01(5)	61.77(1)
γ (deg)					96.57(1)
V (Å^3)	2262.4	4376.0	3091.0	5275.2	1284.2
d measured Z	1.55(1) 4	1.49(1) 8	1.47(1) 4	1.38(1) 8	1.49(1) 2
d calc. g/cm^3	1.55	1.49	1.49	1.40	1.51
Absorption Coefficient $\mu(Mo_{-1}K_\alpha)$ cm	11.23	10.56	8.70	8.72	10.1
T (deg C)	21(1)	21(1)	21(1)	21(1)	21(1)

Table 2.2

Experimental conditions used to collect data on the Ni(II) Hexaazamacrocycles

	(L0)$(NCS)_2$	(L0)(NO_2)	(L2)(H_2O)	(L3)(NO_2)	(L4)
Inner Data 2θ range (deg)	0 - 30	0 - 20	0 - 30	0 - 30	0 - 30
scan width (deg) (deg)	1.6	1.8	1.4	1.7	1.1
bkg time at both scan limits (sec)	10	10	10	20	10
Outer Data 2θ range (deg)	30 - 45	20 - 45	30 - 45	30 - 45	30 - 45
scan width (deg) (deg)	1.6	1.2	1.0	1.0	0.9
bkg time at both scan limits (sec)	10	10	10	10	10
variation of standards	±3%	±3%	±5%	±4%	±1%
max error in F due to neglect of absorption	none	±1.1%	±1.1%	±1.0%	±1.2%
#measured data	2027	2859	4295	3647	3317
#observed data	2257	2539	3254	2347	2517

2iv Structural Determinations

a Common Particulars

Atomic scattering factors used in these calculations were taken from reference 35, and included corrections for anomalous dispersion where relevant for nickel ($\Delta f'=.285$, $\Delta f''=1.113$), chlorine ($\Delta f'=.132, \Delta f''=.159$), and sulphur ($\Delta f'=.110$, $\Delta f''=.124$). Hydrogen atom positions, where calculated, assumed regular tetrahedral and trigonal angles and C-H bond lengths of 0.95 Å and N-H bond lengths of 0.87 Å (reference 36), and were assigned isotropic thermal motion parameters which reflected the degree of motion exhibited by the atom to which each was bonded. Unit weights were assigned to observed data in the early stages of each refinement. In the later stages, counter weights $=1/\sigma_F^2$, given in terms of $\sigma_F = \sigma_I/(Lp)(2F_o)$, were used. All residuals, R, quoted are those given by $\Sigma(|F_o|-|F_c|)/\Sigma(|F_o|)$. Tabulated anisotropic temperature factors are of the form:

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

b $Ni(L0)(NCS)_2$

A three-dimensional Patterson synthesis using an inner set of data ($2\theta<30^\circ$, 422 observed reflections) gave the strongest peaks as $0\ 0\ \frac{1}{2}$, $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$, $\frac{1}{2}\ \frac{1}{2}\ 0$, which do not correspond to the Harker planes and lines expected for the space group P21/n. Clearly, either this space group assignment was incorrect, or some false symmetry was present. Careful re-examination of the photographs confirmed the choice of the space group, and, from the Patterson map, coordinates could be chosen for the nickel atom ($0\ 0\ \frac{1}{4}$) and two sulphur atoms, which were entirely reasonable

and consistent with a trans-,N-bonded $Ni(NCS)_2$ moiety. This model was adopted, therefore, and refinement commenced using only the ℓ-even data, thereby assuming the false symmetry. A Fourier synthesis using the phases thus generated gave the positions of the nitrogen atoms in the coordination shell of the nickel atom. Further refinements and subsequent electron density difference maps quickly gave all of the light atom positions, which, though not entirely chemically sensible, preserved the false center of symmetry at the nickel atom. Refinement was continued using only the ℓ-even data to an R-factor of 0.107. At this stage, displacement of the nickel atom from 0 0 $\frac{1}{4}$ (as suggested by the original Patterson), and the adoption of one of the two possible orientations of the macrocyclic ligand L O (as suggested by the light atom positions already assigned), permitted removal of the false symmetry and inclusion of the ℓ-odd data ($2\theta<30^{\circ}$) into the refinement. The initial R-factor of 0.311 quickly dropped upon refinement of the scale factor, and positional and isotropic thermal motion parameters to 0.092 (140 variables and 816 observations). The outer set of data was then included in the calculations, and anisotropic thermal motion was first assigned to the nickel and sulphur atoms, and then, as the refinement continued, to the lighter atoms. Hydrogen atom positions were found from electron density difference maps, or, in the case of some methyl hydrogens, calculated using a C-H bond length of 0.965 Å. Full matrix, least-squares refinement gave a final R-factor of 0.060 (249 variables, 2257 observed data).

Final atomic parameters are listed in table 2.3 and thermal motion parameters in table 2.4. Calculated hydrogen atom positions are given in table 2.5, and measured and calculated structure factors (x10) in table 2.6.

Table 2.3

Fractional Atomic Coordinates: $Ni(L0)(NCS)_2.H_2O$.
($\times 10^4$, $\times 10^5$ for Ni) Least-squares estimated errors are given in parentheses.

Atom Type	x	y	z
Ni	-1299(6)	-528(6)	25541(4)
S1	3588(2)	746(2)	4344(1)
S2	-3535(2)	-746(2)	470(1)
NS1	1307(5)	305(4)	3495(3)
NS2	-1481(5)	-525(5)	1624(3)
N1	-544(4)	-1379(4)	3309(3)
N2	-1503(4)	951(4)	2923(3)
N3	373(4)	1492(4)	2096(3)
N4	1071(4)	-869(4)	1897(3)
N5	921(5)	-2014(4)	1867(4)
N6	341(5)	-2207(5)	3518(3)
C5	-1416(5)	-1395(5)	3714(4)
C6	-1480(6)	-2218(6)	4379(4)
C7	-2422(6)	-573(5)	3518(4)
C8	-2086(5)	559(5)	3637(4)
C9	-1224(6)	879(5)	4396(4)
C10	-3257(6)	1333(6)	3614(5)
C11	-1115(6)	2128(5)	2886(4)
C12	-628(6)	2283(6)	2120(4)
C13	1046(5)	1548(5)	1398(4)
C14	213(6)	1197(6)	638(4)
C15	1499(6)	2736(6)	1295(4)
C16	2149(6)	784(5)	1598(4)
C17	1928(5)	-451(5)	1601(4)
C18	2771(7)	-1164(6)	1213(5)
CS1	2257(6)	482(5)	3847(4)
CS2	-2325(6)	-610(5)	1151(4)
O_w	-4391(11)	534(10)	1828(8)

Table 2.4

Hydrogen Atom Coordinates: $Ni(L0)(NCS)_2.H_2O$.

($x10^4$)

Atom	x	y	z
HN2	-2268	930	2448
HN3	900	1565	2617
HNS1	4072	2913	1776
HNS2	4369	2840	897
HN61	3857	2521	3594
HN62	4688	2647	2917
H61	-4033	3051	151
H62	-2575	2560	695
H63	-3687	1955	827
H71	-2211	4344	2062
H72	-1975	4245	1113
H91	-3093	2137	3683
H92	-3823	1178	3115
H93	-3530	1094	4128
H101	-1602	581	4870
H102	-366	534	4427
H103	-993	1805	4568
H111	-492	2250	3281
H112	-2000	2559	2820
H121	-1146	2045	1714
H122	-139	2865	2195
H141	-313	1765	417
H142	754	1045	202
H143	-221	434	726
H151	744	3218	1070
H152	1918	2637	835
H153	1939	2935	1781
H161	2650	961	2130
H162	2574	882	1141
H181	1410	4267	3671
H182	2090	2977	3531
H183	2168	4093	4333
HO_w1	-4109	103	1377
HO_w2	-3720	661	2204

Table 2.5

Thermal Motion Parameters: $Ni(L0)(NCS)_2.H_2O$.

(X 10^3, x 10^4 for Ni A^2)

Atom Type	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni	309(6)	292(6)	543(7)	2(4)	53(3)	-6(4)
S1	35(1)	58(1)	80(2)	-6(1)	0(1)	6(1)
S2	77(2)	89(2)	88(2)	-20(1)	-29(1)	28(1)
NS1	38(3)	51(4)	57(4)	1(3)	3(3)	8(3)
NS2	41(3)	47(4)	64(4)	-7(3)	3(3)	-10(3)
N1	36(3)	34(3)	58(4)	4(3)	8(3)	3(3)
N2	35(3)	32(3)	58(4)	3(2)	1(3)	6(3)
N3	43(3)	31(3)	47(3)	4(2)	6(3)	6(3)
N4	39(3)	38(3)	61(4)	-0(3)	11(3)	-9(3)
N5	52(4)	54(4)	71(4)	23(3)	23(3)	16(3)
N6	68(4)	29(3)	83(4)	-6(3)	30(3)	-9(3)
C5	36(4)	30(4)	67(5)	-5(3)	11(3)	-3(3)
C6	51(4)	52(5)	74(5)	-9(4)	8(4)	7(4)
C7	37(4)	44(4)	82(5)	-5(3)	16(4)	-3(4)
C8	31(3)	31(4)	69(5)	3(3)	19(3)	-3(3)
C9	57(4)	49(4)	61(5)	-5(4)	8(4)	1(4)
C10	41(4)	48(5)	123(7)	11(4)	21(4)	-3(5)
C11	58(4)	41(4)	64(5)	13(3)	27(4)	8(4)
C12	65(5)	49(5)	73(5)	16(4)	21(4)	8(4)
C13	39(4)	37(4)	55(4)	-3(3)	13(3)	2(3)
C14	60(5)	58(5)	52(4)	-4(4)	9(4)	1(4)
C15	59(5)	59(5)	68(5)	-7(4)	11(4)	4(4)
C16	41(4)	48(5)	64(5)	-2(3)	12(3)	3(4)
C17	36(4)	43(4)	56(5)	7(3)	6(3)	2(4)
C18	75(5)	47(5)	98(6)	14(4)	48(5)	18(4)
CS1	35(4)	36(4)	51(4)	4(3)	11(3)	9(3)
CS2	46(4)	42(4)	57(5)	-9(3)	9(4)	12(4)
O_w	U = 121(6) (isotropic)					

Table 2.6

Structure Factor Listing: $Ni(L0)(NCS)_2.H_2O$.

(x 10)

Unobserved reflections are denoted by an asterisk.

L	FO	FC
H=	0, K=	0
2	1743	-1854
4	913	-866
6	164	-176
8	53	-38
10	1053	-1030
12	50*	46
14	6*	37
16	289	256
H=	0, K=	1
17	131	-93
16	79	-58
15	61*	-34
14	99	-97
13	367	-305
12	115	123
10	76	-54
9	279	-301
8	98	-72
7	85	133
6	382	369
5	380	434
4	230	215
3	107	12
2	140	-165
H=	0, K=	2
0	1750	1801
2	432	-434
4	416	415
6	715	-682
8	499	483
10	811	-797
1	189	-252
3	31*	5
5	617	-591
7	139	144
9	254	265
11	81	64
12	428	434
13	312	302
14	319	-293
15	179	-184
16	204	193
17	78	-50
H=	0, K=	3
2	1743	1624
4	865	879
6	226	236
8	148	152
10	36*	-25
11	164	170
9	285	-307
7	304	325
5	176	-158
3	3*	-63
1	83	90
17	83	-35
16	7*	-21
15	7*	35
14	190	-216
13	132	-112
12	153	-196
H=	0, K=	4
0	253	267
2	1047	-1043
4	778	755
6	572	-571
8	706	686
10	399	-409
1	75	-90
3	548	-546
5	98	89
7	13*	44
9	189	189
11	94	135
12	329	427
13	49*	92
14	186	-209
15	7*	-32
16	68*	90
17	59*	-93
H=	0, K=	5
0	4*	0
2	979	927
4	105	121
6	139	166
8	152	154
10	64	-85
9	125	-132
7	100	-99
5	69	-76
3	73	83
1	239	-270
16	38*	-14
15	108	171
14	57*	-135
13	42*	-47
12	71	-101
11	50*	227
H=	0, K=	6
0	527	-555
2	955	-968
4	709	694
6	367	-357
1	411	398
3	38*	-46
5	79	89
7	104	114
9	6*	80
10	6*	-185
11	6*	-196
12	6*	366
13	35*	-11
14	78*	-235
15	7*	-36
H=	0, K=	7
0	34*	0
2	186	167
4	5*	-43
3	216	214
1	135	136
15	7*	274
14	7*	48
13	7*	34
12	6*	-36
11	6*	-41
10	76	-117
9	6*	14
8	91	148
H=	0, K=	8
0	32*	59
2	657	-679
4	594	584
3	202	-219
5	253	262
1	89	90
6	395	-412
7	118	-95
8	427	511
9	6*	-61
10	114	-149
11	7*	-172
12	7*	201
13	30*	53
14	7*	-145
H=	0, K=	9
13	52*	-111
12	7*	59
11	32*	138
10	36*	12
9	6*	-10
8	109	107
7	6*	44
6	414	-423
5	168	-161
4	82	-66
3	195	195
2	379	-358
1	76	-85
0	53*	0
H=	0, K=	10
0	223	215
1	209	214
2	368	-358
3	66	50
4	643	644
5	86	67
6	374	-382
7	140	-149
8	84	97
9	43*	109
10	107	-116
11	134	-186
H=	0, K=	11
9	82	-81
8	25*	10
7	255	261
6	89	-81
5	116	-92
4	315	-313
3	78	-99
2	30*	-36
1	99	81
0	6*	0
H=	0, K=	12
0	232	230
1	112	99
2	159	-171
3	186	-180
4	392	401
5	188	154
6	307	-320
7	134	-124
H=	0, K=	13

L	FO	FC
1	74	-87
0	7*	0
H=	1, K=	0
9	123	123
5	528	493
3	278	-249
1	135	134
11	375	415
7	41*	-57
17	167	-137
15	187	170
13	172	-191
H=	1, K=	1
0	1997	1990
2	2173	-2087
4	1692	1636
6	47	-51
8	618	614
10	544	-501
1	148	-104
3	383	338
5	633	-631
7	21*	3
9	114	-115
11	5*	-74
12	411	374
13	210	219
14	211	-251
15	49*	-43
16	21*	30
17	113	92
H=	1, K=	2
0	501	-456
2	1295	-1244
4	421	-420
6	45	38
8	75	-68
10	273	286
11	295	333
9	75	-106
7	145	151
5	431	-460
3	204	220
1	73	65
17	71	-53
16	7*	-1
15	37*	28
14	30*	65
13	50*	-27
12	221	199
H=	1, K=	3
0	92	-103
2	196	202
4	646	614
6	750	-791
8	839	839
10	453	-433
1	68	119
3	774	-787
5	498	-469
7	5*	-28
9	11*	-34
11	102	77
12	371	379
13	200	193
14	374	-399
15	72	50
16	134	135
17	93	54
H=	1, K=	4
2	25*	60
4	310	-333
6	160	-191
8	225	230
10	228	230
9	211	-200
7	153	147
5	253	252
3	54	-47
1	311	-296
16	59*	56
15	55*	15
14	43*	79
13	153	-197
12	61*	64
11	79	103
H=	1, K=	5
0	1165	1159
2	373	-367
4	180	201
6	919	-915
8	438	-422
1	225	247
3	205	-211
5	172	166
7	125	-153
9	95	-97
10	326	-412
11	57*	-74
12	202	261
13	91	124
14	155	-173
15	65*	67
16	156	172
H=	1, K=	6
0	268	-250
2	171	171
4	209	-186
6	70	73
8	116	115
7	5*	5
5	45*	-83
3	133	141
1	50	-63
15	63*	71
14	7*	-2
13	85	-69
12	29*	55
11	65*	-127
10	6*	67
9	144	-152
H=	1, K=	7
0	687	691
2	551	-579
4	154	159
6	596	-594
1	231	252
3	290	-281
5	273	297
7	34*	-11
8	301	354
9	6*	19
10	366	-485
11	41*	-53
12	182	237
13	43*	60
14	87	-77
H=	1, K=	8
0	337	-313
2	295	309
4	441	454
3	143	141
1	43*	17
13	21*	-62
12	7*	36
11	84	-100
10	144	-173
9	81	-92
8	30*	59
7	28*	21
6	196	-210
5	57*	-65
H=	1, K=	9
0	639	614
1	184	172
2	568	-547
3	205	-194
4	362	347
5	141	103
6	567	-583
7	66	10
8	244	248
9	183	214
10	167	-206
11	117	-152
12	111	151
H=	1, K=	10
11	136	171
10	64*	-45
9	115	-150
8	43*	-16
7	79	61
6	57*	-38
5	81	69
4	114	96
3	6*	-25
2	6*	35
1	65	-58
0	224	220
H=	1, K=	11
0	145	142
1	198	218
2	305	-302
3	240	-255
4	422	435
5	82	70
6	298	-298
7	51*	24
8	296	304
9	115	108
H=	1, K=	12
6	34*	27
5	86	-29

L	FO	FC
H=	1, K=	12
4	92	106
3	7*	-50
2	167	185
1	7*	21
0	177	193
H=	2, K=	0
2	2903	-3012
4	1207	1247
6	1817	-1809
8	156	153
10	147	-152
12	625	603
14	118	99
16	145	133
H=	2, K=	1
0	211	182
2	913	-884
4	845	853
6	199	-153
8	512	-511
10	28*	-12
11	65	-60
9	147	-147
7	385	-379
5	297	283
3	81	55
1	203	164
17	7*	-24
16	7*	-16
15	282	244
14	6*	12
13	175	-149
12	6*	3
H=	2, K=	2
0	366	-307
2	427	-456
4	811	791
6	1424	-1401
8	480	483
10	247	-256
1	105	-132
3	367	-338
5	158	-119
7	299	286
9	31*	-22
11	87	-78
11	112	-78
12	457	467
13	97	-62
14	197	-212
15	132	-132
16	239	236
17	51*	36
H=	2, K=	3
0	547	473
2	400	388
4	75	59
6	633	-608
8	468	-463
10	243	-226
9	108	-119
7	232	222
5	169	-147
3	223	-179
1	66	-31
16	150	176
15	80	45
14	114	135
13	56*	-52
12	160	-142
11	92	119
H=	2, K=	4
0	902	882
2	434	-429
4	509	541
6	402	-419
8	771	777
1	280	-282
3	79	-96
5	371	368
7	5*	-20
9	49*	41
10	381	-402
11	105	-68
12	161	190
13	104	-126
14	248	-253
15	105	-93
16	153	145
H=	2, K=	5
0	870	830
2	36*	54
4	86	-78
6	5*	-4
8	209	-232
9	49*	41
7	133	134
5	147	141
3	180	-163
1	41*	-37
15	39*	-37
14	58*	93
13	86	-90
12	125	-122
11	226	233
10	160	-184
H=	2, K=	6
0	1223	1231
2	264	-249
4	801	837
6	62	-60
1	164	168
3	25*	23
5	221	236
7	291	-303
8	478	506
9	51*	41
10	473	-511
11	44*	-32
12	59*	75
13	56*	-48
14	262	-298
15	22*	-6
H=	2, K=	7
0	254	-271
2	105	93
4	5*	-9
6	6*	42
5	146	-132
3	146	-150
1	83	-88
14	7*	-44
13	81	107
12	46*	50
11	91	76
10	6*	-34
9	49*	21
8	93	65
7	187	160
H=	2, K=	8
0	867	876
2	310	-342
1	61	64
3	98	-117
4	513	525
5	113	110
6	101	-116
7	187	-172
8	337	329
9	95	56
10	408	-432
11	7*	-43
12	151	121
13	171	172
H=	2, K=	9
12	128	115
11	135	137
10	100	129
9	75	-77
8	160	167
7	81	-82
6	56*	-41
5	86	83
4	286	291
3	30*	32
2	111	-128
1	122	120
0	766	-749
H=	2, K=	10
0	448	456
1	308	280
2	336	-349
3	285	-274
4	253	254
5	63*	-43
6	456	-443
7	89	-83
8	362	365
9	81	75
10	221	-225
H=	2, K=	11
8	7*	37
7	36*	-3
6	153	149
5	94	98
4	7*	-3
3	7*	-12
2	185	-179
1	66	-32
0	91	-89
H=	2, K=	12
0	241	259

L	FO	FC
1	182	149
2	407	-417
3	194	-194
4	134	123
5	154	152
H=	3, K=	0
9	130	164
7	370	-355
5	502	517
3	475	455
1	301	304
15	7*	70
13	192	-175
11	215	-212
H=	3, K=	1
0	928	900
2	279	282
4	1298	1266
6	1391	-1351
8	510	481
10	661	-649
1	21*	46
3	263	-273
5	47*	-34
7	43*	-46
9	128	148
11	222	207
12	61	28
13	6*	19
14	186	-155
15	38*	-31
16	266	261
H=	3, K=	2
0	117	-87
2	276	-263
4	843	811
6	39*	18
8	149	165
10	238	239
9	53*	55
7	369	366
5	210	-198
3	82	-86
1	270	309
16	66*	-44
15	73	19
14	160	-144
13	96	-104
12	108	-107
11	111	-115
H=	3, K=	3
0	278	272
2	29*	-78
4	641	650
6	734	-706
8	604	595
1	93	-60
3	450	-458
5	272	260
7	215	209
9	123	147
10	462	-448
11	220	191
12	184	159
13	42*	45
14	239	-217
15	79	-58
16	261	256
H=	3, K=	4
0	14*	-31
2	163	-129
4	360	339
6	452	454
8	157	184
9	200	-202
7	48*	-40
5	256	265
3	209	-245
1	53	-19
15	67*	48
14	126	-141
13	62*	-48
12	98	-112
11	205	198
10	47*	64
H=	3, K=	5
0	438	436
2	1123	-1122
4	460	430
6	410	-394
8	624	630
1	360	355
3	94	-106
5	72	58
7	249	-271
9	319	341
10	171	-188
11	98	75
12	292	300
13	29*	-85
14	170	-173
15	7*	29
H=	3, K=	6
0	525	515
2	555	-547
4	146	128
6	546	532
7	35*	-19
5	96	-116
3	157	-173
1	69	82
14	79	-93
13	78	96
12	88	-99
11	122	122
10	57*	-68
9	71	-76
8	100	-78
7	23*	-19
H=	3, K=	7
0	529	552
2	1170	-1194
4	510	516
1	5*	32
3	60	48
5	117	118
6	228	-210
7	196	-180
8	212	203
9	48*	50
10	124	-112
11	100	-91
12	408	445
13	7*	-12
H=	3, K=	8
0	466	-460
1	312	332
12	83	64
11	113	107
10	27*	37
9	82	-70
8	6*	-45
7	158	-128
6	296	-297
5	80	-101
4	121	-123
3	83	-79
2	317	287
H=	3, K=	9
0	532	514
1	6*	-45
2	528	-504
3	6*	12
4	148	121
5	82	89
6	305	-295
7	124	-95
8	407	411
9	7*	-7
10	171	-168
11	194	-196
H=	3, K=	10
9	7*	-28
8	81	-97
7	77	-47
6	172	-182
5	103	91
4	11*	-24
3	71	-70
2	102	-93
1	155	142
0	72	-50
H=	3, K=	11
0	285	302
1	167	142
2	155	-163
3	139	-139
4	302	288
5	186	167
6	299	-294
7	89	-100
H=	3, K=	12
3	69	-84
2	20*	-6
1	35*	-31
0	7*	47
4	89	-108
H=	4, K=	0
2	1107	-1129
4	1003	970
6	431	-415
8	1170	1157

L	FO	FC
H=	4, K=	0
10	142	-127
12	232	226
14	335	-328
H=	4, K=	1
0	328	327
2	506	-491
4	153	-166
6	558	-511
8	99	89
9	188	178
7	226	-216
5	131	-141
3	102	-87
1	280	275
15	124	117
14	42*	18
13	195	204
12	45*	76
11	6*	-35
10	203	185
H=	4, K=	2
0	699	678
2	1053	-982
4	515	500
6	444	-432
8	932	911
1	20*	26
3	114	-129
5	105	127
7	207	-234
9	36*	-69
10	275	-261
11	22*	41
12	208	202
13	44*	-2
14	253	-255
15	50*	60
H=	4, K=	3
0	836	-831
2	646	-648
4	517	-513
6	583	-590
8	95	60
7	78	70
5	146	131
3	121	-131
1	197	210
15	25*	4
14	7*	5
13	60*	-53
12	321	323
11	115	114
10	372	373
9	89	-80
H=	4, K=	4
0	778	776
2	263	-269
4	429	442
6	570	-580
8	433	433
1	287	264
3	123	-133
5	62	96
7	139	-160
9	38*	-28
10	394	-401
11	147	-139
12	152	160
13	37*	24
14	219	-200
15	83	105
H=	4, K=	5
0	219	213
2	669	-669
4	100	-109
6	62	-4
7	49*	8
5	326	330
3	152	-145
1	51	61
14	45*	-1
13	157	-148
12	190	198
11	6*	35
10	202	209
9	125	-83
8	226	-253
H=	4, K=	6
0	874	883
4	826	818
1	86	116
5	116	140
6	802	-801
7	215	-182
8	131	-119
9	136	143
10	361	-350
11	91	-75
12	264	260
13	12*	-9
H=	4, K=	7
0	57	-51
2	146	173
3	167	-166
1	291	288
12	7*	29
11	93	-100
10	20*	22
9	21*	-12
8	120	-115
7	154	151
6	86	90
5	6*	34
4	123	108
H=	4, K=	8
0	630	651
1	81	55
2	440	-441
3	73	83
4	528	512
5	93	-112
6	484	-477
7	46*	54
8	99	-108
9	107	107
10	287	-273
11	95	-86
H=	4, K=	9
10	69*	-57
9	7*	-27
8	48*	55
7	7*	-18
6	40*	42
5	19*	41
4	106	104
3	267	-254
2	427	415
1	241	245
0	45*	-34
H=	4, K=	10
0	170	173
1	6*	31
2	159	-170
3	156	-137
4	206	202
5	7*	23
6	246	-240
7	31*	-45
8	296	279
H=	4, K=	11
6	138	115
5	67	53
4	76	81
3	7*	-11
2	7*	40
1	25*	15
0	127	118
H=	4, K=	12
0	137	127
1	163	158
2	241	-249
H=	5, K=	0
7	270	-307
5	66	-61
3	109	-132
1	78	105
15	69	20
13	154	157
11	212	-206
9	145	-108
H=	5, K=	1
2	984	-984
4	217	235
6	923	-948
8	140	133
1	83	-86
3	137	-180
5	194	187
7	5*	-28
9	173	164
10	241	-211
11	60*	-46
12	547	503
13	95	-105
14	228	-190
15	37*	-31
H=	5, K=	2
0	26*	50

L	FO	FC
2	476	463
4	128	121
6	356	-364
8	111	-104
7	28*	-14
5	65	98
3	192	-216
1	467	439
14	43*	-8
13	45*	23
12	66	-40
11	116	-137
10	204	-204
9	141	-128
H=	5, K=	3
0	1137	1140
2	909	-900
4	307	327
6	341	-342
1	111	-81
3	90	-82
5	252	250
7	62	42
8	357	342
9	52*	-34
10	347	-335
11	145	-132
12	358	346
13	53*	-24
14	202	-186
H=	5, K=	4
0	207	191
2	429	453
4	216	194
6	105	-114
5	132	154
3	225	-222
1	471	495
14	7*	-6
13	112	-110
12	7*	3
11	149	152
10	154	-169
9	114	112
8	386	-357
7	37*	-70
H=	5, K=	5
0	356	361
2	260	-255
4	800	821
1	50*	67
3	146	-161
5	265	260
6	272	-254
7	78	-55
8	543	521
9	149	140
10	353	-343
11	168	-165
12	114	123
13	57*	-55
H=	5, K=	6
0	358	330
2	100	114
3	234	-259
1	177	202
12	7*	51
11	7*	-1
10	77	-104
9	153	131
8	320	-327
7	108	102
6	52*	42
5	177	183
4	183	188
H=	5, K=	7
0	296	322
1	195	184
2	405	-412
3	67	-9
4	993	963
5	27*	-28
6	402	-378
7	44*	-17
8	322	310
9	7*	11
10	166	-148
11	52*	-59
12	61*	69
H=	5, K=	8
10	7*	36
9	62*	39
8	131	143
7	7*	27
6	72	74
5	6*	60
4	183	-185
3	283	-296
2	123	110
1	171	173
0	205	-192
H=	5, K=	9
0	98	108
1	279	280
2	153	-148
3	130	-124
4	334	313
5	134	-161
6	144	-105
7	30*	35
8	280	275
9	26*	35
H=	5, K=	10
7	57*	-62
6	124	122
5	7*	-8
4	111	-116
3	65*	-41
2	193	-192
1	54*	32
0	119	-110
H=	5, K=	11
0	185	177
1	172	145
2	279	-275
3	156	-141
4	122	112
H=	6, K=	0
0	837	858
2	186	211
4	1127	1177
6	393	-388
8	6*	27
10	484	-470
12	158	129
14	358	-332
H=	6, K=	1
0	304	-288
2	38*	30
4	176	-144
6	174	176
5	37*	71
3	145	-177
1	113	145
14	7*	45
13	7*	37
12	7*	-24
11	54*	-6
10	61*	-51
9	121	83
8	363	349
7	6*	10
H=	6, K=	2
0	718	754
2	746	-745
4	1108	1084
6	202	-180
1	190	-180
3	69	55
5	5*	14
7	69	-103
8	39*	-25
9	140	127
10	432	-411
11	75	82
12	301	300
13	139	125
H=	6, K=	3
0	768	-768
2	157	164
4	5*	13
5	206	208
3	390	-435
1	486	498
13	94	-104
12	7*	-59
11	7*	-38
10	6*	31
9	95	81
8	501	511
7	43*	-26
6	444	445
H=	6, K=	4
0	393	384
2	581	-588
4	273	265
1	16*	42
3	72	-58
5	86	-62
6	264	-259
7	48*	-65
8	335	340

L	FO	FC
H=	6, K=	4
9	94	93
10	317	-315
11	66	10
12	335	315
13	198	180
H=	6, K=	5
0	50*	-39
2	215	-202
3	192	-192
1	169	189
12	64*	-27
11	41*	-75
10	38*	-45
9	45*	42
8	140	110
7	125	-115
6	436	423
5	224	220
4	42*	28
H=	6, K=	6
0	184	189
1	228	214
2	824	-795
3	29*	-35
4	194	180
5	80	82
6	583	-606
7	160	-139
8	515	507
9	131	118
10	62*	-62
11	54*	-32
H=	6, K=	7
10	140	-127
9	35*	18
8	7*	2
7	197	-198
6	13*	30
5	117	122
4	141	-149
3	68	-49
2	88	77
1	318	305
0	98	128
3	68	-49
2	88	77
1	318	305
0	98	128
H=	6, K=	8
0	393	391
1	197	186
2	498	-476
0	393	391
1	197	186
2	498	-476
3	186	-200
4	51*	21
5	7*	7
6	423	-421
7	76	106
8	406	404
9	90	-71
H=	6, K=	9
8	110	-88
7	83	-83
6	84	-71
5	34*	38
4	218	-214
3	9*	-44
2	45*	56
1	68*	65
0	173	212
H=	6, K=	10
0	273	264
1	55*	69
2	142	-135
3	103	-129
4	67*	88
5	188	184
H=	6, K=	11
2	7*	21
1	153	143
0	67*	40
H=	7, K=	0
11	85	86
9	73	90
7	6*	-35
5	154	-172
H=	7, K=	1
5	6*	-10
6	166	-194
7	114	-106
8	534	519
9	6*	-15
10	127	-124
11	7*	-49
12	275	265
2	834	-840
4	463	502
1	49*	-68
3	205	215
H=	7, K=	2
0	59	-65
2	128	-127
3	269	-254
1	365	418
12	86	83
11	7*	41
10	33*	-57
9	100	85
8	193	200
7	228	-231
6	61*	-59
5	109	109
4	715	-724
H=	7, K=	3
0	374	378
2	677	-677
1	40*	43
3	138	141
4	447	440
5	222	-237
6	130	-130
7	107	-82
8	245	258
9	7*	-26
10	273	-279
11	64*	-72
12	288	265
H=	7, K=	4
0	145	127
1	57*	62
11	100	-82
10	75	33
9	140	104
8	29*	22
7	88	-84
6	94	-96
5	320	329
4	436	-439
3	226	-233
2	313	-285
H=	7, K=	5
0	534	538
1	87	85
2	93	-105
3	54*	42
4	253	268
5	110	113
6	419	-405
7	185	-156
8	134	147
9	7*	4
10	383	-362
11	116	-112
H=	7, K=	6
10	7*	8
9	131	140
8	45*	27
7	165	-156
6	6*	-24
5	166	187
4	259	-264
3	32*	-20
2	34*	-20
1	147	158
0	180	176
H=	7, K=	7
0	695	703
1	112	89
2	276	-276
3	107	-93
4	312	322
5	129	110
6	477	-482
7	78	-67
8	176	175
9	54*	20
H=	7, K=	8
7	90	-90
6	123	120
5	103	94
4	24*	59
3	112	-106
2	100	97
1	180	174

L	FO	FC
0	108	95
H=	7, K=	9
0	428	445
1	72	77
2	87	-89
3	170	-169
4	147	146
5	164	153
6	278	-265
H=	7, K=	10
3	116	-108
2	142	143
1	124	137
0	35*	-50
H=	8, K=	0
2	298	-307
4	197	-180
6	759	-770
8	319	303
10	399	-386
H=	8, K=	1
0	13*	-30
11	115	-100
10	122	-115
9	47*	23
8	38*	-46
7	66	-68
6	141	139
5	126	127
4	37*	-18
3	217	-224
2	242	235
1	316	319
H=	8, K=	2
0	639	661
1	56*	36
2	374	-383
3	55*	-72
4	150	148
5	192	-192
6	488	-472
7	172	172
8	244	235
9	58*	72
10	299	-296
11	7*	-10
H=	8, K=	3
10	148	-147
9	136	136
8	139	-123
7	244	-237
6	17*	-11
5	243	243
4	211	237
3	117	-114
2	425	428
1	190	193
0	257	276
H=	8, K=	4
0	327	327
1	31*	-14
2	267	-255
3	106	-84
4	268	258
5	6*	-15
6	72	-65
7	77	63
8	289	273
9	78	91
10	218	-215
H=	8, K=	5
9	167	144
8	138	-119
7	167	-171
6	38*	-41
5	117	98
4	112	143
3	6*	27
2	287	279
1	171	180
0	160	164
H=	8, K=	6
0	90	65
1	56*	-18
2	291	-284
3	44*	50
4	535	527
5	117	129
6	82	-66
7	134	-144
8	351	359
H=	8, K=	7
7	194	-189
6	32*	-68
5	57*	46
4	46*	-36
3	178	-175
2	95	85
1	211	219
0	129	-107
H=	8, K=	8
0	77	73
1	62*	34
2	317	-319
3	100	-72
4	394	396
5	153	170
H=	8, K=	9
3	201	-178
2	90	-106
1	131	133
0	236	-229
H=	9, K=	0
9	92	78
7	29*	-31
5	204	207
3	285	-277
1	324	311
H=	9, K=	1
0	544	549
1	14*	-35
2	21*	45
3	6*	-51
4	333	334
5	65	-39
6	206	-219
7	53*	21
8	375	401
9	43*	-56
H=	9, K=	2
9	208	208
8	128	130
7	183	-156
6	154	138
5	185	168
4	97	100
3	244	-261
2	58*	36
1	272	280
0	459	-458
H=	9, K=	3
0	347	351
1	6*	11
2	176	-175
3	202	-203
4	255	253
5	7*	17
6	177	-182
7	94	94
8	212	206
9	54*	-20
H=	9, K=	4
8	65*	76
7	145	-127
6	43*	-26
5	181	178
4	254	251
3	87	-57
2	67	-77
1	158	137
0	384	-384
H=	9, K=	5
0	138	152
1	80	100
2	349	-353
3	33*	25
4	64*	80
5	7*	-12
6	280	-292
7	134	-138
H=	9, K=	6
6	59*	-20
5	83	66
4	58*	36
3	85	-81
2	86	76
1	189	191
0	239	-227
H=	9, K=	7
0	60*	50

L	FO	FC
H=	9, K=	7
1	7*	4
2	411	-423
3	34*	-39
4	145	140
H=	9, K=	8
2	110	133
1	122	106
0	110	-107
H=	10, K=	0
0	138	-120
2	450	-471
4	131	139
6	241	-268
H=	10, K=	1
7	195	-180
6	19*	-55
5	204	207
4	151	-140
3	245	-248
2	109	101
1	369	367
0	32*	-14
H=	10, K=	2
0	140	135
1	172	-163
2	305	-302
3	52*	-50
4	109	120
5	165	159
6	216	-224
7	51*	27
H=	10, K=	3
6	244	-255
5	240	231
4	122	-112
3	152	-151
2	46*	-61
1	139	140
0	66	-50
H=	10, K=	4
0	267	289
1	7*	36
2	88	-99
3	30*	-49
4	245	233
5	157	132
6	224	-221
H=	10, K=	5
4	46*	-38
3	219	-215
2	53*	34
1	146	131
0	10*	-9
H=	10, K=	6
0	342	335
1	45*	49
2	59*	-16
3	7*	-39
H=	10, K=	7
0	123	-103
H=	11, K=	0
3	339	-335
1	81	82
H=	11, K=	1
0	149	154
1	53*	-41
2	147	-151
3	7*	-49
4	218	229
H=	11, K=	2
4	10*	34
3	208	-194
2	189	184
1	127	127
0	103	102
H=	11, K=	3
0	205	218
1	7*	28
2	153	-178
3	92	-99
H=	11, K=	4
2	102	86
1	257	244
0	97	122
H=	11, K=	5
0	110	111
H=	1, K=	0
-1	436	-429
-9	241	-237
-7	328	-304
-5	608	-654
-3	69	48
-17	31*	-38
-15	258	267
-13	44*	-59
-11	193	209
H=	1, K=	1
-6	482	-515
-3	63	-87
-9	99	-94
-11	401	398
-4	471	-399
-8	700	668
-10	372	-340
-12	385	387
-5	479	462
-1	16*	-42
-7	318	-304
-13	146	-187
-14	107	-143
-15	85	84
-16	219	238
-17	7*	18
-18	102	-132
-2	1512	-1398
H=	1, K=	2
-9	527	-557
-6	200	207
-8	231	238
-12	256	-247
-11	166	207
-3	276	346
-2	15*	-58
-5	204	-210
-17	77	-96
-16	7*	6
-15	144	161
-14	12*	-18
-13	35*	-43
-12	209	-247
-4	767	740
-10	352	308
-7	267	250
-1	209	-235
H=	1, K=	3
-8	901	867
-6	716	-704
-10	574	-546
-5	51	-64
-4	760	744
-1	375	-412
-3	178	177
-7	262	240
-9	232	225
-11	105	104
-12	381	469
-14	203	-220
-15	46*	65
-17	7*	-12
H=	1, K=	4
-7	320	310
-4	1072	1023
-10	119	104
-3	219	253
-2	580	-589
-6	327	331
-8	5*	-16
-11	244	241
-9	60	61
-5	382	-381
-1	178	-161
-17	107	-78
-16	64*	-62
-15	7*	31
-14	30*	-5
-11	222	241
H=	1, K=	5
-1	190	-200
-2	1104	-1036
-4	1216	1195
-6	207	-216
-8	435	428
-10	605	-578
-3	41*	62
-5	158	-172
-7	71	-42

L	FO	FC
-9	5*	-23
-12	220	247
-13	6*	94
-14	181	-189
-15	72	21
H=	1, K=	6
-9	10*	-10
-7	226	220
-2	671	-614
-4	589	557
-6	263	267
-8	128	-129
-5	34*	13
-3	101	117
-1	113	87
-14	38*	20
-13	213	-230
-12	38*	-52
-11	125	113
-10	99	87
H=	1, K=	7
-2	60	-78
-4	912	909
-6	695	-704
-1	49	-44
-3	43*	48
-5	121	-132
-7	114	111
H=	1, K=	8
-2	418	414
-4	119	-140
-5	149	-156
-3	303	311
-1	88	-89
-14	79	-104
-13	145	-173
-12	117	153
-11	70	56
-10	6*	-24
-8	303	-316
H=	1, K=	9
-5	6*	-74
-6	345	-346
-7	190	208
-9	178	-169
-10	232	-271
H=	1, K=	10
-8	7*	-87
-3	108	131
-2	151	152
-1	46*	-9
H=	1, K=	11
-2	292	-300
-3	82	69
-4	250	262
-5	100	-79
-7	214	193
-8	158	164
-9	156	-124
H=	1, K=	12
-7	90	107
-6	103	-100
-5	84	-80
-4	7*	-15
-3	20*	-13
-2	114	-126
-1	51*	14
H=	2, K=	0
-2	284	270
-4	2484	2387
-6	573	549
-8	43*	51
-10	448	-450
-12	244	223
-14	443	-475
-16	184	171
-18	113	-78
H=	2, K=	1
-2	664	641
-4	702	665
-6	118	-131
-8	634	-572
-10	277	280
-12	180	-182
-11	267	247
-9	48	49
-7	309	326
-5	574	-577
-3	82	-132
-1	90	134
-18	7*	-10
-17	195	-196
-16	7*	-1
-15	296	291
-14	39*	-15
-13	114	-109
H=	2, K=	2
-2	710	-663
-4	1911	1759
-6	609	-543
-8	458	448
-1	53	-41
-3	184	182
-5	448	414
-7	362	360
-9	98	-84
-10	494	-489
-11	159	178
-12	343	308
-13	288	-319
-14	300	-311
-15	138	-116
-16	181	185
-17	52*	6
-18	128	-133
H=	2, K=	3
-10	140	-138
-2	1746	1718
-4	760	720
-6	656	-594
-8	635	-615
-11	236	255
-9	209	-190
-7	516	518
-5	402	-403
-3	281	245
-1	115	-81
-17	135	-140
-16	34*	89
-15	104	70
-14	58*	-71
-13	201	-201
-12	118	-107
H=	2, K=	4
-10	388	-378
-2	1342	-1296
-4	851	796
-6	861	-812
-8	517	515
-1	422	-399
-3	379	399
-5	142	-141
-7	399	378
-9	124	107
-11	133	-137
-12	285	312
-13	29*	-41
-14	196	-188
-15	134	-89
-16	75	95
-17	138	-119
H=	2, K=	5
-8	273	-283
-2	129	159
-4	135	125
-6	256	-273
-10	6*	41
-9	246	-251
-7	175	181
-5	309	-316
-3	272	289
-1	42*	8
-16	21*	-5
-15	90	86
-14	94	110
-13	278	-267
-12	110	-131
-11	48*	64
H=	2, K=	6
-2	1109	-1069
-4	5*	33
-6	964	-958
-8	391	373
-1	60	-29
-3	59	53
-5	146	-144
-7	106	131
-9	132	-118
-10	243	-242
-11	44*	-66
-12	291	328
-13	50*	-19
-14	77	-49
-15	87	91
-16	110	115
H=	2, K=	7
-2	194	174
-4	168	-147
-6	143	-135
-7	56	68

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	2, K=	7	-6	104	-89	-13	87	-73	-7	277	276
			-7	102	98	-14	293	-308	-5	585	-573
-5	31*	11	-8	286	289	-15	6*	-48	-3	502	503
-3	316	297	-9	202	-174	-16	180	202	-1	333	-360
-1	93	111	-10	231	-251	-17	64*	87	-17	125	-113
-15	176	205	-11	7*	6	-18	39*	-37	-16	7*	-4
-14	7*	4							-15	95	77
-13	308	-295	H=	2, K=	11	H=	3, K=	2	-14	35*	17
-12	49*	64							-13	6*	-35
-11	6*	17	-9	150	-156	-2	376	-366	-12	44*	31
-10	72	77	-8	36*	85	-4	722	-727	-11	243	244
-9	250	-232	-7	171	162	-6	275	240			
-8	24*	-11	-6	100	114	-8	340	-327	H=	3, K=	5
			-5	115	-122	-11	112	133			
H=	2, K=	8	-4	7*	-15	-9	259	-261	-2	1080	-1080
			-3	60*	28	-7	655	656	-4	609	587
-2	709	-724	-2	210	-212	-5	348	-368	-6	303	-282
-4	126	113	-1	78	-51	-3	115	141	-8	670	659
-1	121	103				-1	119	-179	-1	239	-252
-3	6*	-26	H=	2, K=	12	-10	264	265	-3	53	-33
-5	351	-319				-17	177	-139	-5	37*	-30
-6	607	-572	-1	159	-159	-16	42*	17	-7	5*	42
-7	163	145	-2	140	-140	-15	213	236	-9	130	-122
-8	312	290	-3	151	138	-14	6*	-16	-10	144	-151
-9	141	-124	-4	260	254	-13	338	-346	-11	156	-169
-10	264	-254	-5	132	-118	-12	41*	66	-12	240	227
-11	30*	-18	-6	179	-180				-13	82	115
-12	291	299				H=	3, K=	3	-14	159	-192
-13	7*	34	H=	3, K=	0				-15	130	118
-14	85	-73				-10	181	-165	-16	51*	85
			-11	94	-98	-2	1040	-1018	-11	199	-169
H=	2, K=	9	-9	151	133	-4	1590	1518			
			-7	420	-398	-6	1306	-1246	H=	3, K=	6
-13	68*	-13	-5	497	-479	-8	276	228			
-12	60*	80	-3	1099	1128	-1	4*	-4	-2	81	87
-11	120	112	-1	73	28	-3	88	-88	-4	606	-606
-10	100	86	-17	67*	-25	-5	350	-357	-6	337	-334
-9	213	-203	-15	265	301	-7	123	121	-8	263	241
-9	213	-203	-13	468	-480	-9	191	-218	-7	297	295
-8	151	166				-11	50*	-68	-5	256	-270
-7	45*	32	H=	3, K=	1	-12	309	336	-3	88	-77
-6	50*	29				-13	53*	29	-1	32*	-87
-5	130	-132	-3	15*	-6	-14	220	-236	-16	35*	10
-4	191	-157	-5	600	587	-15	39*	62	-15	194	187
-3	275	252	-7	101	-86	-16	141	149	-14	82	65
-2	194	176	-9	399	369	-17	68*	41	-13	97	-128
-1	226	-232	-11	139	128				-12	177	-147
			-10	418	-423	H=	3, K=	4	-11	305	311
H=	2, K=	10	-12	480	473				-10	378	372
			-2	272	-269	-10	229	220	-9	220	-237
-1	119	131	-4	1145	1149	-2	93	-89			
-2	348	-312	-6	1204	-1193	-4	761	-739	H=	3, K=	7
-3	16*	9	-8	189	-166	-6	319	-311			
-4	121	96	-1	195	-195	-8	210	210	-2	607	-622
-5	195	-185	-12	385	473	-9	201	-210	-4	483	483

L	FO	FC
-6	295	-297
-1	26*	-25
-3	133	133
-5	184	-212
-7	170	163
-8	560	570
-9	35*	-56
-10	146	-143
-11	104	99
-12	35*	41
-13	37*	-17
-14	107	-116
-15	74	69
H=	3, K=	8
-2	447	461
-3	53*	45
-1	239	-244
-14	76	15
-13	45*	-70
-12	66	-55
-10	13*	-93
-9	246	-209
-8	172	179
-7	128	90
-6	60	-53
-5	76	-30
-4	182	176
H=	3, K=	9
-1	109	-74
-2	468	-455
-3	183	171
-4	131	115
-5	107	-124
-6	42*	54
-7	180	146
-8	525	550
-9	36*	11
-10	425	-428
-11	91	76
-12	128	124
H=	3, K=	10
-11	93	103
-10	22*	-38
-9	282	-272
-8	35*	15
-7	206	225
-6	64*	94
-5	119	-104
-4	149	152
-3	73	68
-2	205	199
-1	73	-55
H=	3, K=	11
-1	246	-222
-2	158	-167
-3	124	129
-4	186	180
-5	43*	-11
-6	213	-215
-7	125	106
-8	235	244
-9	57*	-49
H=	3, K=	12
-6	102	116
-5	39*	-34
-4	96	93
-3	56*	62
-2	72	60
-1	7*	-34
H=	4, K=	0
-12	577	587
-14	318	-345
-16	62*	-13
-10	195	-197
-2	997	-974
-4	46	48
-6	710	-720
-8	1000	990
H=	4, K=	1
-10	161	-177
-2	197	192
-4	639	-601
-6	912	858
-8	81	86
-11	305	300
-9	417	-393
-7	131	-106
-5	524	-565
-3	336	332
-1	305	302
-17	7*	-11
-16	60*	42
-15	318	303
-14	6*	22
-13	220	-247
-12	130	-142
H=	4, K=	2
-10	123	-83
-2	942	-910
-4	467	446
-6	731	-704
-8	702	692
-1	175	-170
-3	321	-326
-5	28*	57
-7	180	182
-9	65	-77
-11	316	309
-12	177	174
-13	102	73
-14	236	-253
-15	85	-110
-16	151	151
-17	56*	27
H=	4, K=	3
-10	243	-232
-2	795	775
-4	152	133
-6	734	725
-8	503	463
-9	421	-407
-7	509	514
-5	259	-306
-3	244	259
-1	670	-659
-17	187	-179
-16	7*	11
-15	122	121
-14	126	-160
-13	84	-54
-12	185	-199
-11	312	318
H=	4, K=	4
-2	997	-946
-4	834	787
-6	437	-444
-8	423	419
-10	381	-354
-1	95	64
-3	398	-368
-5	319	-356
-7	194	193
-9	152	131
-11	75	20
-12	216	249
-13	173	132
-14	186	-192
-15	101	106
-16	110	122
-17	94	-101
H=	4, K=	5
-2	246	234
-4	67	-63
-6	228	224
-8	188	170
-9	106	-108
-7	532	550
-5	225	-242
-3	360	380
-1	409	-428
-16	7*	-8
-15	51*	61
-14	75	60
-13	165	-151
-12	204	-237
-11	117	112
-10	6*	-2
H=	4, K=	6
-2	11*	41
-4	773	765
-6	517	-506
-1	159	-173
-3	225	235
-5	61	-70
-7	30*	26
-8	6*	-24
-9	52*	19
-10	240	-258
-11	54*	64
-12	6*	17
-13	48*	3
-14	123	-123
-15	16*	-23
H=	4, K=	7
-2	84	73
-4	6*	-36
-5	129	98
-3	121	-114
-14	73	60
-13	271	-271
-12	72	-75
-11	273	290
-10	58*	37
-9	192	-207

L	FO	FC
H=	4, K=	7
-8	82	-59
-7	386	367
-6	110	-90
-1	299	-322
H=	4, K=	8
-1	133	-139
-2	140	-140
-3	306	301
-4	643	610
-5	59*	-14
-6	455	-452
-7	70	59
-8	32*	71
-9	292	-255
-10	281	-315
-11	68	107
-12	88	106
-13	110	-105
H=	4, K=	9
-12	120	-107
-11	18*	16
-10	41*	20
-9	155	-176
-8	20*	44
-7	242	226
-6	246	-247
-5	218	-206
-4	163	-151
-3	124	141
-2	6*	-24
-1	19*	10
H=	4, K=	10
-1	262	-272
-2	255	-267
-3	370	348
-4	223	231
-5	131	143
-6	301	-279
-7	43*	-46
-8	277	292
-9	113	-100
-10	302	-316
H=	4, K=	11
-8	114	-87
-7	151	152
-6	66*	-41
-5	175	-169
-4	228	-214
-3	18*	70
-2	41*	4
-1	39*	-8
H=	4, K=	12
-1	136	-115
-2	402	-404
-3	66*	57
-4	207	206
H=	5, K=	0
-9	375	-388
-7	259	300
-5	85	-131
-3	557	574
-1	57	-87
-17	198	-191
-15	74	76
-13	186	-187
-11	496	431
H=	5, K=	1
-10	707	-682
-2	31*	-72
-4	740	730
-6	342	-331
-8	818	792
-1	63	76
-3	148	-133
-5	276	275
-7	181	192
-9	95	-93
-11	32*	23
-12	54*	53
-13	67	-24
-14	90	-94
-15	140	-154
-16	92	84
-17	45*	33
H=	5, K=	2
-10	353	-340
-2	714	702
-4	248	-209
-6	100	87
-8	127	-121
-9	430	-473
-7	493	523
-5	193	-219
-3	43*	-30
-1	375	-410
-17	208	-183
-16	47*	53
-15	90	65
-14	54*	-17
-13	113	-99
-12	45*	5
-11	466	439
H=	5, K=	3
-2	578	-567
-4	402	413
-6	472	-428
-8	641	609
-1	356	321
-3	5*	24
-5	79	83
-7	206	216
-9	220	-224
-10	295	-313
-11	64	59
-12	6*	-18
-13	151	-126
-14	135	-143
-15	108	-89
-16	183	191
-17	7*	-3
H=	5, K=	4
-2	150	146
-4	40*	48
-6	51	-61
-8	230	-224
-9	326	-321
-7	441	453
-5	284	-276
-3	248	249
-1	558	-561
-16	37*	1
-15	129	134
-14	73	110
-13	67	-76
-12	54*	2
-11	44*	56
-10	224	-231
H=	5, K=	5
-2	614	-623
-4	148	135
-6	656	-641
-1	59	-92
-3	107	151
-5	41*	29
-7	69	-90
-8	292	300
-9	169	171
-10	186	-174
-11	28*	-54
-12	281	303
-13	136	-122
-14	168	-172
-15	40*	15
-16	133	146
H=	5, K=	6
-2	168	-129
-4	135	-150
-6	194	177
-5	214	-205
-3	201	212
-1	125	-126
-15	197	178
-14	160	166
-13	290	-271
-12	28*	80
-11	214	230
-10	57*	-107
-9	274	-278
-8	385	-379
-7	47*	67
H=	5, K=	7
-1	244	-227
-2	640	-674
-3	115	119
-4	392	403
-5	70	-77
-6	358	-341
-7	38*	39
-8	128	-142
-9	175	-209
-10	6*	35
-11	150	148
-12	221	245
-13	7*	20
-14	105	-108
H=	5, K=	8
-13	257	-241
-12	7*	-33
-11	149	173
-10	140	119

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-9	246	-217	-14	270	272	-13	90	-73	-11	59*	80
-8	6*	-12	-16	79	68	-12	206	218	-12	140	133
-7	84	59				-11	142	131	-13	7*	-5
-6	103	112	H=	6, K=	1	-10	175	190	-14	223	-231
-5	220	-208				-9	358	-347			
-4	6*	-8	-2	46*	-16				H=	6, K=	7
-3	330	298	-4	192	-202	H=	6, K=	4			
-2	253	-256	-6	27*	57				-13	177	-182
-1	82	-74	-8	197	207	-2	471	-482	-12	7*	58
			-9	634	-638	-4	444	446	-11	514	471
H=	5, K=	9	-7	503	487	-6	415	-393	-10	30*	-4
			-5	100	-112	-1	80	104	-9	229	-227
-1	231	-216	-3	541	571	-3	177	186	-8	198	-207
-2	406	-428	-1	252	-273	-5	92	-88	-7	70	-49
-3	48*	68	-17	179	-166	-7	232	-228	-6	300	282
-4	397	396	-16	7*	-46	-8	470	463	-5	148	-149
-5	61*	-29	-15	101	111	-9	163	-139	-4	98	-93
-6	418	-439	-14	7*	-37	-10	245	-253	-3	78	96
-7	7*	-13	-13	283	-246	-11	52*	67	-2	6*	-5
-8	206	196	-12	97	96	-12	284	272	-1	304	-287
-9	136	-155	-11	143	157	-13	79	-98			
-10	140	-139	-10	112	-106	-14	205	-206	H=	6, K=	8
-11	153	170				-15	110	95			
			H=	6, K=	2	-16	44*	74	-1	104	-78
H=	5, K=	10							-2	352	-355
			-2	339	-337	H=	6, K=	5	-3	6*	-30
-10	171	170	-4	215	231				-4	372	381
-9	129	-104	-6	657	-662	-2	318	-325	-5	67	-85
-8	7*	51	-8	386	358	-4	117	-140	-6	6*	36
-7	235	218	-1	93	92	-6	111	117	-7	310	307
-6	82	65	-3	188	192	-5	461	-489	-8	201	219
-5	251	-262	-5	62	-64	-3	141	162	-9	58*	-78
-4	70	-53	-7	96	-79	-1	226	-243	-10	200	-227
-3	230	232	-9	355	-361	-15	170	159	-11	42*	73
-2	65	-5	-10	214	-193	-14	53*	34	-12	81	93
-1	90	-77	-11	43*	69	-13	156	-166			
			-12	93	98	-12	47*	113	H=	6, K=	9
H=	5, K=	11	-13	58*	78	-11	404	375			
			-14	38*	10	-10	116	116	-10	7*	23
-1	100	-92	-15	14*	-43	-9	6*	-49	-9	102	-72
-2	229	-224	-16	121	128	-8	65	-58	-8	192	-200
-3	76	77				-7	190	176	-7	122	149
-4	346	364	H=	6, K=	3				-6	125	99
-5	102	-91				H=	6, K=	6	-5	244	-231
-6	217	-237	-2	624	-635				-4	88	96
-7	7*	-15	-4	44*	-39	-1	245	-242	-3	353	374
			-6	57	65	-2	342	-340	-2	166	140
H=	6, K=	0	-8	92	58	-3	127	91	-1	256	-246
			-7	521	525	-4	467	490			
-2	575	-566	-5	458	-464	-5	6*	-70	H=	6, K=	10
-4	36*	-62	-3	31*	54	-6	62	82			
-6	847	-842	-1	191	-227	-7	156	-147	-1	235	-230
-8	520	473	-16	147	-140	-8	254	252	-3	7*	25
-10	785	-740	-15	169	152	-9	109	100	-2	256	-261
-12	233	249	-14	51*	-43	-10	133	-158	-4	362	380

L	FO	FC
H=	6, K=	10
-5	7*	24
-6	348	-368
-7	139	118
-8	188	197
H=	6, K=	11
-5	160	-158
-4	24*	-19
-3	196	191
-2	232	213
-1	180	-165
H=	7, K=	0
3	260	-247
1	380	404
H=	7, K=	0
-7	341	336
-5	487	-513
-3	350	345
-1	402	-397
-15	354	307
-13	238	-250
-11	266	260
-9	408	-368
H=	7, K=	1
-2	660	-667
-4	549	526
-6	346	-327
-1	195	-207
-3	43*	40
-5	72	-64
-7	42*	65
-8	325	355
-9	6*	-1
-10	60*	-72
-11	61*	47
-12	121	128
-13	107	80
-14	7*	-69
-16	43*	12
-15	7*	-57
H=	7, K=	2
-5	391	-427
-3	341	351
-1	275	-317
-7	149	174
-2	254	248
-4	192	191
-6	137	152
-16	64*	-52
-15	251	195
-14	50*	-57
-13	179	-159
-12	44*	-75
-11	251	231
-10	123	-134
-9	326	-296
-8	282	276
H=	7, K=	3
-2	499	-493
-4	489	465
-6	255	-241
-1	148	-163
-3	131	-115
-5	49*	34
-7	329	310
-8	247	266
-9	151	-149
-10	160	-150
-11	156	120
-12	230	250
-13	27*	33
-14	148	-148
-15	7*	-22
H=	7, K=	4
-2	156	155
-4	285	288
-3	372	383
-1	197	-209
-15	170	164
-14	59*	-63
-13	271	-249
-12	107	-112
-11	209	204
-10	181	159
-9	80	-38
-8	109	-126
-7	416	396
-6	127	103
-5	547	-527
H=	7, K=	5
-1	199	-204
-2	203	-222
-3	122	127
-4	418	404
-5	108	-70
-6	298	-304
-7	214	-227
-8	186	175
-9	216	212
-10	389	-399
-11	171	147
-12	225	246
-13	50*	-73
-14	101	-95
H=	7, K=	6
-13	218	-201
-12	38*	33
-11	354	337
-10	89	-93
-9	339	-333
-8	114	-77
-7	264	244
-6	162	160
-5	60*	36
-4	94	-72
-3	201	177
-2	197	178
-2	184	178
-1	308	-300
H=	7, K=	7
-2	25*	-22
-1	6*	9
-3	68	86
-4	86	-79
-5	110	-133
-6	181	-173
-7	47*	83
-8	239	235
-9	49*	-20
-10	241	-280
-11	7*	-42
-12	7*	12
H=	7, K=	8
-11	198	203
-10	138	133
-9	260	-269
-8	217	-190
-7	258	236
-6	32*	-4
-5	39*	-44
-4	245	-239
-3	209	203
-2	86	72
-1	285	-276
H=	7, K=	9
-1	71	-77
-2	209	-222
-3	93	83
-4	177	176
-5	7*	-4
-6	319	-317
-7	99	126
-8	187	193
-9	117	-105
H=	7, K=	10
-6	74	66
-5	250	-238
-4	172	-159
-3	256	268
-2	7*	-56
-1	232	-214
H=	8, K=	0
-2	39*	-39
-4	774	774
-6	258	-259
-8	155	-176
-10	168	-187
-12	72	44
-14	143	-176
H=	8, K=	1
-2	46*	92
-4	6*	-2
-3	356	370
-1	544	-574
-15	140	140
-14	7*	8
-13	353	-361
-12	13*	-5
-11	423	381
-10	6*	-37
-9	58*	-72
-8	170	184
-7	305	285
-6	259	-266
-5	269	-253
H=	8, K=	2
-1	19*	50

L	FO	FC
-2	230	-264
-3	119	103
-4	402	416
-5	60	-73
-6	201	-204
-7	456	448
-8	56*	43
-9	86	-78
-10	154	-179
-11	279	-272
-12	152	149
-13	7*	-25
-14	66*	-118
-15	7*	-18
H=	8, K=	3
-14	7*	62
-13	267	-265
-12	134	-123
-11	211	198
-10	190	190
-9	117	-90
-8	137	-131
-7	188	171
-6	309	-333
-5	358	-339
-4	200	-208
-3	486	478
-2	76	67
-1	411	-408
H=	8, K=	4
-1	131	-120
-2	65*	-512
-3	180	154
-4	246	273
-5	187	161
-6	282	-298
-7	111	117
-8	277	289
-9	44*	-54
-10	219	-200
-11	60*	-70
-12	185	193
-13	123	-80
-14	93	-76
H=	8, K=	5
-13	165	-146
-12	7*	-13
-11	200	177
-10	22*	13
-9	433	-390
-8	66	-56
-7	274	-273
-6	97	-101
-5	404	-377
-4	193	-202
-3	290	289
-2	6*	-20
-1	193	-180
H=	8, K=	6
-1	107	-102
-2	452	-452
-3	199	207
-4	64	-40
-5	6*	-37
-6	200	-231
-8	351	384
-7	164	-186
-9	29*	8
-10	112	-115
-11	7*	-2
-12	125	122
H=	8, K=	7
-11	128	120
-10	62*	29
-9	480	-459
-8	7*	14
-7	211	211
-6	20*	47
-5	170	-132
-4	180	-165
-3	173	176
-2	93	101
-1	9*	-25
H=	8, K=	8
-1	68	-27
-2	211	-204
-3	49*	-40
-4	42*	25
-5	127	-143
-6	161	-186
-7	70	71
-8	255	290
-9	21*	-49
H=	8, K=	9
-7	194	189
-6	144	144
-5	255	-258
-4	60*	39
-3	231	218
-2	96	86
-1	110	-135
H=	9, K=	0
-13	336	-309
-11	321	325
-9	456	-452
-7	151	170
-5	76	-81
-3	425	409
-1	355	-360
H=	9, K=	1
-1	88	101
-2	487	-520
-3	234	229
-4	6*	-25
-5	294	-289
-6	180	-201
-7	6*	21
-8	74	60
-9	59*	67
-10	80	-102
-11	143	-128
-12	104	127
-13	7*	-2
-14	74	-72
H=	9, K=	2
-13	280	-234
-12	7*	-22
-11	213	208
-10	94	137
-9	295	-262
-8	104	119
-7	151	125
-6	35*	-41
-5	63	-47
-4	67	113
-3	417	411
-2	240	-244
-1	410	-409
H=	9, K=	3
-1	136	131
-2	429	-452
-3	45*	66
-4	157	178
-5	327	-311
-6	244	-258
-7	104	99
-8	224	222
-9	50*	64
-10	89	-102
-11	164	-140
-12	126	140
-13	7*	45
H=	9, K=	4
-12	102	-99
-11	266	245
-10	173	182
-9	109	-119
-8	7*	-26
-7	241	231
-6	131	140
-5	532	-522
-4	76	4
-3	383	362
-2	133	-173
-1	269	-275
H=	9, K=	5
-1	81	-71
-2	320	-327
-3	100	94
-4	400	418
-5	60*	12
-6	78	-91
-7	144	-151
-8	175	190
-9	97	-76
-10	34*	-67
-11	7*	14
-12	7*	33
H=	9, K=	6
-10	7*	-15
-9	220	-222
-8	127	143
-7	350	348
-6	42*	30
-5	351	-337
-4	20*	-22
-3	135	112
-2	7*	-10
-1	222	-187
H=	9, K=	7

L	FO	FC
H=	9, K=	7
-1	46*	30
-2	26*	75
-3	31*	4
-4	275	299
-5	78	-86
-6	149	-162
-7	55*	65
-8	165	198
-9	7*	2
H=	9, K=	8
-7	257	268
-6	75	42
-5	287	-269
-4	75	78
-3	154	140
-2	200	205
-1	111	-115
H=	10, K=	0
-2	282	-282
-2	150	148
-1	189	-197
H=	10, K=	6
-1	23*	29
-2	102	-100
-3	39*	30
-4	108	119
-5	100	-67
-6	285	-317
-7	7*	38
-8	7*	8
H=	10, K=	7
-5	128	-132
-4	47*	12
-3	241	221
-2	100	86
-1	196	-181
H=	11, K=	0

L	FO	FC
-4	302	317
-6	140	152
-8	172	192
-10	31*	-67
-12	35*	-44
H=	10, K=	1
-12	47*	8
-11	255	244
-10	90	-87
-9	387	-381
-8	38*	-29
-7	276	281
-6	6*	27
-5	344	-312
-4	171	182
-3	32*	30
-2	17*	-45
-1	159	-150
H=	10, K=	2
-1	160	-152
-9	196	-188
-7	583	574
-5	386	-394
-3	69	47
-1	65*	68
H=	11, K=	1
-1	76	-89
-2	115	115
-3	143	150
-4	292	311
-5	64*	17
-6	162	-204
-7	52*	31
-8	37*	-25
-9	61*	56
-10	105	-113
H=	11, K=	2
-9	112	-128
-8	35*	-83
-7	341	313

L	FO	FC
-2	252	-273
-3	175	186
-4	216	233
-5	187	-185
-6	42*	-73
-7	58*	40
-8	257	279
-9	268	269
-10	189	-195
-11	17*	14
-12	7*	16
H=	10, K=	3
-11	254	252
-10	7*	-12
-9	151	-134
-8	212	-229
-7	130	123
-6	104	109
-5	307	-282
-4	260	280
-3	396	386
-2	258	276
-6	76	-76
-5	295	-273
-4	102	-101
-3	186	176
-2	38*	-47
-1	220	-211
H=	11, K=	3
-1	33*	-54
-2	122	-150
-3	63*	41
-4	148	174
-5	164	175
-6	137	-168
-7	58*	-55
-8	7*	84
-9	7*	-4
H=	11, K=	4
-7	156	140
-6	30*	-26
-5	184	-195

L	FO	FC
-1	310	-312
H=	10, K=	4
-1	109	-131
-2	319	-352
-3	146	-118
-4	246	256
-5	7*	5
-6	112	-121
-7	76	45
-8	7*	-18
-9	142	132
-10	7*	-32
H=	10, K=	5
-9	153	-143
-8	132	-146
-7	300	298
-6	50*	43
-5	295	-300
-4	116	117
-3	392	382
-4	233	-251
-3	295	308
-2	48*	47
-1	288	-284
H=	11, K=	5
-1	44*	-32
-2	289	-301
-3	20*	-4
-4	25*	14
-5	143	124
H=	12, K=	0
-2	157	-150
-4	7*	-7
H=	12, K=	1
-5	300	-308
-4	7*	-20
-3	319	309
-2	85	-73

c $\underline{Ni(LO)NO_2ClO_4}$

The positions of the nickel and chlorine atoms were determined from inspection of a three-dimensional Patterson synthesis based on all the observed data. Refinement of their coordinates and two scale factors gave an R of 0.411. A Fourier synthesis using the phases generated by this model revealed the positions of the perchlorate oxygen atoms and the the atoms in nickel coordination sphere. Refinement of these coordinates and isotropic thermal motion parameters, and a subsequent electron density difference map gave the positions of all the other non-hydrogen atoms in the cation. Further refinement of this model reduced the R to 0.128. Anisotropic thermal motion was then assigned , first to the heavy atoms, then to the light atoms. Hydrogen atom positions were determined from the difference maps or calculated, and included in the structure factor calculation, to give an R of 0.073. At this stage, extremely large anisotropic thermal motion parameters in the carbon atoms of one chelate (C13 through C18) of the macrocycle indicated some disorder, possibly as a result of two alternate conformations of the six-membered ring. Each of these carbon atoms was split into two half-occupied positions as suggested by the thermal motion. Refinement of this model, first with isotropic, and later with anisotropic thermal motion parameters, gave a chemically reasonable picture.

Full matrix, least-squares refinement gave a final R factor fo 0.041 (317 variables).

Final fractional atomic coordinates (table 2.7) and thermal motion parameters (table 2.8) are given, together with hydrogen atom coordinates (table 2.9), and measured and calculated structure factors (x10) (table 2.10).

Table 2.7

Fractional Atomic Coordinates: $Ni(LO)NO_2(ClO_4)$.

(X 10^4, x 10^5 for Ni and Cl)

Atom	Type	x	y	z
Ni		10777(2)	13158(5)	18973(4)
Cl	perchlorate anion	34977(6)	11180(14)	23651(13)
O11		3308(3)	1594(5)	1351(5)
O12		3697(3)	1993(6)	3155(6)
O13		3163(4)	662(6)	2588(5)
O14		3762(3)	70(6)	2567(5)
On1	nitrite ligand	865(2)	-279(3)	983(3)
On2		437(1)	238(3)	1616(3)
Nn		487(2)	-511(4)	1066(4)
N1		1684(1)	1975(3)	1832(3)
N2		532(1)	2299(3)	552(3)
N3		1028(1)	2724(3)	2728(3)
N4		1542(2)	328(4)	3277(4)
N5		2179(1)	1571(4)	2651(3)
N6		1744(2)	-700(4)	3166(4)
C5		1670(2)	2840(4)	1252(4)
C6		2157(2)	3365(3)	1468(5)
C7		1177(2)	3404(4)	385(4)
C8		681(2)	2690(4)	-205(3)
C9		731(2)	1583(5)	-730(4)
C10		262(2)	3487(5)	-1085(4)
C11		358(2)	3286(4)	937(4)
C12		476(2)	3034(5)	2048(4)
C13		1185(10)	2644(24)	3934(18)
C13'		1301(11)	2487(24)	3891(24)
C14		1200(12)	3730(21)	4460(17)
C14'		1036(16)	3436(32)	4232(31)
C15		832(5)	1651(11)	3968(10)
C15'		1848(7)	2872(18)	4443(9)
C16		1727(5)	2002(10)	4426(8)
C16'		1219(6)	1361(13)	4156(10)
C17		1820(5)	781(12)	4264(10)
C17'		1575(6)	470(14)	4134(14)
C18		2154(15)	59(30)	5228(25)
C18'		1966(14)	-55(33)	5172(28)

Table 2.8

Hydrogen Atom Coordinates: $Ni(L0)NO_2(ClO_4)$.

($\times 10^4$)

Atom	x	y	z
HN2	204	1791	111
HN3	1231	3344	2676
HN51	2143	763	2863
HN52	2437	1667	2466
HN61	1531	-1079	2466
HN62	3178	3646	1267
H61	2057	4162	1080
H62	2136	3570	914
H63	2224	4046	1882
H71	1258	3755	-238
H72	1106	4164	813
H91	265	1279	-1283
H92	859	1775	-1204
H93	959	987	-235
H101	271	4199	-726
H102	331	3663	-1521
H103	-16	3129	-1360
H111	-28	3532	425
H112	549	3990	908
H121	317	3787	2287
H122	321	3210	2297
H141	907	4534	3827
H142	1127	3679	878
H143	1517	4207	4622
H141'	1361	3626	5169
H142'	1023	4224	3976
H143'	763	3256	4286
H151	494	1916	3663
H152	775	916	3475
H153	966	1322	4647
H151'	192	3928	4473
H152'	2079	2558	5157
H153'	1877	2538	3998
H161	1926	2518	4239
H162	1889	2107	5205
H161'	1272	1374	4909
H162'	853	1141	3685
H181	2322	63	5205
H182	1914	-91	5172
H183	1999	298	5778
H181'	2022	268	5674
H182'	2399	633	5263
H183'	2220	-696	5145

Table 2.9

Thermal Motion Parameters: $Ni(L0)NO_2(ClO_4)$.

($\times 10^3$, $\times 10^4$ for Ni A^2)

Atom Type	U11	U22	U33	U12	U13	U23
Ni	331(4)	279(4)	343(4)	-3(2)	19(3)	-2(2)
Cl	68(1)	45(1)	80(1)	10(1)	47(9)	11(8)
O11	156(7)	86(4)	116(5)	-1(5)	92(6)	14(3)
O12	191(9)	121(7)	90(6)	-7(5)	90(6)	-9(4)
O13	95(5)	193(10)	106(9)	-57(6)	61(6)	12(4)
O14	182(9)	104(7)	201(10)	62(8)	42(6)	8(4)
On1	52(2)	53(2)	70(2)	-11(2)	33(2)	3(2)
On2	75(3)	46(2)	54(2)	-5(2)	32(2)	-8(2)
Nn	72(3)	45(3)	54(3)	-19(3)	20(3)	-6(2)
N1	32(2)	45(2)	33(2)	-4(2)	18(2)	-5(2)
N2	35(2)	41(2)	35(2)	-2(2)	18(2)	1(2)
N3	51(2)	34(2)	34(2)	2(2)	28(2)	-1(2)
N4	55(3)	44(3)	50(3)	14(2)	31(2)	13(2)
N5	34(2)	67(3)	53(3)	10(2)	24(2)	14(2)
N6	78(3)	49(3)	78(3)	30(3)	36(3)	18(3)
C5	38(3)	38(3)	44(3)	-7(2)	25(2)	-6(2)
C6	71(4)	66(4)	78(4)	-27(3)	47(3)	2(3)
C7	48(3)	43(3)	45(3)	-5(2)	25(3)	5(2)
C8	38(3)	55(3)	26(2)	-3(2)	15(2)	4(2)
C9	64(3)	67(4)	50(3)	-12(3)	36(3)	-19(3)
C10	58(3)	87(4)	38(3)	2(3)	20(3)	14(3)
C11	40(3)	55(3)	46(3)	17(2)	24(2)	13(2)
C12	47(3)	52(3)	55(3)	18(2)	34(3)	11(3)
C13	55(11)	54(8)	27(7)	46(7)	39(7)	9(7)
C13'	55(11)	41(11)	58(11)	8(10)	52(11)	-23(7)
C14	146(15)	35(8)	27(7)	24(9)	13(9)	-35(9)
C14'	131(16)	117(17)	115(11)	-26(9)	58(8)	36(7)
C15	62(8)	81(9)	79(9)	26(7)	9(6)	-11(8)
C15'	59(8)	143(15)	28(6)	-12(9)	17(5)	-1(5)
C16	50(7)	50(7)	28(5)	-12(7)	42(8)	6(7)
C16'	111(13)	103(12)	39(7)	-27(11)	16(6)	12(6)
C17	24(7)	56(8)	40(6)	6(6)	36(9)	32(8)
C17'	49(9)	67(10)	79(10)	17(8)	36(10)	32(10)
C18	96(18)	146(19)	92(15)	76(10)	52(9)	80(8)
C18'	133(19)	71(13)	66(13)	37(10)	21(9)	32(9)

Table 2.10

Structure Factor Listing: $Ni(L0)NO_2(ClO_4)$.

(x 10)

Unobserved reflections are indicated by an asterisk.

L	FO	FC
H=	0, K=	0
2	1499	-1593
4	28	11
6	253	-236
H=	0, K=	2
0	767	-711
1	1755	-1851
2	242	-236
3	1412	1462
4	161	-151
5	106	90
H=	0, K=	4
0	938	-986
1	169	168
2	898	894
3	38	33
4	233	-226
H=	1, K=	5
0	134	-124
1	640	651
2	300	310
H=	1, K=	3
0	914	901
1	458	418
2	247	271
3	418	427
4	885	-904
H=	1, K=	1
0	644	577
1	1307	-1306
2	82	28
3	538	536
4	413	-439
5	529	-531
H=	2, K=	0
2	372	319
4	313	348
H=	2, K=	2
0	327	-331
1	356	349
2	305	-306
3	519	511
4	1056	-1075
5	458	-491
H=	2, K=	4
0	115	111
1	167	-162
2	31	32
3	153	150
H=	3, K=	5
0	101	98
1	297	287
H=	3, K=	3
0	67	-63
1	117	-101
2	376	-360
3	972	927
4	745	-755
H=	3, K=	1
0	63	80
1	333	-332
2	1148	-1165
3	638	668
4	784	775
5	827	-828
H=	4, K=	0
2	52	87
4	124	107
H=	4, K=	2
0	180	195
1	1079	1077
2	657	-637
3	330	-298
4	410	371
H=	4, K=	4
0	888	857
1	179	192
2	441	-476
H=	5, K=	5
0	269	308
H=	5, K=	3
0	804	780
1	672	643
2	1057	-1064
3	20*	-57
H=	5, K=	1
0	424	-400
1	64	-59
2	26*	-38
3	647	-653
4	176	153
H=	6, K=	0
0	198	222
2	741	-724
4	455	-440
H=	6, K=	2
0	305	266
1	320	369
2	342	-351
3	1080	-1070
H=	6, K=	4
0	263	246
1	3*	-28
H=	7, K=	3
0	231	222
1	518	527
2	472	-500
H=	7, K=	1
0	959	-912
1	83	89
2	247	274
3	339	-354
H=	8, K=	0
0	502	-508
2	50	-20
H=	8, K=	2
0	126	-121
1	202	-201
2	725	664
H=	8, K=	4
0	944	-937
H=	9, K=	3
0	714	-730
1	699	-729
H=	9, K=	1
0	179	162
1	957	-946
2	568	-564
H=	10, K=	0
0	142	182
H=	10, K=	2
0	205	-190
1	303	-268
H=	11, K=	1
0	217	240
1	74	40
H=	10, K=	0
0	178	182
H=	1, K=	5
-2	159	177
-1	237	246
H=	1, K=	3
-1	471	-490
-2	203	214
-3	238	254
-4	304	276
-5	876	-862
H=	1, K=	1
-1	483	456
-2	208	172
-3	979	919

L	FO	FC
-4	853	-813
-5	347	-311
-6	732	716
H=	2, K=	0
-2	1001	1020
-4	1735	-1792
-6	242	238
H=	2, K=	2
-1	254	-231
-2	257	-224
-3	947	975
-4	142	133
-5	1636	-1665
-6	316	-310
H=	2, K=	4
-2	395	-397
-1	328	339
-3	662	-651
-4	1092	1063
H=	3, K=	5
-1	369	366
-2	133	-142
-3	821	-816
H=	3, K=	3
-1	682	667
-2	338	-324
-3	140	139
-4	707	707
-5	406	-389
H=	3, K=	1
-1	884	-878
-2	442	404
-3	871	-889
-4	380	-358
-5	532	-506
-6	345	-352
H=	4, K=	0
-4	1138	-1078
-6	423	379
H=	4, K=	2
-1	1561	-1630
-2	1180	1141
-3	1217	1213
-4	611	-620
-5	112	102
-6	86	-58
H=	4, K=	4
-1	236	211
-2	261	-262
-3	82	111
-4	883	909
H=	5, K=	5
-1	357	375
-2	100	-93
H=	5, K=	3
-1	65	59
-2	823	807
-3	2*	18
-4	1061	-1035
-5	502	514
-6	483	494
H=	5, K=	1
-1	1288	-1293
-2	922	920
-3	316	-338
-4	854	837
-5	410	424
-6	347	-353
H=	6, K=	0
-2	200	-174
-4	683	685
-6	460	-492
H=	6, K=	2
-1	773	724
-2	222	-185
-3	798	-775
-4	566	566
-5	791	773
-6	45	-38
H=	6, K=	4
-1	260	-234
-2	574	568
-3	942	867
-4	851	-844
-5	218	-227
H=	7, K=	3
-1	75	51
-2	120	114
-3	22*	-42
-4	623	-639
-5	295	286
-6	205	228
H=	7, K=	1
-1	1109	-1148
-2	252	-237
-3	1102	1074
-4	63	59
-5	491	524
-6	133	115
-7	178	140
H=	8, K=	0
-2	1223	-1349
-4	1220	1247
-6	97	-92
H=	8, K=	2
-1	1217	1260
-2	371	-351
-3	1039	-1034
-4	342	307
-5	35	30
-6	491	-467
H=	8, K=	4
-1	95	34
-2	738	788
-3	198	214
-4	1265	-1226
H=	9, K=	3
-1	715	722
-2	775	717
-3	85	-73
-4	117	-93
-5	167	147
-6	167	-161
H=	9, K=	1
-1	823	815
-2	590	-551
-3	479	-474
-4	579	572
-5	298	286
-6	96	-72
-7	325	323
H=	10, K=	0
-2	604	582
-4	102	-119
-6	925	890
H=	10, K=	2
-1	570	549
-2	711	705
-3	22*	-81
-4	510	-471
-5	583	-563
-6	45	-67
H=	10, K=	4
-2	246	-232
-3	188	164
H=	11, K=	3
-1	548	-528
-2	3*	39
-3	499	511
-4	462	445
-5	93	-76
H=	11, K=	1
-1	27*	-5
-2	454	461
-3	113	135
-4	390	-368
-5	273	-257
-6	200	213
H=	12, K=	0
-2	195	126
-4	1113	-1148
-6	642	701
H=	12, K=	2

L	FO	FC
H= 12, K= 2		
-1	178	-209
-2	51	36
-3	1248	1259
-4	116	114
-5	1183	-1203
-6	289	-293
H= 13, K= 1		
-1	640	-690
-2	691	691
-3	624	634
-4	450	-457
-5	550	-547
-6	288	-294
H= 14, K= 2		
-3	152	-139
-4	411	388
H= 14, K= 0		
-2	344	305
-6	469	-874
H= 0, K= 0		
8	470	-476
10	326	334
12	4*	11
H= 0, K= 2		
6	126	145
7	347	-365
8	69	68
9	275	275
10	3*	41
11	86	-75
12	177	163
13	130	-126
H= 0, K= 4		
5	148	-155
6	22*	-30
7	83	70
8	328	350
9	109	-113
10	170	-160
11	118	119
12	4*	-3
H= 0, K= 6		
0	595	596
1	967	964
2	105	-107
3	451	-445
4	172	-188
5	41	-22
6	120	111
7	135	-138
8	108	-106
9	245	-251
10	67	76
11	220	228
H= 0, K= 8		
0	560	596
1	198	-201
2	401	-390
3	230	252
4	263	275
5	309	319
6	99	94
7	46	-63
8	139	-142
9	74	65
10	82	78
H= 0, K= 10		
0	185	-189
1	405	-414
2	83	-95
3	176	176
4	185	188
5	37*	68
6	52	-48
7	315	-317
H= 0, K= 12		
0	279	-279
1	33*	-37
2	232	237
H= 1, K= 11		
0	281	-281
1	27*	-53
2	271	287
3	80	89
4	79	-79
5	65	52
H= 1, K= 9		
0	63	-55
1	350	-355
2	92	-107
3	244	235
4	52	61
5	35*	-28
6	97	-105
7	214	-218
8	126	-122
H= 1, K= 7		
0	340	340
1	93	97
2	649	-652
3	27*	25
4	333	350
5	109	113
6	123	121
7	184	-195
8	185	-186
9	121	-120
10	275	287
H= 1, K= 5		
3	571	-567
4	295	-292
5	62	51
6	117	-112
7	145	150
8	39	37
9	272	-290
10	184	-173
11	295	317
H= 1, K= 3		
5	139	-107
6	50	-43
7	320	-322
8	445	470
9	106	107
10	328	-318
11	71	-79
12	166	167
H= 1, K= 1		
6	233	244
7	573	-567
8	312	-311
9	460	469
10	194	197
11	199	-209
12	86	-68
13	207	222
H= 2, K= 0		
6	342	-360
8	129	-302
10	483	493
12	400	-430
H= 2, K= 2		
6	312	304
7	15*	-24
8	180	192
9	321	338
10	169	-185
11	403	-398
12	40	15
H= 2, K= 4		
4	718	-712
5	15*	-25
6	331	316
7	374	-380
8	159	154
9	50	57
10	242	-286
11	120	126
12	302	315
H= 2, K= 6		
0	29	14
1	504	486
2	178	-166
3	396	-394
4	3*	31
5	73	68
6	278	-289
7	71	-81
8	39	-40
9	299	-306
10	49	44
11	329	338
H= 2, K= 8		
0	132	138
1	89	82
2	269	-275

L	FO	FC
3	187	190
4	303	300
5	94	-82
6	82	-73
7	25*	-32
8	195	-209
9	27*	14
H=	2, K=	10
0	135	-135
1	237	-237
2	40	-26
3	182	186
4	84	-82
5	255	-261
6	170	175
7	83	69
H=	2, K=	12
0	61	-68
1	119	116
H=	3, K=	11
0	79	78
1	21*	-8
2	155	131
3	194	202
4	144	-146
H=	3, K=	9
0	195	207
H=	20, K=	6
-2	33*	29
H=	17, K=	9
-5	160	167
H=	3, K=	9
3	137	141
4	128	120
5	368	-370
6	360	-372
7	147	146
8	132	125
H=	3, K=	7
0	31	-38
1	315	308
2	231	-223
3	287	-289
4	611	601
5	296	293
6	194	-189
7	127	-122
8	67	47
9	78	64
10	50	45
H=	3, K=	5
2	129	134
3	465	-480
4	530	-533
5	314	322
6	366	359
7	590	609
8	153	-152
9	241	260
10	76	-79
11	155	151
H=	3, K=	3
5	487	-513
6	521	527
7	386	390
8	194	-188
9	242	-229
10	179	189
11	76	-62
12	116	98
H=	3, K=	1
6	474	-484
7	490	508
8	500	511
9	3*	-12
10	116	-123
11	49	-41
12	163	-176
H=	4, K=	0
6	491	-484
8	633	631
10	46	-15
12	28*	22
H=	4, K=	2
5	470	-493
6	275	269
7	448	475
8	83	70
9	228	-226
10	27*	-3
11	119	119
12	119	-140
H=	4, K=	4
3	61	-29
4	91	-91
5	27*	25
6	538	530
7	108	-114
8	423	-431
9	188	187
10	186	188
11	76	-63
H=	4, K=	6
0	82	74
1	525	-535
2	98	-78
3	112	107
4	163	155
5	341	336
6	93	-93
7	276	-271
8	196	194
9	214	220
10	73	-68
H=	4, K=	8
0	640	-661
1	107	101
2	351	342
3	140	140
4	132	128
5	331	-337
6	155	-151
7	4*	9
8	165	168
H=	4, K=	10
0	59	60
1	220	206
2	140	140
3	4*	7
4	107	-108
5	181	-179
6	60	65
H=	4, K=	12
0	275	283
H=	5, K=	11
0	237	225
1	13*	32
2	58	-55
3	62	-68
4	49	41
H=	5, K=	9
0	86	-88
1	288	289
2	126	136
3	45	-31
4	170	-163
5	84	-81
6	44	-34
7	161	163
H=	5, K=	7
0	734	-717
1	382	-379
2	653	645
3	321	333
4	85	88
5	122	-118
6	118	-126
7	4*	19
8	263	270
9	171	166
H=	5, K=	5
1	628	-608
2	403	-422
3	32	27
4	242	244
5	184	-186
6	189	186
7	301	-301
8	245	-229
9	350	351
10	53	42
H=	5, K=	3
4	76	91
5	23*	-10

L	FO	FC
H= 5, K= 3		
6	276	287
7	199	206
8	169	-184
9	107	-95
10	335	336
11	64	51
H= 5, K= 1		
5	142	126
6	168	189
7	302	311
8	58	79
9	197	-190
10	153	-155
11	165	159
H= 6, K= 0		
6	219	219
8	287	291
10	318	-325
H= 6, K= 2		
4	502	507
5	52	-38
6	13*	44
7	172	162
8	200	-189
9	156	-152
10	20*	-30
11	309	321
H= 6, K= 4		
2	962	-918
3	224	215
4	320	309
5	301	-305
6	43	49
7	144	138
8	338	-333
9	88	-91
10	230	228
H= 6, K= 6		
0	112	-124
1	592	-590
2	129	119
3	451	448
4	29*	20
5	88	-94
6	160	160
7	210	-192
8	4*	-9
9	427	436
H= 6, K= 8		
0	372	-356
1	73	78
2	270	267
3	409	-409
4	227	-228
5	66	62
6	102	-102
7	51	-63
8	197	206
H= 6, K= 10		
0	281	291
1	139	132
2	164	-167
3	115	-109
4	236	227
5	120	120
H= 7, K= 11		
0	20*	-2
1	26*	23
2	186	-186
H= 7, K= 9		
0	120	-118
1	3*	-10
2	250	237
3	412	-407
4	168	-162
5	374	375
6	70	70
H= 7, K= 7		
0	229	-235
1	321	-300
2	196	196
3	311	303
4	473	-464
5	289	-292
6	267	254
7	80	77
8	28*	-20
H= 7, K= 5		
0	31	20
1	585	-576
2	519	-491
3	454	439
4	531	544
5	528	-519
6	239	-241
7	309	290
8	93	-95
9	4*	24
10	117	121
H= 7, K= 3		
3	705	-667
4	715	689
5	365	347
6	513	-482
7	275	-280
8	128	138
9	108	117
10	28*	11
H= 7, K= 1		
4	595	-598
5	562	548
6	579	581
7	228	-231
8	249	-253
9	146	-152
10	149	-156
11	48	41
H= 8, K= 0		
4	266	-274
6	372	373
8	105	-95
10	21*	-18
H= 8, K= 2		
3	291	-305
4	96	98
5	446	421
6	209	197
7	364	-345
8	211	-218
9	271	273
10	30*	-40
H= 8, K= 4		
1	215	-201
2	438	-428
3	65	61
4	422	412
5	26*	42
6	467	-475
7	14*	8
8	262	260
9	93	-93
10	41	-32
H= 8, K= 6		
0	60	58
1	177	170
2	211	206
3	186	177
4	58	58
5	327	-333
6	71	67
7	353	354
8	18*	-12
9	55	-53
H= 8, K= 8		
0	502	497
1	65	-76
2	34*	-27
3	91	-83
4	327	-331
5	33*	-25
6	232	232
7	4*	-17
H= 8, K= 10		
0	97	-99
1	130	-113
2	56	-44
3	138	-152
4	94	89
H= 9, K= 11		
0	160	-158
1	13*	34
2	127	125
H= 9, K= 9		
0	288	289
1	279	-281
2	71	-68

L	FO	FC
3	64	57
4	34*	-25
5	94	89
H=	9, K=	7
0	682	665
1	326	334
2	354	-397
H=	9, K=	5
1	813	786
2	471	469
3	56	-53
4	28*	-20
5	53	-50
6	42	-32
7	357	382
8	160	147
9	65	-70
H=	9, K=	3
2	842	811
3	137	142
4	193	190
5	99	104
6	234	-262
7	239	-235
8	96	82
9	98	101
10	138	-143
H=	9, K=	1
3	446	462
4	441	436
5	46	14
6	55	45
7	52	28
8	54	-63
9	8*	21
10	104	97
H=	10, K=	0
2	487	-487
4	222	215
6	70	-72
8	393	-389
10	282	286
H=	3, K=	9
1	161	154
2	316	-310
H=	10, K=	2
2	249	234
3	258	257
4	308	293
5	119	111
6	19*	15
7	261	-267
8	30*	16
9	348	345
10	4*	19
H=	10, K=	4
0	731	-748
1	48	51
2	509	513
3	57	-51
4	33	18
5	18*	5
6	360	-350
7	83	81
8	341	328
9	55	-49
H=	10, K=	6
0	220	197
1	366	376
2	90	-92
3	252	-262
4	3*	17
5	71	84
6	40	40
7	264	257
8	59	-41
H=	10, K=	8
0	328	341
1	59	-49
2	167	-158
3	252	255
4	140	140
5	227	-234
6	62	55
H=	10, K=	10
0	243	-249
1	188	-194
2	302	301
3	218	228
H=	11, K=	11
0	4*	10
H=	11, K=	9
0	31*	23
1	196	-194
2	198	-191
3	498	503
4	148	144
5	245	-241
H=	11, K=	7
0	154	157
1	181	179
2	223	-211
3	269	-263
4	225	219
5	103	108
6	216	-222
7	56	-41
H=	11, K=	5
0	308	-323
1	397	407
2	357	348
3	321	-330
4	310	-299
5	193	164
6	133	143
7	107	107
8	42	65
H=	11, K=	3
0	543	-553
1	529	-521
2	411	408
3	275	296
4	199	-183
5	277	-285
6	48	-42
7	18*	21
8	4*	10
9	90	67
H=	11, K=	1
2	340	-336
3	391	416
4	310	331
5	116	-125
6	168	-171
7	65	-36
8	133	-135
9	142	130
H=	12, K=	0
2	408	-397
4	623	609
6	414	-386
8	31*	44
H=	12, K=	2
0	149	147
1	271	-295
2	132	-133
3	559	566
4	3*	32
5	664	-651
6	169	-165
7	227	212
8	25*	-3
9	33*	-43
H=	12, K=	4
0	223	205
1	54	66
2	275	285
3	50	-50
4	489	-466
5	78	71
6	421	393
7	64	78
8	123	-130
H=	12, K=	6
0	166	-143
1	3*	12
2	32*	-55
3	260	-251
4	34*	-42
5	268	256
6	171	-159
7	233	-239
H=	12, K=	8
0	189	-185
1	63	66
2	213	-218

L	FO	FC
H= 12, K= 8		
3	8*	-7
4	362	350
H= 12, K= 10		
0	163	178
1	4*	-3
2	4*	-14
H= 13, K= 9		
0	320	-317
1	196	204
2	106	106
3	32*	50
H= 13, K= 7		
0	254	-241
1	314	-317
2	42	40
3	94	104
4	15*	14
5	9*	8
6	197	-204
H= 13, K= 5		
0	524	493
1	208	-204
2	287	-293
3	3*	-21
4	149	158
5	207	213
6	37*	-40
7	270	-276
H= 13, K= 3		
0	79	100
1	164	171
2	23*	9
3	136	-179
4	266	-299
5	229	-221
6	300	319
7	207	191
8	125	-131
H= 13, K= 1		
0	292	-308
1	595	592
2	241	256
3	330	340
4	69	73
5	91	83
6	222	-242
7	146	145
8	140	131
H= 14, K= 0		
0	1078	-1050
2	605	638
4	119	122
6	70	-78
8	343	338
H= 14, K= 2		
0	187	167
1	418	425
2	83	80
3	44	-59
4	137	-132
5	328	-297
6	111	-127
7	306	305
8	31*	-12
H= 14, K= 4		
0	353	344
1	112	-119
2	91	-114
3	8*	20
4	79	-74
5	261	249
6	341	341
7	90	-84
H= 14, K= 6		
0	116	-109
1	219	-221
2	68	72
3	86	82
4	6*	-33
5	52	35
6	76	-76
H= 14, K= 8		
0	141	-152
1	196	191
2	156	156
3	166	-167
4	4*	-2
H= 14, K= 10		
0	124	118
1	240	236
H= 15, K= 9		
0	49	-40
1	314	309
20	44*	-5
H= 15, K= 7		
0	190	-186
1	20*	29
2	353	354
3	91	82
4	291	-282
5	31*	-4
H= 15, K= 5		
0	229	214
1	205	-198
2	136	-149
3	182	171
4	97	87
5	137	-115
6	29*	-34
H= 15, K= 3		
0	148	151
1	76	84
2	356	-365
3	248	-253
4	297	303
5	79	74
6	116	95
7	113	110
H= 15, K= 1		
0	289	-289
1	560	561
2	419	425
3	291	-304
4	223	-236
5	222	232
6	134	-119
7	89	87
H= 16, K= 0		
2	1090	1126
4	387	-375
6	273	271
H= 16, K= 2		
0	221	-223
1	484	458
2	273	-270
3	689	-666
4	3*	-32
5	476	460
6	92	-89
7	107	-92
H= 16, K= 4		
0	241	237
1	95	94
2	349	-355
3	35*	-10
4	386	372
5	97	-85
6	262	-235
H= 16, K= 6		
0	149	-146
1	265	-270
2	57	59
3	343	328
4	65	-31
5	279	-274
H= 16, K= 8		
0	94	-81
1	116*	40
3	120	-118
H= 17, K= 9		
0	128	112
1	66	-72
H= 17, K= 7		
0	79	65
1	136	138
2	54	-61
3	43	19
4	194	-193
H= 17, K= 5		

L	FO	FC
0	388	-375
1	90	77
2	51	57
3	94	97
4	38*	29
5	227	-226
H=	17, K=	3
0	385	-392
1	127	-129
2	91	82
3	13*	19
4	236	251
5	158	151
6	205	-186
H=	17, K=	1
0	210	222
1	132	-130
2	36	-7
3	333	-354
4	194	-196
5	89	94
6	134	130
7	138	-159
H=	18, K=	0
0	885	870
2	76	-71
4	97	109
6	224	239
H=	18, K=	2
0	262	-263
1	333	-347
2	13*	-5
3	165	160
4	83	-83
5	145	151
6	44	-47
H=	18, K=	4
0	263	-249
1	84	91
2	136	144
3	50	-45
4	100	82
5	36*	-18

L	FO	FC
H=	18, K=	6
0	51	56
1	156	171
2	77	-85
3	25*	-4
4	28*	43
H=	18, K=	8
0	173	159
1	168	-175
2	47	-49
H=	19, K=	7
0	274	264
1	33*	-28
2	293	-302
H=	19, K=	5
0	82	-76
1	249	237
2	156	157
3	113	-117
4	22*	30
H=	19, K=	3
0	224	-227
1	111	-103
2	266	274
3	98	101
4	111	-111
5	129	129
H=	19, K=	1
0	271	276
1	559	-560
2	99	-103
3	156	164
4	26*	36
5	51	-57
H=	20, K=	0
0	280	268
2	510	-496
4	309	299
H=	20, K=	2
0	174	187

L	FO	FC
1	377	-380
2	177	175
3	368	353
4	132	-121
5	142	-137
H=	20, K=	4
0	173	-167
1	113	-125
2	434	414
3	54	56
4	261	-254
H=	20, K=	6
0	80	-99
1	314	325
2	24*	-11
3	354	-339
H=	20, K=	8
0	265	263
H=	21, K=	7
0	4*	-21
1	67	72
H=	21, K=	5
0	127	139
1	40	-25
2	114	117
3	192	-180
H=	21, K=	3
0	198	191
1	61	53
2	98	101
3	134	118
4	122	-136
H=	21, K=	1
0	3*	11
1	3*	-24
2	4*	-32
3	71	75
4	49	74
H=	22, K=	0

L	FO	FC
0	253	-253
2	24*	10
4	44	37
H=	22, K=	2
0	102	99
1	90	99
2	35*	43
3	59	44
4	4*	4
H=	22, K=	4
0	290	293
1	115	114
2	42	29
3	4*	-8
H=	22, K=	6
0	40	-23
1	75	-76
H=	23, K=	5
0	102	97
1	145	-138
2	43	-35
H=	23, K=	3
0	212	211
1	178	173
2	4*	-39
3	78	79
H=	23, K=	1
0	54	-51
1	124	125
2	59	37
3	107	-99
H=	24, K=	0
0	190	-174
2	166	161
H=	24, K=	2
0	37*	23
1	343	327
2	8*	-6

L	FO	FC
H= 24, K= 4		
0	327	334
1	22*	31
H= 24, K= 6		
0	47	68
H= 25, K= 5		
0	72	59
H= 25, K= 3		
0	135	152
1	108	103
H= 25, K= 1		
0	36	-38
1	131	138
2	91	89
H= 26, K= 0		
0	87	104
H= 26, K= 2		
0	103	93
1	4*	-17
H= 26, K= 4		
0	122	-132
H= 27, K= 3		
0	82	-75
H= 27, K= 1		
0	124	123
H= 28, K= 0		
0	290	283
H= 1, K= 1		
-7	255	258
-8	559	-548
-9	299	-300
-10	291	304
-11	341	-87
-12	192	182
-13	115	110
H= 1, K= 3		
-6	458	-494
-7	752	751
-8	420	412
-9	274	-262
-10	113	104
-11	3*	25
-12	148	-128
-13	126	121
H= 1, K= 5		
-3	565	-542
-4	162	175
-5	136	126
-6	317	-326
-7	411	-429
-8	242	232
-9	263	269
-10	209	-209
-11	78	-77
-12	88	95
H= 1, K= 7		
-1	33	17
-2	33	-44
-3	345	-355
-4	243	-255
-5	294	286
-6	404	399
-7	194	-194
-8	244	-232
-9	210	213
-10	101	93
-11	50	-49
H= 1, K= 9		
-1	282	286
-2	261	275
-3	147	-137
-4	215	-224
-5	296	-292
-6	406	417
-7	303	307
-8	244	-234
-9	66	-53
H= 1, K= 11		
-1	92	95
-2	17*	30
-3	64	56
-4	156	158
-5	198	-206
-6	225	-221
H= 2, K= 12		
-1	25*	-12
-2	147	-146
H= 2, K= 10		
-1	39	-38
-2	34*	-39
-3	303	297
-4	96	96
-5	272	-264
-6	101	-110
-7	231	232
-8	56	54
H= 2, K= 8		
-1	116	109
-2	170	167
-3	139	-130
-4	394	-398
-5	318	-319
-6	366	373
-7	125	119
-8	72	-72
-9	21*	-16
-10	239	-251
H= 2, K= 6		
-1	254	233
-2	282	260
-3	465	-471
-4	470	-466
-5	344	340
-6	208	220
-7	129	-136
-8	142	-133
-9	95	103
-10	153	152
-11	212	205
-12	146	137
H= 2, K= 4		
-5	116	107
-6	635	-651
-7	201	-189
-8	117	112
-9	103	-101
-10	11*	12
-11	47	56
-12	327	-323
-13	18*	8
H= 2, K= 2		
-7	714	692
-8	20*	-62
-8	306	-62
-10	115	119
-11	318	-313
-12	26*	-4
-13	254	265
H= 2, K= 0		
-8	27	-29
-10	74	-90
-12	460	462
H= 3, K= 1		
-7	135	104
-8	314	292
-9	421	411
-10	441	-434
-11	285	-284
-12	127	139
-13	179	183
-14	43	-22
H= 3, K= 3		
-6	491	-497
-7	81	-68
-8	374	-366
-9	312	307
-10	304	323
-11	128	-121
-12	98	-116
-13	106	96
H= 3, K= 5		
-4	88	107
-5	241	260
-6	136	-131
-7	70	72
-8	31*	-40
-9	34	-25

L	FO	FC
-10	200	184
-11	252	247
-12	234	-232
H=	3, K=	7
-1	32	34
-2	248	264
-3	33	44
-4	517	-518
-5	95	-102
-6	170	170
-7	57	63
-8	3*	-29
-9	138	-143
-10	359	-364
-11	204	205
H=	3, K=	9
-1	323	-328
-2	30*	-27
-3	380	389
-4	65	60
-5	334	-340
-6	24*	4
-7	4*	-29
-8	91	81
-9	296	295
H=	3, K=	11
-1	28*	38
-2	416	-424
-3	80	84
-4	243	244
-5	38*	26
-6	111	-109
H=	4, K=	12
-1	37*	21
-2	298	-298
H=	4, K=	10
-1	389	-389
-2	45	-40
-3	489	493
-4	21*	-15
-5	148	-148
-6	172	183
-7	141	-147
-8	182	-180
H=	4, K=	8
-1	53	-59
-2	528	544
-3	133	126
-4	390	-391
-5	35	-26
-6	97	92
-7	205	-200
-8	160	157
-9	276	289
-10	264	-255
-11	132	-127
H=	4, K=	6
-1	950	951
-2	178	-147
-3	760	-735
-4	166	-165
-5	272	279
-6	240	-226
-7	52	-59
-8	306	304
-9	79	-82
-10	46	44
-11	304	321
-12	76	75
H=	4, K=	4
-5	632	-638
-6	107	90
-7	310	305
-8	544	-521
-9	177	-178
-10	54	-53
-11	59	-52
-12	163	-161
-13	4*	22
H=	4, K=	2
-7	302	-330
-8	101	-112
-9	625	634
-10	55	42
-11	62	-55
-12	35*	65
-13	140	-153
-14	84	101
H=	4, K=	0
-8	356	368
-10	559	-557
-12	50	36
-14	80	70
H=	5, K=	1
-7	77	-72
-8	500	502
-9	452	438
-10	515	-503
-11	245	-244
-12	160	156
-13	89	-89
-14	136	130
H=	5, K=	3
-7	874	-862
-8	445	-447
-9	522	506
-10	116	120
-11	217	-194
-12	17*	40
-13	99	-86
-14	23*	-14
H=	5, K=	5
-3	293	260
-4	364	349
-5	615	-609
-6	505	495
-7	409	409
-8	187	-195
-9	207	-200
-10	248	247
-11	245	242
-12	89	-89
-13	82	85
H=	5, K=	7
-1	450	448
-2	231	227
-3	264	235
-4	42	19
-5	346	-352
-6	319	-308
-7	186	178
-8	394	404
-9	270	-269
-10	313	-303
-11	51	51
-12	35*	3
H=	5, K=	9
-1	412	-415
-2	96	99
-3	158	151
-4	108	117
-5	75	92
-6	205	-217
-7	346	-352
-8	267	271
-9	299	295
-10	71	-77
H=	5, K=	11
-1	32*	12
-2	255	-243
-3	88	94
-4	112	-108
-5	56	-48
-6	221	220
H=	6, K=	10
-1	35*	-59
-2	102	-96
-3	189	-191
-4	47	-40
-5	370	367
-6	136	135
-7	322	-315
-8	78	-64
H=	6, K=	8
-1	29*	-45
-2	126	-134
-3	303	321
-4	481	487
-5	166	-170
-6	459	-462
-7	133	-130
-8	422	423
-9	99	93
-10	31*	-15
-11	4*	29
H=	6, K=	6
-1	162	175
-2	58	-49
-3	409	418
-4	30	18
-5	730	-707
-6	3*	-13

L	FO	FC
H=	6, K=	6
-7	428	423
-8	286	283
-9	105	-118
-10	127	-125
-11	138	-140
-12	68	-61
-13	240	246
H=	6, K=	4
-6	915	904
-7	223	-228
-8	551	-554
-9	91	-88
-10	39	41
-11	38	-23
-12	254	246
-13	48	36
-14	236	-227
H=	6, K=	2
-7	907	-899
-8	192	185
-9	385	389
-10	88	-92
-11	84	97
-12	174	170
-13	290	-280
-14	94	75
H=	6, K=	0
-8	238	265
-10	121	-132
-12	317	-311
-14	261	260
H=	7, K=	1
-8	92	-111
-9	526	-524
-10	407	391
-11	373	371
-12	280	-272
-13	144	-138
-14	202	191
H=	7, K=	3
-7	92	-99
-8	191	-185
-9	250	-236
-10	340	-329
-11	127	124
-12	184	177
-13	310	-309
-14	173	-177
H=	7, K=	5
-1	287	298
-2	41	39
-3	484	484
-4	119	-120
-5	980	-973
-6	325	301
-7	83	-78
-8	287	286
-9	301	306
-10	357	-376
-11	83	-73
-12	237	236
-13	376	373
H=	7, K=	7
-1	173	157
-2	83	-85
-3	243	238
-4	117	121
-5	39	44
-6	253	-252
-7	129	-119
-8	53	-40
-9	87	75
-10	316	315
-11	328	-331
-12	311	-304
H=	7, K=	9
-1	124	120
-2	37	21
-3	357	-339
-4	46	34
-5	503	508
-6	50	56
-7	143	-140
-8	38*	-32
-9	161	-157
-10	67	70
H=	7, K=	11
-1	30*	-28
-2	221	227
-3	14*	28
-4	418	-422
-5	76	-80
-6	165	165
H=	8, K=	10
-1	268	261
-2	167	163
-3	425	-439
-4	172	-175
-5	280	291
-6	94	-101
-7	49	-35
-8	192	191
-9	125	-127
H=	8, K=	8
-1	128	138
-2	668	-661
-3	64	50
-4	377	383
-5	78	68
-6	224	-226
-7	82	83
-8	71	-61
-9	308	-313
-10	297	290
-11	223	225
H=	8, K=	6
-1	634	-630
-2	89	76
-3	707	718
-4	160	153
-5	512	-501
-6	208	230
-7	93	-76
-8	320	-331
-9	271	271
-10	82	-84
-11	255	-254
-12	139	-130
-13	86	91
H=	8, K=	4
-5	329	318
-6	78	59
-7	3*	28
-8	465	448
-9	109	97
-10	122	-119
-11	38	9
-12	155	160
-13	104	108
-14	53	-52
H=	8, K=	2
-7	277	-240
-8	264	266
-9	421	-410
-10	217	-213
-11	395	379
-12	84	-90
-13	63	-69
-14	4*	-13
H=	8, K=	0
-8	341	-354
-10	409	440
-12	315	-335
-14	12*	-10
H=	9, K=	1
-8	45	25
-9	264	-281
-10	394	396
-11	334	350
-12	315	-305
-13	22*	46
-14	40	-34
-15	49	63
H=	9, K=	3
-7	312	319
-8	333	340
-9	537	-547
-10	471	-467
-11	136	126
-12	32*	44
-13	100	-97
-14	53	58
H=	9, K=	5
-1	789	-774
-2	175	180
-3	168	154
-4	110	-111
-5	62	-42
-6	395	-389
-7	437	-417
-8	491	491
-9	412	405

L	FO	FC
-10	140	-117
-11	64	78
-12	28*	-19
-13	24*	4
-14	62	51
H=	9, K=	7
-1	599	-595
-2	559	-564
-3	272	283
-4	145	142
-5	230	211
-6	73	79
-7	224	-202
-8	366	-363
-9	248	234
-10	314	317
-11	190	-193
-12	67	-59
H=	9, K=	9
-1	422	408
-2	139	-150
-3	123	-117
-4	38	27
-5	42	68
-6	85	87
-7	188	181
-8	72	-66
-9	291	-287
-10	125	122
H=	9, K=	11
-1	94	-79
-2	171	174
-3	80	-71
-4	72	-33
-5	62	71
-6	174	-177
H=	10, K=	10
-1	139	-143
-2	165	168
-3	115	130
-4	49	-59
-5	334	-342
-6	58	-54
-7	303	304
-8	9*	-16
-9	197	-207
H=	10, K=	8
-1	247	255
-2	173	-183
-3	93	-103
-4	485	-469
-5	192	187
-6	499	518
-7	69	-75
-8	361	-368
-9	32*	44
-10	331	335
-11	73	-82
H=	10, K=	6
-1	513	-524
-2	261	256
-3	228	-234
-4	211	212
-5	718	719
-6	196	-194
-7	835	-826
-8	3*	9
-9	311	309
-10	25*	-10
-11	13*	34
-12	30*	-35
-13	206	-208
H=	10, K=	4
-1	448	-408
-4	537	539
-5	336	323
-6	699	-708
-7	221	208
-8	897	896
-9	184	185
-10	152	-146
-11	63	-61
-12	90	-97
-13	152	-153
-14	292	282
H=	10, K=	2
-7	308	327
-8	152	-147
-9	635	-623
-10	111	115
-11	253	253
-12	118	-100
-13	206	188
-14	4*	-5
-15	266	-269
H=	10, K=	0
-8	64	-76
-10	184	198
-12	3*	-8
-14	143	-139
H=	11, K=	1
-7	152	160
-8	131	-131
-9	71	63
-10	196	-186
-11	353	-333
-12	340	334
-13	389	370
-14	258	-266
-15	171	-178
H=	11, K=	3
-6	629	-634
-7	93	-83
-8	680	657
-9	3*	-6
-10	41	39
-11	211	-212
-12	269	-254
-13	272	278
-14	356	356
-15	99	-86
H=	11, K=	5
-1	134	120
-2	63	62
-3	285	-282
-4	3*	39
-5	595	577
-6	267	-269
-7	403	-419
-8	123	-126
-9	238	243
-10	469	458
-11	145	142
-12	278	-277
-13	460	-447
-14	132	142
H=	11, K=	7
-1	512	-512
-3	99	88
-4	302	-316
-5	157	154
-6	267	258
-7	41	27
-8	18*	-15
-9	184	-189
-10	222	-218
-11	204	204
-12	274	260
H=	11, K=	9
-1	65	-47
-2	36	-31
-3	237	238
-4	11*	10
-5	409	-404
-6	34*	-41
-7	191	193
-8	72	79
-9	25*	-6
-10	4*	8
H=	11, K=	11
-1	100	89
-2	138	-142
-3	35*	-36
-4	282	274
-5	4*	7
-6	262	-266
H=	12, K=	10
-1	281	-284
-2	112	-125
-3	199	190
-4	93	99
-5	279	-271
-6	139	-138
-7	133	140
-8	61	-44
-9	64	55
H=	12, K=	8
-1	117	-119
-2	350	339
-3	256	277
-4	388	-391
-5	157	-146
-6	181	182
-7	25*	-8
-8	145	150
-9	295	290

L	FO	FC
H= 12, K= 8		
-10	160	-156
-11	96	-94
-12	211	204
H= 12, K= 6		
-1	217	230
-2	245	258
-3	519	-524
-4	182	-182
-5	400	405
-6	3*	30
-7	102	-92
-8	62	-56
-9	352	-336
-10	72	-72
-11	267	273
-12	60	43
-13	129	-125
H= 12, K= 4		
-1	329	-333
-2	566	-555
-3	17*	-7
-4	805	814
-5	394	372
-6	759	-769
-7	262	-261
-8	117	102
-9	91	80
-10	263	260
-11	92	-86
-12	91	-87
-13	39	-32
-14	130	135
H= 12, K= 2		
-7	254	253
-8	230	-213
-9	165	161
-10	163	152
-11	247	-246
-12	184	-187
-13	138	157
-14	70	-72
-15	31*	-33
H= 12, K= 0		
-8	107	95
-10	258	-263
-12	459	487
-14	4*	-16
H= 13, K= 1		
-7	575	-549
-8	100	-72
-9	255	253
-10	147	-156
-11	458	-454
-12	175	185
-13	263	266
-14	47	-43
-15	4*	18
H= 13, K= 3		
-1	516	-508
-2	810	-799
-3	333	363
-4	602	588
-5	429	-402
-6	154	151
-7	144	122
-8	310	-303
-9	301	307
-10	381	381
-11	36	35
-12	184	-169
-13	86	79
-14	40	-20
-15	70	58
H= 13, K= 5		
-1	568	578
-2	457	-452
-3	282	-303
-4	72	94
-5	282	281
-6	92	-94
-7	157	163
-8	323	-324
-9	384	-371
-10	275	276
-11	115	106
-12	85	-81
-13	70	-63
-14	37*	-26
H= 13, K= 7		
-1	457	459
-2	808	815
-3	439	-442
-4	176	-170
-5	141	147
-6	189	-168
-7	45	-42
-8	250	245
-9	75	-61
-10	256	-264
-11	156	148
-12	122	125
-13	31*	-7
H= 13, K= 9		
-1	268	-273
-2	118	113
-3	132	129
-4	295	-304
-5	50	-51
-6	151	161
-7	117	-129
-8	96	-99
-9	189	169
-10	103	-107
H= 13, K= 11		
-1	134	-153
-2	161	-159
-3	158	175
-4	164	149
-5	84	-65
H= 14, K= 10		
-4	22*	70
-2	43	-33
-3	31*	-24
-4	73	70
-5	165	177
-6	31*	-33
-7	320	-332
-8	4*	15
H= 14, K= 8		
-1	233	-231
-2	212	216
-3	19*	-22
-4	197	201
-5	92	85
-6	373	-388
-7	36	16
-8	311	300
-9	32*	10
-10	253	-251
-11	95	104
-12	127	129
H= 14, K= 6		
-1	529	539
-2	27*	-30
-3	7*	-20
-4	48	-36
-5	530	-524
-6	3*	9
-7	616	619
-8	38	-15
-9	620	-631
-10	128	-146
-11	346	344
-12	34*	-33
-13	32*	24
H= 14, K= 4		
-1	169	157
-2	138	121
-3	143	-139
-4	103	-108
-5	116	108
-6	399	407
-7	62	63
-8	878	-861
-9	184	-180
-10	736	749
-11	93	73
-12	3*	21
-13	43	55
-14	170	-160
-15	123	-132
H= 14, K= 2		
-1	413	-425
-2	395	-376
-5	461	442
-6	18*	16
-7	735	-739
-8	144	-164
-9	746	739
-10	93	84
-11	324	-310
-12	215	-205
-13	86	74
-14	78	-84
-15	162	157
H= 14, K= 0		

L	FO	FC
-8	928	901
-10	656	-661
-12	382	371
-14	118	131
H= 15, K= 1		
-1	422	-420
-2	106	-106
-3	83	-73
-4	596	599
-5	508	480
-6	507	-524
H= 11, K= 7		
-2	232	224
H= 15, K= 1		
-7	574	-573
-8	190	195
-9	117	131
-10	120	120
-11	113	102
-12	201	-195
-13	403	-407
-14	318	311
-15	163	158
H= 15, K= 3		
-1	114	102
-2	64	-85
-3	311	-303
-4	256	246
-5	351	358
-6	559	540
-7	53	-73
-8	476	-484
-9	169	169
-10	39	17
-11	322	300
-12	84	71
-13	253	-245
-14	325	-301
-15	132	124
H= 15, K= 5		
-1	199	190
-2	197	-182
-3	70	67
-4	71	-56
-5	250	-253
-6	32	57
-7	333	351
-8	78	-93
-9	569	-590
-10	20*	17
-11	69	-54
-12	177	180
-13	330	321
-14	139	-147
H= 15, K= 7		
-1	76	64
-2	85	87
-3	53*	-173
-4	400	385
-5	11*	12
-6	334	-339
-7	17*	16
-8	157	152
-9	141	159
-10	60	66
-11	34*	41
-12	41	-39
-13	103	106
H= 15, K= 9		
-1	87	-75
-2	66	-91
-3	4*	7
-4	59	54
-5	212	206
-6	171	-172
-7	316	-312
-8	31*	8
-9	61	51
-10	37*	20
H= 15, K= 10		
-1	102	95
-2	69	82
-3	177	-182
-4	36*	-48
-5	324	324
-6	124	132
-7	192	-203
-8	52	-34
H= 16, K= 8		
-1	8*	-17
-2	47	-26
-3	235	-244
-4	183	170
-5	56	57
-6	253	-242
-7	134	-120
-8	46	-79
-9	26*	-44
-10	198	208
-11	110	100
-12	176	-184
H= 16, K= 6		
-1	48	53
-2	252	-253
-3	293	307
-4	474	470
-5	87	-93
-6	174	-166
-7	29*	31
-8	23*	39
-9	43	41
-10	33*	25
-11	178	-178
-12	170	-166
-13	252	245
-14	89	85
H= 16, K= 4		
-1	87	-73
-2	121	128
-3	21*	-9
-4	387	-386
-5	49	49
-6	483	467
-7	62	62
-8	218	-208
-9	50	-55
-10	144	-123
-11	3*	-10
-12	300	294
-13	59	36
-14	211	-222
-15	42	-41
H= 16, K= 2		
-1	223	-221
-2	29	9
-3	504	-525
-4	13*	43
-5	692	715
-6	214	212
-7	402	-397
-8	7*	-7
-9	129	-119
-10	3*	-27
-11	415	415
-12	159	164
-13	337	-328
-14	4*	-12
-15	173	184
H= 16, K= 0		
-2	35	-65
-4	841	861
-6	551	-548
-8	174	-180
-10	211	208
-12	627	-647
-14	339	364
-16	25*	18
H= 17, K= 1		
-1	617	627
-2	582	-594
-3	554	-587
-4	415	431
-5	461	462
-6	224	-215
-7	149	141
-8	145	-133
-9	350	-377
-10	254	259
-11	314	325
-12	105	-114
-13	408	-412
-14	74	75
-15	77	-70
-16	83	78
H= 17, K= 3		
-1	176	170
-2	360	368
-3	441	-426
-4	185	-203
-5	695	687
-6	360	350
-7	235	-244
-8	177	182
-9	59	-56
-10	557	-565
-11	89	94
-12	89	86
-13	67	68
-14	69	-59
-15	35*	57

L	FO	FC
H= 17, K= 5		
-1	381	-392
-2	454	459
-3	602	591
-4	307	-291
-5	409	-400
-6	169	167
-7	237	-221
-8	199	-196
-9	110	94
-10	83	-68
-11	272	-272
-12	163	147
-13	112	111
-14	48	-45
H= 17, K= 7		
-1	350	-336
-2	412	-421
-3	238	228
-4	279	283
-5	167	-153
-6	93	-95
-7	267	275
-8	8*	-15
-9	23*	16
-10	279	278
-11	25*	-11
-12	209	-207
-13	46	45
H= 17, K= 9		
-1	166	168
-2	206	-209
-3	169	-160
-4	363	372
-6	211	-215
-7	25*	-10
-8	27*	33
-9	236	-224
-10	52	-55
H= 18, K= 10		
-3	80	-94
-4	69	-72
-5	35*	18
-6	38*	-22
-7	243	249
H= 18, K= 8		
-1	82	81
-2	175	-188
-3	145	-139
-4	72	77
-5	38	28
-6	128	124
-7	59	-61
-8	378	-388
-9	113	-105
-10	263	263
-11	4*	18
H= 18, K= 6		
-1	357	-350
-2	245	-240
-3	444	451
-4	225	228
-5	152	158
-6	175	169
-7	226	-219
-8	20*	23
-9	376	363
-10	59	-57
-11	525	-521
-12	66	74
-13	241	252
H= 18, K= 4		
-1	142	-140
-2	386	385
-3	70	65
-4	202	-197
-5	158	-142
-6	352	-347
-7	159	-167
-8	471	479
-9	110	129
-10	643	-644
-11	103	79
-12	145	130
-13	28*	20
-14	34*	-35
-15	110	119
H= 18, K= 2		
-1	432	427
-2	52	59
-3	262	-258
-4	121	109
-5	9*	11
-6	53	46
-7	639	636
-8	61	73
-9	771	-763
-10	40	40
-11	331	328
-12	204	204
-13	175	-174
-14	45	-46
-15	74	-70
H= 18, K= 0		
-2	1153	-1194
-4	128	123
-6	632	642
-8	840	-834
-10	502	519
-12	598	-578
-14	93	96
-16	144	129
H= 19, K= 1		
-1	341	336
-2	281	-294
-3	41	-16
-4	211	-192
-5	241	-248
-6	467	467
-7	260	263
-8	345	-345
-9	149	-160
-10	164	162
-11	29*	24
-12	145	142
-13	163	159
-14	339	-338
-15	237	-223
-16	202	196
H= 19, K= 3		
-1	144	145
-2	36	34
-3	112	133
-4	89	72
-5	306	-297
-6	67	-72
-7	403	407
-8	332	340
-9	285	-293
-10	122	-121
-11	52	-44
-12	217	-221
-13	309	309
-14	270	269
-15	178	-169
H= 19, K= 5		
-1	276	-256
-2	109	108
-3	3*	22
-4	40	-36
-5	254	254
-6	72	-56
-7	153	-164
-8	110	98
-9	142	145
-10	254	-240
-11	136	-141
-12	105	124
-13	140	-141
-14	101	99
H= 19, K= 7		
-1	21*	21
-2	274	-269
-3	39	-57
-4	30*	-20
-5	159	155
-6	229	217
-7	161	-182
-8	295	-290
-9	104	102
-10	237	229
-11	68	-78
-12	34*	-18
H= 19, K= 9		
-1	262	258
-2	67	96
-3	53	-68
-4	86	-99
-5	63	-69
-6	268	279
-7	289	301
-8	150	-162
-9	245	-239
H= 20, K= 8		
-1	25*	-19
-2	86	-93
-3	4*	13
-4	112	-105
-5	25*	-20
-6	264	252
-7	256	262

L	FO	FC
-8	196	-197
-9	231	-218
-10	148	-155
-11	91	-104
H=	20, K=	6
-1	178	-173
-3	30*	36
-4	267	-265
-5	70	150
-6	365	364
-7	130	-107
-8	34	-18
-9	20*	-8
-10	153	159
-11	118	119
-12	107	116
-13	225	-224
H=	20, K=	4
-1	200	190
-2	23*	-31
-3	437	-435
-4	236	227
-5	149	148
-6	350	-362
-7	37	-57
-8	25*	23
-9	103	-97
-10	3*	-3
-11	190	189
-12	335	-333
-13	14*	7
-14	276	265
-15	16*	8
H=	20, K=	2
-1	212	223
-2	199	-192
-3	126	121
-4	83	-87
-5	301	-332
-6	149	154
-7	632	619
-8	115	105
-9	57	-44
-10	121	121
-11	540	-537
-12	3*	33
-13	365	366
-14	53	-47
-15	281	-293
H=	20, K=	0
-2	232	-230
-4	121	-115
-6	404	415
-8	41	-60
-10	233	-222
-12	370	366
-14	480	-491
-16	117	118
H=	21, K=	1
-1	328	-328
-2	326	329
-3	287	299
-4	564	-560
-5	249	-265
-6	501	510
-7	359	368
-8	113	-121
-9	52	-46
-10	46	-49
-11	114	-117
-12	58	73
-13	158	163
-14	143	-150
-15	33*	35
H=	21, K=	3
-1	150	-147
-2	678	-702
-3	376	385
-4	474	486
-5	572	-578
-6	427	-423
-7	307	306
-8	66	59
-9	234	-223
-10	258	251
-11	56	-56
-12	53	-55
-13	76	61
-14	49	49
-15	94	-93
H=	21, K=	5
-1	173	172
-2	251	-232
-3	590	-590
-4	324	301
-5	660	664
-6	219	-206
-7	21*	17
-8	244	237
-9	43	55
-10	3*	22
-11	77	66
-12	155	-163
-13	153	-149
-14	47	43
H=	21, K=	7
-1	142	138
-2	92	82
-3	285	-303
-4	315	-296
-5	182	160
-6	293	287
-7	156	-158
-8	131	-145
-9	104	-105
-10	170	-168
-11	54	72
-12	211	216
H=	21, K=	9
-3	238	250
-4	168	-169
-5	238	-248
-6	199	182
-7	145	151
-8	42	-49
H=	22, K=	8
-1	70	-57
-2	293	304
-3	14*	9
-4	178	-203
-5	28*	40
-6	19*	32
-7	28*	54
-8	203	190
-9	70	74
-10	346	-326
H=	22, K=	6
-1	219	206
-2	87	-86
-3	427	-433
-4	96	-89
-5	240	245
-6	71	76
-7	117	114
-8	40	33
-9	301	-296
-10	84	88
-11	386	395
-12	36*	-51
-13	233	-248
H=	22, K=	4
-1	115	122
-2	446	-458
-3	166	-172
-4	345	340
-5	84	-94
-6	61	-66
-7	77	77
-8	283	-296
-9	34	-26
-10	361	348
-11	58	-49
-12	325	-308
-13	4*	23
-14	81	77
H=	22, K=	2
-1	499	-499
-2	52	55
-3	428	426
-4	246	-241
-5	22*	15
-6	90	85
-7	156	-158
-8	39	26
-9	421	420
-10	149	151
-11	459	-448
-12	3*	12
-13	137	135
-14	42	-32
-15	34*	42
H=	22, K=	0
-2	321	315
H=	25, K=	3
-3	249	-253
-4	351	-366
-5	251	238
-6	276	274
-7	232	-256
-8	228	-234

L	FO	FC
H= 25, K= 3		
-9	127	145
-10	41	41
-11	88	-88
-12	171	161
-13	163	-169
-14	184	-181
H= 25, K= 5		
-1	4*	-22
-2	118	118
-3	164	155
-4	244	-246
-5	415	-401
-6	255	261
-7	377	368
-8	121	-118
-9	48	45
-10	138	-146
-11	174	-169
-12	173	181
-13	191	192
H= 25, K= 7		
-3	136	146
-4	104	117
-5	276	-267
-6	200	-196
-7	149	127
-8	89	92
-9	34*	-38
-10	139	148
-11	70	-58
H= 26, K= 6		
-2	43	40
-3	229	245
-4	36*	-57
-5	331	-345
-6	33*	-45
-7	36*	18
-8	105	-106
-9	263	265
-10	40	25
-11	291	-286
-12	22*	-11
H= 26, K= 4		
-1	109	121
-2	307	305
-3	4*	50
-4	428	-426
-5	23*	-12
-6	356	370
-7	136	141
-8	124	121
-9	4*	-33
-10	216	-206
-11	31*	-17
-12	330	334
-13	66	55
-14	158	-152
H= 26, K= 2		
-1	227	214
-2	37*	-43
-3	422	-430
-4	33*	-15
-5	209	187
-6	150	-145
-7	143	-137
-8	48	-31
-9	127	-119
-10	212	-224
-11	319	312
-12	103	101
-13	269	-264
-14	33*	36
-15	143	139
H= 26, K= 0		
-2	71	-81
-4	386	367
-6	148	-131
-8	85	-115
-10	356	351
-12	229	-227
-14	144	143
H= 27, K= 1		
-1	164	166
-2	128	-132
-3	204	-190
-4	16*	22
-5	121	-131
-6	113	112
-7	311	296
-8	237	-239
-9	309	-310
-10	276	264
-11	418	416
-12	223	-232
-13	139	-141
-14	99	100
-15	4*	19
H= 27, K= 3		
-1	193	185
-2	246	242
-3	47	-38
-4	76	-89
-5	57	-54
-6	32*	-19
-7	175	169
-8	147	149
-9	282	-282
-10	308	-307
-11	241	241
-12	341	342
-13	80	-69
-14	65	-79
H= 27, K= 5		
-2	51	23
-3	154	149
-4	23*	54
-5	35*	-42
-6	190	-201
-7	153	-149
-8	298	318
-9	210	217
-10	257	-262
-11	234	-239
-12	71	77
H= 27, K= 7		
-6	82	86
-7	176	-177
-8	240	-248
-9	239	240
H= 28, K= 6		
-5	50	76
-6	46	-34
-7	288	-280
-8	21*	-52
-9	217	206
-10	50	47
H= 28, K= 4		
-2	197	195
-3	134	136
-4	29*	0
-5	53	-68
-6	46	-24
-7	82	-68
-8	202	206
-9	13*	21
-10	81	-82
-11	92	-80
-12	127	-146
-13	4*	9
H= 28, K= 2		
-1	288	288
-2	86	74
-3	258	-264
-4	49	-64
-5	69	74
-6	74	-62
-7	118	112
-8	34*	-38
-9	156	-137
-10	87	-93
-11	111	107
-12	16*	-33
-13	140	136
-14	38*	-39
H= 28, K= 0		
-2	273	-264
-4	167	168
-6	192	184
-8	200	-180
-10	160	160
-12	163	163
-14	122	-107
H= 29, K= 1		
-1	112	110
-2	49	-50
-3	4*	-6
-4	59	-78
-5	274	-288
-6	200	206
-7	122	126
-8	143	-144
-9	107	-117
-10	35*	-17
-11	73	-68
-12	62	40
-13	144	135
-14	113	-110

L	FO	FC
1	198	202
0	300	-303
H=	5, K=	15
0	257	-269
1	102	-71
2	67*	-46
3	42*	48
4	117	111
5	281	-298
6	196	-160
7	39*	9
8	84*	-112
H=	5, K=	14
9	132	152
8	207	-189
7	59*	-41
6	55*	49
5	119	105
4	42*	-56
3	58*	-22
2	258	-222
1	395	-392
0	228	242
H=	5, K=	13
0	115	-131
1	10*	12
2	10*	15
3	450	-446
4	92	-79
5	10*	-33
6	109	102
7	10*	12
8	106	109
9	51*	-63
10	43*	-24
H=	5, K=	12
11	92	-69
10	27*	21
9	100	35
8	111	109
7	162	176
6	83*	-113
5	207	-226
4	410	398
3	180	-180
2	173	144
1	362	375
0	509	-510
H=	5, K=	11
0	197	-192
1	200	176
2	70*	-85
3	269	271
4	298	289
5	174	-191
6	169	-180
7	212	220
8	181	-182
9	390	370
10	255	231
11	130	-113
H=	5, K=	10
12	131	133
11	162	177
10	47*	6
9	83	-34
8	230	-288
7	283	-314
6	460	466
5	160	138
4	222	235
3	126	141
2	324	-354
1	612	-617
0	163	171
H=	5, K=	9
0	395	407
1	343	328
2	90	100
3	352	-336
4	334	-341
5	337	340
6	164	187
7	150	120
8	128	95
9	182	-179
10	249	-254
11	87*	26
12	164	-151
H=	5, K=	8
13	11*	12
12	67*	-33
11	324	-307
10	174	-206
9	53*	-38
8	92	-95
7	238	252
6	299	-265
5	202	-230
4	187	175
3	46*	-13
2	420	401
1	1040	1061
0	385	-400
H=	5, K=	7
0	81	124
1	186	-195
2	97	-110
3	393	409
4	427	445
5	445	-440
6	26*	-42
7	136	-175
8	142	-144
9	106	123
10	10*	-29
11	123	-142
12	71*	-37
13	121	-120
H=	5, K=	6
14	11*	20
13	160	-185
12	130	137
11	190	163
10	131	166
9	237	251
8	299	-337
7	307	-328
6	72	14
5	71	27
4	80	-69
3	398	372
2	239	-270
1	442	-432
0	38*	-13
H=	5, K=	5
0	155	-144
1	107	59
2	101	-111
3	1127	-1136
4	347	-365
5	54*	-45
6	325	332
7	41*	-32
8	90	89
9	92	-91
10	10*	-76
11	163	167
12	183	198
13	23*	26
14	129	101
H=	5, K=	4
14	11*	-18
13	314	350
12	10*	38
11	53*	15
10	124	92
9	9*	-6
8	159	-126
7	294	317
6	89	-87
5	326	-333
4	63*	77
3	551	-552
2	85	47
1	372	429
0	193	-161
H=	5, K=	3
0	298	-301
1	387	346
2	105	-129
3	827	805
4	159	154
5	212	-215
6	95	99
7	99	77
8	132	70
9	341	406
10	28*	41
11	200	-191
12	10*	11
13	153	-186
14	38*	49
H=	5, K=	2
14	11*	-72
13	236	-254
12	10*	13
11	338	340
10	62*	-90
9	64*	-26
8	303	310
7	285	-258

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 24, K= 4						-7	237	-250			
			H= 24, K= 2			-8	61	-60	H= 24, K= 0		
-8	128	-124				-9	156	153			
-9	77	73	-1	366	-363	-10	24*	-51	-2	322	334
-10	80	92	-2	29*	32	-11	31*	-2	-4	193	-190
-11	69	89	-3	27*	9	-12	69	81	-6	245	-232
-12	244	248	-4	21*	29	-13	206	-211	-8	274	272
-13	76	-78	-5	134	132	-14	106	110	-10	13*	15
-14	326	-315	-6	68	-60	-15	378	380	-12	229	-226

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-14	224	233	-5	136	133	-13	41	-29			
			-6	268	-265	-14	157	156	H= 16, K= 0		
H= 25, K= 1			-7	250	-261	-15	46	-37			
			-8	184	183				0	530	-584
-1	31*	41	-9	156	156	H= 25, K= 3					
-2	61	-50	-10	62	-71				H= 15, K= 1		
-3	21*	-15	-11	303	313	-1	84	83			
-4	185	191	-12	19*	-15	-2	230	231	8	195	196

d $\underline{Ni(L2)(H_2O)(ClO_4)_2 \cdot 3H_2O}$

This structure was solved using MULTAN based on an inner set of data ($2\theta < 30$ deg). From a Fourier synthesis with 100 reflections whose E values were >1.5, the positions of the nickel, two chlorine, and ten lighter atoms were determined. Refinement of these parameters and a scale factor gave an R of 0.32. Several cycles of refinement and subsequent electron density difference syntheses revealed all non-hydrogen atom positions. Inclusion of the outer set of data, calculated hydrogen atom positions, together with anisotropic thermal motion parameters for all non-hydrogen atoms gave an R-factor of 0.092. Considerable thermal motion was evident in the oxygen atoms of both perchlorate anions. In one case (O11), splitting of the atom with two half-occupied positions, and subsequent refinement using isotropic and then anisotropic parameters gave a model for that perchlorate anion which fitted the data considerably better. Similar attempts to split other oxygen atoms which showed this behaviour were deemed not successful since the resulting pair did not behave well when refined and gave no improved agreement with the data. Full matrix, least-squares refinement gave a final R-factor of 0.079 (370 parameters).

Final atomic coordinates are given in table 2.11, and thermal motion parameters in table 2.12. Hydrogen atom coordinates (table 2.13) and measured and calculated structure factors (x10) are also listed (table 2.14).

Table 2.11

Fractional Atomic Coordinates: $Ni(L2)H_2O(ClO_4)_2.3H_2O$

($\times 10^4$, $\times 10^5$ for Ni)

Atom		x	y	z
Ni		16952(9)	24120(4)	15692(5)
Cl1	perchlorate anions	-2417(3)	4787(1)	1212(2)
Cl2		2923(3)	3782(1)	4604(1)
O11		-2720(22)	5437(9)	1387(15)
O11'		-3586(19)	5221(12)	1140(13)
O12		-2306(8)	4426(5)	1930(6)
O13		-1148(9)	4947(5)	973(6)
O14		-2936(11)	4338(6)	655(7)
O21		3251(7)	3219(4)	4088(4)
O22		4026(10)	4257(5)	4690(6)
O23		2819(8)	3525(4)	4617(4)
O24		1707(8)	4093(4)	4323(5)
O1		2583(5)	2015(2)	518(3)
O2		-280(5)	2517(3)	908(3)
O3		-415(6)	3656(3)	-26(3)
O4		724(6)	3512(3)	-152(3)
O5		1111(6)	2184(3)	-99(3)
N1		3786(6)	2358(3)	1888(3)
N2		1726(6)	3504(3)	1491(3)
N3		1022(7)	2594(3)	2697(4)
N4		1183(6)	1359(3)	1598(3)
N5		4436(6)	1692(3)	1901(4)
N6		1714(6)	956(3)	998(3)
C1		4050(8)	1243(4)	1374(5)
C2		4756(9)	559(4)	1476(6)
C3		4050(8)	1243(4)	1374(5)
C4		3204(8)	935(4)	-89(5)
C5		4640(8)	2863(4)	1949(4)
C6		6220(8)	2763(4)	1916(6)
C7		4176(8)	3595(4)	2020(5)
C8		3068(8)	3855(4)	1375(4)
C9		3432(8)	3671(4)	541(5)
C10		2941(8)	4647(4)	1440(5)
C11		1059(8)	3771(4)	2214(4)
C12		232(9)	3223(4)	2593(5)
C13		442(8)	1993(4)	3128(5)
C14		-393(10)	2244(5)	3807(5)
C15		1700(10)	1590(4)	3507(5)
C16		-449(8)	1531(4)	2576(5)
C17		195(8)	1098(4)	1950(4)
C18		-379(8)	395(4)	1766(5)

Table 2.12

Thermal Motion Parameters: $Ni(L2)H_2O(ClO_4)_2.3H_2O$.

($\times 10^3$, $\times 10^4$ for Ni A^2)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni	407(7)	317(7)	356(7)	-11(5)	152(4)	-9(4)
Cl1	76(2)	49(2)	80(2)	1(1)	29(1)	0(1)
Cl2	77(2)	60(2)	62(2)	11(1)	3(1)	4(1)
O11	143(22)	57(10)	219(21)	-23(12)	132(18)	-31(10)
O11'	114(16)	143(22)	99(14)	95(14)	47(12)	77(15)
O12	120(7)	176(9)	205(10)	36(6)	38(6)	113(8)
O13	158(8)	125(7)	271(12)	33(6)	138(8)	-17(7)
O14	207(11)	198(11)	210(11)	-78(9)	22(9)	-89(9)
O21	106(6)	106(6)	91(5)	31(4)	4(4)	-39(4)
O22	180(9)	164(9)	184(10)	-68(8)	47(7)	-27(7)
O23	158(4)	133(7)	82(6)	-43(6)	24(5)	-32(5)
O24	144(7)	134(7)	113(6)	85(6)	-31(5)	-10(5)
O1	48(3)	31(3)	40(3)	-0(2)	14(2)	0(2)
O2	52(3)	62(4)	53(3)	5(3)	-1(3)	3(3)
O3	96(5)	74(4)	49(4)	20(4)	-1(3)	-3(3)
O4	105(5)	55(4)	66(4)	19(3)	3(4)	-1(3)
O5	82(4)	61(4)	49(4)	-2(3)	10(3)	-8(3)
N1	44(4)	35(4)	53(4)	1(3)	15(3)	-6(3)
N2	47(4)	39(4)	44(4)	-2(3)	10(3)	-6(3)
N3	71(5)	46(4)	46(4)	21(4)	27(3)	12(3)
N4	41(4)	35(3)	52(4)	-6(3)	24(3)	-3(3)
N5	52(4)	33(4)	52(4)	-4(3)	16(3)	-1(3)
N6	44(4)	50(4)	47(4)	-9(3)	17(3)	-13(3)
C1	43(5)	38(5)	54(5)	2(4)	16(4)	6(4)
C2	71(6)	41(50)	96(7)	11(5)	2(5)	-2(5)
C3	43(5)	40(5)	51(5)	-3(4)	21(4)	-8(4)
C4	73(6)	54(5)	57(6)	-4(5)	31(5)	-25(4)
C5	56(5)	46(5)	30(4)	-4(4)	8(4)	-17(4)
C6	26(5)	69(6)	117(8)	11(4)	6(5)	18(6)
C7	45(5)	35(4)	63(6)	-4(4)	10(4)	-4(4)
C8	47(5)	36(4)	47(5)	-3(4)	17(4)	0(4)
C9	76(6)	49(5)	48(5)	-12(4)	25(4)	1(4)
C10	69(6)	39(5)	77(6)	3(4)	4(5)	-0(4)
C11	58(5)	46(5)	49(5)	-1(4)	9(4)	-3(4)
C12	86(7)	60(6)	51(6)	7(5)	32(5)	14(4)
C13	56(8)	47(5)	44(5)	1(4)	28(4)	9(5)
C14	108(5)	85(7)	54(6)	-5(6)	48(6)	10(4)
C15	98(7)	63(6)	44(5)	4(5)	1(5)	13(4)
C16	58(6)	68(6)	56(6)	-14(5)	30(5)	-3(5)
C17	48(5)	46(5)	41(5)	-7(4)	5(4)	4(4)
C18	59(6)	56(6)	66(6)	-17(4)	12(5)	1(4)

Table 2.13

Hydrogen Atom Coordinates: $Ni(L2)H_2O(ClO_4)_2.3H_2O$.

($\times 10^4$)

Atom	x	y	z
H(01)	2083	2290	-5
H(02)	-329	2927	570
H(02)'	-937	2157	727
H(03)	-1200	3868	180
H(03)'	-22	3606	-510
H(04)	870	4029	-1327
H(04)'	279	3442	-2065
H(05)	153	2049	-963
H(05)'	977	2642	-1173
H(N2)	1173	3455	1028
H(N3)	1890	2716	2990
H(N6)	999	881	567
H(C2)1	5408	457	1949
H(C2)2	5265	496	1008
H(C2)3	4033	214	1475
H(C4)1	3083	459	-231
H(C4)2	4178	1091	-128
H(C4)3	2671	1183	-513
H(C6)1	6666	2292	2143
H(C6)2	6682	3138	2221
H(C6)3	6422	2800	1359
H(C7)1	3807	3645	2538
H(C7)2	4978	3889	2000
H(C9)1	2655	3796	169
H(C9)2	4227	3946	430
H(C9)3	3636	3222	454
H(C10)1	2223	4814	1071
H(C10)2	2741	4769	1980
H(C10)3	3804	4859	1322
H(C11)1	1774	3933	2608
H(C11)2	454	4152	2048
H(C12)1	-9	3384	3112
H(C12)2	-602	3132	2251
H(C14)1	-1155	2426	3539
H(C14)2	-628	1862	4146
H(C14)3	108	2592	4131
H(C15)1	2302	1533	3079
H(C15)2	2133	1896	3913
H(C15)3	1692	1116	3776
H(C16)1	-907	1212	2913
H(C16)2	-1129	1827	2289
H(C18)1	-1342	409	1565
H(C18)2	141	144	1391
H(C18)3	-258	226	2260

Table 2.14

Structure Factor Listing: $Ni(L2)H_2O(ClO_4)_2.3H_2O$.

(x10)

Unobserved reflections are indicated by an asterisk.

L	FO	FC
H=	0, K=	0
2	327	-358
4	1691	-1791
6	931	951
8	259	-295
10	545	-644
12	100	135
14	97	75
16	159	-209
18	11*	-9
H=	0, K=	1
19	76*	-6
18	205	245
17	11*	-56
16	77*	-87
15	202	-200
14	70*	-44
13	53*	-55
12	261	256
11	197	158
10	546	538
9	567	-593
8	832	-802
7	519	-485
6	277	-239
5	477	482
4	1708	1552
3	1618	1468
2	2058	-1903
1	109	123
H=	0, K=	2
0	1608	-1651
1	70	-147
2	1262	1175
3	450	411
4	211	-207
5	1547	1457
6	361	-355
7	34*	-65
8	700	647
9	100	91
10	406	371
11	303	277
12	678	-562
13	116	-107
14	90	-73
15	10*	4
16	329	304
17	86	-45
18	27*	-9
19	12*	-15
H=	0, K=	3
19	12*	16
18	270	-242
17	73*	-17
16	79*	-37
15	167	152
14	328	292
13	312	260
12	142	-119
11	139	141
10	348	-299
9	83	56
8	1144	1136
7	476	428
6	526	516
5	1065	1014
4	88	68
3	352	-328
2	351	-384
1	1505	-1407
H=	0, K=	4
0	411	-400
1	533	509
2	1354	-1263
3	614	574
4	1882	-1763
5	43*	109
6	64	36
7	745	746
8	95	174
9	427	397
10	170	144
11	79	-66
12	425	359
13	155	-159
14	10*	-37
15	76*	-64
16	175	-152
17	11*	-10
18	135	94
19	12*	40
H=	0, K=	5
19	102	71
18	251	208
17	11*	-13
16	92	62
15	23*	-77
13	519	427
12	128	99
11	45*	40
10	285	273
9	220	-238
8	671	-665
7	184	-214
6	491	449
5	365	320
4	896	849
3	86	49
2	1562	-1512
1	1017	-954
H=	0, K=	6
0	558	-564
1	47*	144
2	151	-192
3	55	4
4	146	110
5	129	-129
6	360	-422
7	768	-724
8	330	339
9	338	-358
10	108	109
11	107	70
H=	0, K=	5
14	333	-326
H=	0, K=	6
12	434	-360
13	71*	98
14	132	-104
15	116	83
16	330	281
17	202	181
18	79*	-77
19	12*	-7
H=	0, K=	7
18	189	-192
17	60*	13
16	133	103
15	53*	24
14	149	373
13	151	-430
12	247	-236
11	96	48
10	518	-508
9	145	-166
8	115	91
7	391	-383
6	554	-534
5	292	257
4	816	-757
3	405	372
2	754	675
1	1081	-1016
H=	0, K=	8
0	675*	2072
1	5*	28
2	5*	-14
3	255	251
4	588	-565
5	507	-513
6	558	570
7	265	-303
8	187	195
9	101	99
10	577	-473
11	49*	47
12	70*	67
13	92	-96
14	169	151
15	60*	-76
16	330	-292
17	140	-106
18	57*	93
H=	0, K=	9
18	92*	88
17	183	-147
16	191	-114
15	193	-141
14	279	-211
13	307	247
12	177	190
11	193	-144
10	272	233
9	509	-494
8	406	-368
7	129	99
6	395	432
5	95	107
4	546	549
3	33*	-26
2	1517	-1455
1	450	467
H=	0, K=	10
0	1004	-1014

L	FO	FC
1	6*	39
2	768	748
3	53*	86
4	485	482
5	410	437
6	829	-837
7	149	-150
8	96	-77
9	9*	34
10	665	574
11	532	459
12	424	-362
13	203	-183
14	214	-190
15	178	-126
16	330	281
17	77*	34

H= 0, K= 11

L	FO	FC
17	58*	67
16	64*	-7
15	218	181
14	326	286
13	133	-123
12	41*	76
11	128	96
10	450	-359
9	559	474
8	567	488
7	215	-172
6	161	155
5	111	100
4	189	-124
3	291	298
2	48*	131
1	6*	-17

H= 0, K= 12

L	FO	FC
0	106	-99
1	500	506
2	391	-359
3	356	335
4	350	-333
5	548	-529
6	88	111
7	12*	14
8	254	219
9	643	553
10	82	-38
11	274	-242
12	512	434
13	35*	59
14	68*	28
15	113	92
16	208	-195

H= 0, K= 13

L	FO	FC
16	64*	36
15	89	-33
14	179	-131
13	205	187
12	159	-112
11	105	54
10	10*	50
9	41*	34
8	224	-186
7	253	211
6	564	442
5	74	111
4	129	144
3	381	-355
2	479	-484
1	7*	-56

H= 0, K= 14

L	FO	FC
0	374	-357
1	164	-165
2	281	247
3	167	140
4	312	260
5	65*	62
6	185	-163
7	413	-338
8	187	-139
9	127	-119
10	115	127
11	138	142
12	141	-107
13	98	-98
14	11*	31
15	106	-60

H= 0, K= 15

L	FO	FC
14	230	204
13	154	-120
12	187	-170
11	311	-269
10	256	-238
9	42*	26
8	171	163
7	20*	30
6	197	-185
5	472	-415
4	386	-338
3	413	356
2	242	227
1	96	-99

H= 0, K= 16

L	FO	FC
0	327	259
1	421	374
2	101	57
3	68*	48
4	92	61
5	598	-525
6	105	79
7	135	101
8	172	-130
9	45*	-44
10	313	-283
11	96	-42
12	11*	62
13	12*	24
14	93*	31

H= 0, K= 17

L	FO	FC
13	146	79
12	191	185
11	88*	-82
10	54*	12
9	224	-196
8	142	-154
7	285	239
6	280	251
5	198	197
4	55*	-30
3	648	-577
2	422	-392
1	396	345

H= 0, K= 18

L	FO	FC
0	338	-307
1	39*	-69
2	73*	-26
3	62*	62
4	233	166
5	523	411
6	128	-113
7	186	-168
8	11*	-50
9	39*	19
10	160	167
11	201	163
12	152	-114

H= 0, K= 19

L	FO	FC
11	79*	38
10	17*	-66
9	285	267
8	194	168
7	173	-153
6	45*	29
5	192	-148
4	165	133
3	343	301
2	192	138
1	103	-108

H= 0, K= 20

L	FO	FC
0	79*	12
1	234	231
2	90	-79
3	153	142
4	52*	-59
5	296	-266
6	170	138
7	163	137
8	72*	-44
9	90	79

H= 0, K= 21

L	FO	FC
7	202	188
6	56*	67
5	64*	-4
4	101	-64
3	382	-302
2	84*	-95
1	157	132

H= 0, K= 22

L	FO	FC
0	134	-131
1	260	-215
2	57*	22
3	41*	-64
4	147	120
5	111	112

H= 1, K= 22

L	FO	FC
4	132	117
3	12*	-5
2	106	-88
1	75*	-17
0	268	-240

H= 1, K= 21

L	FO	FC
0	65*	64

L	FO	FC
H=	1, K=	21
2	109	-194
3	11*	-17
4	120	112
5	12*	-33
6	162	132
7	108	-70
H=	1, K=	20
9	72*	-57
8	126	99
7	160	107
6	165	158
5	189	153
4	191	-147
3	217	-184
2	120	144
1	11*	-54
0	198	171
H=	1, K=	19
0	70*	-30
1	480	439
2	383	350
3	11*	-25
4	11*	-9
5	115	-78
6	317	-268
7	258	220
8	250	216
9	135	-117
10	125	115
H=	1, K=	18
11	185	-162
10	122	141
9	11*	37
8	164	-138
7	53*	-15
6	237	-218
5	81*	-39
4	475	420
3	190	187
2	288	256
1	43*	15
0	219	-237
H=	1, K=	17
0	10*	-68
1	117	-132
2	74*	-86
3	183	140
4	123	105
5	10*	-28
6	10*	24
7	97	-49
8	256	-229
9	267	242
10	11*	-23
11	97	84
12	134	93
H=	1, K=	16
13	40*	31
12	100	73
11	128	92
10	120	-81
9	207	-189
8	100	-80
7	155	-153
6	239	212
5	161	138
4	98	-97
3	274	-218
2	170	-164
1	253	-251
0	9*	18
H=	1, K=	15
0	114	-87
1	364	334
2	179	177
3	602	-550
4	135	-148
5	140	-97
6	299	-263
7	358	337
8	233	-193
9	209	-196
10	43*	70
11	96	-101
12	74*	-62
13	185	148
14	75*	11
H=	1, K=	14
15	126	111
14	11*	-57
13	153	135
12	184	133
11	271	-218
10	95	58
9	168	161
8	237	-207
7	197	160
6	273	-250
5	256	-267
4	398	367
3	283	279
2	170	-147
1	289	257
0	649	-606
H=	1, K=	13
0	42*	-32
1	392	-388
2	231	-212
3	141	-140
4	478	474
5	423	-370
6	163	144
7	176	-183
8	74*	91
9	198	166
10	36*	16
11	10*	-11
12	173	138
13	106	-99
14	132	-87
15	37*	34
16	96*	-79
H=	1, K=	12
16	128	-128
15	156	-127
14	84	99
13	108	-127
12	134	182
11	115	147
10	202	-205
9	85	-91
8	82	-87
7	243	285
6	321	361
5	320	321
4	262	-262
3	115	-106
2	116	-51
1	57*	-93
0	103	95
H=	1, K=	11
0	342	-312
1	285	320
2	327	337
3	327	-316
4	336	-361
5	80	65
6	7*	-28
7	343	325
8	539	566
9	30*	34
10	116	113
11	340	-284
12	172	-148
13	91	79
14	179	150
15	11*	3
16	59*	4
17	165	-116
H=	1, K=	10
17	84*	-53
16	11*	-31
15	315	262
14	61*	-84
13	109	-91
12	264	-265
11	417	-391
10	88	127
9	501	451
8	345	-332
7	261	-271
6	217	-217
5	809	-781
4	1064	1040
3	107	103
2	146	-120
1	179	173
0	280	-281
H=	1, K=	9
0	586	562
1	521	-492
2	886	-865
3	978	906
4	247	-275
5	44*	53
6	274	263
7	279	-250
8	624	-618
9	449	425
10	9*	-35
11	184	166
12	153	108
13	655	-558
14	10*	-93

L	FO	FC
15	123	-106
16	59*	55
17	320	258
H=	1, K=	8
18	12*	-12
17	136	92
16	111	-96
15	291	-266
14	10*	-8
13	217	180
12	208	204
11	478	444
10	144	-123
9	509	-531
8	208	-189
7	337	-345
6	264	256
5	561	526
4	357	-354
3	338	-323
2	108	134
1	314	-311
0	785	719
H=	1, K=	7
0	740	-751
1	1053	1026
2	232	222
3	771	-768
4	118	111
5	376	-350
6	83	78
7	488	505
8	222	233
9	118	-135
10	286	-269
11	40*	-16
12	309	-302
13	383	355
14	42*	-14
15	196	149
16	71*	-6
17	181	-181
18	84*	-66
H=	1, K=	6
18	12*	-17
17	71*	-74
16	151	125
15	208	183
14	62*	63
13	63*	17
12	456	452
11	266	-257
10	262	243
9	561	557
8	203	150
7	210	173
6	178	-166
5	411	-453
4	77	63
3	468	434
2	158	170
1	536	551
0	1431	-1422
H=	1, K=	5
0	393	405
1	725	-727
2	325	-302
3	547	-552
4	117	107
5	221	224
6	453	490
7	702	-749
8	72	97
9	443	396
10	50*	-75
12	228	238
13	168	-198
14	181	166
15	172	156
16	56*	15
17	241	252
18	11*	-36
19	161	-160
H=	1, K=	4
19	44*	10
18	70*	-32
17	73*	23
16	18*	-33
15	284	-286
14	72*	94
13	9*	19
12	110	-126
11	530	505
10	97*	-99
9	415	-373
8	17*	-27
7	578	-544
6	313	338
5	121	-88
4	279	-249
3	1190	1179
2	351	-350
1	753	717
0	105	-38
H=	1, K=	3
0	348	-378
1	1270	1275
2	334	-327
3	548	550
4	393	358
5	109	-108
6	306	805
7	85	144
8	440	449
9	157	-203
10	341	-350
11	421	-410
12	9*	-4
13	64*	37
14	187	179
15	78*	-62
16	26*	-36
17	188	-209
18	38*	-9
19	105	141
H=	1, K=	2
19	92*	-117
18	11*	-46
17	11*	18
16	87*	-114
15	141	198
14	61*	-110
13	381	-428
12	240	-316
11	241	-299
10	212	-222
9	528	552
8	145	-176
7	134	-166
6	361	-372
5	147	120
4	737	755
3	133	110
2	299	245
1	1393	1457
0	538	541
H=	1, K=	1
0	329	337
1	1284	-1342
2	1622	-1661
3	1635	1774
4	781	-798
5	95	66
6	73	-80
7	267	-323
8	203	-174
9	191	181
10	76	-45
11	362	363
12	124	-182
13	492	-600
14	10*	-70
15	120	-116
16	98	111
17	163	242
18	50*	-31
19	240	-230
H=	1, K=	0
19	269	326
17	100	105
15	400	-501
13	380	499
11	834	924
9	558	-662
7	540	-574
5	306	-330
3	75	-32
1	794	-865
H=	2, K=	0
0	1210	-1108
2	1485	-1560
4	915	914
6	238	233
8	592	-597
10	702	743
12	300	331
14	339	-385
16	280	329
18	72*	64
H=	2, K=	1
19	90*	-2
18	66*	-115
17	41*	65
16	259	268
15	108	95
14	48*	-16
13	52*	-76
12	684	-826

L	FO	FC
H=	2, K=	1
11	104	-121
10	469	482
9	45*	-19
8	385	382
7	168	158
6	749	795
5	109	-156
4	815	868
3	1991	-2095
2	1566	1625
1	148	-109
0	630	-571
H=	2, K=	2
0	1081	-1103
1	509	-492
2	675	706
3	391	-427
4	388	-367
5	572	568
6	5*	8
7	50*	-99
8	435	439
9	299	-296
10	635	-674
11	227	-244
12	84	-136
13	9*	-31
14	251	313
15	10*	17
16	180	-202
17	66*	-101
18	11*	-33
19	43*	22
H=	2, K=	3
19	36*	1
18	109	137
17	11*	-29
16	98	-81
15	45*	-2
14	33*	17
13	128	-107
12	247	312
11	262	-234
10	432	-452
9	100	69
8	330	-376
7	324	364
6	433	461
5	280	-327
4	419	430
3	239	191
2	209	-179
1	1623	1713
0	1559	1514
H=	2, K=	4
0	70	-27
1	741	-841
2	653	661
3	218	229
4	626	668
5	112	93
6	212	-250
7	184	-175
8	1070	-1078
9	110	-145
10	209	227
11	59*	51
12	188	185
13	175	201
14	184	-209
15	73*	-38
16	88*	-86
17	11*	24
18	12*	16
H=	2, K=	5
18	165	-148
17	70*	27
16	85*	61
15	151	-160
14	10*	-30
13	68*	71
12	142	-154
11	106	120
10	342	312
9	242	244
8	420	371
7	147	181
6	99	46
5	113	94
4	597	-613
3	410	416
2	268	236
1	474	404
0	696	-720
H=	2, K=	6
0	222	230
1	364	-331
2	283	247
3	189	249
4	185	-218
5	660	639
6	333	328
7	129	153
8	547	538
9	277	258
10	271	-273
11	119	140
12	141	137
13	153	-132
14	191	172
15	120	106
16	72*	-55
17	62*	27
18	107	-101
H=	2, K=	7
18	141	130
17	11*	7
16	237	-210
15	72*	101
14	131	-149
13	60*	12
12	416	419
11	47*	-26
10	136	136
9	171	170
8	215	-209
7	118	116
6	456	484
5	307	-313
4	52*	11
3	849	-872
2	673	-654
1	235	-280
0	821	882
H=	2, K=	8
0	358	-443
1	245	-284
2	94	-136
3	691	-669
4	864	829
5	6*	51
6	318	-296
7	123	153
8	511	-518
9	303	-296
10	553	521
11	79	61
12	206	152
13	212	195
14	161	-132
15	101	-100
16	177	132
17	58*	-56
H=	2, K=	9
17	96	75
16	324	285
15	99	84
14	32*	-47
13	10*	-76
12	476	-469
11	167	156
10	461	447
9	9*	20
8	81	97
7	310	-290
6	1001	-989
5	116	-135
4	51*	-70
3	145	130
2	817	804
1	683	-656
0	128	-144
H=	2, K=	10
0	114	-48
1	451	-501
2	6*	24
3	172	175
4	320	-267
5	56*	23
6	100	89
7	114	-112
8	259	247
9	283	-321
10	284	-269
11	317	-313
12	179	-167
13	138	-131
14	229	165
15	199	138
16	93*	-51
17	12*	34
H=	2, K=	11
16	133	-113
15	25*	12
14	11*	-35
13	11*	-16
12	148	113
11	309	-264

L	FO	FC
10	484	-450
9	104	86
8	175	-173
7	325	322
6	97	100
5	7*	-32
4	130	-156
3	85	-57
2	91	44
1	173	214
0	631	624

H= 2, K= 12

0	55*	55
1	233	-204
2	77	-77
3	237	-220
4	340	353
5	384	377
6	135	-96
7	48*	-43
8	323	-291
9	116	-70
10	22*	38
11	93	-95
12	111	-106
13	135	159
14	213	-176
15	116	-99
16	49*	-8

H= 2, K= 13

15	131	-128
14	43*	-11
13	112	-91
12	108	-87
11	171	160
10	446	418
9	187	-186
8	181	172
7	308	-279
6	424	-403
5	373	356
4	192	-182
3	431	440
2	292	276
1	147	-160
0	298	-297

H= 2, K= 14

0	240	252
1	173	-150
2	206	209
3	83	97
4	193	-218
5	53*	52
6	225	238
7	271	276
8	313	301
9	191	147
10	160	-158
11	56*	67
12	11*	-16
13	44*	-51
14	174	137

H= 2, K= 15

14	100	-38
13	168	148
12	181	145
11	107	-100
10	88*	96
9	172	171
8	10*	31
7	112	104
6	94	48
5	346	-340
4	348	329
3	107	122
2	9*	57
1	163	-143
0	60*	-28

H= 2, K= 16

0	10*	-72
1	96	-75
2	182	-208
3	232	-202
4	37*	36
5	190	196
6	51*	-97
7	362	321
8	61*	35
9	258	-237
10	231	201
11	11*	15
12	96	96
13	112	143

H= 2, K= 17

12	114	-72
11	214	201
10	48*	72
9	11*	-97
8	36*	39
7	285	-248
6	244	-211
5	224	207
4	127	-102
3	138	-109
2	412	422
1	140	-103
0	10*	-49

H= 2, K= 18

0	261	231
1	10*	3
2	113	100
3	10*	45
4	318	-287
5	255	-211
6	118	-111
7	251	-227
8	136	119
9	200	161
10	144	-106
11	147	-128

H= 2, K= 19

10	148	-119
9	12*	-35
8	161	-118
7	179	156
6	54*	8
5	136	-79
4	139	-141
3	57*	16
2	131	-137
1	192	198
0	207	214

H= 2, K= 20

0	75*	74
1	41*	-33
2	11*	-64
3	251	-241
4	57*	-10
5	146	162
6	64*	38
7	123	95
8	12*	-46

H= 2, K= 21

6	41*	-77
5	222	189
4	58*	34
3	174	163
2	82*	94
1	274	-273
0	142	-149

H= 2, K= 22

0	103	118
1	12*	-30
2	80*	31
3	176	178

H= 3, K= 22

1	73*	70
0	27*	107

H= 3, K= 21

0	131	-121
1	135	143
2	35*	22
3	61*	89
4	119	117
5	80*	-68

H= 3, K= 20

7	165	-160
6	12*	52
5	72*	-78
4	69*	57
3	194	185
2	211	-216
1	78*	48
0	54*	-6

H= 3, K= 19

0	256	261
1	325	-320
2	146	-133
3	73*	-86
4	142	-142
5	90*	94
6	257	225
7	65*	-54
8	95	-38
9	114	-123

H= 3, K= 18

10	47*	-67
9	72*	-51

L	FO	FC
H= 3, K= 18		
8	315	297
7	148	82
6	190	-211
5	57*	-6
4	334	-327
3	218	-208
2	124	137
1	59*	51
0	86	-51
H= 3, K= 17		
0	440	-433
1	37*	79
2	134	-136
3	23*	52
4	223	206
5	210	-206
6	200	-220
7	11*	-59
8	95	95
9	116	90
10	220	221
11	12*	-18
H= 3, K= 16		
12	12*	16
11	159	158
10	45*	58
9	186	179
8	253	-242
7	167	-145
6	217	214
5	52*	-58
4	72*	39
3	324	326
2	248	-248
1	215	-222
0	252	272
H= 3, K= 15		
0	210	222
1	80*	-149
2	104	-67
3	386	354
4	315	-317
5	408	378
6	452	444
7	98	-69
8	21*	-8
9	146	-123
10	180	-142
11	135	129
12	150	129
13	61*	-61
H= 3, K= 14		
14	86*	93
13	116	121
12	109	-86
11	50*	-50
10	158	-118
9	152	-146
8	444	426
7	10*	-26
6	165	158
5	112	114
4	182	-202
3	56*	-25
2	306	279
1	146	154
0	244	259
H= 3, K= 13		
0	80	-108
1	189	207
2	47*	11
3	219	198
4	160	192
5	9*	-19
6	463	-464
7	101	84
8	33*	63
9	77*	76
10	10*	-22
11	227	-195
12	224	-181
H= 3, K= 12		
13	202	-176
12	107	76
11	36*	38
10	10*	49
9	168	119
8	102	-76
7	521	-469
6	61*	-40
5	297	-287
4	51*	-18
3	312	298
2	7*	-62
1	170	-169
0	95	89
H= 3, K= 11		
0	439	460
1	633	-642
2	243	280
3	172	-149
4	262	-271
5	715	714
6	148	159
7	552	-532
8	89	75
9	566	-557
10	255	-239
11	369	351
12	74*	32
13	120	90
H= 3, K= 10		
14	220	205
13	162	177
12	264	-271
11	102	-97
10	82*	60
9	302	-272
8	305	288
7	548	493
6	480	-467
5	443	472
4	388	-391
3	373	-390
2	120	-139
1	225	234
0	99	-95
H= 3, K= 9		
0	86	34
1	48*	102
2	95	-70
3	88	73
4	365	344
5	746	-748
6	60*	-48
7	128	115
8	62*	62
9	375	329
10	287	274
11	70*	-63
12	92	-125
13	239	208
14	51*	50
H= 3, K= 8		
15	232	189
14	192	-211
13	31*	-82
12	120	122
11	244	237
10	128	110
9	438	405
8	100	-75
7	259	-234
6	257	244
5	29*	-7
4	117	-121
3	469	465
2	897	-915
1	272	-296
0	227	223
H= 3, K= 7		
0	21*	-43
1	416	-438
2	603	-607
3	172	173
4	368	-366
5	547	563
6	47*	-36
7	185	-186
8	42*	8
9	346	-389
10	98	110
11	305	323
12	229	210
13	220	-215
14	35*	5
15	188	-203
H= 3, K= 6		
15	112	-121
14	73*	-44
13	213	204
12	321	-322
11	264	-273
10	168	-125
9	302	-335
8	497	500
7	684	709
6	258	258
5	187	194
4	242	-193
3	677	-704
2	758	774
1	85	68
0	483	523

L	FO	FC
H=	3, K=	5
0	61	42
1	722	769
2	462	483
3	273	-254
4	112	108
5	234	217
6	222	-265
7	97	121
8	77	89
9	141	126
10	55*	-10
11	402	-443
12	230	-226
13	37*	16
14	164	-198
15	52*	-78
16	86*	66
H=	3, K=	4
16	116	82
15	51*	13
14	20*	-24
13	295	-326
12	49*	-41
11	58*	-69
10	214	267
9	43*	44
8	267	-229
7	543	-557
6	45*	-20
5	142	-93
4	374	396
3	610	622
2	341	357
1	229	-244
0	342	344
H=	3, K=	3
0	796	706
1	577	-612
2	731	794
3	567	622
4	625	-661
5	318	342
6	422	-415
7	454	-466
8	108	115
9	358	-374
10	34*	18
11	547	688
12	50*	75
13	80*	108
14	65*	-39
15	15*	-14
16	62*	-76
H=	3, K=	2
16	11*	8
15	113	-112
14	112	96
13	309	342
12	62*	3
11	46*	-25
10	79	-77
9	565	-558
8	6*	-61
7	739	792
6	532	-543
5	190	-206
4	207	179
3	1615	-1736
2	485	-492
1	339	347
0	134	123
H=	3, K=	1
0	665	-577
1	68	36
2	228	-237
3	423	452
4	490	533
5	1217	-1282
6	202	158
7	420	423
8	352	-361
9	469	506
10	276	243
11	341	-424
12	121	133
13	137	185
14	85	-55
15	282	309
H=	3, K=	0
15	378	408
13	97	-74
11	125	-147
9	459	452
7	495	-513
5	370	309
3	1788	1815
1	979	-959
H=	4, K=	0
0	152	37
2	1633	1622
4	296	-301
6	288	-260
8	397	440
10	94	-76
12	253	-224
14	73*	112
H=	4, K=	1
15	46*	-44
14	147	200
13	10*	7
12	215	233
11	69*	-4
10	101	-82
9	7*	19
8	436	437
7	297	-278
6	517	526
5	81	121
4	1203	-1225
3	249	281
2	416	-436
1	229	258
0	786	720
H=	4, K=	2
0	836	795
1	378	-383
2	1565	-1569
3	643	-664
4	116	92
5	597	-619
6	460	501
7	109	80
8	190	-161
9	223	177
10	110	124
11	9*	17
12	182	227
13	111	100
14	118	-144
15	11*	27
H=	4, K=	3
15	65*	-14
14	10*	-18
13	70*	75
12	70*	-40
11	241	257
10	396	479
9	64*	-58
8	265	-224
7	227	245
6	452	-467
5	323	-363
4	1018	1023
3	307	-329
2	222	-229
1	307	-421
0	849	-833
H=	4, K=	4
0	139	-49
1	538	517
2	571	527
3	226	228
4	696	-711
5	104	-111
6	287	-294
7	175	-167
8	340	335
9	63*	65
10	178	-213
11	9*	50
12	301	-335
13	23*	-21
14	242	259
15	11*	-35
H=	4, K=	5
15	83*	71
14	11*	-16
13	127	95
12	122	123
11	171	-196
10	538	-586
9	174	-201
8	79	-51
7	7*	-56
6	138	157
5	148	-147
4	668	-664
3	334	339
2	65	-68
1	199	179
0	767	782
H=	4, K=	6
0	468	506

L	FO	FC
H=	4, K=	6
1	543	578
2	566	-579
3	351	-344
4	173	129
5	353	343
6	335	340
7	79	32
8	233	-247
9	287	-272
10	9*	-94
11	48*	35
12	152	173
13	72*	-48
14	249	-261
15	51*	-58
H=	4, K=	7
14	54*	-76
13	42*	-49
12	217	-206
11	168	174
10	82	19
9	82*	-101
8	426	-483
7	203	-210
6	38*	-25
5	566	576
4	838	824
3	140	-116
2	499	-470
1	167	157
0	392	-453
H=	4, K=	8
0	619	-609
1	6*	-47
2	869	896
3	265	233
4	82	31
5	81	70
6	325	-310
7	246	-261
8	493	526
9	167	124
10	194	212
11	88	96
12	219	-246
13	208	-227
14	117	127
H=	4, K=	9
14	118	131
13	126	-124
12	159	155
11	89*	-105
10	155	-188
9	292	287
8	384	403
7	87	-99
6	671	711
5	7*	-14
4	387	-341
3	642	674
2	163	-157
1	7*	10
0	306	321
H=	4, K=	10
0	307	295
1	93	90
2	735	-732
3	184	-173
4	327	318
5	464	-465
6	471	482
7	409	388
8	351	-346
9	163	159
10	71*	-77
11	10*	-13
12	202	190
13	233	208
H=	4, K=	11
12	50*	-34
11	191	194
10	348	321
9	168	-158
8	52*	15
7	39*	-63
6	158	-132
5	176	170
4	401	384
3	274	-282
2	273	-262
1	130	-105
0	836	-863
H=	4, K=	12
0	369	-389
1	37*	32
2	261	248
3	215	208
4	196	-206
5	57*	-1
6	435	-407
7	407	-432
8	131	118
9	283	293
10	63*	38
11	97	112
12	145	-124
H=	4, K=	13
11	124	-90
10	341	-334
9	21*	12
8	135	-85
7	87	91
6	157	149
5	303	-302
4	276	-267
3	139	-117
2	157	-105
1	9*	-60
0	356	355
H=	4, K=	14
0	52*	-56
1	468	478
2	225	-180
3	80	80
4	50*	-7
5	128	-137
6	70*	25
7	10*	13
8	163	-142
9	229	-186
10	11*	-35
H=	4, K=	15
9	77*	-59
8	126	-110
7	197	-184
6	118	-118
5	180	177
4	152	199
3	113	-71
2	126	-138
1	166	-155
0	10*	32
H=	4, K=	16
0	64*	-69
1	184	-173
2	339	339
3	302	298
4	10*	40
5	185	-157
6	150	-126
7	312	-273
8	146	120
H=	4, K=	17
7	209	195
6	237	210
5	222	-224
4	221	-234
3	129	127
2	65*	65
1	361	343
0	73*	30
H=	4, K=	18
0	59*	-12
1	187	229
2	224	-216
3	99	-117
4	211	181
5	51*	-10
H=	4, K=	19
1	65*	-67
0	201	-170
H=	5, K=	18
1	220	-211
0	82*	57
H=	5, K=	17
0	322	320
1	175	191
2	162	146
3	196	-195
4	55*	-67
H=	5, K=	16
6	167	-132
5	87*	-75
4	55*	-40
3	21*	-68
2	169	180

L	FO	FC
H= 29, K= 3		
-2	112	110
-3	123	116
-4	119	129
-5	114	-105
-6	274	-261
-7	112	121
-8	270	291
-9	38	8
-10	27*	-40
-11	4*	29
-12	123	-115
-13	116	116
H= 29, K= 5		
-4	112	117
-5	162	170
-6	157	-156
-7	276	-274
-8	87	84
-9	92	84
-10	41	-32
-11	58	61
H= 30, K= 4		
-4	313	320
-5	36*	45
-6	317	-321
-7	175	-186
-8	241	244
-9	15*	38
-10	28*	11
-11	10*	-3
-12	202	-204
H= 30, K= 2		
-3	313	308
-4	86	95
-5	429	-423
-6	4*	-13
-7	394	391
-8	33*	41
-9	4*	-7
-10	90	-89
-11	140	-134
-12	173	-166
-13	170	156
H= 30, K= 0		
10	25*	50
-2	239	240
-4	420	-428
-6	320	321
-8	122	-114
-12	279	275
H= 31, K= 1		
-4	131	-128
-5	117	-114
-6	72	52
-7	154	-164
-8	197	198
-9	149	159
-10	295	-285
-11	383	-388
-12	151	149
-13	221	226
H= 31, K= 3		
-5	16*	-9
-6	125	-118
-7	52	44
-8	104	-111
-9	214	220
-10	192	192
-11	170	-169
-12	189	-192
H= 32, K= 2		
-5	34*	18
-6	125	112
-7	168	-149
-8	15*	-26
-9	240	240
-10	42	54
-11	156	-155
H= 32, K= 0		
-6	239	-248
-8	277	274
-10	332	-332
-12	220	229
H= 33, K= 1		
-7	234	-213
-8	166	173
-9	120	115
-10	14*	-16
H= 22, K= 0		
-4	342	-324
-6	31*	30
-8	204	208
-10	478	-482
-12	341	326
-14	190	-189
H= 23, K= 1		
-1	53	58
-2	159	161
-3	86	92
-4	99	103
-5	165	158
-6	378	-371
-7	334	-350
-8	404	387
-9	436	435
-10	277	-279
-11	177	-167
-12	128	138
-13	55	69
-14	37	38
-15	79	71
H= 23, K= 3		
-1	135	-132
-2	222	-211
-3	50	-41
-4	330	-328
-5	128	120
-6	257	254
-7	435	-437
-8	313	-316
-9	308	302
-10	294	303
-11	293	-290
-12	47	-46
-13	83	-92
-14	45	-33
-15	184	170
H= 23, K= 5		
-1	17*	44
-2	4*	33
-3	151	-140
-4	67	73
-5	67	-59
-6	213	208
-7	436	454
-8	261	-282
-9	154	-154
-10	198	190
-11	201	205
-12	97	-98
-13	34*	-26
-14	97	-90
H= 23, K= 7		
-1	153	139
-2	178	166
-3	13*	-5
-4	72	-78
-5	218	-221
-6	194	-181
-7	215	212
-8	360	378
-9	232	-226
-10	300	-306
-11	76	90
-12	105	103
H= 24, K= 8		
-4	84	93
-5	57	66
-6	198	-181
-7	105	-127
-8	230	221
-9	148	146
H= 24, K= 6		
-1	231	214
-2	23*	3
-3	108	-110
-4	4*	9
-5	212	-198
-6	182	-197
-7	326	323
-8	102	97
-9	44	-39
-10	172	-171
-11	183	-203
-12	4*	12
-13	191	185
H= 24, K= 4		
-1	14*	31
-2	156	-156
-3	188	195
-4	125	-120
-5	242	-228
-6	314	309
-7	110	100

L	FO	FC
H=	5, K=	2
6	144	144
5	229	234
4	117	97
3	241	196
2	154	-115
1	536	-542
0	143	-161
H=	5, K=	1
0	281	313
1	150	-139
2	223	-230
3	364	-396
4	86	-42
5	569	579
6	135	161
7	330	320
8	118	-121
9	127	-88
10	256	-241
11	172	179
12	64*	-42
13	86*	123
14	11*	6
H=	5, K=	0
13	77*	-21
11	312	-338
9	147	179
8	58*	0
7	114	-95
5	382	-391
3	254	247
1	1023	1030
H=	6, K=	0
0	372	360
2	202	187
4	696	-728
6	203	225
8	96	-90
10	354	-329
12	277	249
H=	6, K=	1
13	22*	15
12	96	104
11	98	-66
10	139	159
9	88	65
8	332	-347
7	46*	-74
6	131	131
5	65*	-11
4	426	427
3	252	-257
2	238	-229
1	136	141
0	713	663
H=	6, K=	2
0	610	-573
1	313	299
2	308	312
3	319	327
4	462	439
5	7*	31
6	438	-490
7	9*	-5
8	120	-45
9	152	-172
10	233	233
11	192	-177
12	203	-216
13	68*	-108
H=	6, K=	3
13	11*	-45
12	191	-174
12	191	-174
11	59*	-28
10	237	-243
9	96	-97
8	224	255
7	219	251
6	132	164
5	107	-112
4	272	-229
3	7*	-17
2	561	535
1	277	244
0	233	248
H=	6, K=	4
0	189	229
1	344	-346
2	265	-234
3	73	-99
4	63*	32
5	51*	59
6	494	549
7	79	71
8	44*	-24
9	10*	46
10	145	-130
11	69*	-48
12	251	259
13	11*	2
H=	6, K=	5
13	33*	24
12	130	134
11	10*	-24
10	170	180
9	160	162
8	66*	-106
7	308	315
6	83	-50
5	37*	44
4	69*	86
3	189	-184
2	599	-589
1	81	-102
0	126	-144
H=	6, K=	6
0	701	-717
1	455	-450
2	234	224
3	210	-211
4	234	228
5	261	302
6	213	-220
7	33*	57
8	35*	72
9	10*	-19
10	81*	123
11	229	193
12	80*	-65
H=	6, K=	7
12	80*	-38
11	11*	-3
10	15*	-17
9	10*	-13
8	112	101
7	160	-151
6	35*	9
5	88	-65
4	324	-340
3	41*	-10
2	361	348
1	136	144
0	101	-96
H=	6, K=	8
0	302	306
1	171	185
2	81	-91
3	273	-282
4	98	-104
5	9*	-42
6	71*	47
7	49*	77
8	280	-301
9	60*	-74
10	228	-208
11	127	-69
12	110	79
H=	6, K=	9
11	67*	-51
10	153	128
9	86*	-73
8	247	-291
7	85	-68
6	77*	-113
5	10*	-7
4	128	163
3	211	-197
2	147	-206
1	271	-281
0	358	372
H=	6, K=	10
0	244	-265
1	295	-250
2	71*	-72
3	221	251
4	217	218
5	10*	-15
6	194	-195
7	86	-98
8	34*	-32
9	128	-112
10	280	261
H=	6, K=	11
10	98	-71
9	63*	88
8	195	175
7	65*	-52
6	133	-125
5	98	-127

L	FO	FC
4	118	-90
3	150	122
2	566	553
1	153	171
0	238	240
H=	6, K=	12
0	375	371
1	116	121
2	124	-109
3	10*	-17
4	10*	24
5	106	91
6	141	166
7	105	104
8	11*	-4
9	11*	54
H=	6, K=	13
8	43*	-46
7	185	167
6	52*	-57
5	102	77
4	147	151
3	73*	-61
2	132	-110
1	168	168
0	163	-195
H=	6, K=	14
0	372	-329
1	414	-385
2	43*	33
3	160	-145
4	62*	93
5	188	165
6	47*	-14
7	51*	17
H=	6, K=	15
5	11*	6
4	85*	-66
3	181	178
2	103	97
1	162	-159
0	62*	-57
H=	6, K=	16
0	130	114
1	165	160
2	27*	-52
3	72*	-85
H=	7, K=	15
0	29*	-55
1	80*	66
H=	7, K=	14
4	188	194
3	179	146
2	11*	-8
1	114	85
0	106	-120
H=	7, K=	13
0	114	104
1	266	-255
2	108	-112
3	228	199
4	48*	-18
5	82*	54
6	188	175
H=	7, K=	12
7	59*	-91
6	51*	9
5	220	233
4	139	-134
3	52*	-51
2	56*	1
1	106	-130
0	186	172
H=	7, K=	11
0	30*	-29
1	147	139
2	74*	30
3	145	-174
4	41*	57
5	46*	-9
6	89	-92
7	72*	81
8	53*	68
H=	7, K=	10
9	233	217
8	105	-99
7	113	131
6	10*	-61
5	229	-218
4	251	-215
3	157	119
2	97	-90
1	10*	-36
0	115	144
H=	7, K=	9
0	58*	28
1	322	-337
2	187	-159
3	181	144
4	86	-78
5	229	213
6	10*	49
7	236	-240
8	59*	-55
9	94*	102
H=	7, K=	8
10	99	-71
9	144	-144
8	236	219
7	45*	-66
6	95	91
5	173	181
4	216	-222
3	424	-440
2	43*	-8
1	105	-114
0	215	210
H=	7, K=	7
0	50*	12
1	241	255
2	260	266
3	13*	-59
4	87	-65
5	77*	102
6	334	-346
7	226	199
8	181	187
9	82*	-105
10	53*	12
H=	7, K=	6
11	142	-127
10	222	236
9	58*	92
8	10*	-20
7	10*	69
6	34*	-32
5	83	-101
4	272	301
3	68*	73
2	60*	78
1	66*	56
0	129	122
H=	7, K=	5
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1	153	-139
2	241	201
3	381	354
4	42*	13
5	16*	-56
6	193	199
7	240	-215
8	95	-119
9	10*	31
10	11*	-44
11	199	181
H=	7, K=	4
11	11*	28
10	105	-64
9	278	-296
8	82	46
7	29*	17
6	146	153
5	407	397
4	157	-111
3	168	179
2	77	-36
1	142	-154
0	9*	-41
H=	7, K=	3
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1	59*	-47
2	183	140
3	344	-329
4	199	145
5	77*	121
6	120	-99
7	112	145
8	97	-107
9	178	-169
10	11*	43
11	215	-187
12	75*	-18
H=	7, K=	2

L	FO	FC
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12	11*	-56
11	197	-168
10	164	-155
9	74*	81
8	10*	-55
7	209	226
6	306	-283
5	288	-280
4	272	-269
3	51*	29
2	155	-123
1	42*	77
0	166	157
H=	7, K=	1
0	65*	36
1	318	-286
2	70*	106
3	288	246
4	221	-199
5	87	-57
6	171	-150
7	429	-435
8	118	130
9	10*	38
10	131	103
11	160	143
12	11*	27
H=	7, K=	0
11	215	189
9	145	-119
7	131	-113
5	411	452
3	681	-615
1	557	-509
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2	342	-342
4	290	286
6	10*	29
8	118	-132
10	193	153
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9	71*	36
8	120	112
7	29*	102
6	370	-408
5	51*	28
4	44*	46
3	10*	-49
2	120	128
1	54*	-22
0	348	-325
H=	8, K=	2
0	216	193
1	197	-181
2	112	66
3	274	-222
4	365	-353
5	89	-30
6	157	119
7	29*	-10
8	279	288
9	46*	-38
10	84*	-134
H=	8, K=	3
10	165	-148
9	79*	-69
8	128	-108
7	21*	-67
6	307	303
5	20*	-46
4	44*	-6
3	231	202
2	331	-288
1	46*	5
0	69*	-24
H=	8, K=	4
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1	10*	-16
2	87	-28
3	10*	4
4	118	102
5	30*	73
6	150	-137
7	10*	17
8	198	-203
9	72*	-53
H=	8, K=	5
9	54*	-33
8	103	94
7	266	-242
6	250	-235
5	10*	-8
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3	178	184
2	207	209
1	91	14
0	55*	-56
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2	235	220
3	130	112
4	386	-346
5	148	-134
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7	11*	-3
8	196	208
9	94	45
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7	216	196
6	403	375
5	39*	27
4	145	-156
3	126	-140
2	223	-199
1	187	194
0	229	255
H=	8, K=	8
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2	290	-293
3	231	-217
4	307	303
5	114	127
6	99	26
7	69*	51
8	145	-133
H=	8, K=	9
7	149	-117
6	168	-163
5	135	146
4	146	119
3	75*	82
2	92	96
1	336	-348
0	190	-182
H=	8, K=	10
0	170	176
1	107	-124
2	101	44
3	118	97
4	269	-243
5	130	-101
6	120	95
H=	8, K=	11
5	11*	7
4	19*	10
3	11*	6
2	319	-265
1	11*	-12
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H=	8, K=	12
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1	36*	0
2	48*	-41
3	101	-75
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1	106	-107
0	134	-125
H=	9, K=	10
1	25*	42
0	124	-102
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0	134	-134
1	265	246
2	71*	47
3	110	-68
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3	335	321
2	114	-155
1	96	60
0	55*	-7
H=	9, K=	7
0	155	155

L	FO	FC
1	246	-228
2	107	-72
3	137	-135
4	11*	18
5	221	220
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6	11*	-10
5	46*	44
4	11*	-42
3	354	-338
2	64*	20
1	133	136
0	15*	16
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0	174	-131
1	323	308
2	69*	-60
3	11*	13
4	159	-143
5	307	-279
H=	9, K=	4
7	158	-129
6	15*	10
5	311	-280
4	85*	-7
3	261	254
2	89	72
1	153	-113
0	57*	-15
H=	9, K=	3
0	10*	-16
1	260	-241
2	148	-92
3	63*	-2
4	11*	-62
5	257	235
6	11*	6
7	128	-108
H=	9, K=	2
7	179	151
6	19*	-23
5	99	73
4	119	150
3	227	-214
2	78*	56
L	FO	FC
1	208	206
0	180	-166
H=	9, K=	1
0	76*	-47
1	282	320
2	10*	-42
3	79*	29
4	161	142
5	244	-225
6	155	139
7	221	194
H=	9, K=	0
7	211	-238
5	88	-45
3	456	415
1	109	76
H=	10, K=	0
0	58*	-52
2	321	280
H=	10, K=	1
3	11*	34
2	93	64
1	27*	93
0	263	242
H=	10, K=	2
0	78*	67
1	88*	96
2	201	-170
3	22*	23
H=	10, K=	3
3	76*	-46
2	11*	-3
1	59*	-86
0	209	-190
H=	10, K=	4
0	183	-202
1	75*	-62
2	270	258
H=	10, K=	5
L	FO	FC
1	66*	20
0	280	273
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-3	123	-79
-2	199	-222
-1	177	169
H=	1, K=	19
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-2	403	-406
-3	205	-185
-4	303	321
-5	87*	96
-6	51*	-3
-7	40*	71
H=	1, K=	18
-8	56*	34
-7	325	-335
-6	335	-376
-5	62*	33
-4	300	331
-3	182	166
-2	237	244
-1	228	-243
H=	1, K=	17
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-2	394	428
-3	106	118
-4	322	-356
-5	253	-256
-6	217	229
-7	78*	-27
-8	271	308
-9	172	200
-10	198	-241
H=	1, K=	16
-11	27*	-74
-10	32*	-77
-9	159	193
-8	207	-213
-7	169	190
-6	296	323
-5	96	101
-4	10*	19
-3	167	165
L	FO	FC
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-1	446	424
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-1	110	-120
-2	287	-299
-3	282	-316
-4	537	592
-5	71*	-54
-6	40*	49
-7	234	241
-8	124	-153
-9	10*	68
-10	146	160
-11	37*	-29
-12	108	-103
H=	1, K=	14
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-12	83*	-141
-11	82*	93
-10	107	134
-9	41*	10
-8	31*	15
-7	37*	31
-6	276	-301
-5	146	168
-4	197	202
-3	120	132
-2	160	176
-1	342	-334
H=	1, K=	13
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-2	213	210
-3	278	273
-4	545	-545
-5	374	-389
-6	213	-273
-7	241	-272
-8	208	247
-9	286	312
-10	230	-264
-11	214	-221
-12	10*	-4
-13	11*	-90
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-13	179	196
-12	287	352

L	FO	FC
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-10	82*	-129
-9	177	-211
-8	364	-392
-7	103	108
-6	259	262
-5	862	-870
-4	139	123
-3	512	-496
-2	298	-295
-1	412	420
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-2	65	51
-3	627	-658
-4	479	532
-5	128	121
-6	113	-99
-7	564	580
-8	224	-275
-9	389	-436
-10	93	158
-11	174	193
-12	32*	73
-13	10*	-12
-14	73*	-37
-15	220	-260
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-15	132	-204
-14	10*	-45
-13	225	-241
-12	210	-268
-11	190	231
-10	180	-210
-9	9*	48
-8	139	131
-7	499	-531
-6	125	96
-5	684	700
-4	79	75
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-2	349	373
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-2	262	296
-3	1205	1143
-4	350	-363
-5	342	-385
-6	277	288
-7	394	-433
-8	254	262
-9	674	678
-10	9*	23
-11	226	-274
-12	101	-104
-13	316	-348
-14	10*	14
-15	160	189
-16	86*	-106
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-15	110	127
-14	30*	-10
-13	169	179
-12	246	298
-11	270	-306
-10	136	-130
-9	136	162
-8	137	-142
-7	888	968
-6	267	295
-5	187	-190
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-3	521	-500
-2	104	-85
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-2	575	-574
-3	1353	-1399
-4	646	626
-5	130	109
-6	618	-645
-7	487	523
-8	275	-306
-9	55*	97
-10	34*	-23
-11	204	263
-12	66*	109
-13	180	248
-14	70*	-139
-15	221	-234
-16	11*	-6
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-16	11*	23
-15	54*	38
-14	190	206
-13	133	-130
-12	142	140
-11	87	92
-10	442	477
-9	188	-206
-8	352	381
-7	88	63
-6	26*	54
-5	358	322
-4	373	-366
-3	37*	-44
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-1	792	-778
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-2	410	371
-3	573	569
-4	700	-698
-5	509	-475
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-7	593	-563
-8	129	76
-9	412	453
-10	262	274
-11	138	-122
-12	9*	22
-13	158	-166
-14	14*	49
-15	302	341
-16	11*	-18
-17	24*	56
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-16	46*	-29
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-13	449	471
-12	245	259
-11	481	-525
-10	517	-525
-9	193	-213
-8	562	-586
-7	472	528
-6	305	296
-5	1334	-1351
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-3	1436	-1425
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-1	725	-669
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-2	387	390
-3	706	-672
-4	243	267
-5	446	428
-6	167	-168
-7	229	183
-8	66	61
-9	1399	-1422
-10	290	310
-11	209	190
-12	182	165
-13	94	63
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-15	382	-370
-16	109	115
-17	82*	46
H=	1, K=	2
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-16	85*	-95
-15	120	86
-14	131	-85
-13	489	-436
-12	362	-345
-11	351	327
-10	608	-577
-9	60*	-42
-8	134	100
-7	1058	-921
-6	5*	25
-5	1987	1854
-4	258	253
-3	882	-882
-2	380	329
-1	2037	-2049
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-3	1372	1272
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-5	115	-119
-6	184	-155
-7	1270	-1210
-8	582	-508
-9	1111	1027
-10	71	69
-11	388	-384

L	FO	FC
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-13	348	-304
-14	392	-314
-15	176	140
-16	163	-158
-17	67*	-83
H=	1, K=	0
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-11	558	-584
-9	159	135
-7	1619	1722
-5	662	-711
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-15	117	140
-14	373	-405
-13	9*	-18
-12	108	-122
-11	7*	-6
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-9	277	306
-8	677	-655
-7	804	756
-6	161	-153
-5	417	-400
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-3	1346	-1200
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-5	90	-18
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-7	513	550
-8	1257	-1212
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-10	480	-409
-11	87	-72
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-14	168	-127
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-16	308	-275
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-16	367	-319
-15	49*	-35
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-13	256	-237
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-11	68	-85
-10	589	-609
-9	129	-104
-8	922	852
-7	415	-375
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-4	294	-268
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-6	1301	-1168
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-8	439	394
-9	286	204
-10	152	-186
-11	103	-107
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-14	96	-129
-15	129	-100
-16	73*	54
-17	24*	6
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-16	234	214
-15	75*	18
-14	78	-29
-13	130	-126
-12	183	-181
-11	308	-305
-10	143	168
-9	322	331
-8	73	-49
-7	42*	-39
-6	236	259
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-5	56*	-105
-6	524	557
-7	657	-654
-8	773	-816
-9	378	-399
-10	192	-169
-11	520	451
-12	483	503
-13	110	-138
-14	114	-122
-15	92	70
-16	69*	-96
-17	209	186
H=	2, K=	7
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-15	69*	12
-14	321	323
-13	111	-127
-12	132	158
-11	112	57
-10	537	-566
-9	217	-168
-8	208	202
-7	152	139
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-5	104	-102
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-2	595	-637
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-2	369	375
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-4	493	-492
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-6	444	-431
-7	80	35
-8	613	625
-9	103	-119
-10	280	319
-11	69*	-93
-12	119	-87
-13	220	215
-14	368	382
-15	137	-137
-16	48*	16
H=	2, K=	9
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-15	56*	79
-14	252	-283
-13	76*	56
-12	116	-129
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-8	368	-354
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-4	532	535
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-1	453	-458
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-2	691	-699
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-4	59*	40
-5	110	113
-6	761	777
-7	444	-438
-8	564	-563
-9	453	488
-10	18*	14
-11	165	189
-12	270	275

L	FO	FC
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-13	283	-304
-14	135	-122
-15	80*	-139
H=	2, K=	11
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-12	10*	-8
-11	184	196
-10	605	-646
-9	251	-265
-8	465	519
-7	277	-310
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-2	145	-157
-1	177	160
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-3	131	117
-4	130	-114
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-7	153	153
-8	189	185
-9	9*	-71
-10	259	-310
-11	99	130
-12	297	-334
-13	130	133
-14	50*	34
H=	2, K=	13
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-12	47*	49
-11	173	-207
-10	77*	111
-9	45*	81
-8	135	-146
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-6	132	140
-5	288	-335
-4	278	304
-3	507	512
-2	250	-229
-1	54*	41
H=	2, K=	14
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-2	254	-293
-3	178	173
-4	259	-266
-5	149	187
-6	236	273
-7	288	-324
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-9	10*	10
-10	10*	29
-11	223	255
-12	62*	40
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-10	188	-201
-9	181	-219
-8	74*	92
-7	201	235
-6	115	169
-5	145	152
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-3	199	-221
-2	401	-426
-1	194	-209
H=	2, K=	16
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-2	158	157
-3	137	-127
-4	185	-215
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-6	86	-54
-7	41*	52
-8	383	436
-9	55*	39
-10	87	58
-11	198	-232
H=	2, K=	17
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-8	127	-155
-7	87	-93
-6	188	-221
-5	34*	-18
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-3	276	271
-2	10*	-16
-1	86	-93
H=	2, K=	18
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-2	154	-191
-3	364	396
-4	10*	-22
-5	111	96
-6	199	210
-7	272	-295
-8	117	-154
H=	2, K=	19
-6	245	279
-5	240	267
-4	226	-230
-3	145	-174
-2	100	67
-1	66*	-48
H=	2, K=	20
-1	303	316
-2	174	147
-3	153	-147
H=	3, K=	19
-1	11*	-38
-2	11*	6
-3	139	153
-4	11*	-32
-5	81*	-88
H=	3, K=	18
-7	218	240
-6	67*	53
-5	103	118
-4	204	212
-3	257	-266
-2	249	-254
-1	80*	-88
H=	3, K=	17
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-2	163	200
-3	190	182
-4	71*	68
-5	274	335
-6	280	-285
-7	166	-192
-8	11*	-116
-9	118	-121
H=	3, K=	16
-10	35*	-29
-9	203	235
-8	158	206
-7	211	-267
-6	187	-203
-5	262	-287
-4	313	-313
-3	52*	-15
-2	266	290
-1	17*	-43
H=	3, K=	15
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-2	262	-282
-3	64*	103
-4	271	-333
-5	60*	-71
-6	198	-235
-7	41*	-16
-8	86	57
-9	69*	-31
-10	103	-107
-11	141	-177
H=	3, K=	14
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-11	67*	-38
-10	95	-58
-9	159	-193
-8	202	194
-7	214	248
-6	10*	-7
-5	73*	-28
-4	188	-210
-3	86	-77
-2	197	-202
-1	9*	16
H=	3, K=	13
-1	229	-257
-2	409	444
-3	267	-293
-4	213	191
-5	216	219
-6	56*	-47

L	FO	FC
-7	270	-292
-8	171	210
-9	178	-198
-10	85	107
-11	124	131
-12	125	-146
-13	129	136
H=	3, K=	12
-14	60*	74
-13	237	-254
-12	175	-165
-11	38*	53
-10	44*	-8
-9	244	244
-8	347	342
-7	134	-138
-6	52*	-46
-5	313	339
-4	344	-327
-3	618	621
-2	437	460
-1	168	-197
H=	3, K=	11
-1	450	463
-2	240	259
-3	144	166
-4	47*	26
-5	318	-327
-6	671	729
-7	410	440
-8	154	-164
-9	50*	25
-10	342	-367
-11	217	-245
-12	166	208
-13	57*	-34
-14	99	88
H=	3, K=	10
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-13	424	397
-12	122	109
-11	204	-228
-10	250	237
-9	361	-337
-8	154	-175
-7	420	452
-6	167	167
-5	7*	-17
-4	113	113
-3	507	-574
-2	384	-426
-1	44*	78
H=	3, K=	9
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-2	283	-261
-3	315	342
-4	131	-83
-5	658	686
-6	407	-428
-7	326	-350
-8	139	-114
-9	323	-321
-10	276	286
-11	692	671
-12	155	-137
-13	235	198
-14	28*	-23
-15	276	-274
H=	3, K=	8
-16	76*	27
-15	292	285
-14	165	170
-14	194	170
-13	351	-371
-12	208	-165
-11	285	277
-10	143	127
-9	554	542
-8	288	285
-7	745	-739
-6	590	-602
-5	161	-117
-4	365	-401
-3	52*	68
-2	328	320
-1	59*	-111
H=	3, K=	7
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-2	138	105
-3	40*	-27
-4	542	-551
-5	145	-135
-6	221	-194
-7	7*	-17
-8	276	269
-9	85	-61
-10	514	-484
-11	632	-577
-12	168	169
-13	176	176
-14	235	212
-15	249	246
-16	154	-155
H=	3, K=	6
-16	34*	54
-15	278	-248
-14	202	-198
-13	335	285
-12	126	-162
-11	22*	-5
-10	252	-273
-9	525	-529
-8	110	-147
-7	644	660
-6	212	206
-5	278	-272
-4	347	299
-3	275	-254
-2	297	335
-1	24*	30
H=	3, K=	5
-1	127	-161
-2	78	-67
-3	376	-346
-4	112	-126
-5	647	679
-6	299	256
-7	241	-205
-8	187	-146
-9	683	-674
-10	29*	45
-11	205	216
-12	325	-280
-13	90	90
-14	78*	-49
-15	323	-302
-16	32*	41
-17	104	102
H=	3, K=	4
-17	124	98
-16	74*	-63
-15	260	-267
-14	179	-164
-13	539	-522
-12	96	106
-11	76	47
-10	411	394
-9	728	728
-8	6*	58
-7	709	-774
-6	451	401
-5	92	-39
-4	534	-499
-3	293	324
-2	265	-279
-1	622	-541
H=	3, K=	3
-1	109	-73
-2	70	-38
-3	81	30
-4	824	773
-5	796	-773
-6	663	617
-7	1121	982
-8	207	-210
-9	634	642
-10	358	-349
-11	147	-188
-12	99	115
-13	64*	-78
-14	103	-73
-15	303	300
-16	90	-111
-17	217	-224
H=	3, K=	2
-17	147	-153
-16	48*	39
-15	157	-174
-14	10*	18
-13	295	287
-12	67*	20
-11	26*	-12
-10	106	98
-9	336	-288
-8	57*	-22
-7	422	380
-6	452	-338
-5	146	132
-4	19*	43
-3	98	40
-2	522	-514
-1	841	882
H=	3, K=	1
-1	765	-797
-2	709	-682

L	FO	FC
H=	3, K=	1
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-4	123	108
-5	1483	1356
-6	258	-264
-7	591	-536
-8	63	98
-9	509	-524
-10	144	136
-11	539	526
-12	9*	-37
-13	167	156
-14	208	245
-15	408	-469
-16	192	227
-17	346	425
H=	3, K=	0
-17	285	348
-15	356	407
-13	288	-333
-11	514	553
-9	418	464
-7	267	-278
-5	339	-352
-3	114	208
-1	239	206
H=	4, K=	0
-2	916	-799
-4	1054	974
-6	155	-182
-8	418	-393
-10	447	467
-12	396	-454
-14	592	-678
-16	315	385
H=	4, K=	1
-17	43*	-13
-16	139	-171
-15	10*	-23
-14	10*	28
-13	64*	-63
-12	462	463
-11	126	-114
-10	103	-134
-9	496	-493
-8	354	-327
-7	364	-384
-6	877	832
-5	291	286
-4	180	123
-3	203	219
-2	776	-713
-1	608	-534
H=	4, K=	2
-1	328	-416
-2	226	191
-3	794	-766
-4	1376	-1286
-5	312	300
-6	636	555
-7	252	263
-8	507	473
-9	275	-285
-10	434	-446
-11	73	81
-12	177	-162
-13	43*	-80
-14	377	422
-15	47*	2
-16	49*	-66
-17	11*	39
H=	4, K=	3
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-15	112	-79
-14	159	-164
-13	335	303
-12	72	30
-11	396	379
-10	359	351
-9	193	205
-8	391	375
-7	165	-147
-6	934	-909
-5	226	254
-4	245	-295
-3	63	121
-2	534	497
-1	186	-185
H=	4, K=	4
-1	206	239
-2	480	-493
-3	633	-593
-4	38*	-74
-5	587	-564
-6	131	-137
-7	95	82
-8	105	50
-9	267	297
-10	539	467
-11	356	-281
-12	163	131
-13	126	109
-14	369	-314
-15	99	94
-16	137	114
H=	4, K=	5
-16	372	-361
-15	110	-110
-14	123	-74
-13	119	95
-12	183	168
-11	269	288
-10	229	-186
-9	71	-50
-8	608	-602
-7	155	151
-6	267	294
-5	134	107
-4	325	-288
-3	389	372
-2	632	657
-1	164	-217
H=	4, K=	6
-1	277	293
-2	242	217
-3	173	150
-4	117	75
-5	572	582
-6	52*	-26
-7	431	435
-8	511	529
-9	217	-231
-10	288	-266
-11	120	-137
-12	224	-219
-13	89	85
-14	341	329
-15	41*	-53
-16	72*	-60
H=	4, K=	7
-16	168	162
-15	197	166
-14	156	-125
-13	95	66
-12	364	-343
-11	129	-117
-10	250	222
-9	53*	-27
-8	288	258
-7	326	-351
-6	378	-397
-5	400	-379
-4	462	489
-3	44*	-7
-2	770	816
-1	501	487
H=	4, K=	8
-1	273	-279
-2	215	206
-3	52*	-78
-4	352	379
-5	64*	40
-6	159	-170
-7	156	140
-8	414	-389
-9	86	81
-10	308	301
-11	144	-95
-12	70*	52
-13	162	-156
-14	409	-375
-15	204	214
H=	4, K=	9
-15	134	-131
-14	48*	17
-13	98	-77
-12	544	562
-11	20*	57
-10	153	139
-9	394	-411
-8	357	-408
-7	361	-360
-6	249	229
-5	252	253
-4	68	-36
-3	75	-72
-2	518	-519
-1	288	-307
H=	4, K=	10
-1	159	-196
-2	289	275
-3	772	-787
-4	522	-518
-5	281	292
-6	118	89

L	FO	FC
-7	283	314
-8	272	260
-9	331	-349
-10	356	-367
-11	191	-186
-12	275	-314
-13	324	324
-14	204	204
H=	4, K=	11
-14	97	-125
-13	106	122
-12	64*	-120
-11	146	-156
-10	307	315
-9	164	215
-8	184	189
-7	314	375
-6	525	-543
-5	112	-132
-4	113	145
-3	239	-239
-2	361	373
-1	250	227
H=	4, K=	12
-1	93	-93
-2	358	-408
-3	86	-68
-4	247	321
-5	195	-169
-6	9*	-8
-7	227	237
-8	55*	-18
-9	72*	123
-10	234	246
-11	159	-166
-12	185	203
-13	35*	-94
H=	4, K=	13
-12	182	196
-11	147	173
-10	23*	-43
-9	150	180
-8	280	-329
-7	169	138
-6	14*	20
-5	48*	53
-4	223	-244
-3	214	177
-2	128	151
-1	199	-208
H=	4, K=	14
-1	9*	15
-2	220	246
-3	190	-206
-4	101	100
-5	213	221
-6	126	112
-7	66*	44
-8	89	138
-9	225	-254
-10	150	-188
-11	11*	19
H=	4, K=	15
-10	139	167
-9	11*	-18
-8	112	103
-7	71*	68
-6	316	-357
-5	340	-409
-4	209	258
-3	10*	-25
-2	281	296
-1	597	659
H=	4, K=	16
-1	141	-145
-2	40*	-17
-3	298	322
-4	153	186
-5	18*	-40
-6	10*	-70
-7	42*	-35
-8	260	-287
-9	174	187
H=	4, K=	17
-8	68*	-57
-7	256	-281
-6	126	86
-5	82*	137
-4	41*	26
-3	10*	-30
-2	44*	-104
-1	325	-381
H=	4, K=	18
-1	80*	-126
-2	11*	-8
-3	311	-381
-4	131	-151
-5	201	223
-6	11*	50
H=	4, K=	19
-2	58*	72
-1	287	314
H=	5, K=	18
-3	192	194
-2	54*	57
-1	128	144
H=	5, K=	17
-1	189	209
-2	203	-218
-3	215	-269
-4	47*	-13
-5	137	-118
-6	224	267
H=	5, K=	16
-8	170	-198
-6	11*	-79
-5	150	151
-4	388	431
-3	46*	24
-2	198	-254
-1	90	113
H=	5, K=	15
-1	73*	30
-2	301	336
-3	219	261
-4	177	222
-5	29*	7
-6	165	-160
-7	58*	-34
-8	217	261
-9	187	237
H=	5, K=	14
-10	299	-326
-9	67*	81
-8	79*	58
-7	87	89
-6	268	289
-5	106	-142
-4	109	104
-3	259	301
-2	109	139
-1	66*	-16
H=	5, K=	13
-1	426	455
-2	252	-299
-3	181	-206
-4	68*	24
-5	233	-260
-6	10*	20
-7	352	406
-8	91	-114
-9	78*	99
-10	37*	-29
-11	206	-237
H=	5, K=	12
-12	41*	18
-11	186	198
-10	146	163
-9	128	-174
-8	135	-81
-7	69*	-93
-6	175	-168
-5	76*	81
-4	144	180
-3	550	-605
-2	190	225
-1	215	-222
H=	5, K=	11
-1	334	-393
-2	126	126
-3	77*	-104
-4	461	-507
-5	119	-92
-6	89	-89
-7	350	-367
-8	55*	82
-9	215	220
-10	136	132
-11	139	210
-12	58*	36
-13	202	-225
H=	5, K=	10
-13	89	-45
-12	63*	80

L	FO	FC
H=	5, K=	10
-11	289	-329
-10	158	-162
-9	197	213
-8	301	-297
-7	344	334
-6	56*	82
-5	416	-457
-4	388	-407
-3	240	260
-2	52*	-79
-1	368	405
H=	5, K=	9
-1	814	816
-2	405	-407
-3	316	-348
-4	472	455
-5	477	-527
-6	118	138
-7	398	400
-8	156	-145
-9	260	-251
-10	10*	-5
-11	228	-249
-12	62*	-21
-13	109	109
-14	164	-175
H=	5, K=	8
-14	95	-112
-13	71*	-7
-12	25*	78
-11	132	168
-10	102	-111
-9	415	-397
-8	273	-269
-7	36*	2
-6	59*	10
-5	703	700
-4	597	596
-3	401	-374
-2	459	-467
-1	54*	-83
H=	5, K=	7
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-2	681	710
-3	101	73
-4	190	-183
-5	326	325
-6	215	-212
-7	288	-311
-8	186	164
-9	625	597
-10	55*	-49
-11	114	110
-12	195	-177
-13	513	-499
-14	11*	-29
-15	80*	30
H=	5, K=	6
-15	327	314
-14	241	247
-13	97	-81
-12	208	139
-11	276	-239
-10	257	-250
-9	73*	81
-8	227	166
-7	211	217
-6	394	391
-5	378	-395
-4	160	164
-3	594	577
-2	54*	82
-1	302	262
H=	5, K=	5
-1	640	655
-2	67	-63
-3	449	-445
-4	361	315
-5	178	-192
-6	15*	-20
-7	449	463
-8	194	-191
-9	211	-236
-10	293	284
-11	45*	-14
-12	219	201
-13	305	305
-14	10*	7
-15	88	-66
H=	5, K=	4
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-15	183	-207
-14	10*	-35
-13	400	397
-12	10*	1
-11	40*	23
-10	136	142
-9	324	-340
-8	276	-266
-7	80	47
-6	47*	25
-5	739	730
-4	330	346
-3	715	-733
-2	444	439
-1	294	-312
H=	5, K=	3
-1	443	-407
-2	76	-32
-3	193	196
-4	193	-156
-5	222	213
-6	391	-391
-7	544	-569
-8	138	-127
-9	413	373
-10	106	109
-11	304	297
-12	454	407
-13	461	-449
-14	53*	42
-15	61*	23
-16	74*	79
H=	5, K=	2
-16	91	-79
-15	434	491
-14	36*	-67
-13	146	-140
-12	188	210
-11	475	-454
-10	9*	-7
-9	509	532
-8	62*	-42
-7	109	-108
-6	46*	-47
-5	698	-628
-4	102	-40
-3	591	530
-2	311	-285
-1	199	-228
H=	5, K=	1
-1	1068	1037
-2	307	311
-3	283	-286
-4	256	-235
-5	656	-590
-6	205	-200
-7	689	684
-8	117	129
-9	388	-366
-10	193	173
-11	83	-82
-12	262	-301
-13	532	571
-14	172	-214
-15	110	-108
-16	50*	-73
H=	5, K=	0
-15	355	-422
-13	206	-220
-11	343	427
-9	695	-722
-7	327	355
-5	1304	1277
-3	1089	-941
-1	612	-640
H=	6, K=	0
-2	338	-310
-4	40*	31
-6	500	481
-8	72*	-42
-10	209	-182
-12	482	530
-14	162	204
H=	6, K=	1
-15	11*	-17
-13	150	-166
-12	344	-321
-11	350	326
-10	224	-203
-9	400	374
-8	527	457
-7	7*	24
-6	512	-503
-5	169	-162
-4	375	-345
-3	222	-233
-2	722	728
-1	308	284
H=	6, K=	2
-1	264	293
-2	145	124

L	FO	FC
-3	7*	44
-4	795	772
-5	104	-77
-6	290	-272
-7	237	-226
-8	306	-280
-9	627	-588
-10	220	212
-11	178	179
-12	120	-98
-13	47*	7
-14	126	-137
-15	36*	-56
H=	6, K=	3
-15	40*	54
-14	328	-350
-13	139	-140
-12	277	266
-11	347	-331
-10	186	-165
-9	131	135
-8	343	-338
-7	9*	12
-6	615	611
-5	196	-198
-4	526	521
-3	163	-152
-2	539	-526
-1	229	239
H=	6, K=	4
-1	120	136
-2	316	-291
-3	264	274
-4	361	-340
-5	181	190
-6	429	402
-7	86	-58
-8	274	-259
-9	72*	50
-10	491	-481
-11	169	115
-12	185	166
-13	10*	11
-14	258	251
-15	167	-189
H=	6, K=	5
-14	435	425
-13	131	113
-12	278	-274
-11	147	-182
-10	79*	-69
-9	269	-242
-8	467	461
-7	336	341
-6	131	-121
-5	329	-344
-4	693	-672
-3	309	-339
-2	229	231
-1	93	97
H=	6, K=	6
-1	25*	26
-2	134	-106
-3	238	229
-4	646	688
-5	447	-465
-6	503	-501
-7	50*	-86
-8	124	-124
-9	495	460
-10	144	143
-11	39*	21
-12	200	-201
-13	63*	86
-14	11*	-19
H=	6, K=	7
-14	167	-186
-13	332	-349
-12	178	157
-11	102	106
-10	91	117
-9	522	520
-8	250	-241
-7	327	-365
-6	441	438
-5	29*	-50
-4	70*	35
-3	342	341
-2	998	-977
-1	338	-312
H=	6, K=	8
-1	115	-127
-2	93	93
-3	186	-223
-4	270	-282
-5	303	335
-6	662	685
-7	134	-145
-8	69*	-84
-9	157	-173
-10	292	-301
-11	345	349
-12	305	317
-13	235	-246
H=	6, K=	9
-13	98	88
-12	289	-315
-11	80*	96
-10	303	-296
-9	82*	-72
-8	452	510
-7	366	372
-6	56*	27
-5	112	138
-4	81	-99
-3	231	-257
-2	306	313
-1	500	547
H=	6, K=	10
-1	366	394
-2	104	117
-3	302	338
-4	471	489
-5	259	-289
-6	298	-309
-7	203	-196
-8	10*	19
-9	120	-162
-10	311	337
-11	132	-99
-12	95	-96
H=	6, K=	11
-12	143	151
-11	73*	-35
-10	192	-195
-9	213	236
-8	289	-324
-7	153	-176
-6	297	303
-5	264	-269
-4	91	54
-3	296	319
-2	296	-317
-1	78*	-43
H=	6, K=	12
-1	81*	-76
-2	31*	62
-3	141	152
-4	463	-518
-5	80*	151
-6	177	173
-7	262	-298
-8	10*	30
-9	85*	-41
-10	263	-293
-11	316	334
H=	6, K=	13
-10	84*	-80
-9	287	-293
-8	224	253
-7	173	197
-6	10*	-8
-5	85*	-66
-4	225	-267
-3	218	-258
-2	111	105
-1	72*	81
H=	6, K=	14
-1	79*	83
-2	10*	28
-3	246	269
-4	160	188
-5	213	-235
-6	243	-286
-7	11*	46
-8	22*	-24
-9	273	311
H=	6, K=	15
-7	152	-175
-6	124	120
-5	48*	79
-4	114	146
-3	87	64
-2	313	-348
-1	293	-329
H=	6, K=	16
-1	86*	-68
-2	11*	-11
-3	97	-133
-4	169	-169
-5	125	139

L	FO	FC
H=	7, K=	15
-1	114	-107
-2	145	-143
-3	138	-166
-4	85*	69
H=	7, K=	14
-6	282	-296
-5	46*	127
-4	74*	-59
-3	29*	74
-2	48*	-39
-1	194	-209
H=	7, K=	13
-1	141	-167
-2	157	209
-3	171	204
-4	68*	-118
-5	103	-142
-6	39*	-16
-7	148	-163
-8	161	207
H=	7, K=	12
-9	81*	95
-8	11*	43
-7	76*	105
-6	91	122
-5	179	-208
-4	89*	-149
-3	82*	85
-2	117	99
-1	273	291
H=	7, K=	11
-1	30*	84
-2	27*	-20
-3	91	-86
-4	51*	49
-5	398	431
-6	132	96
-7	162	126
-8	75*	-108
-9	265	-281
-10	107	103
H=	7, K=	10
-11	301	319
-10	139	136
-9	209	-239
-8	170	174
-7	299	-311
-6	10*	15
-5	267	274
-4	46*	-56
-3	49*	56
-2	228	253
-1	10*	-60
H=	7, K=	9
-1	10*	10
-2	61*	-66
-3	314	358
-4	134	-135
-5	83	-79
-6	10*	-54
-7	10*	-14
-8	210	212
-9	276	266
-10	154	-164
-11	99	87
H=	7, K=	8
-12	172	187
-11	175	-171
-10	99	-94
-9	189	187
-8	145	140
-7	304	302
-6	89	94
-5	257	-270
-4	126	-154
-3	9*	-25
-2	179	-230
-1	76*	67
H=	7, K=	7
-1	90	-59
-2	312	-324
-3	468	-500
-4	175	-168
-5	213	235
-6	482	502
-7	127	113
-8	149	-158
-9	419	-417
-10	10*	15
-11	46*	63
-12	145	163
H=	7, K=	6
-13	177	-190
-12	144	-125
-11	460	457
-10	419	416
-9	60*	-92
-8	86	-102
-7	489	-503
-6	375	-381
-5	363	391
-4	120	-122
-3	105	109
-2	9*	21
-1	243	-268
H=	7, K=	5
-1	436	-449
-2	50*	-20
-3	445	456
-4	9*	-39
-5	167	-171
-6	23*	-88
-7	491	-496
-8	209	229
-9	164	168
-10	148	-126
-11	51*	25
-12	246	-270
-13	193	-185
H=	7, K=	4
-13	168	167
-12	61*	20
-11	405	-380
-10	38*	42
-9	10*	18
-8	23*	-60
-7	226	211
-6	133	130
-5	516	-503
-4	52*	-81
-3	202	179
-2	118	-168
-1	500	489
H=	7, K=	3
-1	58*	56
-2	99	-106
-3	319	-351
-4	54*	63
-5	555	481
-6	9*	33
-7	392	374
-8	388	385
-9	431	-392
-10	115	-80
-11	48*	-26
-12	212	-216
-13	280	267
-14	163	-158
H=	7, K=	2
-14	120	-93
-13	247	-228
-12	53*	-60
-11	457	441
-10	328	-335
-9	40*	36
-8	108	83
-7	653	-613
-6	157	136
-5	472	447
-4	74*	-65
-3	372	349
-2	170	173
-1	373	-356
H=	7, K=	1
-1	225	216
-2	367	-340
-3	742	711
-4	89	-66
-5	362	-309
-6	251	210
-7	220	-233
-8	164	-187
-9	369	320
-10	10*	-4
-11	49*	-53
-12	21*	44
-13	245	-257
-14	120	129
H=	7, K=	0
-13	260	286
-11	99	-94
-9	7*	-22
-7	200	216
-5	675	-723
-3	57*	-9
-1	614	618
H=	8, K=	0

L	FO	FC
-2	384	386
-4	218	-171
-6	621	-632
-8	135	138
-10	192	222
-12	353	-411
H=	8, K=	1
-12	41*	78
-11	98	-75
-10	463	405
-9	294	-285
-8	39*	-32
-7	57*	13
-6	193	-147
-5	164	169
-4	384	371
-3	59*	-37
-2	43*	-34
-1	201	-208
H=	8, K=	2
-1	259	-239
-2	307	-299
-3	58*	-86
-4	137	-135
-5	10*	-3
-6	269	250
-7	311	274
-8	186	-171
-9	140	139
-10	61*	-46
-11	120	114
-12	307	308
H=	8, K=	3
-12	125	105
-11	78*	65
-10	258	-261
-9	96	36
-8	204	213
-7	114	-124
-6	279	278
-5	201	208
-4	202	-202
-3	64*	24
-2	53*	8
-1	280	-262
H=	8, K=	4
-1	138	142
-2	370	361
-3	199	-182
-4	90	-55
-5	56*	-4
-6	266	-283
-7	142	159
-8	390	389
-9	34*	-32
-10	268	255
-11	164	-159
-12	394	-395
H=	8, K=	5
-11	11*	-53
-10	265	268
-9	10*	-19
-8	311	-300
-7	68*	56
-6	215	-208
-5	93	97
-4	230	223
-3	243	264
-2	38*	17
-1	21*	31
H=	8, K=	6
-1	63*	-21
-2	80	-56
-3	10*	42
-4	81	44
-5	176	188
-6	149	125
-7	173	-167
-8	46*	-54
-9	11*	-61
-10	102	-61
-11	123	-67
H=	8, K=	7
-11	74*	41
-10	190	-187
-9	120	-125
-8	46*	-20
-7	56*	99
-6	10*	31
-5	219	213
-4	169	-196
-3	67*	-124
-2	148	176
-1	215	-189
H=	8, K=	8
-1	154	192
-2	180	190
-3	314	-311
-4	299	-310
-5	110	-105
-6	268	-292
-7	128	135
-8	133	154
-9	137	-107
-10	199	225
H=	8, K=	9
-9	41*	-22
-8	167	-182
-7	11*	-43
-6	312	-321
-5	104	-110
-4	258	286
-3	115	-56
-2	10*	-48
-1	157	159
H=	8, K=	10
-1	207	-228
-2	195	-206
-3	45*	-41
-4	58*	97
-5	11*	-14
-6	85*	72
-7	84*	75
-8	139	-165
H=	8, K=	11
-7	40*	-2
-6	223	243
-5	66*	68
-4	133	-149
-3	41*	-15
-2	98	94
-1	131	-120
H=	8, K=	12
-1	98	113
-2	178	200
-3	38*	-64
-4	79*	-87
-5	33*	28
-6	52*	-66
H=	8, K=	13
-3	117	151
-2	11*	-2
-1	56*	26
H=	9, K=	10
-4	42*	-7
-3	245	-280
-2	195	-197
-1	192	203
H=	9, K=	9
-1	11*	-25
-2	66*	100
-3	118	-120
-4	90*	108
-5	119	126
-6	145	-134
H=	9, K=	8
-7	153	-140
-6	103	-88
-5	107	-102
-4	19*	44
-3	172	174
-2	172	175
-1	214	-234
H=	9, K=	7
-1	215	214
-2	37*	-20
-3	162	128
-4	166	-181
-5	179	-165
-6	164	168
-7	97	90
-8	132	-129
H=	9, K=	6
-8	155	-140
-7	165	171
-6	234	211
-5	98	125
-4	216	204
-3	333	-349
-2	123	-112
-1	158	168
H=	9, K=	5

L	FO	FC
H=	9, K=	5
-1	203	-203
-2	71*	70
-3	10*	-26
-4	159	184
-5	259	280
-6	175	-169
-7	209	-212
-8	91	-6
-9	51*	-50
H=	9, K=	4
-9	318	313
-8	78*	-51
-7	40*	-65
-6	59*	12
-5	191	-175
-4	72*	101
-3	214	241
-2	72*	-21
-1	218	-212
H=	9, K=	3
-1	260	279
-2	82	45
-3	47*	-42
-4	105	113
-5	399	-369
-6	207	-206
-7	236	258
-8	105	11
-9	170	164
-10	61*	-35
H=	9, K=	2
-10	74*	-42
-9	211	-197
-8	11*	75
-7	220	213
-6	150	-154
-5	100	93
-4	183	-169
-3	324	-340
-2	118	-68
-1	129	149
H=	9, K=	1
-1	259	-269
-2	170	153
-3	294	-305
-4	61*	-2
-5	259	247
-6	55*	20
-7	129	-94
-8	76*	-68
-9	116	-106
-10	35*	77

L	FO	FC
H=	9, K=	0
-9	108	127
-7	101	-98
-5	96	115
-3	151	139
-1	257	-310
H=	10, K=	0
-2	259	-238
-4	197	148
-6	89	69
H=	10, K=	1
-6	137	120
-5	83*	-92
-4	255	-243
-3	11*	23
-2	81*	-69
-1	54*	79
H=	10, K=	2
-1	15*	-43
-2	205	175
-3	120	82
-4	154	-120
-5	132	-100
-6	92*	88
H=	10, K=	3
-6	293	-292
-5	19*	5
-4	88	44
-3	85	-3
-2	209	211
-1	63*	36
H=	10, K=	4
-1	62*	44
-2	346	-322
-3	27*	8
-4	349	365
-5	11*	-56
H=	10, K=	5
-4	110	-111
-3	61*	-52
-2	282	-286
-1	88*	-123
H=	10, K=	6
-1	11*	-14
-2	168	202

e $\underline{Ni(L3)NO_2ClO_4.\frac{1}{2}H_2O}$

A Patterson synthesis based on the inner set of data ($2\theta < 30$ deg, 937 observed data) revealed the position of the nickel atom. Its coordinates, isotropic thermal motion parameter and scale were refined to give an R of 0.496. A Fourier synthesis using the phases generated by this model gave the positions of the atoms in the coordination sphere of the nickel atom. Several cycles of refinement using isotropic thermal motion parameters, and subsequent electron density difference maps using the complete set of data (2512 observed reflections) gave the positions of all the non-hydrogen atoms, and an R of 0.190. Anisotropic thermal motion was assigned to first the heavy atoms and then the atoms coordinated to the metal (R=0.130) and then to all the non-hydrogen atoms. Inclusion of determined and calculated hydrogen atom positions in the structure factor calculation reduced the R to 0.085. Some problems existed at this stage. The perchlorate anion was disordered between two alternate positions (labelled as Cl and Cl'), one of which was occupied together with a ½-occupied water molecule of solvation, connecting it via hydrogen bonding to two, symmetry-related cations, and the other perchlorate position being occupied when the water molecule was not present.

A further problem lay in the high anisotropic thermal motion exhibited by the terminal methyl (C4) and carbonyl oxygen (O1) atoms. Attempts were made to again assign split atoms to better represent this motion, but this model did not behave upon further refinement, and the single, highly anisotropic atoms

were retained. Full-matrix, least-squares refinement gave a final R of 0.071 for 358 variables.

Final fractional atomic coordinates (table 2.15) and thermal motion parameters (table 2.16 are listed, together with hydrogen atom positions (table 2.17) and a table of measured and calculated structure factors (x10) (table 2.18).

Table 2.15

Fractional Atomic Coordinates: $Ni(L3)NO_2(ClO_4).\frac{1}{2}H_2O$.

Atom Type	x	y	z
Ni	9505(4)	14964(6)	9200(7)
Cl1	4050(4)	683(6)	1269(7)
Cl2	3422(4)	265(5)	216(6)
O11	3932(6)	1135(9)	408(8)
O12	4399(6)	-20(8)	1154(8)
O13	4260(7)	1280(8)	2141(8)
O14	3610(7)	215(9)	1248(9)
O21	3920(6)	-208(10)	-0055(9)
O22	3198(6)	-155(8)	709(8)
O23	3048(7)	-354(8)	-580(8)
O24	3568(6)	1181(9)	232(8)
On1	758(2)	759(5)	1929(4)
On2	700(2)	21(4)	697(5)
N1	1056(3)	2879(4)	1439(4)
N2	104(2)	1825(4)	-44(4)
N3	1054(2)	1700(4)	-295(4)
N4	1794(3)	1121(5)	1778(4)
N5	1628(2)	3109(5)	2061(5)
N6	1943(3)	827(5)	2716(5)
Nn	640(3)	-12(6)	1488(7)
C1	1806(3)	2990(6)	2956(7)
C2	1489(4)	2690(7)	3454(7)
C3	2412(5)	3225(9)	3550(9)
C4	2756(8)	3518(9)	3061(9)
C5	714(3)	3570(6)	1152(6)
C6	891(4)	4546(6)	1508(7)
C7	106(3)	3482(6)	440(7)
C8	-191(3)	2533(6)	243(6)
C9	-795(4)	2667(7)	-556(7)
C10	-211(4)	2205(7)	1157(7)
C11	68(3)	1989(6)	-996(6)
C12	509(3)	1434(6)	-1129(6)
C13	1553(3)	1267(5)	-333(5)
C14	1520(4)	223(7)	-371(7)
C15	1590(4)	1687(7)	-1231(6)
C16	2072(3)	1634(6)	586(6)
C17	2195(3)	1269(6)	1567(6)
C18	2801(4)	1112(8)	2290(7)
O1	2599(7)	3119(10)	4317(10)
Ow	2184	4279(10)	980(10)

Cl1, Cl2, O11, O12, O13, O14, O21, O22, O23, O24: perchlorate anions

On1, On2, N1, N2, N3, N4, N5, N6, Nn: nitrite ligand

Table 2.16

Hydrogen Atom Coordinates: $Ni(L3)NO_2(ClO_4.\frac{1}{2}H_2O$.

($\times 10^4$)

Atom	x	y	z
HN2	1096	2365	-351
HN3	-113	1236	-144
HN61	2203	466	3104
HN62	1657	599	2835
H21	1372	3271	3609
H22	1723	2344	4066
H23	1165	2293	3070
H41	2568	3769	2361
H42	2951	3989	3540
H43	3011	2999	3144
H61	1063	4705	2268
H62	588	4968	1170
H63	1196	4713	1350
H71	-829	3908	674
H72	740	3710	-165
H91	-952	1964	-850
H92	-824	3082	-1071
H93	-1036	2931	-293
H101	-339	2769	1341
H102	182	2043	1711
H103	-433	1657	1101
H111	102	2654	-1112
H112	-319	1807	-1541
H121	443	744	-1118
H122	505	1551	-1755
H141	1510	3	215
H142	1894	-15	-295
H143	1167	-165	-1063
H151	3529	2685	1290
H152	3676	3530	1881
H153	3061	3475	1191
H161	2399	1556	478
H162	2016	2335	582
H181	2889	788	1702
H182	3006	1691	2546
H183	2858	693	2802
HOw1	1785	4131	484
HOw2	2457	4763	1388

Table 2.17

Thermal Motion Parameters: $Ni(L3)NO_2(ClO_4).\frac{1}{2}H_2O$.

($\times 10^3$, $\times 10^4$ for Ni A^2)

Atom Type	U11	U22	U33	U12	U13	U23
Ni	317(8)	390(8)	391(8)	-12(5)	121(5)	27(5)
Cl1	126(6)	67(5)	106(7)	11(5)	79(6)	27(5)
Cl2	104(7)	85(5)	100(6)	20(4)	51(5)	2(4)
O11	106(5)	40(2)	69(3)	-30(3)	82(4)	18(1)
O12	167(8)	54(7)	157(8)	49(2)	61(4)	38(2)
O13	133(5)	59(2)	58(2)	25(2)	7(1)	-11(1)
O14	88(4)	138(5)	75(3)	15(1)	19(2)	-45(3)
O21	66(4)	136(6)	183(7)	-13(2)	-55(4)	81(5)
O22	94(4)	137(6)	130(6)	14(2)	-8(1)	-14(2)
O23	181(7)	69(4)	72(5)	52(3)	48(3)	21(2)
O24	133(6)	79(5)	125(6)	-18(2)	29(3)	-21(2)
On1	58(4)	64(4)	62(4)	-7(3)	27(3)	6(3)
On2	53(4)	55(4)	86(5)	-12(3)	22(4)	-10(4)
N1	44(4)	61(4)	96(7)	-2(3)	32(5)	24(5)
N2	42(4)	48(4)	27(4)	-11(3)	13(3)	1(3)
N3	40(4)	43(4)	32(4)	-2(3)	12(3)	0(3)
N4	46(4)	45(4)	41(4)	-4(4)	15(3)	3(3)
N5	46(4)	90(6)	38(4)	9(4)	20(3)	0(3)
N6	34(4)	50(4)	64(5)	-5(3)	20(4)	30(4)
Nn	62(5)	64(6)	53(5)	-6(5)	11(4)	-6(4)
C1	46(5)	51(5)	52(6)	-6(4)	14(5)	-7(5)
C2	89(7)	76(7)	53(6)	-5(6)	29(6)	-8(5)
C3	72(8)	116(10)	45(7)	-10(7)	-21(6)	-11(7)
C4	92(9)	101(10)	91(9)	-17(8)	31(7)	-23(7)
C5	301(4)	57(6)	52(5)	10(4)	15(4)	6(4)
C6	41(5)	120(8)	73(7)	8(6)	18(5)	27(6)
C7	39(4)	60(6)	63(6)	15(4)	25(4)	8(4)
C8	41(5)	47(5)	51(5)	3(4)	27(4)	-6(4)
C9	72(7)	73(7)	82(7)	15(5)	38(6)	0(5)
C10	66(6)	107(8)	57(6)	17(6)	36(5)	5(5)
C11	48(5)	83(6)	39(5)	-5(5)	12(4)	9(5)
C12	41(5)	58(5)	40(5)	-3(4)	7(4)	8(4)
C13	35(5)	69(6)	61(6)	14(4)	13(4)	4(5)
C14	43(5)	87(7)	84(7)	11(5)	16(5)	1(6)
C15	54(6)	104(8)	80(7)	10(5)	40(5)	7(6)
C16	43(5)	53(6)	88(7)	8(5)	19(5)	-13(5)
C17	47(4)	50(5)	65(6)	9(5)	21(5)	-2(5)
C18	75(7)	42(6)	104(8)	-5(5)	28(6)	-22(5)
Cl	118(10)	151(13)	99(9)	-25(9)	23(9)	-25(9)

Table 2.18

Structure Factor Listing: $Ni(L3)NO_2(ClO_4).\frac{1}{2}H_2O$.

(x 10)

Unobserved reflections are denoted by an asterisk.

L	FO	FC
H=	0, K=	0
2	1481	1478
4	1240	-1252
6	253	-242
8	28*	44
10	346	328
12	94	49
14	42*	-79
H=	0, K=	2
1	679	-484
2	168	-146
3	207	166
4	311	308
5	381	-376
6	89	114
7	365	365
8	66*	-70
9	603	627
10	146	-163
11	155	187
12	12*	-14
13	226	-257
14	54*	-18
H=	0, K=	4
0	717	-651
1	1136	-1214
2	392	411
3	508	448
4	100	117
5	223	227
6	430	457
7	404	-437
8	76	100
9	317	-324
10	322	-354
11	216	-214
12	97*	-142
13	136	143
14	137	140
H=	0, K=	6
0	1338	1355
1	849	764
2	914	910
3	153	169
4	401	-416
5	172	-132
6	463	-470
7	66*	-96
8	22*	26
9	222	-264
10	213	255
11	114	-121
12	112	118
13	106	87
H=	0, K=	8
0	322	285
1	63*	18
2	348	363
3	423	-457
4	109	-105
5	109	-95
6	175	-147
7	255	331
8	108	-127
9	238	310
10	29*	-90
11	12*	62
12	96*	90
H=	0, K=	10
0	386	-387
1	126	44
2	366	-366
3	10*	-17
4	233	308
5	51*	-90
6	281	362
7	83*	-89
8	12*	-41
9	47*	16
10	116	-141
11	93*	-23
H=	0, K=	12
0	112	127
1	196	225
2	133	111
3	244	287
4	12*	-19
5	114	98
6	141	-119
7	196	-240
8	49*	-20
9	191	-213
H=	0, K=	14
0	274	273
1	71*	-126
2	55*	8
3	123	-109
4	272	-288
5	66*	-68
6	217	-232
H=	1, K=	1
0	3*	569
1	1928	-1835
2	774	-713
3	172	-177
4	268	-224
5	543	536
6	296	-314
7	279	287
8	92	-96
9	209	217
10	453	491
11	64*	-79
12	110	124
13	75*	-51
14	159	-152
H=	1, K=	3
0	1091	-1146
1	1196	-1247
2	369	-260
3	432	361
4	590	549
5	102	-87
6	419	398
7	67*	54
8	495	-507
9	431	449
10	733	-749
11	11*	-12
12	274	-255
13	115	-66
14	218	253
H=	1, K=	5
0	299	249
1	624	622
2	612	579
3	796	787
4	304	-357
5	79	-18
6	96	-109
7	716	-720
8	207	179
9	290	-293
10	91	18
11	130	91
12	79*	87
13	185	152
H=	1, K=	7
0	792	808
1	364	-349
2	162	-157
3	184	-208
4	703	-741
5	111	106
6	222	-240
7	176	184
8	203	200
9	48*	50
10	225	198
11	74*	74
12	186	153
H=	1, K=	9
0	201	-217
1	496	-519
2	116	-105
3	549	-610
4	178	207
5	134	143
6	42*	-9
7	361	376
8	127	-148
9	57*	58
10	138	-137
11	112	-45
H=	1, K=	11
0	161	148
1	175	180
2	109	103
3	212	210
4	143	155
5	50*	-54
6	215	225
7	225	-220
8	90*	-66
9	71*	-50
10	123	-129
H=	1, K=	13
0	273	279
1	114	95
2	93*	-146
3	61*	-23

L	FO	FC
4	230	-240
5	121	-122
6	156	-136
7	12*	20
H=	1, K=	15
0	12*	30
1	211	-213
2	33*	0
H=	2, K=	0
2	568	456
4	696	-632
6	196	155
8	849	876
10	909	928
12	76*	24
14	218	-213
H=	2, K=	2
0	540	-510
1	970	-975
2	650	-554
3	255	-293
4	280	252
5	616	602
6	143	140
7	424	415
8	395	-389
9	192	205
10	70*	-108
11	420	-438
12	79*	-29
13	26*	29
14	125	127
H=	2, K=	4
0	504	489
1	1425	1472
2	142	110
3	192	-176
4	156	154
5	527	-575
6	36*	47
7	135	-140
8	378	-387
9	136	118
10	430	-453
11	73*	69
12	183	213
13	43*	19

L	FO	FC
H=	2, K=	6
0	326	344
1	241	275
2	448	-496
3	273	-251
4	442	-423
5	269	-274
6	66*	50
7	109	-101
8	526	505
9	90*	49
10	249	275
11	175	158
12	151	119
13	99*	131
H=	2, K=	8
0	152	153
1	522	-552
2	186	-192
3	8*	-24
4	245	-250
5	441	463
6	79*	-17
7	331	354
8	113	85
9	11*	-6
10	83*	62
11	115	-78
12	46*	-83
H=	2, K=	10
2	248	271
0	215	-206
1	174	167
3	86*	59
4	308	324
5	146	-169
6	11*	28
7	44*	35
8	284	-283
9	12*	78
10	214	-191
H=	2, K=	12
0	131	147
1	326	345
2	11*	5
3	109	121
4	36*	-89

L	FO	FC
5	166	-186
6	12*	-23
7	248	-255
8	102*	86
H=	2, K=	14
0	208	173
1	197	-190
2	152	-209
3	94*	-5
4	340	-334
5	188	190
H=	3, K=	1
0	312	305
1	552	-591
2	517	-462
3	259	270
4	431	-451
5	158	165
6	59*	34
7	8*	67
8	541	556
9	603	-598
10	281	264
11	280	-276
12	82*	-103
13	27*	5
H=	3, K=	3
0	550	573
1	907	-817
2	66	-49
3	125	103
4	59*	38
5	25*	-13
6	342	-350
7	97	101
8	721	-742
9	169	-138
10	366	-345
11	139	-129
12	217	199
13	139	109
H=	3, K=	5
0	1002	983
1	857	849
2	116	33
3	101	-75
4	107	19

L	FO	FC
5	669	-695
6	276	273
7	324	-343
H=	3, K=	15
0	88*	66
1	202	-195
H=	3, K=	5
8	31*	32
9	360	371
10	248	223
11	226	215
12	17*	44
13	38*	-62
H=	3, K=	7
0	688	-699
1	413	-410
2	545	-550
3	112	108
4	289	-318
5	181	180
6	105	90
7	129	-163
8	398	372
9	131	-100
10	162	134
11	21*	26
12	12*	-26
H=	3, K=	9
0	104	108
1	466	-438
2	215	207
3	8*	21
4	79*	-51
5	261	217
6	306	-300
7	109	47
8	245	-229
9	249	-236
10	114	-86
11	342	-296
H=	3, K=	11
0	141	157
1	371	356
2	10*	47
3	272	-262

L	FO	FC
H=	3, K=	11
4	230	239
5	360	-368
6	46*	9
7	92*	-59
8	185	-185
9	86*	91
H=	3, K=	13
0	187	-185
1	103*	76
2	401	-420
3	123	-153
4	164	-158
5	106*	-152
6	78*	170
H=	4, K=	0
0	1268	-1061
2	1410	-1358
4	93	-24
6	238	247
8	426	437
10	135	-116
12	99*	-38
H=	4, K=	2
0	896	-898
1	153	156
2	864	-863
3	771	789
4	199	-211
5	377	388
6	475	-478
7	121	108
8	204	-210
9	676	-682
10	81*	-76
11	251	-221
12	26*	17
13	126	110
H=	4, K=	4
0	161	-173
1	210	192
2	28*	28
3	6*	-52
4	71	86
5	454	-423
6	520	-531
7	230	213
8	478	-453
9	247	244
10	317	323
11	188	214
12	180	196
13	64*	-106
H=	4, K=	6
0	378	-350
1	309	-287
2	763	-770
3	363	-379
4	368	-383
5	322	-313
6	694	709
7	33*	29
8	103	110
9	282	273
10	110	-125
11	79*	72
12	157	-116
H=	4, K=	8
0	153	-160
1	64*	-29
2	472	-480
3	357	362
4	353	-377
5	287	244
6	174	163
7	181	-192
8	77*	87
9	231	-225
10	66*	-84
11	228	-218
H=	4, K=	10
0	290	323
1	97	-72
2	323	307
3	197	-190
4	124	-128
5	344	352
6	365	-374
7	11*	53
8	118	-97
9	67*	-61
H=	4, K=	12
0	89*	22
1	11*	-36
2	118	-62
3	247	-227
4	103*	111
5	264	-273
6	111	130
7	74*	6
H=	4, K=	14
0	190	-166
1	91*	-64
2	222	-224
3	130	97
4	12*	54
H=	5, K=	1
0	26*	-98
1	419	441
2	837	-784
3	643	629
4	179	195
5	160	-142
6	278	281
7	634	-634
8	201	184
9	447	-426
10	166	-195
11	90*	-113
12	35*	-12
13	151	149
H=	5, K=	3
0	213	117
1	180	-180
2	147	127
3	409	406
4	133	-123
5	350	349
6	394	-403
7	98	66
8	10*	-41
9	281	-260
10	306	294
11	128	123
12	85*	71
H=	5, K=	5
0	117	-102
1	49*	-71
2	100	-100
3	405	-394
4	175	-185
5	378	-358
6	38*	40
7	599	615
8	96*	94
9	415	412
10	89*	86
11	23*	-31
12	92*	81
H=	5, K=	7
0	860	-916
1	312	302
2	618	-664
3	79	55
4	324	307
5	87	-85
6	494	437
7	10*	-20
8	158	-148
9	90*	-10
10	72*	-73
11	82*	-85
H=	5, K=	9
0	329	345
1	369	351
2	136	147
3	475	487
4	236	-217
5	243	256
6	115	-123
7	251	-260
8	91*	-82
9	177	-194
10	12*	60
H=	5, K=	11
0	56*	67
1	10*	40
2	31*	-12
3	86*	-91
4	11*	37
5	11*	29
6	164	-151
7	131	113
8	12*	14
H=	5, K=	13
0	343	-369
1	94*	11

L	FO	FC
2	243	-229
3	159	-133
4	125	145
5	12*	-57
6	153	112
H=	5, K=	15
0	12*	9
H=	6, K=	0
0	773	-808
2	98	-77
4	880	1014
6	299	328
8	402	-397
10	69*	30
12	65*	-120
H=	6, K=	2
0	447	-434
1	731	720
2	41*	48
3	715	698
4	58*	23
5	190	190
6	86	-58
7	516	-512
9	211	-189
10	96*	-95
11	153	155
12	12*	-5
H=	6, K=	4
0	708	783
1	580	-550
2	71	26
3	287	-276
4	457	-485
5	74	-56
6	232	-244
7	207	211
8	435	423
9	258	251
10	371	336
11	160	-151
12	93*	102
H=	6, K=	6
0	380	-379
1	238	-247
2	87	-67
3	390	-396
4	392	429
5	113	-94
6	166	156
7	244	246
8	147	-169
9	152	-148
10	154	-175
11	12*	39
H=	6, K=	8
0	206	-202
1	336	330
2	88	-24
3	342	330
4	209	183
5	10*	-41
6	258	263
7	291	-298
8	71*	-91
9	194	-185
10	167	-131
H=	6, K=	10
0	506	472
1	165	-155
2	100	-105
3	84*	20
4	352	-367
5	124	122
6	157	-167
7	11*	23
8	12*	63
9	12*	67
H=	6, K=	12
0	193	-215
1	297	-295
2	56*	-124
3	302	-300
4	11*	16
5	12*	24
6	12*	65
7	141	120
H=	6, K=	14
0	348	-343
1	142	117
2	48*	-9
3	65*	62
H=	7, K=	1
0	638	-604
1	602	553
2	446	415
3	437	429
4	497	463
5	392	-407
6	55*	3
7	329	-344
8	129	-145
9	11*	14
10	56*	-59
11	165	135
12	70*	-39
H=	7, K=	3
0	49*	43
1	605	548
2	898	-946
3	266	273
4	604	-655
5	141	-126
6	74	61
7	9*	-10
8	177	210
9	156	98
10	142	132
11	12*	33
12	47*	-45
H=	7, K=	5
0	67	-104
1	319	-334
2	148	-132
3	800	-818
4	54*	-22
5	460	436
6	66*	-25
7	523	488
8	21*	10
9	25*	-23
10	12*	-20
11	236	-212
H=	7, K=	7
0	500	-547
1	82	100
2	135	122
3	195	194
4	640	635
5	82*	-13
6	114	108
7	87*	-107
8	184	-170
9	12*	-9
10	177	-180
H=	7, K=	9
0	56*	86
1	255	280
2	347	-324
3	256	240
4	48*	65
5	238	-227
6	63*	-39
7	141	-142
8	12*	50
9	51*	24
H=	7, K=	11
0	64*	19
1	387	-359
2	81*	-35
3	11*	-10
4	263	-233
5	138	140
6	109	36
7	220	213
H=	7, K=	13
0	232	-252
1	112	-137
2	161	160
3	90*	96
4	138	154
5	155	109
H=	8, K=	0
0	483	-317
2	2508	2621
4	908	931
6	153	-153
8	62*	-39
10	194	-185
12	186	199
H=	8, K=	2
0	1034	-1031
1	855	832
2	636	-656

L	FO	FC
H=	8, K=	2
3	55*	57
4	53*	-28
5	306	-325
6	169	170
7	118	-109
8	48*	62
9	40*	77
10	96*	77
11	213	186
H=	8, K=	4
0	103	-80
1	374	-358
2	568	-598
3	318	-341
4	311	-324
5	265	278
6	317	323
7	191	204
8	474	455
9	189	-184
10	227	225
11	71*	-15
H=	8, K=	6
0	71	17
1	310	-315
2	460	445
3	443	456
4	584	553
5	401	383
6	101	-129
7	134	-131
8	368	-358
9	12*	74
10	21*	-82
H=	8, K=	8
0	246	-234
1	377	388
2	116	107
3	102	-84
4	356	324
5	152	-149
6	27*	-22
7	72*	-57
8	56*	-43
9	106*	99
H=	8, K=	10
0	108	-136
1	37*	-91
2	379	-364
3	28*	2
4	250	-256
5	112	-101
6	87*	-8
7	68*	89
8	341	321
H=	8, K=	12
0	95*	-73
1	181	-209
2	75*	9
3	78*	28
4	125	126
5	157	133
6	83*	57
H=	8, K=	14
0	86*	-93
1	173	204
2	111*	151
H=	9, K=	1
0	238	-227
1	560	597
2	710	750
3	1016	-1028
4	229	230
5	310	-332
6	92	-88
7	210	193
8	192	-170
9	34*	20
10	12*	27
11	217	208
H=	9, K=	3
0	972	-936
1	125	127
2	600	-552
3	593	-609
4	149	-134
5	206	-200
6	302	286
7	112	-77
8	447	456
9	127	54
10	87*	-127
11	136	106
H=	9, K=	5
0	531	553
1	155	-148
2	26*	-53
3	412	383
4	384	386
5	399	416
6	83*	45
7	11*	55
8	201	-200
9	270	-259
10	200	185
H=	9, K=	7
0	254	276
1	74	-83
2	441	438
3	174	-173
4	167	139
5	187	-190
6	126	-104
7	11*	0
8	149	-97
9	12*	19
H=	9, K=	9
0	351	-329
1	135	-136
2	244	-263
3	347	-322
4	168	-180
5	323	-323
6	133	92
7	116	-101
8	174	162
H=	9, K=	11
0	108	-86
1	188	-196
2	73*	-18
3	84*	110
4	12*	66
5	190	196
6	158	115
H=	9, K=	13
0	12*	30
1	12*	-17
2	259	259
3	92*	99
H=	10, K=	0
0	1162	1091
2	899	923
4	69*	-78
6	487	-471
8	195	-176
10	165	175
H=	10, K=	2
0	633	-607
1	580	-589
2	530	-562
3	668	-686
4	248	-255
5	76*	-87
6	68*	94
7	140	157
8	11*	9
9	239	236
10	202	-175
11	68*	90
H=	10, K=	4
0	741	-760
1	204	211
2	155	-171
3	331	351
4	204	205
5	180	192
6	287	280
7	115	-132
8	186	224
9	191	-200
10	91*	-84
H=	10, K=	6
0	126	107
1	270	246
2	476	501
3	333	341
4	61*	53
5	54*	25
6	472	-433
7	129	-101
8	208	-173
9	164	-134
H=	10, K=	8

L	FO	FC
0	132	-161
1	263	-235
2	99	72
3	385	-337
4	101	96
5	141	-151
6	153	-114
7	173	204
8	140	-133

H= 10, K= 10

L	FO	FC
0	389	-363
1	140	162
2	219	-211
3	11*	41
4	125	109
5	24*	-20
6	293	274
7	109*	-82

H= 10, K= 12

L	FO	FC
0	113	90
1	50*	76
2	213	213
3	272	267
4	109*	111
5	86*	96

H= 10, K= 14

L	FO	FC
0	176	174

H= 11, K= 1

L	FO	FC
0	347	339
1	358	-348
2	133	152
3	322	-341
4	118	-121
5	71*	44
6	166	-158
7	187	179
8	78*	47
9	370	374
10	193	173

H= 11, K= 3

L	FO	FC
0	570	-574
1	185	-202
2	113	92
3	197	-173
4	416	420
5	52*	-18
6	294	294
7	92*	78
8	212	-210
9	114	-63
10	278	-241

H= 11, K= 5

L	FO	FC
0	163	-172
1	670	672
2	526	516
3	763	781
4	111	59
5	195	179
6	145	-117
7	379	-366
8	246	254
9	277	-268

H= 11, K= 7

L	FO	FC
0	333	330
1	187	-171
2	85*	-87
3	203	-194
4	225	-251
5	27*	26
6	136	-146
7	36*	33
8	42*	34

H= 11, K= 9

L	FO	FC
0	193	-235
1	98	-56
2	11*	9
3	258	-287
4	92*	36
5	88*	-36
6	66*	-11
7	355	343

H= 11, K= 11

L	FO	FC
0	47*	-20
1	208	200
2	117	96
3	331	322
4	165	170
5	13*	46

H= 11, K= 13

L	FO	FC
0	156	180
1	99*	63
2	33*	4

H= 12, K= 0

L	FO	FC
0	1313	1305
2	132	124
4	377	-388
6	110	117
8	120	75
10	330	322

H= 12, K= 2

L	FO	FC
0	236	-233
1	348	-363
2	227	238
3	293	-299
4	9*	43
5	254	254
6	73*	-71
7	413	406
8	70*	-81
9	27*	70
10	164	-165

H= 12, K= 4

L	FO	FC
0	17*	-91
1	129	135
2	345	369
3	133	130
4	544	525
5	10*	13
6	128	133
7	319	-315
8	191	-191
9	12*	91

H= 12, K= 6

L	FO	FC
1	292	313
2	86	-94
0	426	411
3	171	-145
4	303	-276
5	287	-278
6	94*	-75
7	131	-157
8	238	242

H= 12, K= 8

L	FO	FC
0	37*	-45
1	408	-418
2	120	90
3	123	-94
4	19*	-35
5	82*	146
6	181	-183
7	235	235

H= 12, K= 10

L	FO	FC
0	134	-136
1	84*	104
2	192	199
3	78*	54
4	316	304
5	12*	-28
6	104*	96

H= 12, K= 12

L	FO	FC
0	12*	26
1	205	231
2	38*	41
3	165	148

H= 13, K= 1

L	FO	FC
1	338	-354
2	145	-138
3	60*	64
0	66*	43
4	272	-269
5	352	341
6	153	118
7	164	104
8	131	131
9	94*	-103

H= 13, K= 3

L	FO	FC
1	298	-296
2	409	437
3	214	-201
0	176	166
4	188	198
5	172	178
6	282	-266
7	41*	75
8	393	-389
9	74*	41

H= 13, K= 5

L	FO	FC
1	544	567
2	221	233

L	FO	FC
H= 13, K= 5		
0	186	203
3	326	-310
4	10*	-25
5	189	-161
6	129	-133
7	271	-246
8	109	43
H= 13, K= 7		
0	77*	53
1	317	-321
2	315	-310
3	54*	20
4	190	-193
5	81*	-14
6	56*	113
7	64*	-70
H= 13, K= 9		
0	106	113
1	170	-168
2	317	324
3	11*	-5
4	97*	79
5	236	273
6	148	-174
H= 13, K= 11		
0	16*	71
1	247	269
2	220	233
3	57*	50
4	107*	126
H= 13, K= 13		
0	54*	-18
H= 14, K= 0		
0	170	162
2	299	-322
4	47*	58
6	112	103
8	349	369
H= 14, K= 2		
0	405	396
1	324	-340
2	86	107
3	260	311
4	78*	26
5	303	293
6	98	76
7	98	-78
8	69*	-102
9	202	-227
H= 14, K= 4		
0	249	227
1	347	350
2	601	649
3	50*	-54
4	81*	72
5	261	-246
6	212	-217
7	169	196
8	222	-236
H= 14, K= 6		
0	89	-86
1	124	86
2	249	-233
3	210	-202
4	124	-132
5	99*	-134
6	106*	136
7	66*	-116
H= 14, K= 8		
0	97	125
1	76*	-33
2	132	-123
3	198	208
4	142	-127
5	261	242
6	136	157
H= 14, K= 10		
0	91*	105
1	62*	49
2	356	366
3	35*	36
4	110	110
H= 14, K= 12		
0	12*	37
1	107*	34
2	59*	-62
H= 15, K= 1		
0	61*	25
1	8*	60
2	275	-292
3	324	343
4	129	121
5	90	-24
6	222	186
7	108	-81
8	155	118
H= 15, K= 3		
0	664	673
1	478	-478
2	453	455
3	122	98
4	155	-134
5	11*	-12
6	362	-347
7	44*	-46
8	108*	-98
H= 15, K= 5		
0	200	203
1	91	43
2	142	137
3	192	-191
5	162	-169
6	12*	55
7	162	151
H= 15, K= 7		
0	528	-514
1	169	-165
2	178	-186
3	81*	-58
4	99	84
5	12*	-36
6	230	247
H= 15, K= 9		
0	213	235
1	91*	25
2	176	169
3	63*	98
4	12*	-14
5	139	153
H= 15, K= 11		
0	297	304
1	59*	29
2	106	106
H= 16, K= 0		
0	711	-715
2	312	-314
4	122	72
6	174	142
8	12*	-44
H= 16, K= 2		
0	216	231
1	351	362
2	180	-156
3	423	420
4	113	-99
5	11*	-35
6	87*	-69
7	240	-256
H= 16, K= 4		
0	390	417
1	183	-182
2	128	131
3	247	-240
4	204	-193
5	11*	-36
6	298	-300
7	142	136
H= 16, K= 6		
0	229	-204
1	366	-369
2	180	-161
3	119	-114
4	63*	-17
5	56*	2
6	175	168
H= 16, K= 8		
0	78*	-63
1	325	335
2	73*	-53
3	245	240
4	105*	-94
5	12*	-20
H= 16, K= 10		

L	FO	FC
0	416	395
1	63*	45
2	175	182
3	12*	-76
H=	16, K=	12
0	12*	16
H=	17, K=	1
0	109	-124
1	564	531
2	88*	-40
3	213	192
4	126	134
5	11*	-37
6	103*	101
7	232	-245
H=	17, K=	3
0	445	477
1	81*	107
2	154	-151
3	102	47
4	458	-431
5	62*	-65
6	166	-83
7	129	-97
H=	17, K=	5
0	79*	-6
1	268	-237
2	47*	-37
3	171	-159
4	91*	95
5	84*	52
6	53*	-52
H=	17, K=	7
0	274	-281
1	80*	102
2	11*	22
3	12*	33
4	143	144
5	96*	-30
H=	17, K=	9
0	170	148
1	315	303
2	85*	-62
3	201	185
H=	17, K=	11
0	78*	90
1	181	-184
H=	18, K=	0
0	89*	115
2	207	212
4	232	211
6	12*	-33
H=	18, K=	2
0	77*	-24
1	541	524
4	61*	-93
2	183	-186
3	212	208
5	283	-282
6	73*	-36
H=	18, K=	4
0	71*	-62
1	365	-370
2	195	-219
3	123	-118
4	263	-260
5	117	161
6	30*	13
H=	18, K=	6
0	179	171
1	266	-267
2	197	202
3	58*	-32
4	150	135
5	58*	106
H=	18, K=	8
0	23*	-24
1	309	293
2	119	-133
3	97*	-13
H=	18, K=	10
0	148	137
1	91*	-58
H=	19, K=	1
0	64*	56
1	185	191
2	235	227
3	78*	-12
4	97*	89
5	258	-262
6	81*	-137
H=	19, K=	3
0	365	-376
1	205	180
2	631	-627
3	11*	-32
4	211	-205
5	103*	-139
H=	19, K=	5
0	81*	47
1	118	-91
2	11*	18
3	77*	74
4	12*	-52
5	291	288
H=	19, K=	7
0	229	254
1	75*	-5
2	166	164
3	123	-84
H=	19, K=	9
0	95*	-117
1	152	155
H=	20, K=	0
0	312	332
2	379	377
4	80*	78
H=	20, K=	2
1	11*	83
2	119	-76
3	289	-291
4	56*	-10
5	195	-197
H=	20, K=	4
0	269	-264
1	82*	18
2	348	-340
3	197	193
4	80*	27
H=	20, K=	6
0	342	341
1	103	-21
2	201	197
3	164	148
H=	20, K=	8
0	12*	-46
1	12*	-46
2	103*	35
H=	21, K=	1
0	164	186
1	267	-284
2	155	127
3	220	-243
4	92*	-77
H=	21, K=	3
0	414	-420
1	101	-38
2	268	-276
3	174	-177
4	180	183
H=	21, K=	5
0	11*	-41
1	195	211
2	32*	8
3	284	280
H=	21, K=	7
0	263	257
1	116*	-169
2	103*	65
H=	22, K=	0
0	111	73
2	12*	-7

L	FO	FC
H= 22, K= 2		
0	114	-82
1	363	-362
2	12*	-43
3	251	-223
H= 22, K= 4		
0	331	-329
1	201	226
2	12*	-7
H= 22, K= 6		
0	62*	68
1	183	168
H= 23, K= 1		
0	57*	-19
1	205	-223
2	83*	-92
H= 23, K= 3		
0	203	-183
1	66*	-87
2	177	210
H= 23, K= 5		
0	12*	-5
1	285	302
H= 24, K= 0		
0	127	-149
H= 24, K= 2		
0	12*	12
1	185	-172
H= 24, K= 4		
0	84*	-16
H= 25, K= 1		
0	135	-118
H= 25, K= 3		
0	189	167
H= 1, K= 1		
-1	231	-251
-2	1101	1064
-3	424	397
-4	165	-153
-5	69	-32
-6	342	-302
-7	143	-164
-8	291	-299
-9	468	-467
-10	73*	18
-11	185	-205
-12	254	239
-13	121	155
-14	12*	15
-15	224	211
H= 1, K= 3		
-1	1244	-1217
-2	1248	-1239
-3	419	405
-4	503	511
-5	197	221
-6	266	282
-7	152	-134
-8	40*	-22
-9	302	-289
-10	153	-168
-11	163	-180
-12	182	-220
-13	98*	142
-14	49*	6
H= 1, K= 5		
-1	593	563
-2	543	554
-3	818	-823
-4	258	258
-5	486	-514
-6	203	-200
-7	209	172
-8	90	82
-9	452	468
-10	67*	49
-11	163	184
-12	72*	4
-13	102*	-121
-14	13*	-9
H= 1, K= 7		
-1	173	-192
-2	790	785
-3	165	-185
-4	316	-300
-5	201	202
-6	309	-301
-7	22*	-43
-8	244	-241
-9	286	-258
-10	83*	-72
-11	100*	-97
-12	127	119
-13	64*	-33
H= 1, K= 9		
-1	291	-285
-2	164	-168
-3	431	444
-4	238	-259
-5	183	181
-6	208	220
-7	155	-170
-8	92*	97
-9	217	-196
-10	146	-107
-11	107*	-93
-12	96*	-74
H= 1, K= 11		
-1	111	-37
-2	10*	-15
-3	303	-348
-4	64*	81
-5	502	-482
-6	173	210
-7	32*	-31
-8	192	164
-9	243	232
-10	143	-87
H= 1, K= 13		
-1	56*	-43
-2	188	184
-3	203	-199
-4	12*	-25
-5	156	-107
-6	225	-246
-7	12*	28
-8	180	-150
H= 1, K= 15		
-1	13*	11
-2	47*	55
-3	182	186
H= 2, K= 0		
-2	1825	1917
-4	693	-760
-6	435	-515
-8	309	-375
-10	385	-372
-12	133	129
-14	62*	83
H= 2, K= 2		
-1	1021	-1032
-2	1121	-1068
-3	72	87
-4	1045	-1028
-5	381	345
-6	91	50
-7	146	157
-8	94	-92
-9	265	-294
-10	277	-259
-15	222	258
-11	344	-393
-12	11*	-87
-13	20*	27
-14	85*	39
H= 2, K= 4		
-1	614	565
-2	854	-995
-3	334	292
-4	312	-300
-5	510	-508
-6	549	513
-7	128	106
-8	335	371
-9	324	317
-10	20*	12
-11	80*	102
-12	270	-274
-13	31*	45
-14	144	-151
H= 2, K= 6		
-1	767	798
-2	640	644
-3	471	-466
-4	166	149

L	FO	FC
-5	569	-568
-6	496	-516
-7	167	149
-8	348	-371
-9	160	160
-10	11*	-23
-11	165	168
-12	118	120
-13	12*	-33
-14	151	132
H=	2, K=	8
-1	468	-438
-2	256	247
-3	66*	-25
-4	100	129
-5	500	513
-6	445	-459
-7	10*	30
-8	224	-192
-9	334	-314
-10	118	-95
-11	185	-175
-12	57*	-43
-13	13*	20
H=	2, K=	10
-1	45*	-22
-2	8*	-243
-3	130	107
-4	259	-277
-5	243	229
-6	155	163
-7	83*	56
-8	347	339
-9	89*	63
-10	49*	14
-11	12*	-17
H=	2, K=	12
-1	179	210
-2	99*	94
-3	92*	-91
-4	210	185
-5	183	-175
-6	160	173
-7	98*	-96
-8	114	-159
-9	173	168
H=	2, K=	14
-1	151	-113
-2	196	198
-3	106*	119
-4	93*	51
-5	83*	59
-6	123	-104
H=	3, K=	1
-1	2170	-2094
-2	1220	965
-3	1040	946
-4	324	291
-5	890	914
-6	66	63
-7	318	320
-8	274	-265
-9	8*	28
-10	69*	-79
-11	146	-145
-12	11*	103
-13	64*	-31
-14	156	192
-15	77*	28
H=	3, K=	3
-1	879	-773
-2	1467	1519
-3	405	355
-4	464	-471
-5	242	217
-6	106	56
-7	411	431
-8	562	565
-9	105	-81
-10	134	160
-11	36*	-50
-12	162	-187
-13	64*	8
-14	289	-313
-15	54*	81
H=	3, K=	5
-1	1035	980
-2	555	-506
-3	445	491
-4	21*	28
-5	712	-710
-6	88	84
-7	394	-397
-8	83	-32
-9	167	182
-10	10*	11
-11	413	432
-12	25*	58
-13	122	107
-14	114	77
H=	3, K=	7
-1	449	-450
-2	342	349
-3	219	237
-4	724	742
-5	20*	-64
-6	189	-181
-7	57*	14
-8	313	-280
-9	56*	72
-10	337	-333
-11	149	-103
-12	88*	59
-13	12*	5
H=	3, K=	9
-1	134	-174
-2	114	-156
-3	72*	-78
-4	198	-188
-5	656	701
-6	64*	13
-7	426	412
-8	286	292
-9	11*	-43
-10	90*	-8
-11	132	-77
-12	142	-113
H=	3, K=	11
-1	202	191
-2	65*	62
-3	81*	-101
-4	184	-158
-5	134	-139
-6	15*	-16
-7	181	-159
-8	155	159
-9	181	186
-10	127	128
-11	166	160
H=	3, K=	13
-1	175	163
-2	272	271
-3	103	-77
-4	11*	-21
-5	153	-148
-6	76*	-27
-7	42*	-40
-8	213	-195
H=	3, K=	15
-1	170	-181
-2	28*	54
-3	60*	37
H=	4, K=	0
-8	296	-318
-10	161	-210
-12	10*	17
-14	254	273
-4	1044	1004
-2	628	810
H=	4, K=	2
-5	102	78
-6	371	375
-7	1006	1027
-8	32*	-53
-9	50*	74
-10	64*	51
-11	272	-381
-12	60*	52
-13	243	-305
-14	82*	34
-15	12*	40
-4	166	-146
-3	1271	-1176
-2	693	-621
-1	420	-505
H=	4, K=	4
-5	82	-60
-6	252	-258
-7	215	-216
-8	509	496
-9	238	-249
-10	286	325
-11	67*	100
-12	11*	-56
-13	136	181
-14	197	-242
-15	76*	-30
-4	544	-566
-3	430	460
-2	655	637

L	FO	FC
H=	4, K=	4
-1	98	87
H=	4, K=	6
-5	489	-528
-6	58*	-12
-7	94	-98
-8	133	-141
-9	119	11
-10	319	-306
-11	11*	-11
-12	78*	65
-13	12*	93
-14	202	202
-4	693	707
-3	117	-39
-2	377	367
-1	277	309
H=	4, K=	8
-5	273	272
-6	139	136
-7	296	321
-8	25*	-33
-9	101	100
-10	85*	-54
-11	274	-260
-12	137	-118
-13	190	-158
-4	514	519
-3	281	-308
-2	120	-84
-1	571	-556
H=	4, K=	10
-3	120	-136
-4	414	-437
-5	20*	-46
-6	160	-139
-7	11*	-65
-8	242	241
-9	117	76
-10	311	331
-11	12*	-29
-12	12*	-24
-2	8*	-72
-1	215	188
H=	4, K=	12
-1	262	248
-2	160	145
-3	169	154
-4	93*	90
-5	78*	-84
-6	97*	63
-7	283	-295
-8	136	-124
-9	135	-142
-10	154	-150
H=	4, K=	14
-1	175	-202
-2	124	148
-3	96*	-18
-4	192	202
-5	12*	11
-6	72*	135
H=	5, K=	1
-6	987	1022
-7	959	974
-8	332	337
-9	332	349
-10	338	-381
-11	10*	-102
-12	244	-301
-13	287	-361
-14	12*	38
-15	75*	-126
-5	638	564
-4	342	-273
-3	69	-79
-2	85	-48
-1	252	254
H=	5, K=	3
-6	867	-901
-7	127	100
-8	13*	11
-9	84	90
-10	246	225
-11	61*	-70
-12	11*	117
-13	88*	-77
-14	90*	-170
-15	49*	-80
-5	213	-181
-4	70	-71
-3	254	227
-2	50*	-128
-1	225	-213
H=	5, K=	5
-6	170	-190
-7	912	-924
-8	227	240
-9	216	-207
-10	66*	-24
-11	178	155
-12	11*	3
-13	243	258
-14	12*	0
-15	49*	67
-5	122	-99
-4	177	-173
-3	1026	1071
-2	473	531
-1	580	595
H=	5, K=	7
-6	569	595
-7	132	118
-8	104	-119
-9	128	115
-10	254	-241
-11	46*	-82
-12	290	-300
-13	103*	-112
-14	113	93
-5	171	164
-4	682	684
-3	484	-503
-2	186	-214
-1	216	-234
H=	5, K=	9
-6	110	-126
-7	428	399
-8	68*	-58
-9	217	180
-10	139	150
-11	115	-65
-12	70*	22
-13	191	-157
-5	164	178
-4	107	-80
-3	53*	-40
-2	8*	106
-1	181	-204
H=	5, K=	11
-2	323	329
-3	139	137
-4	11*	-52
-5	11*	-8
-1	363	364
-6	224	-223
-7	134	-132
-8	11*	45
-9	284	-305
-10	171	198
-11	47*	48
H=	5, K=	13
-1	197	177
-2	98*	-108
-3	88*	116
-4	180	179
-5	113	56
-6	160	142
-7	90*	25
-8	12*	33
H=	5, K=	15
-1	179	-185
-2	135	76
-3	155	-158
H=	6, K=	0
-8	1058	1050
-10	141	-151
-12	248	-301
-14	181	-194
-16	100*	120
-6	1451	1456
-4	2200	2068
-2	680	714
H=	6, K=	2
-8	65*	-134
-9	770	772
-10	8*	-8
-7	67	-41
-11	75*	-94
-12	142	184
-13	52*	-111
-14	61*	-66
-15	186	-276
-6	542	-541
-5	688	-650
-4	781	736
-3	603	-491
-2	1383	1365
-1	527	-449

L	FO	FC
H=	6, K=	4
-7	378	-338
-8	321	-310
-9	318	-345
-10	379	380
-6	621	-600
-11	79*	-43
-12	144	147
-13	242	263
-14	64*	43
-15	173	174
-5	522	510
-4	6*	-11
-3	331	337
-2	338	330
-1	278	252
H=	6, K=	6
-7	58*	-53
-8	268	272
-9	86	-102
-10	53*	30
-11	104	-104
-12	393	-387
-13	102*	70
-14	70*	20
-6	795	800
-5	220	235
-4	634	642
-3	620	621
-2	200	-230
-1	90	-56
H=	6, K=	8
-7	264	277
-8	198	164
-9	299	301
-10	227	-234
-11	178	175
-12	184	-161
-13	171	-167
-6	393	412
-5	213	-217
-4	78	-87
-3	426	-468
-2	118	132
-1	103	112
H=	6, K=	10
-1	108	119
-2	139	129
-3	41*	42
-4	162	-160
-5	246	-259
-6	407	-408
-7	119	-150
-8	155	-136
-9	34*	-10
-10	266	257
-11	66*	128
-12	193	224
H=	6, K=	12
-1	49*	-5
-2	90*	-28
-3	350	318
-4	49*	11
-5	133	114
-6	93*	45
-7	47*	-43
-8	136	96
-9	203	-169
-10	99*	-89
H=	6, K=	14
-1	92*	38
-2	153	-155
-3	188	-196
-4	109	97
-5	12*	-14
-6	125	108
H=	7, K=	1
-9	380	410
-10	194	-188
-11	92	66
-8	870	914
-12	162	-224
-13	11*	-75
-14	58*	-85
-15	133	-185
-16	99*	51
-7	232	213
-6	265	228
-5	390	-352
-4	581	-516
-3	823	-835
-2	750	-692
-1	380	346
H=	7, K=	3
-8	993	-1006
-9	131	162
-10	70*	-76
-11	72*	-15
-12	262	269
-13	70*	3
-14	76*	156
-15	74*	-52
-7	652	-633
-6	783	-717
-5	306	-323
-4	410	363
-2	1106	1086
-1	617	-576
H=	7, K=	5
-8	216	263
-9	158	-145
-10	313	344
-11	432	-421
-12	86*	-54
-13	43*	5
-14	12*	-2
-15	224	244
-7	197	203
-6	258	239
-5	449	411
-4	102	-23
-3	315	321
-2	184	168
-1	168	-134
H=	7, K=	7
-8	297	286
-9	114	-112
-10	140	115
-11	106	103
-12	264	-251
-13	96*	-93
-14	155	-161
-7	64*	-19
-6	477	443
-5	259	-259
-4	131	98
-3	518	-493
-2	890	-908
-1	233	-245
H=	7, K=	9
-6	402	-429
-7	159	-123
-8	298	-284
-9	11*	104
-10	93*	6
-11	233	239
-12	87*	40
-13	12*	22
-5	336	-378
-4	141	92
-3	341	-331
-2	467	501
-1	89	75
H=	7, K=	11
-1	189	-213
-2	288	281
-3	80*	-17
-4	251	237
-5	156	146
-6	73*	12
-7	79*	-86
-8	11*	-35
-9	295	-289
-10	12*	10
-11	217	-207
H=	7, K=	13
-1	116	-71
-2	340	-329
-3	148	167
-4	99*	-24
-5	88*	61
-6	221	233
-7	75*	-12
-8	231	231
H=	8, K=	0
-10	88	88
-12	188	-210
-14	248	-274
-16	90*	-154
-8	687	696
-6	854	765
-4	1020	-999
-2	1385	-1331
H=	8, K=	2
-9	50*	27
-10	51*	56
-11	577	593
-12	151	-143
-13	95*	92
-14	11*	21

L	FO	FC
H=	8, K=	2
-15	165	-170
-16	39*	19
-8	324	-310
-7	1027	-1015
-6	742	-790
-5	813	-812
-4	535	491
-3	416	416
-2	350	360
-1	68	-60
H=	8, K=	4
-9	136	140
-10	130	-131
-11	111	-162
-12	131	169
-13	75*	10
-14	46*	68
-15	138	183
-8	461	-449
-7	445	379
-6	321	-325
-5	466	485
-4	138	107
-3	592	595
-2	246	-214
-1	767	-777
H=	8, K=	6
-9	118	-106
-10	134	158
-11	136	-165
-12	49*	-77
-13	244	-231
-14	160	-173
-15	12*	24
-8	422	411
-7	148	88
-6	377	379
-5	464	495
-4	184	-143
-3	111	-94
-2	581	-630
-1	302	-301
H=	8, K=	8
-8	127	-117
-9	64*	51
-10	104	-55
-11	235	207
-12	140	-120
-13	169	153
-14	121	-83
-7	319	-327
-6	72*	-44
-5	525	-529
-4	66*	-9
-3	8*	5
-2	471	-492
-1	718	742
H=	8, K=	10
-1	44*	34
-2	470	500
-3	92*	57
-4	144	147
-5	93*	-82
-6	50*	-90
-7	83*	76
-8	141	-172
-9	116	129
-10	121	-86
-11	63*	114
-12	116	136
H=	8, K=	12
-1	245	-246
-2	11*	14
-3	156	-107
-4	60*	-16
-5	300	308
-6	11*	32
-7	322	300
-8	191	196
-9	12*	-38
-10	130	130
H=	8, K=	14
-1	131	150
-2	256	-240
-3	83*	54
-4	120	-120
-5	183	-184
-6	12*	3
H=	9, K=	1
-10	588	596
-11	136	113
-12	10*	18
-13	162	126
-14	11*	11
-15	60*	-54
-16	92*	-127
-9	96	72
-8	343	329
-7	376	-355
-6	186	-181
-5	862	-819
-4	132	-107
-3	355	360
-2	479	-484
-1	794	777
H=	9, K=	3
-10	426	-473
-11	285	305
-12	20*	59
-13	11*	69
-14	128	134
-15	115	131
-16	104*	147
-9	127	-122
-8	304	-270
-7	373	-384
-6	411	427
-5	86	113
-4	460	461
-3	83	101
-2	257	262
-1	246	239
H=	9, K=	5
-10	219	252
-11	200	-182
-12	79*	-37
-13	186	-180
-14	60*	-95
-15	94*	102
-9	171	161
-8	216	228
-7	879	849
-6	83	47
-5	698	709
-4	194	202
-3	434	-475
-2	130	123
-1	613	-621
H=	9, K=	7
-9	70*	-39
-10	348	341
-11	44*	-82
-12	166	146
-13	96*	69
-14	245	-207
-8	301	274
-7	184	-175
-6	160	-165
-5	302	-283
-4	764	-806
-3	165	170
-2	450	-438
-1	110	124
H=	9, K=	9
-5	90	-62
-6	10*	-35
-7	238	-235
-8	106	-130
-9	51*	64
-10	109	-84
-11	392	374
-12	12*	-13
-13	226	240
-4	117	89
-3	208	212
-2	26*	-61
-1	494	523
H=	9, K=	11
-1	424	-436
-2	64*	54
-3	128	-109
-4	309	332
-5	11*	43
-6	97*	101
-7	210	218
-8	124	-122
-9	156	131
-10	12*	-54
-11	111	-117
H=	9, K=	13
-1	165	-143
-2	156	-180
-3	68*	27
-4	276	-261
-5	102*	106
-6	93*	-45
-7	12*	-38
-8	96*	96
H=	10, K=	0
-12	103	121

L	FO	FC
-14	78*	-73
-16	111	-146
-10	509	521
-8	127	135
-6	879	-880
-4	295	-319
-2	360	-329
H=	10, K=	2
-12	83*	39
-14	113	125
-15	104	-10
-16	12*	74
-11	230	229
-10	147	111
-13	128	85
-9	441	-422
-8	67	-64
-7	939	-901
-6	76	-80
-5	72	83
-4	215	196
-3	514	491
-2	833	-804
-1	1127	1107
H=	10, K=	4
-11	118	120
-12	103	-91
-13	189	-164
-14	117	74
-15	12*	-18
-16	141	150
-10	242	-239
-9	318	309
-8	111	-115
-7	262	262
-6	250	243
-5	454	394
-4	36*	-26
-3	536	-510
-2	384	-383
-1	282	-283
H=	10, K=	6
-12	335	325
-13	211	-238
-15	12*	-53
-11	169	-166
-10	298	293
-14	130	-140
-9	112	96

L	FO	FC
-8	40*	62
-7	199	192
-6	86	-84
-5	214	-194
-4	261	-281
-3	731	-731
-2	286	272
-1	482	-495
H=	10, K=	8
-7	536	-533
-8	113	-123
-12	171	113
-14	82*	19
-10	136	130
-9	348	-342
-11	11*	45
-13	212	201
-6	169	-162
-5	190	-210
-4	227	-237
-3	580	599
-2	269	-227
-1	142	137
H=	10, K=	10
-2	142	-134
-3	91*	129
-4	306	296
-5	141	129
-6	260	257
-7	96*	122
-8	29*	61
-11	12*	-27
-12	63*	-90
-9	109	-9
-10	137	-116
H=	10, K=	12
-1	267	-274
-2	83*	76
-3	414	-415
-4	120	147
-5	109	12
-6	78*	-135
-7	320	314
-8	56*	-14
-9	95*	117
-10	67*	61
H=	10, K=	14

L	FO	FC
-4	166	-216
-5	12*	-94
-6	100*	-112
-1	84*	130
-2	62*	-20
-3	12*	54
H=	11, K=	1
-12	337	329
-13	73*	-28
-15	116	109
-16	187	-157
-11	86	66
-10	410	368
-14	85*	-104
-9	246	-226
-8	170	-172
-7	410	-368
-6	532	-556
-5	452	461
-4	235	219
-3	56*	-36
-2	237	-204
-1	279	269
H=	11, K=	3
-12	419	-410
-11	29*	-54
-13	185	207
-15	101*	14
-16	187	184
-10	337	-323
-14	11*	74
-9	312	-307
-8	101	115
-6	489	488
-5	425	420
-4	184	157
-3	28*	16
-2	993	-1000
-1	550	540
-7	39*	-42
H=	11, K=	5
-13	206	-206
-14	131	-116
-10	98	-92
-11	98	65
-12	11*	50
-15	184	-143
-9	426	438
-8	88	-83

L	FO	FC
-7	371	369
-6	284	251
-5	19*	-51
-4	430	-467
-3	358	-366
-2	86	-50
-1	51*	58
H=	11, K=	7
-9	10*	-97
-11	61*	-92
-12	256	233
-13	61*	-37
-14	12*	46
-8	155	-158
-10	289	256
-7	87	-83
-6	558	-552
-5	8*	-51
-4	342	-361
-3	60*	41
-2	408	411
-1	61*	-43
H=	11, K=	9
-1	263	273
-3	727	753
-5	122	122
-6	354	361
-7	107	-69
-8	153	89
-9	97*	-75
-10	52*	-65
-11	11*	29
-13	130	136
-2	419	-444
-4	110	52
-12	12*	-14
H=	11, K=	11
-1	11*	58
-3	11*	-110
-4	70*	-38
-5	136	-128
-9	222	204
-11	57*	38
-2	195	-200
-6	200	190
-7	142	120
-8	98*	67
-10	100*	-81

L	FO	FC
H=	11, K=	13
-7	76*	3
-2	12*	-13
-6	295	-299
-1	78*	-54
-3	87*	-123
-4	82*	-52
-5	39*	-42
-8	102*	-143
H=	12, K=	0
-10	231	236
-12	166	160
-14	202	199
-8	203	-214
-6	503	-463
-4	95	-98
-2	727	725
H=	12, K=	2
-12	188	166
-14	77*	-59
-15	211	190
-10	54*	41
-13	145	166
-16	43*	26
-11	479	-456
-9	734	-729
-8	57*	66
-7	154	151
-6	693	687
-5	138	137
-4	185	172
-3	253	257
-2	372	340
-1	381	-333
H=	12, K=	4
-11	397	371
-13	147	-154
-14	56*	-70
-16	100*	86
-10	77	-63
-12	295	-321
-15	137	-151
-6	158	173
-9	292	304
-8	490	501
-7	90	-114
-5	90	112
-2	551	-561
-4	283	-262
-3	147	83
-1	560	563
H=	12, K=	6
-2	446	538
-10	285	261
-12	288	250
-14	120	71
-15	100*	-100
-9	341	320
-13	11*	17
-11	105	103
-7	163	121
-6	379	-381
-5	309	-289
-4	199	201
-3	458	-460
-1	53*	-31
-8	191	-201
H=	12, K=	8
-7	172	-194
-8	251	-266
-10	73*	-11
-1	303	-290
-9	443	-430
-12	213	210
-13	141	134
-6	10*	-73
-11	105	-63
-14	12*	-10
-5	411	431
-4	70*	49
-3	219	240
-2	309	326
H=	12, K=	0
-16	92*	-108
H=	12, K=	10
-12	168	-148
-11	59*	-61
-8	226	239
-3	101	88
-5	98*	122
-7	55*	91
-1	82*	99
-10	58*	37
-2	421	-414
-4	10*	-47
-6	200	186
-9	104*	-109
H=	12, K=	12
-4	64*	-55
-5	263	-249
-6	93*	-114
-8	125	-145
-1	99*	-88
-3	155	-139
-7	88*	-8
-2	51*	-34
-9	211	180
-10	37*	-70
H=	13, K=	1
-11	377	-379
-12	306	288
-13	91*	-72
-14	137	119
-15	130	149
-16	72*	-6
-10	122	-130
-9	221	-201
-8	784	-792
-7	210	203
-6	171	-204
-5	73	106
-4	294	328
-3	58*	11
-2	475	447
-1	495	-487
H=	13, K=	3
-11	102	-121
-12	236	-265
-13	64*	15
-14	267	-244
-15	16*	-5
-16	12*	5
-10	258	255
-6	262	260
-5	119	-101
-4	226	-230
-3	224	223
-2	567	-604
-1	31*	-212
-9	240	-243
-8	311	278
-7	30*	40
H=	13, K=	5
-10	36*	-32
-11	368	372
-12	44*	86
-13	40*	-8
-14	142	99
-15	214	-201
-1	409	423
-9	71*	72
-8	50*	24
-7	368	-317
-6	102	-59
-5	523	-577
-4	174	-174
-3	30*	-86
-2	400	-407
H=	13, K=	7
-1	209	-205
-7	93	-12
-8	494	-484
-9	281	-280
-10	305	-305
-12	263	282
-13	57*	-34
-14	264	239
-11	122	-103
-4	333	348
-3	226	-206
-2	434	440
-6	295	-326
-5	71*	80
H=	13, K=	9
-1	132	-85
-2	214	-193
-4	141	-133
-5	165	151
-6	336	320
-7	92*	72
-8	241	255
-9	88*	-42
-10	11*	-74
-11	311	-297
-12	12*	-69
-3	44*	79
-13	12*	-59
H=	13, K=	11
-2	107	-110
-4	211	-221
-5	283	-272

L	FO	FC
-7	211	-186
-8	262	253
-9	58*	122
-11	47*	30
-1	81*	65
-3	147	-142
-6	96	40
-10	76*	110
H=	13, K=	13
-1	12*	78
-2	105*	122
-4	152	105
-6	115	-132
-7	12*	-42
-3	12*	-34
-5	137	-101
H=	14, K=	0
-12	87*	16
-14	301	283
-10	707	-657
-16	149	117
-8	823	-803
-6	182	194
-4	210	191
-2	540	508
H=	14, K=	2
-13	395	-362
-15	182	213
-10	69*	79
-1	380	-406
-12	108	-106
-11	414	-406
-14	11*	-7
-16	107*	-98
-9	36*	38
-8	45*	75
-7	564	548
-6	97	-94
-5	403	396
-4	260	-281
-3	569	-569
-2	195	-187
H=	14, K=	4
-1	356	406
-2	7*	-326
-3	90	73
-4	467	-552

L	FO	FC
-13	251	230
-14	328	-290
-16	98*	-81
-11	264	277
-10	100	118
-12	11*	-50
-15	67*	-62
-9	59*	-65
-8	160	156
-7	28*	26
-6	64*	-49
-5	376	-395
H=	14, K=	6
-7	32*	-62
-6	57*	-60
-5	172	-171
-4	210	237
-3	17*	71
-8	255	-263
-10	295	-283
-11	166	179
-12	106	102
-2	358	370
-1	457	437
-9	25*	-3
-13	123	55
-14	167	169
-15	12*	-59
H=	14, K=	8
-1	380	-375
-2	57*	42
-6	206	-187
-8	98*	-65
-10	223	-227
-11	249	-220
-5	404	426
-3	25*	-33
-4	100	114
-7	321	293
-9	11*	-22
-12	74*	-73
-13	72*	-50
-14	25*	57
H=	14, K=	10
-1	11*	-19
-5	11*	-39
-6	86*	-76
-8	253	221
-12	12*	25

L	FO	FC
-2	174	-187
-3	11*	-35
-4	334	-343
-7	69*	-78
-9	210	157
-10	270	262
-11	12*	20
H=	14, K=	12
-2	12*	-49
-3	12*	61
-8	195	-204
-5	138	-97
-6	105	66
-7	306	-326
-1	200	195
-4	51*	55
-9	12*	-39
H=	15, K=	1
-9	188	186
-8	208	-233
-7	592	662
-6	202	216
-5	237	232
-4	183	208
-3	220	-238
-1	459	-588
-12	88*	-113
-13	259	-275
-15	198	-186
-10	230	-196
-2	89	-67
-16	158	173
-11	138	-117
-14	224	232
H=	15, K=	3
-9	154	166
-8	120	127
-7	7*	9
-6	248	-288
-5	69	65
-4	498	-499
-3	28*	-49
-1	191	-211
-10	407	400
-11	304	276
-13	173	-159
-15	12*	15
-16	182	-182
-2	231	234

L	FO	FC
-2	231	234
-12	225	230
-14	300	-332
H=	15, K=	5
-8	140	140
-7	417	-432
-6	91	96
-5	193	-172
-4	192	112
-4	7*	112
-9	390	-393
-10	80*	-69
-11	124	91
-12	117	139
-13	405	381
-14	126	122
-15	125	92
-1	558	581
-3	379	364
H=	15, K=	7
-1	439	-433
-2	179	185
-3	10*	7
-4	525	518
-5	56*	32
-6	182	185
-7	101	131
-8	396	-387
-9	140	136
-10	416	-386
-11	122	-107
-12	64*	25
-13	63*	34
-14	184	152
H=	15, K=	9
-1	196	-187
-2	31*	31
-3	286	-249
-5	123	156
-6	228	-201
-9	230	219
-13	85*	-119
-10	140	83
-7	206	226
-11	29*	-14
-4	198	-241
-8	74*	82
-12	27*	-84

L	FO	FC
H= 15, K= 11		
-5	88*	-65
-8	94*	5
-10	138	154
-11	12*	67
-3	53*	35
-9	156	-166
-1	92*	35
-2	12*	-1
-4	95*	-35
-6	12*	-55
-7	165	-150
H= 15, K= 13		
-3	76*	64
-6	131	158
-4	142	119
-5	41*	35
H= 16, K= 0		
-10	249	-254
-8	64*	-121
-6	636	624
-4	647	668
-2	223	-226
-12	23*	-75
-14	19*	-90
-16	223	231
H= 16, K= 2		
-9	433	430
-8	149	-110
-7	627	617
-6	297	-291
-5	271	-238
-4	291	-320
-2	178	172
-1	190	-206
-3	720	-720
-10	10*	-45
-11	76*	1
-12	120	141
-13	303	-307
-14	104*	80
-15	275	-288
-16	98*	15
H= 16, K= 4		
-9	371	-376
-10	10*	-78
-11	76*	-81
-12	191	182
-15	108	98
-8	234	-207
-7	214	-191
-6	348	-340
-5	145	139
-4	8*	-415
-2	37*	50
-1	219	212
-3	361	367
-13	371	385
-14	54*	69
-16	136	-156
H= 16, K= 6		
-2	87*	58
-7	263	-263
-8	283	269
-3	216	-198
-10	203	-196
-11	232	-236
-13	46*	45
-14	149	130
-5	37*	-44
-4	175	179
-6	324	335
-1	36*	-8
-3	316	300
-12	217	-205
-15	135	124
H= 16, K= 8		
-2	123	-105
-3	445	-406
-4	57*	-17
-6	61*	35
-8	28*	-28
-10	32*	-38
-11	36*	-40
-12	184	-189
-14	12*	15
-1	67*	-45
-5	162	-150
-7	312	276
-9	222	236
-13	252	-251
H= 16, K= 10		
-1	83*	-30
-4	251	-250
-6	196	-227
-7	11*	19
-8	36*	-67
-10	144	173
-11	12*	90
-2	91*	57
-3	11*	9
-5	66*	10
-9	126	120
-12	179	182
H= 16, K= 12		
-6	121	128
-7	137	-169
-8	12*	39
-1	122	80
-2	60*	54
-3	170	206
-4	60*	68
-5	107*	94
H= 17, K= 1		
-9	391	372
-8	323	320
-7	255	222
-6	467	462
-5	405	-381
-3	606	-611
-2	199	-217
-1	327	349
-4	196	-200
-10	147	-141
-11	100	-84
-12	96*	-70
-13	209	-205
-14	135	-155
-15	253	-227
-16	141	133
H= 17, K= 3		
-8	384	-444
-7	129	128
-6	553	-542
-5	272	-269
-3	64*	59
-2	446	467
-1	30*	57
-4	8*	-30
-9	325	333
-10	188	-175
-11	82*	64
-12	139	99
-13	66*	126
-14	188	195
-15	178	-174
-16	134	-153
H= 17, K= 5		
-6	49*	-50
-3	562	583
-4	99	-91
-1	10*	27
-2	265	251
-3	560	583
-7	47*	-13
-8	41*	38
-9	245	-263
-10	76*	70
-11	169	-159
-12	70*	-119
-13	122	101
-14	12*	25
-15	210	190
H= 17, K= 7		
-1	11*	6
-2	487	-482
-3	212	-217
-4	189	178
-5	93*	-68
-6	285	280
-7	10*	-4
-8	169	158
-9	186	163
-10	11*	20
-11	48*	105
-12	225	-219
-13	85*	-152
-14	86*	-73
H= 17, K= 9		
-1	90*	87
-2	151	133
-3	11*	-61
-4	11*	-28
-5	58*	-74
-6	215	-239
-7	145	129
-8	211	-215
-9	154	165
-10	67*	-12
-11	242	231
-12	114*	139
H= 17, K= 11		

L	FO	FC
-1	12*	46
-2	281	267
-3	123	97
-4	98*	10
-5	288	293
-6	56*	-135
-7	36*	74
-8	133	-111
-9	208	-225
-10	40*	2
H= 18, K= 0		
-8	769	777
-6	475	449
-4	200	-202
-2	223	-243
-10	211	225
-12	159	-156
-14	293	-287
-16	119	-138
H= 18, K= 2		
-8	131	-112
-7	191	-177
-6	8*	9
-4	119	83
-3	87	-49
-2	503	501
-5	775	-773
-1	259	263
-9	215	223
-10	10*	5
-11	49*	-53
-12	160	168
-13	19*	-24
-14	12*	15
-15	214	-221
-16	93*	46
H= 18, K= 4		
-4	266	273
-6	210	-174
-5	404	401
-1	169	-190
-2	214	201
-3	290	280
-7	123	117
-8	304	-307
-9	90*	-50
-10	147	-154
-11	11*	-18
-12	74*	59
-13	120	134
-14	305	280
-15	168	154
H= 18, K= 6		
-1	484*	-499
-2	258	-244
-3	61*	82
-4	134	110
-5	267	247
-6	275	267
-7	83*	88
-8	383	394
-9	259	-255
-10	174	168
-11	133	-120
-12	205	-191
-13	67*	38
-14	160	-118
H= 18, K= 8		
-1	375	385
-2	39*	-52
-3	143	-146
-4	101*	-98
-5	346	-374
-6	178	195
-7	246	-226
-8	155	149
-9	149	134
-10	12*	-97
-11	126	114
-12	12*	-29
-13	92*	-87
H= 18, K= 10		
-1	132	130
-2	215	219
-3	85*	-58
-4	141	144
-5	23*	26
-6	65*	-28
-7	126	89
-8	201	-162
-9	91*	83
-10	185	-167
-11	12*	17
H= 18, K= 12		
-4	107*	-86
-5	167	205
-6	13*	-4
H= 19, K= 1		
-7	321	-293
-5	432	-413
-4	443	-443
-3	81	100
-6	140*	159
-1	161	130
-2	58*	63
-8	364	398
-9	48*	-79
-10	33*	-11
-11	37*	-77
-12	165	-192
-13	83*	-102
-14	12*	-78
-15	74*	25
-16	127	-110
H= 19, K= 3		
-1	10*	-46
-2	253	260
-3	89*	65
-4	567	582
-5	226	-229
-6	85*	82
-7	122	-140
-8	378	-369
-9	75*	-63
-10	280	-311
-11	11*	62
-12	94*	112
-13	25*	68
-14	296	278
-15	12*	58
H= 19, K= 5		
-1	209	-210
-2	50*	-79
-3	50*	6
-4	189	196
-5	291	298
-6	38*	-69
-7	395	384
-8	85*	-1
-9	121	79
-10	78*	34
-11	334	-329
-12	141	-60
-13	217	-195
-14	117	-98
-15	69*	74
H= 19, K= 7		
-1	43*	63
-2	139	-139
-3	206	-196
-4	443	-428
-5	76*	-56
-6	109	-63
-7	95*	-89
-8	431	411
-9	157	-132
-10	214	185
-11	65*	-31
-12	215	-195
-13	12*	-5
-14	202	-198
H= 19, K= 9		
-1	272	269
-2	164	176
-3	80*	19
-4	243	229
-5	172	-156
-6	55*	29
-8	139	-124
-9	73*	-11
-10	12*	9
-11	130	151
-12	13*	29
H= 19, K= 11		
-2	152	145
-3	48*	-15
-4	182	151
-5	59*	78
-6	91*	54
-7	12*	88
-8	12*	-75
H= 20, K= 0		
-2	209	221
-4	576	-585
-6	307	-326
-8	331	352
-10	98*	111
-12	219	-245
-14	279	-269
-16	189	-183

L	FO	FC
H= 20, K= 2		
-1	157	153
-2	91*	113
-3	128	135
-4	387	379
-5	40*	-54
-6	47*	-49
-7	584	-567
-8	10*	-33
-9	201	-181
-10	21*	-35
-11	220	208
-12	85*	-82
-13	102*	115
-14	26*	13
-15	12*	48
-16	50*	19
H= 20, K= 4		
-1	132	-104
-2	155	-117
-3	242	226
-4	137	176
-5	20*	22
-6	313	315
-7	156	162
-8	117	-158
-9	313	334
-10	289	-296
-11	54*	62
-12	80*	-6
-13	101*	-114
-14	125	132
-15	60*	-16
H= 20, K= 6		
-1	192	-160
-2	130	127
-3	301	-307
-4	190	-195
-5	145	123
-6	11*	-22
-7	254	251
-8	90*	73
-9	125	125
-10	188	166
-11	66*	-90
-12	12*	-31
-13	68*	-92
-14	226	-244
H= 20, K= 8		
-1	267	275
-2	74*	-53
-3	284	276
-4	70*	-34
-5	177	-172
-6	184	-174
-7	315	-282
-8	12*	-13
-9	101*	-87
-10	12*	55
-11	132	142
-12	12*	-6
H= 20, K= 10		
-1	13*	4
-2	150	104
-3	67*	13
-4	201	180
-5	70*	22
-6	187	202
-7	12*	49
-8	93*	-43
-9	50*	-28
-10	168	-190
H= 21, K= 1		
-1	150	-144
-2	46*	-14
-3	96	59
-4	60*	40
-5	42*	90
-6	444	-462
-7	231	-213
-8	10*	80
-9	240	-267
-10	192	196
-11	11*	-34
-12	103	68
-13	243	238
-14	106*	-80
-15	141	106
H= 21, K= 3		
-1	103	89
-2	108	106
-3	157	-168
-4	194	226
-5	210	226
-6	437	470
-7	178	-180
-8	102	151
-9	96*	-98
-10	187	-212
-11	83*	44
-12	66*	-97
-13	148	195
-14	12*	112
-15	163	134
H= 21, K= 5		
-1	78*	-52
-2	72*	20
-3	284	-290
-4	11*	19
-5	74*	-56
-6	161	177
-7	258	267
-8	11*	57
-9	316	287
-10	50*	-5
-11	140	-152
-12	86*	-41
-13	287	-266
-14	12*	20
H= 21, K= 7		
-1	105*	-148
-2	129	112
-3	66*	109
-4	357	-358
-5	202	-201
-6	242	-234
-7	72*	-77
-8	11*	10
-9	54*	-69
-10	256	251
-11	12*	-24
-12	12*	21
-13	87*	84
H= 21, K= 9		
-1	112	77
-2	12*	-53
-3	145	98
-4	188	206
-5	17*	81
-6	145	154
-7	55*	-50
-8	97*	25
-9	205	-154
-10	12*	-82
-11	17*	68
H= 22, K= 10		
-5	77*	38
-6	145	134
-7	162	140
H= 22, K= 8		
-1	98*	-21
-2	17*	-36
-3	309	283
-4	33*	-27
-5	159	153
-6	52*	-37
-7	188	-164
-8	174	-181
-9	258	-244
-10	78*	84
-11	12*	19
H= 22, K= 6		
-1	80*	-91
-2	195	186
-3	204	-220
-4	25*	-44
-5	181	-207
-6	176	-193
-7	11*	-16
-8	161	-135
-9	212	205
-10	156	164
-11	96*	-39
-12	188	176
-13	184	-212
H= 22, K= 4		
-1	80*	50
-2	150	-173
-3	152	-153
-4	19*	-13
-5	11*	35
-6	124	115
-7	75*	65
-8	131	175
-9	258	281
-10	64*	-69
-11	115	103
-12	253	-265
-13	141	-145
-14	12*	-70
H= 22, K= 2		

L	FO	FC
-1	11*	5
-1	11*	5
-2	59*	-94
-3	217	223
-4	73*	35
-5	241	236
-6	154	172
-7	113	-113
-8	150	174
-9	312	-325
-10	46*	-75
-11	147	-139
-12	132	-126
-13	166	183
-14	12*	13
-15	214	208
H= 22, K= 0		
-2	130	-138
-6	408	-442
-8	241	-255
-10	127	133
-12	263	280
-14	94*	80
H= 23, K= 1		
-1	284	-275
-2	178	169
-3	84*	58
-4	95*	-81
-5	356	383
-6	157	-172
-7	26*	88
-8	204	-231
-9	216	-213
-10	83*	80
-11	241	-225
-12	177	179
-13	35*	-7
-14	54*	72
-15	166	166
H= 23, K= 3		
-1	53*	15
-2	303	-282
-3	281	271
-4	164	156
-5	11*	28
-6	105	113
-7	135	131
-8	333	343
-9	72*	19
-10	93*	80
-11	98*	-13
-12	308	-319
-13	111	64
-14	193	-193
H= 23, K= 5		
-1	151	146
-2	123	-60
-3	128	-159
-4	45*	-72
-5	208	-230
-6	11*	-23
-7	96*	-121
-8	23*	-21
-9	130	146
-10	12*	0
-11	338	326
-12	12*	5
-13	67*	11
H= 23, K= 7		
-1	12*	-26
-2	191	159
-3	90*	-14
-4	24*	-13
-5	184	178
-6	271	-278
-7	96*	-57
-8	227	-206
-9	12*	-31
-10	34*	13
-11	88*	5
-12	180	193
H= 23, K= 9		
-4	12*	-64
-5	110*	109
-6	266	254
-7	150	156
-8	146	170
H= 24, K= 8		
-4	120	24
-5	282	283
-6	12*	47
-7	142	124
-8	12*	36
-9	126	-109
H= 24, K= 6		
-1	126	96
-2	183	135
-3	67*	-144
-4	205	206
-5	258	-252
-6	100*	-39
-7	12*	-16
-8	94*	-88
-9	12*	-18
-10	71*	-39
-11	112	77
-12	12*	72
H= 24, K= 4		
-1	174	184
-2	282	-275
-3	118	-111
-4	161	-181
-5	168	-176
-6	11*	-82
-7	180	-170
-8	79*	104
-9	74*	52
-10	225	240
-11	259	251
-12	12*	-33
-13	105*	45
H= 24, K= 2		
-1	304	-297
-2	12*	-39
-3	121	143
-4	66*	-89
-5	308	315
-6	183	173
-7	251	269
-8	166	174
-9	79*	-107
-10	164	136
-11	381	-392
-12	12*	20
-13	210	-196
-14	76*	-17
H= 24, K= 0		
-2	188	200
-4	303	293
-6	105	-119
-8	162	-195
-10	61*	-73
-12	119	135
-14	305	319
H= 25, K= 1		
-1	303	-306
-2	72*	-5
-3	245	-260
-4	222	245
-5	173	185
-6	55*	7
-7	244	259
-8	11*	-43
-9	11*	-28
-10	53*	-45
-11	204	-208
-12	126	-116
-13	222	-232
-14	120	98
H= 25, K= 3		
-1	12*	7
-2	166	-188
-3	12*	-10
-5	83*	124
-6	12*	-86
-7	12*	-11
H= 25, K= 2		
-8	47*	84
H= 25, K= 3		
-9	71*	57
-10	254	271
-11	12*	60
-12	140	106
-13	137	-178
H= 25, K= 5		
-1	251	257
-2	12*	-56
-3	145	151
-4	123	-93
-5	184	-187
-6	12*	-41
-7	318	-314
-8	12*	17
-9	127	-113
-10	12*	-3
-11	170	171
-12	47*	76

L	FO	FC
H= 25, K= 7		
-4	262	252
-5	12*	50
-6	113	64
-7	161	175
-8	155	-157
-9	84*	11
-10	198	-192
H= 26, K= 6		
-4	131	120
-5	85*	64
-6	270	272
-7	143	-140
-8	12*	54
-9	12*	-41
-10	136	-143
H= 26, K= 4		
-2	103*	90
-3	186	121
-4	214	-249
-5	82*	-60
-7	74*	-48
-8	67*	-72
-9	99*	-106
-10	84*	112
-11	117	92
-12	204	225
H= 26, K= 2		
-1	201	-189
-2	12*	34
-3	325	-354
-4	12*	7
-5	113	126
-6	201	-204
-7	184	189
-8	12*	1
-9	97*	17
-10	130	116
-11	64*	-43
-12	12*	15
-13	176	-172
H= 26, K= 0		
-2	181	-164
-4	341	320
-6	409	423
-8	12*	-116
-10	183	-214
-12	196	-216
H= 27, K= 1		
-2	184	-195
-3	243	-256

L	FO	FC
-4	74*	60
-5	295	-291
-6	187	188
-7	108	47
-8	12*	-10
-9	74*	61
-10	108*	-110
-11	53*	-34
-12	79*	-64
H= 27, K= 3		
-3	115	-93
-4	77*	-100
-5	41*	-70
-6	258	-236
-7	77*	-7
-9	114	107
-10	111*	147
-11	132	126
-12	148	202
H= 27, K= 5		
-5	150	159
-6	107*	-72
-7	80*	-86
-8	66*	73
-9	205	-204
-10	45*	71
H= 28, K= 4		
-7	13*	83
-8	178	-202
-9	13*	-10
H= 28, K= 2		
-4	13*	-26
-5	231	-240
-6	133	-104
-7	12*	-25
-8	98*	-128
-9	115	118
-10	77*	46
-11	124	100
H= 28, K= 0		
-4	103*	-157
-6	175	167
-8	156	130
-10	78*	-105
H= 29, K= 1		
-7	175	-193
-8	70*	21
-9	13*	52

f $\underline{Ni(L4)(ClO_4)_2}$

The structure was solved using the inner set of data ($2\theta < 30$ deg, 902 observed data). Direct methods (SAP programs-see Appendix) and a Patterson synthesis were used to determine the positions of the nickel, one chlorine and fourteen lighter atoms. Refinement of these atomic positions and a scale factor gave R=0.47 Several cycles of refinement and subsequent electron density difference maps gave the positions of all non-hydrogen atoms, with an R of 0.086 (all atoms isotropic). Inclusion of the outer shell of data and calculated hydrogen atom positions gave an R of 0.089 after refinement of all non-hydrogen atom coordinates and their anisotropic thermal motion parameters. Careful analysis of one perchlorate anion (Cl(2) etc) indicated some disorder in the oxygen atom positions. This anion was best described by allowing one oxygen atom (O(22)) anisotropic thermal motion, and splitting each of the other three oxygen atoms into two half-occupied isotropic positions. Full matrix, least-squares refinement of this model gave a final *R* of 0.066 for the 2514 observed data, using 314 varables. Final fractional atomic coordinates are given in table 2.19, with thermal motion parameters in table 2.20. Hydrogen atom coordinates are given in table 2.21, and measured and calculated structure factors (x10) in table 2.22.

g Summary of Refinements

Table 2.23 summarises the conclusions to these structure determinations: residuals, # variables, # reflections used, and the remaining outstanding features of the final electron density difference maps.

Table 2.19

Fractional Atomic Coordinates: $Ni(L4)(ClO_4)_2$.

(x 10^4, x 10^5 for Ni)

Atom	Type	x	y	z
Ni		22708(7)	1783(8)	3267(8)
Cl1	perchlorate anions	3695(2)	4462(2)	2898(2)
Cl2		1076(2)	2231(2)	-2745(2)
O11		3610(6)	2985(7)	2394(8)
O12		4127(7)	4712(9)	1713(8)
O13		2613(6)	5116(9)	3891(8)
O14		4438(6)	4893(7)	3517(7)
O21		2061(6)	2322(7)	-2534(7)
O22		1580(15)	2431(18)	-4002(18)
O22'		1089(14)	2779(17)	-3653(17)
O23		261(13)	3498(17)	-1478(17)
O23'		65(15)	2876(19)	-1474(19)
O24		906(10)	740(13)	-3562(14)
O24'		661(12)	991(16)	-2645(17)
N1		2574(4)	-1723(5)	-1272(5)
N2		1728(5)	-563(5)	1675(5)
N3		1576(4)	2057(5)	1973(5)
N4		3192(4)	997(5)	-909(5)
N5		2436(5)	-1750(5)	-2422(5)
N6		4300(4)	166(6)	-2030(5)
C1		3241(6)	-1396(6)	-3276(7)
C2		3182(7)	-1318(8)	-4463(7)
C3		4291(6)	-978(7)	-3112(7)
C4		5397(6)	-1978(8)	-4292(7)
C5		2665(6)	-2948(7)	-1356(7)
C6		2722(7)	-4337(7)	-2622(8)
C7		2663(6)	-3058(7)	-130(8)
C8		2609(7)	-1707(7)	1199(7)
C9		2770(7)	-1146(8)	795(9)
C10		2321(8)	-2071(8)	2408(9)
C11		1344(6)	687(7)	3179(7)
C12		764(6)	1876(7)	3269(7)
C13		1072(6)	2912(7)	1590(7)
C14		397(6)	1957(8)	822(7)
C15		289(6)	4272(7)	2970(7)
C16		764(6)	3363(7)	571(7)
C17		3090(6)	2308(7)	-664(7)
C18		4015(6)	2867(7)	-1568(7)

Table 2.20

Thermal Motion Parameters (x 10^3 A^2, x 10^4 A^2 for Ni) in $Ni(L4)(ClO_4)_2$.

Anisotropic Parameters

Atom Type	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni	374(7)	259(6)	266(6)	-23(4)	-109(4)	95(4)
Cl1	64(2)	56(1)	60(1)	-14(1)	-34(1)	24(1)
Cl2	71(2)	60(1)	55(1)	-10(1)	-27(1)	31(1)
O11	130(6)	67(4)	184(7)	-32(4)	-104(6)	58(5)
O12	66(5)	142(7)	138(7)	-92(6)	-97(6)	131(7)
O13	157(7)	202(8)	140(7)	9(5)	-28(5)	1(6)
O14	126(6)	116(5)	131(6)	-37(5)	-103(5)	52(5)
O21	916(5)	122(5)	120(5)	-27(4)	-76(4)	59(5)
N1	34(4)	34(3)	33(3)	0(3)	-10(3)	15(3)
N2	53(4)	33(3)	37(3)	0(3)	-22(3)	13(3)
N3	36(3)	37(3)	29(3)	-3(3)	-15(3)	13(3)
N4	39(4)	31(3)	30(3)	-4(3)	-17(3)	8(3)
N5	45(4)	29(3)	29(3)	0(3)	-15(3)	5(3)
N6	32(4)	38(3)	33(3)	0(3)	-5(3)	14(3)
C1	30(5)	30(4)	26(4)	7(3)	-11(3)	2(3)
C2	56(6)	56(5)	37(4)	0(4)	-23(4)	15(4)
C3	47(5)	40(4)	25(5)	6(4)	-1(3)	16(4)
C4	48(5)	59(5)	46(5)	8(4)	-9(4)	15(4)
C5	37(4)	32(4)	41(4)	-8(3)	-18(3)	15(3)
C6	72(6)	24(4)	59(5)	-4(4)	-27(4)	10(4)
C7	56(5)	35(4)	55(5)	2(4)	-21(4)	20(4)
C8	58(6)	43(4)	52(5)	-7(4)	-25(4)	26(4)
C9	67(6)	64(5)	78(6)	2(5)	-44(5)	29(5)
C10	111(8)	62(5)	72(6)	-8(5)	-50(5)	38(5)
C11	66(5)	43(4)	31(4)	-12(4)	-21(4)	15(4)
C12	59(5)	43(4)	25(4)	-2(4)	-8(4)	11(3)
C13	43(5)	37(4)	33(4)	1(4)	-15(3)	11(3)
C14	32(5)	68(5)	52(5)	-5(4)	-18(4)	25(4)
C15	60(5)	45(4)	43(4)	13(4)	-10(4)	12(4)
C16	43(5)	35(4)	42(4)	1(4)	-20(4)	16(3)
C17	42(5)	33(4)	35(4)	-6(3)	-23(3)	15(3)
C18	49(5)	51(5)	54(5)	-13(4)	-14(4)	37(4)

Isotropic Parameters (x10^3)

Atom Type	U
O22	108(6)
O22'	89(5)
O23	97(5)
O23'	110(6)
O24	79(4)
O24'	106(5)

Table 2.21

Hydrogen Atom Coordinates: $Ni(L4)(ClO_4)_2$.

($\times 10^4$)

Atom	x	y	z
H(N2)	1038	-989	1706
H(N3)	2142	5567	2228
H21	2551	-1782	-4596
H22	3045	-206	-4155
H23	3884	-1785	-5363
H41	5573	-2087	-5230
H42	5333	-2905	-4325
H43	5872	-1530	-3999
H61	2313	-5001	-2274
H62	3506	-4763	-3322
H63	2368	-4145	-3091
H71	2007	-3512	232
H72	3353	-3682	-564
H91	3969	-1072	-69
H92	4345	-1825	575
H93	3719	-217	1586
H101	2373	-1234	3211
H102	2877	-2867	2024
H103	1599	-2330	2770
H111	814	426	3914
H112	1990	1002	3338
H121	590	2767	4172
H122	56	1620	3234
H141	1096	1144	-246
H142	-100	1443	1319
H143	-6	2451	639
H151	805	4906	3523
H152	581	4849	2680
H153	-343	4030	3609
H161	1615	3715	297
H162	2156	4204	1350
H181	4487	3257	-1094
H182	3653	3629	-1521
H183	4551	2264	-2602

Table 2.22

Structure Factor Listing: $Ni(L4)(ClO_4)_2$.

(x 10)

Unobserved reflections are denoted by an asterisk.

L	FO	FC
H=	0, K=	0
1	924	923
2	937	-928
3	550	566
4	198	225
5	122	-139
6	52	56
8	95	-115
9	82	-77
H=	0, K=	1
9	75	78
8	65	-50
7	256	-257
6	65	74
5	209	205
4	166	179
3	25*	14
2	687	683
1	530	524
0	672	656
H=	0, K=	2
0	197	-213
1	323	320
2	607	578
3	392	353
4	268	276
5	199	227
6	110	113
7	96	-119
8	26*	-15
H=	0, K=	3
8	119	-126
7	69	-76
6	290	294
5	131	122
4	206	-210
3	304	325
2	1001	982
1	273	250
0	374	-372
H=	0, K=	4
0	686	710
1	590	564
2	22*	-26
3	30*	46
4	139	125
5	83	93
6	77	-71
7	42*	-21
H=	0, K=	5
6	60	-54
5	8*	19
4	132	123
3	159	149
2	44	39
1	253	252
0	247	250
H=	0, K=	6
0	173	192
1	500	510
2	186	177
3	210	-198
4	35*	14
5	81	88
H=	0, K=	7
4	105	-103
3	13*	4
2	7*	21
1	55	-62
0	185	188
H=	0, K=	8
0	89	-93
1	7*	-28
2	119	132
3	37*	5
H=	0, K=	9
1	144	133
0	198	186
H=	1, K=	10
0	166	-167
H=	1, K=	9
0	176	-177
1	144	-144
H=	1, K=	8
3	82	-71
2	185	-171
1	106	-113
0	17*	12
H=	1, K=	7
0	247	-236
1	94	-85
2	7*	-18
3	175	-188
4	281	-278
H=	1, K=	6
5	252	-241
4	320	-326
3	283	-288
2	127	-131
1	179	-186
0	334	-340
H=	1, K=	5
0	328	-339
1	50	95
2	254	-258
3	379	-362
4	142	-150
5	93	-100
6	186	-176
H=	1, K=	4
7	70	-68
6	71	-60
5	304	-295
4	91	-106
3	81	-83
2	90	-101
1	303	-308
0	174	-157
H=	1, K=	3
0	375	386
1	320	-330
2	161	-158
3	193	-190
4	407	-405
5	374	-373
6	193	-174
7	49*	-67
8	167	-179
H=	1, K=	2
9	116	-106
8	227	-222
7	126	-121
6	102	-118
5	222	-236
4	562	-550
3	565	-565
2	23*	11
1	641	-631
0	350	-323
H=	1, K=	1
0	17*	-28
1	578	554
2	918	-887
3	443	-458
4	278	-278
5	110	-103
6	300	-310
7	217	-216
8	32*	37
9	89	-70
H=	1, K=	0
10	128	-137
9	142	-131
8	178	-180
7	374	-376
6	328	-345
5	132	-141
4	192	-170
3	75	-69
2	403	-404
1	34	43
0	108	100
H=	2, K=	0
0	1078	-1066
1	796	-757
2	1208	-1132
3	750	-755
4	350	-341
5	34	-25
6	127	-138
7	358	-363
8	33*	-6
9	35*	33
10	36*	-4
H=	2, K=	1

L	FO	FC
9	176	180
8	48*	41
7	242	-236
6	150	-171
5	7*	-19
4	334	-339
3	426	-419
2	181	190
1	1075	-1034
0	1346	-1310

H= 2, K= 2

L	FO	FC
0	820	-776
1	110	-124
2	344	-343
3	623	-610
4	298	-302
5	113	-104
6	121	-115
7	66	-60
8	56*	74
9	43*	47

H= 2, K= 3

L	FO	FC
8	34*	-31
7	59	50
6	69	-67
5	63	-57
4	137	-157
3	561	-543
2	1027	-1028
1	626	-628
0	26*	43

H= 2, K= 4

L	FO	FC
0	267	-273
1	85	103
2	585	-559
3	340	-329
5	26*	-23
6	141	-136
7	49*	-30

H= 2, K= 5

L	FO	FC
6	109	-97
5	121	-115
4	102	-104
3	196	-185
2	128	-121
1	263	-271
0	171	-174

H= 2, K= 6

L	FO	FC
0	509	-511
1	349	-350
2	37*	45
3	176	-193
4	193	-181
5	11*	34
6	59*	57

H= 2, K= 7

L	FO	FC
4	81	90
3	84	-89
2	156	-146
1	149	-141
0	135	-137

H= 2, K= 8

L	FO	FC
0	7*	-29
1	19*	12
2	144	-148
3	72	-66

H= 2, K= 9

L	FO	FC
2	179	-183
1	8*	17
0	56*	-70

H= 2, K= 10

L	FO	FC
0	71	-83

H= 3, K= 10

L	FO	FC
0	103	93

H= 3, K= 9

L	FO	FC
0	241	245
1	165	166
2	127	118

H= 3, K= 8

L	FO	FC
3	41*	20
2	112	99
1	144	150
0	7*	11

H= 3, K= 7

L	FO	FC
0	72	78
1	193	-198
2	34*	28
3	276	280
4	124	111
5	105	98

H= 3, K= 6

L	FO	FC
6	235	239
5	254	252
4	149	149
3	102	107
2	76	82
1	96	99
0	118	120

H= 3, K= 5

L	FO	FC
0	383	-383
1	7*	-7
2	474	469
3	238	236
4	7*	11
5	148	141
6	276	252
7	124	129

H= 3, K= 4

L	FO	FC
8	152	166
7	169	151
6	66	-73
5	135	144
4	522	543
3	167	190
0	98	98

H= 3, K= 3

L	FO	FC
0	47	-32
1	421	414
2	119	124
3	28*	26
4	346	339
5	404	402
6	248	264
7	126	153
8	147	136

H= 3, K= 2

L	FO	FC
9	48*	-14
8	70	74
7	328	325
6	272	270
5	224	229
4	395	381
3	462	444
2	66	-66
1	190	-214
0	108	124

H= 3, K= 1

L	FO	FC
0	1803	-1753
1	276	240
2	1503	1463
3	40	50
4	4*	-37
5	161	176
6	184	176
7	13*	-36
8	130	131
9	185	175
10	81	98

H= 3, K= 0

L	FO	FC
10	115	120
9	223	225
8	197	207
7	230	232
6	251	250
5	252	-219
4	34	-35
3	77	62
2	9*	-8

H= 4, K= 0

L	FO	FC
4	284	264

H= 3, K= 0

L	FO	FC
1	217	-201
0	135	112

H= 4, K= 0

L	FO	FC
0	185	176
1	985	924
2	1130	1030
3	603	569
5	455	451
6	127	117
7	160	162
8	307	319
9	241	238
10	112	-113

L	FO	FC
H=	4, K=	1
10	35*	-4
9	7*	-14
8	69	71
7	369	346
6	154	154
5	325	342
4	310	324
3	66	-53
2	398	367
1	253	243
0	226	236
H=	4, K=	2
0	35	25
1	279	-273
2	199	181
3	375	377
4	378	349
5	200	198
6	220	239
7	171	178
8	48*	-24
9	26*	37
H=	4, K=	3
9	14*	-36
8	56	68
7	61	76
6	15*	-7
5	128	124
4	704	669
3	568	543
2	318	276
1	327	353
0	160	174
H=	4, K=	4
0	77	89
1	359	358
2	514	505
3	302	289
4	238	245
5	142	140
6	68	36
7	82	-83
8	8*	15
H=	4, K=	5
7	8*	-4
6	8*	-4
5	186	185
4	94	119
3	32*	14
2	153	164
1	309	313
0	355	340
H=	4, K=	6
0	456	442
1	102	99
2	165	155
3	273	265
4	85	82
5	27*	-7
6	60	44
H=	4, K=	7
5	27*	-5
4	159	159
3	119	121
2	49*	35
1	218	232
0	372	343
H=	4, K=	8
0	269	243
1	102	96
2	35*	12
3	167	174
H=	4, K=	9
2	169	150
1	140	116
0	106	105
H=	5, K=	9
0	136	-139
1	93	-100
H=	5, K=	8
3	87	-87
2	40*	28
1	17*	-17
0	89	-85
H=	5, K=	7
0	132	119
1	55	70
2	181	-170
3	66	-59
4	31*	-10
5	156	-159
H=	5, K=	6
6	142	-154
5	93	-86
4	172	-172
3	155	-164
2	36*	7
1	54	-59
0	28*	-40
H=	5, K=	5
0	117	125
1	244	-244
2	25*	18
3	6*	14
4	298	-304
5	233	-221
6	15*	-11
7	152	-153
H=	5, K=	4
8	114	-106
7	138	-131
6	181	-167
5	138	-154
4	312	-286
3	219	-227
2	355	350
1	131	143
0	17*	-50
H=	5, K=	3
0	150	164
1	62	71
2	20*	-48
3	264	248
4	118	-117
5	324	-342
6	146	-145
7	98	-94
8	265	-262
9	136	-129
H=	5, K=	2
9	292	-288
8	125	-142
7	7*	23
6	220	-215
5	133	-123
4	16*	-6
3	184	-172
2	389	-401
1	342	331
0	388	374
H=	5, K=	1
0	310	288
1	532	458
2	73	-48
3	74	-54
4	387	-397
5	332	-319
6	62	-63
7	16*	-48
8	92	-83
9	89	-94
10	19*	-19
H=	5, K=	0
11	109	-95
10	106	-109
9	195	-203
8	129	-121
7	136	-150
6	190	-187
5	68	77
4	34	-16
3	903	-887
2	361	310
1	816	786
0	310	284
H=	6, K=	0
0	568	-563
1	695	-648
2	165	-144
3	343	-319
4	800	-779
5	692	-677
6	149	-141
7	270	-265
8	457	-448
9	7*	-24
10	109	110
11	23*	-23
H=	6, K=	1

L	FO	FC
10	47*	-33
9	137	-118
8	7*	-48
7	245	-242
6	365	-375
5	125	-126
4	449	-398
3	554	-476
2	95	-70
1	401	-413
0	287	-266

H= 6, K= 2

0	91	102
1	184	-182
2	558	-550
3	92	-98
4	72	86
5	495	-487
6	186	-168
7	7*	-20
8	108	-116
9	111	-113

H= 6, K= 3

9	35*	-3
8	93	93
7	253	-239
6	334	-330

H= 6, K= 4

4	255	-245

H= 6, K= 3

5	120	-129
4	345	-328
3	580	-559
2	106	-89
1	40	-25
0	328	-297

H= 6, K= 4

0	332	-327
1	283	-270
2	279	-268
3	11*	-26
5	375	-377
6	128	-132
7	31*	16
8	65	-64

H= 6, K= 5

7	86	-74
6	36*	46
5	41*	-38
4	366	-385
3	66	-71
2	22*	14
1	314	-316

H= 6, K= 6

0	93	-121
1	287	-308
2	461	-489
3	51*	-69
4	77	74
5	148	-143
6	131	-117

H= 6, K= 7

5	75	-54
4	96	-104
3	44*	-62
2	119	-116
1	421	-416
0	331	-354

H= 6, K= 8

0	158	-161
1	57	-57
2	111	-106
3	182	-189

H= 6, K= 9

1	206	-206
0	76	-70

H= 7, K= 9

0	8*	26

H= 7, K= 8

3	97	77
2	104	107
1	101	90
0	44*	20

H= 7, K= 7

0	89	-102
1	206	196
2	11*	12
3	63	-53
4	96	98

H= 7, K= 6

6	92	99
5	36*	42
4	21*	41
3	61	76
2	34*	-20
1	56	-66
0	51*	-99

H= 7, K= 5

0	29*	34
1	47*	-68
2	129	-164
3	28*	-60
4	116	107
5	36*	32
6	47*	68
7	169	162

H= 7, K= 4

8	91	98
7	32*	-19
6	323	303
5	271	280
4	312	-308

H= 7, K= 3

4	6*	15
5	169	170
6	170	166
7	65	87
8	115	115
9	173	182

H= 7, K= 2

9	203	195
8	126	131
7	25*	-14
6	140	154
5	242	227
4	101	75
3	122	116
2	236	-224
1	384	-340
0	273	-263

H= 7, K= 1

0	292	-271
1	485	-458
2	508	-461
3	228	225
4	384	352
5	40	-24
6	262	262
7	310	304
8	104	-120
9	25*	-18
10	194	187

H= 7, K= 0

11	97	96
10	180	177
9	73	82
8	24*	-9
7	148	135
6	274	264
5	180	176
4	347	-315
3	175	-164
2	104	-81
1	259	-253
0	151	-145

H= 8, K= 0

0	230	234
1	114	103
2	48	55
3	360	360
4	310	296
5	86	63
6	179	181
7	480	511
8	393	394
9	92	104
10	190	185
11	41*	17

H= 8, K= 1

10	8*	6
9	57	62
8	274	278
7	256	262
6	212	200
5	161	145

L	FO	FC
H= 8, K= 1		
4	211	197
3	412	383
2	124	109
H= 8, K= 2		
6	7*	41
7	195	203
8	79	49
9	8*	-8
H= 8, K= 3		
9	134	140
8	43*	-10
7	35*	46
6	377	383
5	252	281
4	6*	-38
H= 8, K= 4		
0	129	269
1	52*	197
2	6*	175
3	106	221
4	198	250
5	194	217
6	133	136
7	99	100
8	53*	59
H= 8, K= 5		
7	62	58
6	127	119
5	37*	30
4	128	144
3	248	313
2	32*	-24
1	55*	-96
0	165	243
H= 8, K= 6		
0	107	123
1	215	288
2	143	207
3	33*	27
4	173	177
5	150	137
H= 8, K= 7		
4	45*	59
3	174	167
2	215	244
1	218	244
0	199	256
H= 8, K= 8		
0	19*	-20
1	91	93
2	211	199
H= 9, K= 8		
0	148	163
H= 9, K= 7		
0	8*	11
1	56*	35
2	53*	60
3	85	-72
H= 9, K= 6		
5	23*	-31
4	158	148
3	23*	28
2	63	-63
1	117	138
0	108	118
H= 9, K= 5		
0	65	61
1	82	194
2	7*	4
3	53*	-114
4	127	143
5	106	115
6	168	-161
H= 9, K= 4		
7	25*	-52
6	62	-80
5	158	-158
4	7*	42
3	153	270
2	7*	-9
1	27*	-69
0	113	189
H= 9, K= 3		
0	24*	53
1	7*	155
2	6*	234
3	44*	49
4	7*	-15
5	131	137
6	107	-149
7	192	-199
8	45*	-45
H= 9, K= 2		
9	43*	14
8	77	-81
7	212	-211
6	92	124
5	7*	60
4	6*	-146
1	24*	167
0	141	189
H= 9, K= 1		
0	384	383
5	25*	56
6	214	-231
7	119	-137
8	150	126
9	38*	-56
10	191	-175
H= 9, K= 0		
10	98	-101
9	78	98
8	54	-31
7	62	-85
6	61	47
0	278	259
H= 10, K= 0		
0	74	-73
1	187	158
2	125	-131
3	6*	-178
4	6*	-80
5	78	-145
6	245	-271
7	108	-118
8	172	-186
9	367	-368
10	227	-212
H= 10, K= 1		
10	112	-93
9	69	-63
8	209	-221
7	207	-209
6	136	-142
5	7*	-84
4	7*	-133
3	7*	-16
2	39*	-41
1	7*	-54
0	109	-107
H= 10, K= 2		
0	134	-126
1	26*	-64
2	7*	49
3	7*	-175
4	7*	-188
5	7*	-21
6	95	-110
7	166	-174
8	83	-75
9	8*	-7
H= 10, K= 3		
8	154	-122
7	8*	-70
6	76	-72
5	204	-324
4	69*	-258
3	24*	-87
2	7*	-162
1	84*	-258
0	23*	59
H= 10, K= 4		
0	50*	-156
1	7*	-165
2	21*	-186
3	7*	-208
4	25*	-163
5	152	-209
6	150	-176
7	106	-99
H= 10, K= 5		
6	151	-152
5	142	-183
4	23*	-44

L	FO	FC
3	44*	-88
2	93	-151
1	37*	-56
0	61*	-180
H=	10, K=	6
0	153	-211
1	45*	-82
2	43*	-69
3	108	-185
4	195	-199
H=	10, K=	7
2	118	-175
1	77	-117
0	92	-108
H=	11, K=	6
3	75	-82
2	8*	-39
1	14*	-7
0	40*	-64
H=	11, K=	5
0	49*	-123
1	8*	-106
2	32*	-18
3	48*	-82
4	53*	-78
5	11*	-37
H=	11, K=	4
6	102	-107
5	70	-66
4	93	126
3	44*	-63
2	8*	-271
1	35*	-71
0	8*	-32
H=	11, K=	3
0	33*	-94
1	10*	-77
2	7*	-78
3	7*	-85
4	7*	-96
5	7*	-62
6	55*	-70
7	8*	16
8	66	74
H=	11, K=	2
8	8*	-25
7	26*	-2
6	7*	-40
5	62*	-131
4	7*	-90
3	7*	21
2	7*	-148
1	57*	-141
0	115	-116
H=	11, K=	1
0	431	-397
1	190	-201
2	7*	-65
3	7*	-284
4	7*	-122
5	7*	144
6	7*	19
7	109	-86
8	52*	21
9	78	58
H=	11, K=	0
10	18*	6
9	49*	12
8	117	107
7	91	94
6	7*	23
5	32*	-124
4	7*	-145
3	59*	-155
2	270	-271
1	207	-201
0	80	-78
H=	12, K=	0
0	31*	-4
1	8*	34
2	11*	11
3	64*	-111
4	13*	-24
5	7*	222
6	144	224
7	83	88
8	221	190
9	235	221
H=	12, K=	1
9	55*	63
8	105	110
7	157	166
6	20*	179
5	7*	62
4	62	68
3	7*	72
2	7*	-4
1	86	105
0	89	91
H=	12, K=	2
1	8*	-36
2	8*	161
4	18*	-25
5	40*	88
6	96	158
7	62	76
8	37*	25
H=	12, K=	3
7	108	149
6	27*	39
5	22*	76
4	8*	221
3	8*	86
2	50*	7
1	70	111
0	58	11
H=	12, K=	4
0	42*	48
1	8*	125
2	30*	113
3	14*	62
4	8*	66
5	46*	107
H=	12, K=	5
3	22*	-9
2	52*	70
1	56*	190
H=	13, K=	3
2	8*	40
3	8*	94
4	8*	53
5	8*	20
H=	13, K=	2
7	87	89
6	8*	58
5	8*	24
4	47*	145
3	8*	86
2	45*	61
1	87	85
H=	13, K=	1
1	59*	74
2	174	202
3	8*	252
4	13*	139
5	37*	57
6	8*	40
7	8*	-8
8	8*	-26
H=	13, K=	0
9	11*	21
8	57	-59
7	44*	-27
6	40*	-20
5	38*	140
4	8*	230
3	84	132
2	162	124
1	155	142
H=	14, K=	0
3	47*	71
4	41*	21
5	8*	-6
6	35*	11
7	108	-123
H=	14, K=	1
6	8*	-111
5	58	-17
4	44*	-17
H=	11, K=	-2
-1	35*	-10
H=	11, K=	-1
-1	87	-66

L	FO	FC
H= 11, K= 0		
-2	140	-119
-1	140	-122
H= 10, K= 0		
-1	131	-120
-2	105	94
-3	93	103
H= 10, K= -1		
-2	68	65
-1	203	170
H= 10, K= -2		
-1	138	129
-2	107	94
H= 10, K= -3		
-1	105	105
H= 9, K= -5		
-1	165	170
H= 9, K= -4		
-1	78	73
H= 9, K= -3		
-1	79	89
-2	68	78
H= 9, K= -2		
-3	67	63
-2	291	261
-1	243	237
H= 9, K= -1		
-1	123	107
-2	176	167
-3	216	185
H= 9, K= 0		
-4	217	198
-3	184	178
-2	71	63
-1	325	288
H= 8, K= 0		
-1	118	120
-2	180	-161
-3	97	-86
-4	43*	12
-5	90	-85
H= 8, K= -1		
-4	50*	-51
-3	115	-109
-2	50	20
-1	125	123
H= 8, K= -2		
-1	48*	-17
-2	7*	-51
-3	103	85
-4	46*	-39
H= 8, K= -3		
-3	54*	46
-2	71	-53
-1	277	-251
H= 8, K= -4		
-1	142	-155
-2	116	-119
H= 8, K= -5		
-1	44*	-56
H= 7, K= -6		
-1	168	-176
H= 7, K= -5		
-1	94	-76
-2	90	-88
H= 7, K= -4		
-3	76	-67
-2	77	-60
-1	133	-135
H= 7, K= -3		
-1	242	-227
-2	318	-304
-3	95	-97
-4	99	-92
H= 7, K= -2		
-4	205	-203
-3	212	-215
-2	198	-181
-1	423	-406
H= 7, K= -1		
-1	43	-35
-2	185	-181
-3	267	-251
-4	207	-182
-5	140	-134
H= 7, K= 0		
-5	68	-50
-4	311	-270
-3	448	-410
-2	206	-177
-1	118	-103
H= 6, K= 0		
-1	139	159
-2	102	93
-3	108	-89
-4	238	238
-5	187	168
-6	8*	8
H= 6, K= -1		
-6	164	157
-5	20*	-6
-4	102	-90
-3	195	171
-2	229	212
-1	104	-124
H= 6, K= -2		
-1	26*	-21
-2	29*	42
-3	61	-67
-4	7*	-26
-5	52*	12
H= 6, K= -3		
-5	8*	25
-4	48*	54
-3	131	123
-2	103	-99
-1	199	-201
H= 6, K= -4		
-1	131	110
-2	144	155
-3	38*	-25
-4	99	101
H= 6, K= -5		
-3	82	77
-2	45*	49
-1	7*	-5
H= 6, K= -6		
-1	48*	-63
-2	110	107
H= 6, K= -7		
-1	79	61
H= 5, K= -7		
-1	117	121
-2	105	110
H= 5, K= -6		
-3	124	122
-2	58	67
-1	244	246
H= 5, K= -5		
-1	253	246
-2	326	306
-3	92	84
-4	90	78
H= 5, K= -4		
-4	181	172
-3	62	22
-2	97	90
-1	412	405

L	FO	FC
H= 5, K= -3		
-1	251	243
-2	251	271
-3	7*	-15
-4	168	164
-5	275	274
H= 5, K= -2		
-6	175	177
-5	97	104
-4	221	215
-3	414	394
-2	168	145
-1	130	134
H= 5, K= -1		
-1	19*	48
-2	524	540
-3	272	268
-4	106	107
-5	213	215
-6	114	94
H= 5, K= 0		
-7	57*	67
-6	222	208
-5	310	288
-4	352	338
-3	455	442
-2	69	-55
-1	176	176
H= 4, K= 0		
-1	251	244
-2	414	440
-3	207	-210
-4	59	-52
-5	17*	-2
-6	122	-132
-7	96	-90
H= 4, K= -1		
-7	22*	10
-6	38*	-20
-5	277	-266
-4	12*	5
-3	28*	16
-2	43	38
-1	247	218
H= 4, K= -2		
-1	86	60
-2	25*	-20
-3	116	97
-4	7*	1
-5	7*	-21
-6	54	-49
H= 4, K= -3		
-6	91	-90
-5	63	-56
-4	40*	3
-3	31*	8
-2	128	-110
-1	380	409
H= 4, K= -4		
-1	121	109
-2	174	163
-3	80	-72
-4	142	-164
-5	24*	12
H= 4, K= -5		
-4	42*	-47
-3	7*	4
-2	46*	31
-1	161	154
H= 4, K= -6		
-1	27*	20
-2	85	78
-3	8*	24
H= 4, K= -7		
-2	70	-56
-1	85	68
H= 4, K= -8		
-1	110	-104
H= 3, K= -8		
-1	242	-232
H= 3, K= -7		
-1	119	-123
-2	373	-378
-3	165	-167
H= 3, K= -6		
-4	126	-118
-3	215	-213
-2	394	-387
-1	201	-201
H= 3, K= -5		
-1	465	-466
-2	422	-429
-3	17*	29
-4	129	-115
-5	209	-208
H= 3, K= -4		
-6	127	-124
-5	55*	-41
-4	25*	-55
-3	320	-314
-2	93	-90
-1	30*	-37
H= 3, K= -3		
-1	714	-710
-2	394	-418
-3	252	-242
-4	119	-113
-5	107	-110
-6	151	-176
H= 3, K= -2		
-7	171	-186
-6	374	-386
-5	140	-130
-4	88	77
-3	444	-485
-2	630	-634
-1	427	-398
H= 3, K= -1		
-1	681	-723
-2	51	32
-3	74	76
-4	488	-514
-5	317	-322
-6	131	-126
-7	126	-121
H= 3, K= 0		
-8	143	-148
-7	148	-141
-6	344	-351
-5	505	-486
-4	304	-308
-3	123	-128
-2	75	-74
-1	168	171
H= 2, K= 0		
-1	939	-930
-2	70	96
-3	124	144
-4	337	-356
-5	277	-291
-6	218	193
-7	246	230
-8	157	-144
H= 2, K= -1		
-8	49*	48
-7	142	136
-6	61	-50
-5	131	-114
-4	33	-15
-3	84	-98
-2	329	-358
-1	93	79
H= 2, K= -2		
-1	364	-356
-2	976	-975
-3	197	-189
-4	12*	-21
-5	49	-43
-6	65	75
-7	8*	20
H= 2, K= -3		
-7	40*	-14
-6	46*	44
-5	165	153
-4	108	-127
-3	234	-251
-2	142	-125
-1	171	-148

L	FO	FC
H=	2, K=	-4
-1	342	-365
-2	153	130
-3	210	211
-4	103	-82
-5	57	-68
-6	130	140
H=	2, K=	-5
-5	78	63
-4	48*	-36
-3	7*	-24
-2	36*	16
-1	350	-339
H=	2, K=	-6
-1	103	-119
-2	222	-225
-3	50*	-42
-4	96	97
H=	2, K=	-7
-3	21*	-47
-2	120	105
-1	88	90
H=	2, K=	-8
-1	94	88
-2	50*	-14
-2	50*	-14
H=	2, K=	-9
-1	48*	-78
H=	1, K=	-9
-1	205	205
H=	1, K=	-8
-2	252	243
-1	84	-81
H=	1, K=	-7
-1	59	41
-2	292	281
-3	207	206
-4	163	170
H=	1, K=	-6
-6	143	157
-5	176	175
-4	354	351
-3	359	369
-2	227	221
-1		
H=	1, K=	-5
-6	73	80
-5	8*	-21
-4	303	304
-3	396	401
-2	10*	33
-1	289	287
H=	1, K=	-4
-6	127	114
-5	68	47
-4	131	146
-3	291	308
-2	235	243
-1	256	241
H=	1, K=	-3
-7	250	251
-6	190	191
-5	136	155
-4	159	185
-3	339	330
-2	645	624
-1	320	292
H=	1, K=	-2
-8	269	276
-7	125	135
-6	76	82
-5	365	367
-4	347	326
-3	342	323
-2	382	395
-1	484	511
H=	1, K=	-1
-1	35	-35
-2	343	-360
-3	304	310
-4	239	248
-5	211	221
-6	169	165
-7	152	157
-8	158	159
H=	1, K=	0
-9	8*	12
-6	357	373
-5	95	103
-4	218	229
-3	413	410
-3	413	410
-2	3*	18
-1	252	234
H=	1, K=	-11
3	28*	35
5	59	37
4	93	-71
6	115	100
7	91	-89
H=	1, K=	-10
9	186	-169
8	8*	-6
7	48*	44
6	49*	-51
5	79	-84
4	137	126
3	161	155
2	109	121
1	159	163
H=	1, K=	-9
1	183	176
2	125	126
9	60	-161
4	133	122
5	117	135
6	82	-75
7	7*	-30
8	62	74
9	161	-161
10	175	-169
H=	1, K=	-8
11	128	-117
10	199	-204
9	238	-239
8	119	115
7	108	96
6	232	-210
5	161	142
4	193	182
3	99	-87
2	97	78
1	289	288
0	58	-71
H=	1, K=	-7
0	92	-82
1	116	125
2	297	299
3	179	186
4	173	-173
5	73	-80
6	176	166
7	74	-80
8	403	-401
9	101	-104
10	7*	10
11	193	-188
H=	1, K=	-6
11	91	-89
10	7*	-15
9	139	-139
8	333	-336
7	31*	-16
6	139	-137
5	295	-300
4	55	-35
3	19*	17
2	277	275
1	305	305
0	217	196
H=	1, K=	-5
0	770	785
1	101	85
2	225	-241
3	254	261
4	72	-57
5	434	-410
6	115	-122
7	71	-69
8	226	-239
9	160	-163
10	97	-88
11	155	-148
H=	1, K=	-4

L	FO	FC
11	162	-170
10	341	-339
9	99	-84
8	171	156
7	395	-404
6	582	-599
5	143	-115
4	56	-54
3	95	-97
2	141	148
1	100	115
0	326	329

H= 1, K= -3

L	FO	FC
0	24*	-10
1	23*	14
2	240	233
3	196	197
4	494	-535
5	406	-393
6	27*	12
7	270	-276
8	209	-208
9	156	-172
10	118	-129
11	84	-87

H= 1, K= -2

L	FO	FC
10	89	-108
9	196	-215
8	448	-435
7	337	-351
6	69	-63
5	4*	-15
4	219	-230
3	44	62
2	1156	1129
1	517	-501
0	879	-870

H= 1, K= -1

L	FO	FC
0	752	738
1	118	-109
2	574	-570
3	584	579
4	43	69
5	328	-363
6	203	-199
7	179	-192
9	491	-470
9	449	-470
10	123	-131

H= 2, K= -1

L	FO	FC
10	35*	-6
9	63	-46
8	164	-161
7	312	-313
6	111	-121
5	44	-70
4	86	-64
3	425	424
2	677	-730
0	150	159

H= 2, K= -2

L	FO	FC
0	449	457
1	372	-354
2	545	-523
3	429	425
4	157	163
5	769	-798
6	184	-190
7	5*	-14
8	129	-106
9	25*	-15
10	7*	20
11	69	-57

H= 2, K= -3

L	FO	FC
11	66	-75
10	45*	-19
9	129	131
8	211	-219
7	275	-305
6	366	-346
5	650	-632
4	508	-528
3	604	-593
2	391	-380
1	760	-733
0	395	-412

H= 2, K= -4

L	FO	FC
0	189	-204
1	345	-302
2	541	-558
3	517	-513
4	491	-491
5	407	-397
6	367	-375
7	231	-220
8	173	-165
9	55	-71
10	96	-98
11	34*	-13

H= 2, K= -5

L	FO	FC
11	73	-57
10	37*	-35
9	28*	-23
8	80	82
7	204	-206
6	653	-671
5	200	-199
4	280	-267
3	66	-62
2	103	-120
1	233	-239
0	312	-317

H= 2, K= -6

L	FO	FC
0	102	-109
1	279	-283
2	403	-415
3	83	-86
4	208	-218
5	450	-447
6	393	-387
7	152	-165
8	260	-273
9	233	-237
10	64	74
11	8*	-15

H= 2, K= -7

L	FO	FC
11	63	-68
10	107	-91
9	249	-237
8	295	-307
7	381	-360
6	201	-198
5	223	-223
4	321	-322
3	304	-322
2	127	-122
1	123	-120
0	262	-259

H= 2, K= -8

L	FO	FC
1	120	-102
2	66	-80
3	230	-236
4	328	-310
5	301	-303
6	119	-117
7	116	-133
8	20*	-15
9	91	-79
10	159	-165
11	82	-105

H= 2, K= -9

L	FO	FC
11	77	-84
10	182	-193
9	8*	14
8	178	175
7	100	-105
6	391	-379
5	224	-225
4	177	-161
3	355	-336
2	113	-110
1	8*	-15
0	49*	-49

H= 2, K= -10

L	FO	FC
1	142	-136
2	137	-123
3	97	-81
4	127	-122
5	181	-174
6	166	-163
7	163	-148
8	223	-216
9	133	-135
10	116	-111

H= 2, K= -11

L	FO	FC
8	243	-238
7	101	-107
6	70	-53
5	71	-63
4	66	-60

H= 3, K= -11

L	FO	FC
4	89	-95
5	61	-56
6	8*	31
7	8*	31
8	62	-53

H= 3, K= -10

L	FO	FC
10	78	89

L	FO	FC
H=	3, K=	-10
9	14*	-24
8	84	97
7	8*	-19
6	243	-237
5	24*	-23
4	41*	28
3	269	-262
2	247	-238
H=	3, K=	-9
0	189	-180
1	111	-99
2	172	-168
3	162	-149
4	205	-195
5	130	-127
6	7*	-36
7	33*	8
8	92	-96
9	40*	15
10	202	202
11	120	127
H=	3, K=	-8
11	45*	28
10	100	96
9	94	113
8	93	-70
7	7*	-17
6	85	76
5	7*	59
4	264	-265
3	327	-330
2	36*	-34
1	132	127
0	93	-79
H=	3, K=	-7
0	275	267
1	288	-290
2	370	-358
3	39	34
4	57	-34
5	294	-295
6	199	194
7	319	304
8	135	-134
9	7*	41
10	174	185
11	95	86
12	82	66
H=	3, K=	-6
12	157	140
11	89	99
10	77	69
9	199	204
8	169	160
7	41	-37
6	12*	32
5	5*	-18
4	69	-73
3	75	-52
2	36*	-46
1	441	-461
0	277	-256
H=	3, K=	-5
0	218	-219
1	154	-144
2	95	-125
3	46	-75
4	176	-159
5	5*	-11
6	175	163
7	19*	46
8	236	250
9	35*	-24
10	33*	15
11	234	239
12	178	185
H=	3, K=	-4
12	205	199
11	78	89
10	114	128
9	215	195
8	101	94
7	28*	-61
6	710	715
5	522	520
4	703	-700
3	230	-231
2	335	336
1	233	-218
0	834	-836
H=	3, K=	-3
0	562	-536
1	66	-81
2	292	-286
3	56	-57
4	28*	27
5	206	184
6	211	233
7	481	497
8	233	-254
9	105	93
10	168	175
11	105	111
H=	3, K=	-2
11	55*	69
10	320	306
9	287	300
8	157	170
7	346	368
6	32	40
5	22*	-50
4	144	-131
3	618	636
2	191	-186
1	844	-861
0	37	-24
H=	3, K=	-1
0	631	672
1	765	759
2	605	-628
3	911	-1068
4	120	140
5	181	205
6	93	-105
7	279	290
8	547	534
9	319	329
10	49*	33
11	208	214
9	7*	329
H=	4, K=	-1
11	35*	-10
10	32*	-11
9	7*	27
8	288	267
7	113	115
6	47	-46
5	196	209
4	716	706
3	881	832
2	88	71
1	823	706
0	177	179
H=	4, K=	-2
0	339	334
1	602	611
2	433	426
3	701	688
4	371	368
5	230	223
6	93	80
7	26*	-27
8	252	247
9	7*	17
10	57	-50
11	21*	27
H=	4, K=	-3
12	76	-91
11	46*	36
10	270	258
9	91	105
8	61	-55
7	336	355
6	672	678
5	321	290
4	550	516
3	622	628
2	726	713
1	57	57
0	203	221
H=	4, K=	-4
0	110	108
1	54	45
2	404	424
3	274	264
4	254	278
5	286	303
6	459	438
7	305	307
8	272	286
9	238	221
10	40*	30
11	96	112
12	87	73
H=	4, K=	-5
12	122	113
11	8*	16
10	47*	-24
9	233	228
8	286	288

L	FO	FC
7	164	150
6	210	211
5	147	145
4	33	-20
3	190	209
2	230	227
1	124	135
0	310	324
H=	4, K=	-6
0	346	347
1	268	280
2	46	-47
3	171	177
4	201	199
5	159	165
6	106	114
7	463	481
8	537	513
9	94	94
10	25*	-36
11	125	115
12	59	76
H=	4, K=	-7
12	8*	9
11	58	66
10	294	286
9	316	308
8	158	169
7	317	293
6	319	312
5	214	220
4	217	199
3	273	285
2	40*	34
1	123	-114
0	20*	8
H=	4, K=	-8
0	111	-113
1	7*	7
2	34*	25
3	159	151
4	250	261
5	232	229
6	305	281
7	235	223
8	24*	14
9	88	72
10	186	201
11	93	88
12	48*	-12
H=	4, K=	-9
11	6*	16
10	30*	10
9	110	103
8	141	134
7	87	73
6	298	291
5	434	424
4	111	119
3	60	36
2	206	211
1	59	41
1	116	41
H=	4, K=	-10
2	44*	34
3	121	119
4	166	160
5	129	122
6	67	83
7	184	179
8	220	212
9	55*	67
10	113	101
H=	4, K=	-11
8	188	196
7	57	59
6	29*	-30
5	8*	11
H=	5, K=	-11
6	57	-21
7	101	84
8	14*	13
H=	5, K=	-10
10	50*	-45
9	113	107
8	110	108
7	43*	56
6	91	75
5	98	84
4	94	110
3	95	95
H=	5, K=	-9
1	182	167
2	50*	88
3	121	126
4	163	161
5	139	127
6	158	155
7	45*	37
8	101	77
9	60	74
10	59	-40
11	90	-118
H=	5, K=	-8
12	82	-97
11	58*	-74
10	123	130
9	16*	-10
8	236	-243
7	85	-96
6	249	256
5	143	156
4	82	82
3	263	268
2	77	84
1	76	-89
0	130	150
H=	5, K=	-7
0	154	150
1	141	148
2	175	177
3	235	249
4	188	170
5	197	193
6	45*	51
7	151	-162
8	133	-140
9	119	-124
10	41*	-50
11	64	-41
12	84	-75
H=	5, K=	-6
12	86	-85
11	69	-76
10	134	-137
9	103	-112
8	6*	-6
7	110	-101
6	52	-50
5	163	157
4	26*	62
3	256	253
2	405	404
1	287	289
0	351	341
H=	5, K=	-5
0	181	174
1	423	419
2	145	146
3	134	-119
4	46	67
5	275	277
6	119	102
7	122	-109
8	17*	24
9	7*	7
10	247	-242
11	71	-69
12	27*	-21
H=	5, K=	-4
12	164	-165
11	128	-93
10	21*	-18
9	131	-139
8	296	-314
7	35*	-56
6	76	85
5	301	317
4	177	164
3	159	-184
2	83	-78
1	57	78
0	348	368
H=	5, K=	-3
0	501	460
1	672	644
2	149	166
3	104	123
4	16*	-13
5	138	-143
6	108	-74
7	81	-77
8	141	-142
9	150	-135
10	145	-160
11	156	-152
12	163	-146
H=	5, K=	-2

L	FO	FC
H=	5, K=	-2
11	35*	-32
10	190	-211
9	432	-405
8	206	-208
7	25*	7
6	72	-102
5	20*	-19
4	341	327
3	278	298
2	179	142
1	219	209
0	537	583
H=	5, K=	-1
0	245	-264
1	263	290
2	442	408
3	48	-40
4	136	138
5	106	111
6	180	168
7	309	-317
8	312	-318
9	221	-231
10	301	-299
11	97	-92
H=	6, K=	-1
11	36*	50
10	188	-162
9	160	-170
8	58	-72
7	169	-184
6	319	-322
5	27*	30
4	381	-347
3	956	-971
2	538	-507
1	36	-25
0	104	-108
H=	6, K=	-2
0	357	-349
1	202	-197
2	314	-299
3	236	-259
4	328	-292
5	483	-476
6	61	-81
7	79	-96
8	121	-125
9	7*	41
10	197	-177
11	105	-120
12	42*	47
H=	6, K=	-3
12	145	-128
11	45*	-62
10	154	-159
9	399	-385
H=	6, K=	-4
9	115	-106
H=	6, K=	-3
8	82	-74
7	73	93
6	675	-675
5	584	-584
4	19*	29
3	60	-66
2	642	-639
1	317	-325
0	155	154
H=	6, K=	-4
0	236	-242
1	171	-177
2	124	-135
3	254	-221
4	114	-116
5	105	-95
6	287	-256
7	318	-333
8	336	-348
10	97	-108
11	275	-263
12	87	-102
H=	6, K=	-5
12	59	-86
11	43*	-19
10	7*	39
9	249	-267
8	348	-340
7	241	-251
6	30*	-59
5	78	-66
4	196	-203
3	78	-98
2	184	-173
1	137	-154
0	101	-87
H=	6, K=	-6
0	265	-273
1	68	44
2	96	80
3	226	-224
4	224	-240
5	135	-141
6	278	-261
7	499	-487
8	115	-129
9	196	-200
10	302	-298
11	15*	-24
12	26*	59
H=	6, K=	-7
12	121	-125
11	64	-69
10	213	-212
9	304	-314
8	250	-245
7	230	-225
6	251	-259
5	359	-373
4	45*	-48
3	195	203
2	7*	14
1	153	-141
0	64	60
H=	6, K=	-8
0	100	119
1	39*	27
2	7*	-37
3	58	-55
4	34*	-11
5	238	-236
6	267	-280
7	91	-93
8	77	-66
9	101	-102
10	222	-209
11	95	-93
12	67	-77
H=	6, K=	-9
11	151	-149
10	29*	-22
9	8*	-15
8	221	-224
7	159	-136
6	100	-105
5	211	-212
4	273	-273
3	66	-53
2	48*	20
H=	6, K=	-10
4	37*	-56
5	8*	-53
6	197	-205
7	119	-115
8	55*	-47
9	116	-112
10	131	-123
H=	7, K=	-10
10	8*	15
9	45*	-50
8	171	-177
7	157	-158
6	25*	-12
5	80	-80
H=	7, K=	-9
3	105	-93
4	160	-145
5	80	-65
6	53*	-63
7	190	-193
8	142	-118
9	40*	-16
10	19*	-8
11	86	-62
H=	7, K=	-8
12	74	-62
11	8*	5
10	47*	44
9	91	-59
8	41*	37
7	56	46
6	169	-176
5	191	-183
4	28*	-11
3	55*	48
2	199	-194

L	FO	FC
1	156	-140

H= 7, K= -7

L	FO	FC
0	53*	-84
1	160	-145
2	176	-169
3	210	-215
4	204	-233
5	82	-96
6	147	-154
7	25*	16
8	195	207
9	94	111
10	106	-134
11	8*	-5
12	139	141

H= 7, K= -6

L	FO	FC
12	93	99
11	143	137
10	25*	9
9	139	107
8	101	108
7	48*	-33
6	146	-161
5	63	-87
4	213	-265
3	413	-480
2	315	-321
1	145	-168
0	138	-143

H= 7, K= -5

L	FO	FC
0	324	-296
1	406	-409
2	88	-120
3	200	-200
4	123	-120
5	110	-107
6	22*	-46
7	234	-241
8	209	-185
9	324	321
10	232	225
11	26*	23
12	49*	9

H= 7, K= -4

L	FO	FC
12	36*	-36
11	236	233
10	255	226
9	69	-49
8	48	37
7	19*	37
6	89	-76
5	192	-186
4	83	49
3	56	-75
2	262	-276
1	269	-259
0	270	-273

H= 7, K= -3

L	FO	FC
0	200	-208
1	182	-187
2	421	-406
3	159	-170
4	17*	-24
5	257	-272
6	61	-45
7	59	72
8	106	112
9	77	78
10	179	175
11	131	109
12	104	106

H= 7, K= -2

L	FO	FC
12	212	207
11	191	189
10	7*	50
9	91	90
8	278	284
7	237	-241
6	407	-419
5	164	154
4	55	72
3	450	-383
2	363	-402
1	161	164
0	164	-178

H= 7, K= -1

L	FO	FC
0	56	-35
1	79	-77
2	122	-123
3	291	-289
4	41	37
5	57	-67
6	181	-183
7	6*	-12
8	131	-126
9	251	238
10	342	329
11	33*	57

H= 8, K= -1

L	FO	FC
11	46*	34
10	125	109
9	258	252
8	208	195
7	79	-87
6	381	401
5	438	457
4	29*	-30
3	63	40
2	473	477
1	104	132
0	275	-275

H= 8, K= -2

L	FO	FC
0	37*	-12
1	30*	-10
2	334	324
3	271	261
4	430	393
5	346	306
6	232	214
7	37	-37
8	71	-60
9	170	167
10	97	94
11	86	75
12	78	95

H= 8, K= -3

L	FO	FC
12	171	184
11	179	158
10	70	-68
9	192	179
8	337	337
7	262	271
6	253	242
5	260	257
4	255	274
3	99	120
2	231	251
1	230	225
0	7*	-31

H= 8, K= -4

L	FO	FC
0	27*	9
1	119	-124
2	31*	52
3	402	375
4	86	109
5	127	-124
6	244	248
7	574	558
8	128	124
9	153	151
10	274	250
11	100	82
12	56	48

H= 8, K= -5

L	FO	FC
12	44*	14
11	42*	69
10	210	200
9	98	103
8	126	122
7	299	304
6	153	154
5	82	87
4	122	184
3	138	174
2	7*	-17
1	40*	35
0	50*	-57

H= 8, K= -6

L	FO	FC
0	8*	-4
1	102	113
2	86	78
3	20*	45
4	7*	44
5	104	136
6	169	213
7	181	216
8	182	214
9	288	281
10	191	191
11	35*	-11
12	86	72

H= 8, K= -7

L	FO	FC
12	162	168
11	226	216
10	62	67
9	127	119
8	323	331
7	126	138
6	35*	13
5	67	58
4	17*	26
3	122	-126

L	FO	FC
H=	8, K=	-7
2	33*	43
1	177	181
H=	8, K=	-8
2	65	61
3	41*	21
4	20*	4
5	15*	32
6	102	121
7	92	117
8	57	67
9	7*	28
10	109	102
11	168	184
12	120	129
H=	8, K=	-9
11	173	173
10	140	137
9	46*	14
8	88	83
7	185	219
6	147	183
5	48*	71
4	68	73
H=	8, K=	-10
7	78	84
8	101	108
9	169	162
H=	9, K=	-9
5	41*	60
6	132	176
7	152	170
8	65	91
9	106	102
10	27*	19
H=	9, K=	-8
11	92	99
10	81	-85
9	41*	-34
8	100	111
H=	9, K=	-7
1	20*	82
H=	9, K=	-8
6	8*	10
5	70	100
4	146	177
3	86	95
H=	9, K=	-7
2	170	186
3	141	146
4	40*	72
5	118	204
6	139	194
7	70	-81
8	62	-93
9	73	78
10	8*	34
11	54*	-45
12	8*	12
H=	9, K=	-6
12	43*	-45
11	31*	-21
10	7*	-23
9	53*	25
8	72	79
7	7*	24
6	59*	105
5	280	275
4	133	203
3	75	111
2	219	224
1	163	184
0	52*	92
H=	9, K=	-5
0	182	187
2	110	105
3	210	289
4	124	239
5	49*	-88
6	7*	66
7	205	272
8	22*	20
9	69	-39
10	125	107
11	110	-107
12	175	-166
H=	9, K=	-4
12	14*	-15
11	98	-100
10	269	-271
9	86	-77
8	319	295
7	95	107
6	68	-90
5	60*	147
4	305	312
3	49*	52
2	57	99
1	244	253
0	151	122
H=	9, K=	-3
0	276	276
1	374	356
2	62	93
3	285	271
4	383	345
5	91	89
6	31*	35
7	175	168
8	7*	-42
9	147	-154
10	98	-70
11	143	-142
12	134	-125
H=	9, K=	-2
11	253	-224
10	52*	-50
9	163	147
8	172	-165
7	162	-164
6	296	294
5	432	395
4	102	-87
3	98	131
2	435	420
1	192	183
0	45*	62
H=	9, K=	-1
0	222	202
1	98	-75
2	6*	13
3	296	284
4	224	212
5	14*	20
6	18*	-6
7	157	169
8	122	-99
9	84	-54
10	81	69
11	100	-79
H=	10, K=	-1
11	75	-61
10	80	-81
9	249	-238
8	204	-174
7	45*	-44
6	100	-120
5	376	-390
4	6*	-329
3	77	48
2	21*	33
1	91	-69
0	68	61
H=	10, K=	-2
0	74	-62
1	7*	45
2	86	63
3	220	-220
4	115	-231
5	252	-243
6	328	-324
7	217	-199
8	113	-97
9	116	-109
10	8*	23
11	22*	8
H=	10, K=	-3
11	206	-177
10	238	-217
9	7*	-24
8	167	-163
7	438	-403
6	74	-88
5	26*	-9
3	228	-250
2	105	94
1	59	42
0	91	97
H=	10, K=	-4
0	141	144
1	137	149
2	96	-81
3	142	-188

L	FO	FC
4	24*	-63
5	7*	-22
6	75	-83
7	69	-64
8	61	-78
9	278	-264
10	269	-253
11	85	-88
12	33*	-29

H= 10, K= -5

L	FO	FC
12	59	-27
11	66	-68
10	128	-133
9	123	-95
8	93	-101
7	61*	-101
6	35*	-43
5	84	-160
4	63*	-129
3	7*	28
2	21*	-19
1	8*	-49
0	34*	36

H= 10, K= -6

L	FO	FC
1	37*	-37
2	8*	-60
3	8*	13
4	32*	-32
5	123	-202
6	7*	-20
7	40*	-43
8	247	-332
9	175	-164
10	67	47
11	93	-96
12	188	-180

H= 10, K= -7

L	FO	FC
11	183	-165
10	155	-160
9	77	-97
8	137	-199
7	7*	-78
6	70	111
5	39*	89
4	68	-48
3	72	-68

H= 10, K= -8

L	FO	FC
4	41*	60
5	8*	8
6	51*	-50
7	8*	12
8	57*	-102
9	56*	-113
10	100	-97
11	120	-134

H= 10, K= -9

L	FO	FC
9	141	-172
8	58*	-61
7	24*	-98

H= 11, K= -8

L	FO	FC
9	8*	59
9	8*	59
8	35*	35
7	74*	-183
6	85	-117

H= 11, K= -7

L	FO	FC
4	95	-116
5	94	-164
6	89	-198
7	60	-66
8	52*	-14
9	51*	-49
10	47*	44
11	8*	-23

H= 11, K= -6

L	FO	FC
11	8*	3
10	8*	19
9	73	-84
8	78	-108
7	58	-72
6	97	-197
5	112	-221
4	79	-154
3	52*	-78

H= 11, K= -5

L	FO	FC
2	166	-168
3	110	-119
4	28*	12
5	69*	-144
6	98	-200
7	7*	45
8	19*	-85

L	FO	FC
9	178	-164
10	8*	-16
11	102	77

H= 11, K= -4

L	FO	FC
11	44*	-23
10	42*	-58
10	69	-58
9	79	52
8	162	-164
7	121	-173
6	7*	62
5	7*	-18
4	80	-137
3	113	-110
2	77	-76
1	75	-99

H= 11, K= -3

L	FO	FC
0	153	-130
1	169	-166
2	152	-159
3	196	-209
4	47*	-79
5	7*	-19
6	106	-144
7	268	-242
8	111	-101
9	21*	32
10	8*	24
11	48*	58

H= 11, K= -2

L	FO	FC
11	8*	14
10	79	55
9	60	35
8	102	-72
7	111	-123
6	38*	-38
5	261	-258
4	192	-226
3	92	78
2	169	-167
1	370	-333
0	152	-117

H= 11, K= -1

L	FO	FC
0	78	-73
1	99	-84
2	157	-125
3	236	-242
4	7*	-148
5	88	-90
6	142	-158
7	54*	47
8	198	190
9	62	-58
10	72	-84

H= 12, K= -1

L	FO	FC
10	120	112
9	94	84
8	119	112
7	231	214
6	117	128
5	19*	13
4	141	189
3	7*	-7
2	210	-176
1	8*	4
0	45*	38

H= 12, K= -2

L	FO	FC
0	89	-63
1	21*	-11
2	85	79
3	41*	7
4	123	131
5	137	219
6	87	70
7	126	117
8	132	125
9	45*	67
10	19*	37

H= 12, K= -3

L	FO	FC
11	103	95
10	253	221
9	96	97
8	90	49
7	133	125
6	115	172
5	35*	74
4	59	33
3	117	121
2	33*	33
1	99	-71

H= 12, K= -4

L	FO	FC
2	8*	-25
3	95	-101
4	8*	10

L	FO	FC
H= 12, K= -4		
5	154	242
6	7*	-7
7	55*	-64
8	128	99
9	88	47
10	81	91
11	175	161
H= 12, K= -5		
11	55*	46
10	81	86
9	129	142
8	86	109
7	8*	20
6	52*	130
5	30*	94
4	40*	-18
3	8*	-29
H= 12, K= -6		
4	8*	38
5	29*	-8
6	8*	-5
7	87	139
8	143	238
9	70	87
10	93	84
H= 12, K= -7		
9	107	154
8	8*	-20
7	16*	-54
6	8*	44
H= 13, K= -6		
8	47*	110
7	80	168
H= 13, K= -5		
5	107	164
6	76	114
7	32*	61
8	116	149
9	91	107
H= 13, K= -4		
10	49*	4
9	76	76
8	47*	85
7	35*	81
6	61*	115
5	25*	66
4	38*	86
H= 13, K= -3		
3	194	185
4	32*	45
5	8*	51
6	49*	73
7	51*	49
8	161	168
9	106	97
10	54*	40
H= 13, K= -2		
10	79	65
9	43*	-26
8	122	108
7	189	142
6	8*	9
5	23*	-7
4	152	117
3	176	126
2	82	96
H= 13, K= -1		
1	116	92
2	82	53
3	65	68
4	45*	36
5	8*	149
6	40*	84
7	8*	23
8	8*	-26
H= 14, K= -1		
8	31*	-49
7	62	-56
6	8*	-40
5	8*	17
4	70	46
H= 14, K= -2		
4	78	-87
5	132	-107
6	25*	-37
7	37*	-58
8	101	-96
H= 14, K= -3		
8	67	-57
7	8*	-33
6	74	-137
5	62*	-81
H= 14, K= -4		
7	58*	-107
H= 0, K= 1		
-10	87	87
-9	37*	52
-8	123	-121
-7	121	124
-6	102	95
-5	128	138
-4	185	188
-3	260	271
-2	466	468
-1	804	811
H= 0, K= 2		
-1	383	-367
-2	58	34
-3	913	951
-4	96	-118
-5	13*	22
-6	391	416
-7	142	142
-8	200	-209
-9	7*	-11
-10	182	199
H= 0, K= 3		
-10	87	-86
-9	65	-69
-8	245	251
-7	78	98
-6	113	102
-5	820	839
-4	793	776
-3	481	-488
-2	205	200
H= 0, K= 4		
-1	175	-176
H= 0, K= 3		
-1	1460	1478
H= 0, K= 4		
-2	109	-105
-3	310	299
-4	608	578
-5	754	769
-6	238	259
-7	89	106
-8	153	149
-9	55	-33
-10	8*	17
-11	8*	20
H= 0, K= 5		
-11	95	89
-10	70	61
-9	65	-36
-8	169	167
-7	177	202
-6	198	-211
-5	125	113
-4	762	789
-3	213	199
-2	115	123
-1	159	148
H= 0, K= 6		
-1	16*	-13
-2	561	569
-3	458	469
-4	70	83
-5	363	362
-6	509	526
-7	40*	46
-8	7*	-28
-9	147	156
-10	46*	46
-11	67	-82
H= 0, K= 7		
-11	8*	-54
-10	15*	-13
-9	127	127
-8	236	231
-7	216	226
-6	249	268
-5	406	411
-4	418	418

L	FO	FC
-3	181	170
-2	294	262
-1	472	483
H=	0, K=	8
-1	214	218
-2	387	373
-3	193	187
-4	299	271
-5	455	448
-6	31*	46
-7	144	-146
-8	138	131
-9	202	194
-10	34*	17
H=	0, K=	9
-10	87	102
-9	42*	26
-8	7*	15
-7	170	155
-6	31*	13
-5	48*	38
-4	441	417
-3	394	386
-2	43*	51
-1	7*	10
H=	0, K=	10
-1	97	86
-2	112	115
-3	147	135
-4	115	110
-5	187	172
-6	188	176
-7	142	148
-8	145	138
-9	164	156
H=	0, K=	11
-7	165	162
-6	182	180
-5	36*	29
-4	24*	-13
-3	144	140
H=	1, K=	11
-3	8*	-9
-4	33*	-38
-5	18*	12
-6	30*	20
H=	1, K=	10
-8	63	-57
-7	65	53
-6	250	237
-5	50*	19
-4	97	-96
-3	8*	25
-2	92	-88
-1	222	-217
H=	1, K=	9
-1	193	-206
-2	100	-93
-3	80	-83
-4	55	-51
-5	62	66
-5	62	66
-6	111	100
-7	32*	49
-8	100	82
-9	146	127
H=	1, K=	8
-10	142	114
-9	158	163
-8	303	312
-7	231	207
-6	105	-111
-5	126	-106
-4	102	77
-3	78	-87
-2	137	-135
-1	71	-71
H=	1, K=	7
-1	31*	-36
-2	58	74
-3	249	-229
-4	59	39
-5	266	252
-6	6*	9
-7	38*	59
-8	331	344
-9	199	185
-10	45*	42
H=	1, K=	6
-10	122	116
-9	47*	39
-8	92	98
-7	218	223
-6	255	274
-5	121	111
-4	232	207
-3	73	-46
-2	96	-111
-1	155	151
H=	1, K=	5
-1	267	-276
-2	195	194
-3	380	379
-4	39	-21
-5	36	43
-6	287	293
-7	218	217
-8	7*	22
-9	112	105
-10	250	267
H=	1, K=	4
-10	225	223
-9	60	59
-8	176	170
-7	403	424
-6	96	97
-5	74	73
-4	167	194
-3	280	253
-2	68	-64
-1	78	79
H=	1, K=	3
-1	242	-254
-2	61	73
-3	33	-33
-4	206	189
-5	685	686
-6	206	212
-7	114	139
-8	157	142
-9	145	148
-10	33*	42
H=	1, K=	2
-10	24*	10
-9	225	230
-8	293	282
-7	226	250
-6	168	169
-5	205	208
-4	411	409
-3	59	62
-2	619	598
-1	579	570
H=	1, K=	1
-1	636	-601
-2	898	907
-3	485	507
-4	135	130
-5	65	66
-6	565	561
-7	438	426
-8	235	250
-9	210	227
-8	7*	250
-7	40*	426
H=	2, K=	1
-6	139	-150
-5	17*	7
-4	29*	14
-3	402	-424
-2	403	-415
-1	150	146
H=	2, K=	2
-1	146	153
-2	167	-179
-3	564	-601
-4	121	-121
-5	205	210
-6	139	-147
-7	238	-221
-8	167	148
-9	45*	45
H=	2, K=	3
-9	37*	-9
-8	289	290
-7	83	69
-6	325	-325
-5	316	-326
-4	282	-266
-3	769	-736
-2	739	-733
-1	133	-140
H=	2, K=	4

L	FO	FC
H=	2, K=	4
-1	634	-634
-3	727	-717
-7	151	-148
-8	50*	-58
-9	64	77
-10	8*	17
H=	2, K=	5
-10	82	82
-9	8*	-8
-8	301	-317
-7	7*	-38
H=	2, K=	6
-6	159	-158
-7	300	-305
-8	78	-79
-9	96	93
-10	11*	-24
H=	2, K=	7
-10	8*	-6
-9	77	-59
-8	71	-65
-7	89	-105
-6	241	-243
-5	260	-228
H=	2, K=	8
-1	197	-190
-2	508	-497
-3	353	-335
-4	7*	-34
-5	80	-74
-6	200	-192
-7	78	-61
-8	28*	33
-9	112	-95
H=	2, K=	9
-9	8*	17
-8	190	-176
-7	109	-96
-6	126	110
-5	212	-194
-4	306	-289
-3	145	-140
-2	209	-196
-1	239	-240
H=	2, K=	10
-1	96	-99
-2	100	-103
-3	164	-148
-4	197	-193
-5	194	-200
-6	167	-144
-7	209	-181
-8	135	-134
H=	2, K=	11
-5	48*	-44
-4	99	-96
H=	3, K=	10
-7	159	-141
-6	72	-76
-5	70	-55
-4	181	-183
-3	33*	-44
-2	136	132
-1	189	183
H=	3, K=	9
-1	88	84
-2	7*	-21
-3	87	87
-4	104	-90
-5	177	-194
-6	98	-94
-7	8*	-22
-8	145	-128
H=	3, K=	8
-9	180	-173
-8	301	-280
-7	131	-137
-6	22*	-17
-5	108	-110
-4	81	-67
-3	192	178
-2	101	110
-1	161	-153
H=	3, K=	7
-1	128	128
-1	128	128
-3	101	-105
-4	240	224
-5	59	-46
-6	309	-314
-7	141	-143
-8	101	-93
-9	198	-188
H=	3, K=	6
-9	102	-76
-8	98	-92
-7	130	-137
-6	7*	-14
-5	179	-161
H=	3, K=	5
-6	209	-227
-7	298	-278
-8	59	-63
-9	88	-91
H=	3, K=	4
-9	153	-151
-8	236	-225
-7	83	-92
-6	165	-173
H=	3, K=	3
-1	252	-284
-2	321	-317
-3	524	-561
-4	356	-353
-5	175	-178
-6	316	-312
-7	80	-72
-8	50*	32
-9	132	-122
H=	3, K=	2
-9	150	-142
-8	98	-96
-7	79	-71
-6	372	-352
-5	308	-332
-4	77	-80
-2	539	-533
-1	229	-268
H=	3, K=	1
-1	340	-325
-2	308	304
-3	113	-144
-4	352	-351
-5	149	-144
-6	350	-359
-7	514	-505
-8	199	-218
H=	4, K=	1
-8	8*	-13
-7	77	-67
-6	29*	-17
-5	188	192
-4	173	184
-3	14*	-19
-2	281	304
-1	348	344
H=	4, K=	2
-1	17*	-21
-2	263	265
-3	75	93
-4	148	177
-5	338	364
-6	40*	-7
-7	59	-56
-8	35*	-33
H=	4, K=	3
-8	188	-182
-7	7*	-12
-6	181	174
-5	18*	5
-4	24*	-15
-3	408	390
-2	601	580
-1	360	363
H=	4, K=	4
-1	425	456
-2	616	608
-3	537	539
-4	151	165
-5	21*	-7
-6	73	74
-7	7*	-25
-8	87	-94
-9	39*	-33
H=	4, K=	5

L	FO	FC
-9	53*	28
-8	64	-49
-7	68	-57
-6	100	111
-5	120	122
-4	127	117
-3	182	186
-2	170	178
-1	317	322
H=	4, K=	6
-1	492	490
-2	163	182
-3	90	100
-4	264	257
-5	168	164
-6	71	-64
-7	7*	17
-8	74	62
-9	8*	-31
H=	4, K=	7
-8	34*	40
-7	105	89
-6	170	154
-5	80	96
-4	83	93
-3	249	249
-2	367	357
-1	366	356
H=	4, K=	8
-1	177	184
-2	147	150
-3	243	218
-4	7*	39
-5	23*	-34
-6	187	191
-7	114	109
-8	8*	-30
H=	4, K=	9
-7	8*	12
-6	194	199
-5	125	124
-4	46*	52
-3	98	116
-2	154	158
-1	85	97

L	FO	FC
H=	4, K=	10
-1	148	148
-4	237	221
-5	113	126
-6	110	88
H=	5, K=	10
-4	167	171
-3	37*	36
-2	26*	-3
H=	5, K=	9
-1	62	-66
-2	170	156
-3	161	145
-4	8*	-9
-5	8*	51
-6	111	106
H=	5, K=	8
-7	106	105
-6	148	150
-5	162	144
-4	7*	-7
-3	7*	-36
-2	72	40
-1	7*	33
H=	5, K=	7
-1	70	-88
-2	121	-115
-3	183	170
-4	194	181
-5	16*	-12
-6	130	121
-7	279	280
-8	167	163
H=	5, K=	6
-8	172	182
-7	103	87
-6	37*	20
-5	195	207
-4	276	291
-3	139	148
-2	67	77
-1	149	141
H=	5, K=	5

L	FO	FC
-1	134	130
-2	5*	42
-3	302	302
-4	451	437
-5	220	213
-6	24*	24
-7	162	148
-8	141	143
H=	5, K=	4
-8	8*	-11
-7	47*	66
-6	355	357
-5	305	299
-4	198	212
-3	347	329
-2	95	95
-1	93	-90
H=	5, K=	3
-1	27*	18
-2	251	297
-3	256	276
-4	245	241
-5	13*	29
-6	99	108
-7	158	156
-8	89	87
H=	5, K=	2
-8	115	120
-7	120	117
-6	229	228
-5	7*	38
-4	118	149
-3	282	294
-2	310	298
-1	259	255
H=	5, K=	1
-1	338	393
-2	71	69
-3	58	66
-4	571	577
-5	551	522
-6	116	129
-7	22*	51
H=	6, K=	1

L	FO	FC
-7	89	81
-6	85	93
-5	116	102
-4	143	-127
-3	82	-62
-3	87	-62
-2	54	-54
-1	324	-293
H=	6, K=	2
-1	5*	-15
-2	291	-270
-3	133	-124
-4	60	-100
-5	155	-154
-6	27*	22
-7	235	234
H=	6, K=	3
-7	39*	18
-6	138	131
-5	20*	-12
-4	252	-247
-3	73	-61
-2	198	-186
-1	239	-230
H=	6, K=	4
-1	243	-229
-2	273	-276
-3	154	-138
-4	73	-92
-5	87	-107
-6	45*	52
-7	8*	-11
H=	6, K=	5
-7	8*	-27
-6	36*	41
-5	78	76
-4	108	-130
-3	317	-334
-2	97	-99
-1	35*	-32
H=	6, K=	6
-1	361	-388
-2	223	-239
-3	7*	-24
-4	7*	-6

L	FO	FC
H=	6, K=	6
-5	111	-107
-6	49*	52
-7	114	121
H=	6, K=	7
-7	38*	15
-6	8*	-37
-5	47*	-50
-4	29*	-23
-3	66	-87
-2	262	-285
-1	314	-336
H=	6, K=	8
-1	239	-240
-2	65	-86
-3	7*	-10
-4	187	-180
-5	131	-128
-6	33*	18
H=	6, K=	9
-5	59	-50
-4	39*	-42
-3	169	-189
-2	124	-118
-1	22*	94
H=	7, K=	9
-1	95	-87
-2	96	-96
-3	134	-120
H=	7, K=	8
-5	80	-71
-4	62	-72
-3	103	-100
-2	91	-97
-1	141	-136
H=	7, K=	7
-1	179	-179
-2	7*	17
-3	29*	-54
-4	226	-222
-5	166	-152
-6	71	-66
H=	7, K=	6
-6	158	-153
-5	96	-92
-4	88	-93
-3	151	-152
-2	151	-140
-1	44*	-44
H=	7, K=	5
-1	34*	53
-2	208	-229
-3	257	-278
-4	100	-111
-5	90	-82
-6	214	-205
H=	7, K=	4
-6	250	-254
-5	35*	-73
-4	114	-117
-3	364	-367
-2	263	-309
-1	48	34
H=	7, K=	3
-1	245	-229
-2	6*	-292
-3	90	-95
-4	125	-108
-5	185	-190
-6	76	-83
H=	7, K=	2
-6	8*	-43
-5	163	-157
-4	110	-98
-3	126	-110
-2	6*	-317
-1	460	-445
H=	7, K=	1
-1	364	-348
-2	479	-455
-3	239	-212
-4	200	-201
-5	215	-214
-6	59	-28
H=	8, K=	1
-5	84	-88
-4	50*	-50
-3	20*	2
-2	235	232
-1	189	194
H=	8, K=	2
-1	64	-81
-2	240	238
-3	266	256
-4	152	-136
-5	197	-184
H=	8, K=	3
-5	8*	2
-4	40*	-43
-3	66	-66
-2	54	45
-1	94	104
H=	8, K=	4
-1	120	196
-2	105	115
-3	41*	68
-4	7*	-19
-5	63	-45
-6	26*	-5
H=	8, K=	5
-5	81	-85
-4	150	150
-3	54*	80
-2	7*	46
-1	176	238

L	FO	FC
H=	8, K=	6
-1	47*	49
-2	132	148
-3	79	82
-4	84	-76
-5	38*	-49
H=	8, K=	7
-5	8*	6
-4	33*	9
-3	52*	49
-2	66	63
-1	123	156
H=	8, K=	8
-1	194	201
-2	184	185
-3	43*	-34
-4	57*	-16
H=	9, K=	8
-1	99	131
H=	9, K=	7
-1	102	96
-2	126	118
-3	29*	24
H=	9, K=	6
-4	95	117
-3	214	221
-2	54*	47
-1	85	-104
H=	9, K=	5
-1	18*	46
-2	202	245
-3	155	151
-4	78	86
H=	9, K=	4
-5	146	153
-4	212	198
-3	68	70
-2	137	178
-1	254	324
H=	9, K=	3
-1	265	275
-2	258	248
-3	41*	-23
-4	58*	62
-5	156	154
H=	9, K=	2
-4	124	128
-3	63	54
-2	82	73
-1	340	352
H=	9, K=	1
-1	172	171
-2	179	161
-3	307	278
-4	86	85
H=	10, K=	1
-3	127	132
-2	94	-80
-1	342	-348
H=	10, K=	2
-1	117	-131
-2	8*	-22
-3	8*	-4
H=	10, K=	3
-3	8*	35
-2	34*	-52
-1	69	82
H=	10, K=	4
-1	7*	7
-2	27*	-9
-3	61	22
H=	10, K=	5
-3	132	117
-2	35*	-6
-1	161	-187
H=	10, K=	6
-1	65	-93
-2	52*	56
H=	10, K=	7
-1	102	-112
H=	11, K=	5
-1	45*	-114
-2	66	-97
H=	11, K=	4
-2	81	-82
-1	192	-238
H=	11, K=	3
-1	8*	-34
-2	97	-85
H=	11, K=	2
-2	138	-126
-1	117	-120
H=	11, K=	1
-1	132	-136
-2	8*	-23
H=	12, K=	1
-1	8*	12
H=	12, K=	2
-1	101	87

Table 2.3

Summary of the Final Refinements for the Ni(II) Hexaazamacrocycles.

	(L0)$(NCS)_2$	(L0)(NO_2)	(L2)(H_2O)	(L3)(NO_2)	(L4)
Final R	0.060	0.041	0.079	0.071	0.066
# variables	249	353	370	389	314
# observations	2257	2539	3254	2347	2517
Largest peaks in final difference map (e^{-} $Å^{-3}$)	0.6±0.1	0.4±0.1	0.4±0.1	0.4±0.1	0.5±0.1
located near:	Ni	Ni/ClO_4	Ni	ClO_4	Ni

Chapter 3

The Ni(II)-Dihydrazone/2,3-Butanedione Condensation: Discussion of the Structures

3i. Outline

The structures of the complexes comprising this investigation are discussed individually in sections 3ii through 3vi, with a final section of discussion (3vii), where an interpretation of the crystallographic results in terms of the sequence of steps involved in the condensation reaction is offered.

A listing of the bond lengths and angles within the coordination spheres is given in table 3.1. Tables 3.2 (bond lengths) and 3.3 (bond angles) give the parameters in the remainder of the ligands.

Table 3.1

Bond Lengths and Angles within the Coordination Spheres of the Ni(II) Hexaazamacrocycles

Bond Lengths (Å)	$Ni(L0)(NCS)_2$	$Ni(L0)NC_2^+$	$Ni(L2)H_2O^{2+}$	$Ni(L3)NO_2^+$	$Ni(L4)^{2+}$
Ni-N1	2.150(7)	2.081(3)	2.053(6)	2.095(6)	1.904(5)
N2	2.131(7)	2.097(4)	2.104(6)	2.115(6)	1.904(5)
N3	2.134(7)	2.072(4)	2.070(6)	2.051(6)	1.908(5)
N4	2.138(7)	2.074(4)	2.085(6)	2.100(6)	1.911(5)
C1			2.154(4)		
C2			2.135(5)		
O_n1		2.132(4)		2.144(6)	
O_n2		2.171(4)		2.183(6)	
N(S1)	2.116(8)				
N(S2)	2.077(8)				
Bond Angles (deg)					
N1NiN2	90.7(3)	92.5(1)	92.7(2)	88.4(2)	90.8(2)
N1NiN3	164.7(3)	97.0(2)	98.9(2)	99.7(2)	164.9(2)
N1NiN4	100.5(3)	94.8(2)	100.2(2)	94.9(2)	94.2(2)
N1NiC1			74.9(2)		
N1NiC2			163.7(2)		
$N1NiO_n1$		104.0(2)		102.5(3)	
$N1NiO_n2$		162.2(2)		160.2(3)	
N1NiN(S1)	85.0(3)				
N1NiN(S2)	92.6(3)				
N2NiN3	81.9(3)	83.0(1)	83.9(2)	83.5(2)	88.1(2)
N2NiN4	165.2(3)	158.6(1)	167.0(2)	175.2(2)	162.8(3)
N2NiC1			107.1(2)		
N2NiC2			83.7(2)		
$N2NiO_n1$		91.8(1)		94.1(2)	
$N2NiO_n2$		86.3(1)		87.1(2)	
N2NiN(S1)	99.8(3)				
N2NiN(S2)	94.2(3)				

Table 3.1(continued)

Bond Angles	$Ni(L0)(NCS)_2$	$Ni(L0)NO_2^+$	$Ni(L2)H_2O^{2+}$	$Ni(L3)NO_2^+$	$Ni(L4)^{2+}$
N3NiN4	89.3(3)	93.4(2)	92.8(2)	92.5(2)	91.2(2)
N3NiO1			167.3(2)		
N3NiO2			96.5(2)		
$N3NiO_n1$		158.6(2)		157.7(2)	
$N3NiO_n2$		100.4(2)		99.0(3)	
N3NiN(S1)	83.0(3)				
N3NiN(S2)	99.9(3)				
N4NiO1			77.7(2)		
N4NiO2			84.2(2)		
$N4NiO_n1$		89.0(2)		88.6(2)	
$N4NiO_n2$		87.5(2)		91.0(3)	
N4NiN(S1)	91.0(3)				
N4NiN(S2)	85.6(3)				
O1NiO2			91.0(2)		
O_n1NiO_n2		58.4(2)		58.8(3)	
N(S1)NiN(S2)	175.4(3)				

Table 3.2

Bond Lengths in the Ligands of the Ni(II) Hexaazamacrocycles

Bond Length (A)	$Ni(L0)(NCS)_2$	$Ni(L0)NO_2^+$	$Ni(L2)H_2O^{2+}$	$Ni(L3)NO_2^+$	$Ni(L4)^{2+}$
N1 - N5	1.42(1)	1.418(5)	1.426(8)	1.40(1)	1.437(6)
N4 - N6	1.39(1)	1.372(6)	1.397(7)	1.42(1)	1.438(7)
N5 - C1			1.266(9)	1.25(1)	1.248(8)
N6 - C3			1.462(8)		1.278(8)
C1 - C2			1.48(1)	1.46(1)	1.476(9)
C1 - C3			1.55(1)	1.50(2)	1.50(1)
C3 - C4			1.52(1)	1.51(2)	1.51(1)
C3 - O1		1.07(2)*	1.41(1)		
N1 - C5	1.27(1)	1.289(6)	1.274(8)	1.27(1)	1.272(7)
C5 - C6	1.51(1)	1.489(7)	1.55(1)	1.49(1)	1.49(1)
C5 - C7	1.51(1)	1.501(6)	1.49(1)	1.50(1)	1.50(1)
C7 - C8	1.55(1)	1.519(7)	1.54(1)	1.53(1)	1.51(1)
C8 - C9	1.51(1)	1.501(6)	1.50(1)	1.53(1)	1.54(1)
C8 - C10	1.54(1)	1.532(7)	1.53(1)	1.52(1)	1.51(1)
N2 - C8	1.50(1)	1.504(6)	1.49(1)	1.48(1)	1.50(1)
N2 - C11	1.50(1)	1.484(6)	1.50(1)	1.46(1)	1.49(1)
C11 - C12	1.47(1)	1.515(7)	1.50(1)	1.52(1)	1.48(1)
N3 - C12	1.49(1)	1.479(6)	1.43(1)	1.48(1)	1.49(1)
N3 - C13	1.50(1)	1.58(2)	1.50(1)	1.51(1)	1.52(1)
N3 - C13'		1.48(3)			
C13 - C14	1.51(1)	1.39(4)	1.52(1)	1.55(1)	1.53(1)
C13'- C14'		1.60(4)			
C13 - C15	1.53(1)	1.59(3)	1.53(1)	1.49(1)	1.53(1)
C13'- C15'		1.49(3)			
C13 - C16	1.55(1)	1.60(3)	1.50(1)	1.56(1)	1.53(1)
C13'- C16'		1.48(3)			
C16 - C17	1.50(1)	1.46(3)	1.51(1)	1.49(1)	1.47(1)
C16'- C17'		1.51(3)			
C17 - C18	1.52(1)	1.48(4)	1.48(1)	1.51(1)	1.49(1)
C17'- C18'		1.47(4)			
N4 - C17	1.25(1)	1.33(2)	1.269(8)	1.29(1)	1.289(7)
N4 - C17'		1.24(2)			
N(S1)- C(S1)	1.16(1)				
N(S2)- C(S2)	1.14(1)				
C(S1)- S1	1.61(1)				
C(S2)- S2	1.64(1)				
O_n1 - N_n		1.276(6)		1.31(1)	
O_n2 - N_n		1.246(6)		1.25(1)	
O_n1....O_n2		2.096(5)		2.13(1)	

*1.22(2) when corrected for thermal motion, O1 riding on C3

Table 3.3

Bond Angles in the Ligands of the Ni(II) Hexaazamacrocycles

Bond Angle (deg)	$Ni(L0)(NCS)_2$	$Ni(L0)NO_2^+$	$Ni(L2)H_2O^{2+}$	$Ni(L3)NO_2^+$	$Ni(L4)^{2+}$
Ni N1 N5	117.6(5)	115.2(3)	118.3(4)	112.6(4)	112.9(4)
Ni N1 C5	126.2(6)	127.3(3)	127.1(5)	130.1(5)	130.1(5)
Ni N2 C8	122.1(5)	116.8(3)	118.4(4)	119.6(5)	110.4(4)
Ni N2 C11	106.8(5)	107.6(3)	106.3(4)	106.7(4)	107.9(4)
Ni N3 C12	107.4(5)	102.3(3)	103.9(4)	105.0(4)	108.0(4)
Ni N3 C13	121.6(5)	123(1)/ 112(1)	117.7(5)	119.2(4)	109.9(3)
Ni N4 C17	126.9(6)	124.6(6)/ 125.0(7)	125.8(5)	126.1(5)	128.8(4)
Ni N4 N6	113.2(5)	116.7(3)	114.8(4)	116.0(5)	113.8(4)
Ni O1 C3			106.2(2)		
N5 N1 C5	115.0(7)	116.4(4)	113.5(6)	115.9(6)	115.5(5)
N1 N5 C1			119.9(6)	116.9(7)	116.0(6)
N5 C1 C2			114.7(7)	127.7(8)	121.7(6)
N5 C1 C3			128.1(7)	113.3(9)	121.3(7)
C2 C1 C3			117.1(7)	119.0(9)	117.0(6)
C1 C3 C4			113.8(6)	120(1)	117.6(6)
C1 C3 O1			110.2(6)	118(2)	
O1 C3 C4			110.5(6)	122(2)	
N6 C3 O1			111.0(5)		
N6 C3 C4			107.9(5)		118.3(7)
N6 C3 C1			103.3(6)		124.0(5)
N4 N6 C3			110.4(5)		114.2(5)
N1 C5 C6	122.9(8)	120.2(4)	122.7(7)	122.4(7)	122.6(6)
N1 C5 C7	118.9(8)	122.6(4)	121.9(7)	123.8(7)	120.9(6)
C6 C5 C7	118.3(8)	117.1(4)	115.3(7)	113.8(7)	116.4(6)
C5 C7 C8	116.7(7)	120.5(4)	116.8(6)	121.0(7)	120.1(5)
C7 C8 C9	112.7(8)	111.9(4)	111.6(6)	108.2(7)	110.0(6)
C7 C8 C10	108.3(7)	107.5(4)	109.2(6)	109.3(8)	108.8(6)
C9 C8 C10	110.6(8)	108.6(4)	108.9(2)	107.7(7)	109.3(6)
N2 C8 C7	103.9(7)	110.8(3)	109.1(6)	111.8(4)	108.0(6)
N2 C8 C9	111.2(7)	107.8(4)	106.7(6)	110.9(5)	108.4(5)
N2 C8 C10	109.9(8)	110.2(4)	111.3(6)	107.9(5)	111.5(6)
C8 N2 C11	114.6(7)	113.6(4)	112.9(5)	114.1(6)	115.5(5)
N2 C11 C12	108.3(8)	111.2(4)	112.4(6)	116.7(4)	106.9(5)
N3 C12 C11	109.4(7)	106.6(4)	110.1(7)	105.8(4)	106.1(5)
C12 N3 C13	118.4(7)	107(1)/ 123(1)	119.4(6)	113.7(6)	115.8(5)
" " C13'					
N3 C13 C14	109.7(7)	114(2)/ 100(2)	110.9(6)	111.2(5)	109.4(5)
" C13' C14'					
N3 C13 C15	110.7(7)	107(2)/ 110(2)	105.6(6)	109.3(5)	110.8(5)
" C13' C15'					
N3 C13 C16	106.4(7)	98(1)/ 116(2)	112.6(6)	105.3(4)	107.0(5)
" C13' C16'					
C14 C13 C15	110.3(8)	116(2)/ 105(2)	108.0(7)	11.9(7)	109.8(6)
C14' C13' C15'					

Table 3.3 (continued)

Bond Angle	$Ni(L0)(NCS)_2$	$Ni(L0)NO_2^+$	$Ni(L2)H_2O^{2+}$	$Ni(L3)NO_2^+$	$Ni(L4)^{2+}$
C15 C13 C16 C15'C13'C16'	107.9(7)	104(2)/ 118(3)	110.5(7)	106.5(6)	108.7(5)
C13 C16 C17 C13'C16'C17'	117.4(7)	118(2)/ 110(2)	120.0(6)	119.6(7)	120.4(5)
C16 C17 C18 C16'C17'C18'	115.8(8)	118(2) 113(2)	118.4(7)	117.1(7)	115.9(5)
N4 C17 C16 N4 C17'C16'	123.8(8)	119(1)/ 118(1)	118.3(7)	118.9(5)	121.9(6)
N4 C17 C18 N4 C17'C18'	120.3(9)	123(1)/ 126(2)	123.3(7)	125.1(5)	127.2(6)
N6 N4 C17 N6 N4 C17'	119.7(8)	113.2(7) 116.9(8)	116.7(6)	117.0(6)	114.9(5)
NiN(S1)C(S1)	161.9(7)				
NiN(S2)C(S2)	166.6(8)				
N(S1)C(S1)S1	179(1)				
N(S2)C(S2)S2	178(1)				
Ni O_n1 N_n		94.1(3)		96.6(5)	
Ni O_n2 N_n		95.1(3)		92.9(5)	
O_n1 N_n O_n2		112.5(4)		111.7(7)	

Table 3.4

Bond Lengths in the Perchlorate Anions of the Ni(II) Hexaazamacrocycles (Å)

	$Ni(L0)(NCS)_2$	$Ni(L0)NO_2^+$	$Ni(L2)H_2O^{2+}$	$Ni(L3)NO_2^+$	$Ni(L4)^{2+}$
Cl1 - O11		1.39(1)	1.37(2)	1.39(2)	1.400(6)
O11'			1.40(2)		
O12		1.39(1)	1.38(1)	1.36(2)	1.379(7)
O13		1.36(1)	1.37(1)	1.45(2)	1.373(7)
O14		1.38(1)	1.33(1)	1.35(2)	1.414(6)
Cl2 - O21			1.43(1)	1.36(2)	1.441(6)
O22			1.40(1)	1.33(2)	1.42(2)
O22'					1.43(2)
O23			1.40(1)	1.42(2)	1.45(2)
O23'					1.37(2)
O24			1.37(1)	1.35(2)	1.47(1)
O24'					1.40(2)

Cl1 and Cl2 in this instance refer to the alternate positions of a disordered anion

3ii. $Ni(LO)(NCS)_2 \cdot H_2O$

A perspective view of the metal complex is shown in figure 3.1. In the unit cell, the nickel atom lies close to the c axis, with the trans SCN-Ni-NCS system arranged approximately along the c axis. These molecules are well separated from each other, affording no unusually short contacts, but n-glide-related molecules are connected via hydrogen bonding with the water molecule of crystallization. Specifically, hydrogen atoms on the water interact with N5 on one molecule (O_w.....N5 = 2.95A), and S2 on the symmetry related molecule (O_w.....S2 = 3.06A), which also provides the remaining close contacts with O_w (O_w.....H(N2) = 2.49A, and O_w.....H92 = 2.30A); the four interactions forming a roughly tetrahedral array about O_w.

As indicated in the introduction to this work (section 1vi), the original intention of studying this crystalline sample was to determine the identity of ligand L1, which was identified as the first product of the reaction of the complex of the dihydrazone L0 with 2,3 butanedione. The reaction of $Ni(L1)(ClO_4)_2$ (a poorly crystalline product) with sodium thiocyanate (section Aii, Appendix) clearly results in the elimination and/or hydrolysis of the diketone to give a derivative of the starting L0. This result raises several questions, the most immediate of which concerns the evidence upon which the assignment of the ligand in the NCS derivative as L1 was made. (This information is given in the Appendix.) In particular, found and calculated analytical data for

$Ni(L0)(NCS)_2 \cdot H_2O$ (section Aii) show a clear discrepancy between, for instance, the % nickel for $Ni(L0)(NCS)_2 \cdot H_2O$ and "$Ni(L1)(NCS)_2 \cdot H_2O$" formulations, and these figures should have been sufficient to suggest the correct assignment of L0 for the tetradentate ligand. Furthermore, the absence of a band in the i.r. (figure A.3) attributable to $\nu(c=o)$, as observed in $Ni(L1)^{2+}$ at 1685 cm^{-1} (figure A.1) also indicates some fundamental change in ligand structure.

Despite the incorrect ligand assignment, the structure of $Ni(L0)(NCS)_2$ would provide useful comparative data for the other products in this study, and it was considered therefore to be profitable to complete the determination and analysis of the data.

The trans configuration of the NCS ligands appears to warrant some rationale, in light of the fact that the other octahedral complexes in this series are cis. With one eye on the results of these other complexes, one can see that the trans arrangement is adopted because there is no particular interaction available to stabilize a cis arrangement (e.g., bidentate cis donors as in NO_2^-, or extensive hydrogen bonding as in $Ni(L2)H_2O^{2+}$). Presumably there is a small but significant destabilization for the N_4 ligand in going from a planar to a non-planar configuration as a result of some bond angle or torsional source of strain. (This is, in fact, borne out by the conformational analyses on the cis octahedral complexes, sections 3iii through 3v.)

Bond lengths and angles within the coordination sphere of the Ni(II) ion (table 3.1) show the geometry to be very nearly regular octahedral, save for the N1NiN4 angle (no chelate ring) which is 100.5(3) deg, and the N2NiN3 angle (five-membered chelate ring) which is 81.9(3) deg. The six-membered rings subtend right angles (within error) at the metal (N1NiN2 = 90.7(3) deg and N3NiN4 = 89.3(3) deg). Some bond angle strain in the six-membered rings is apparent from the rather large angles seen at the central methylene groups (116.7(7) deg at C7, and 117.4(7) deg at C16). Similar effects have been seen in related complexes, with distortions as high as 120-121 deg.[37]

Further distortion from the equatorial sites in a regular octahedral geometry occur as a result of a small tetrahedral distortion of the L0 donors: the angle of twist (the angle between the planes defined by NiN1N2 and N3NiN4) is 16.7 deg. The extent of this distortion is shown in figure 3.2, where the displacements of the L0 atoms from the best least-squares plane calculated for the NiN1N2N3N4 atoms are sketched. Equations of the planes used in this discussion are given in table 3.5. The tetrahedral distortion (as measured by the angle between the NiN1N2 and NiN3N4 planes of 16.7 deg) is reflected in the angles subtended at the metal ion by equatorially and axially bonded donors (table 3.1). A consistent lack of planarity of the four nitrogen donors about a Ni(II) ion has been noted previously,[23] and interpreted as being a mode of imparting some flexibility to the tetradentate

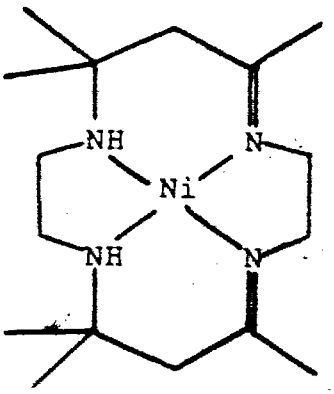
ligand, while costing practically nothing in terms of Ni-N bond energy, as suggested by the ready equilibrium between some planar and tetrahedral complexes.[23]

Within the configuration of L0 about the metal atom, the conformations of the six-membered chelate rings approximate the half-chair conformation of cyclohexene,[38] and that of the five-membered ring approximates a cyclopentane[38] half-chair. Torsion angles about the bonds within each chelate are shown in figure 3.3. An alternative schematic analysis of these chelates is given in figure 3.4, where displacements from the planes defined by the donor atoms of each chelate and the metal ion are plotted.

The asymmetric nitrogen atoms N2 and N3 have the same chirality, and, thus, by virtue of the centrosymmetric space group, the crystal contains a racemic mixture of RR and SS enantiomers. This continues a trend for cis bonded chiral N-centres, which have yet to be found in an RS, meso arrangement. One rationale for this was based on possible methyl-methyl steric interactions (those bonded to C8 and C12 in this instance[39]), but this was subsequently stated[37] to be unlikely on the basis that a scale model shows small changes in conformation would easily separate the methyl groups to compatible distances. An alternative argument was put forward,[37] and is reiterated here, in terms of the ligand conformation. If the molecule is considered in two halves, divided by a line bisecting C11 and C12 and passing through the metal ion, the optimal conformations of these halves must

be identical since they both correspond to a minimum in strain energy. If the two halves are related by a diad axis, i.e., an N-RR or -SS arrangement, there is no symmetry restriction on the torsion angle about C11-C12, and the strain-free angle can be adopted. If they are related by a mirror plane, however (to given the N-meso, RS configuration), the C11-C12 torsion angle is restricted to 0 deg, corresponding to an extra 25-30 kJ mole^{-1} in strain energy.

The Ni-N bond lengths to the tetradentate ligands are equal within error, and their mean (2.136(9)Å) lies within the range of bond lengths previously observed for such ligands.[23] However, there is no suggestion of Ni-N(imine) bond lengths being shorter than Ni-N(amine) bond lengths, as recorded for XVIII.[37]



XVIII

The C=N distances of 1.27(1)A(C5=N1) and 1.25(1)A(C17=N4) are equal within error to the standard C=N distance of 1.27A and imply no delocalization of electrons around the ring systems. The Ni-NCS distances of 2.116(8)Å and 2.077(8)A are somewhat shorter than those of the Ni-N distances within the tetradentate ligand.

Previous structural studies of Ni(II)-bonded NCS^- ligands[40] show a striking consistency in dimensions, e.g., for trans-$Ni(NCS)_2(tu)$ (tu = thiourea or substituted thiourea) complexes, N=C = 1.16(2) - 1.17(2)Å, C-S = 1.64(1)Å, and the NCS angle = 178(1) - 179(1) deg. The only exceptional dimensions are the angle about the nitrogen atom (NiN(S1)C(S1) = 161.9(7) deg and NiN(S2)C(S2) = 166.8(8) deg), which may be the result of packing environments, and presumably reflects an electronic structure which can be described in resonance terms as some hybrid of

$$M{\leftarrow}N{\equiv}C{-}\bar{S} \longleftrightarrow \overset{M}{\bar{N}}{=}C{=}S$$

The variation in the valence angle at the thiocyanate nitrogen has been noted previously,[40] varying from 111 deg in tetrahedral $K_2Co(NCS)_4$, through 160 deg in binuclear $Cu(py)_2(NCS)_2$ to 180 deg in $Ni(NH_3)_4(NCS)_2$.

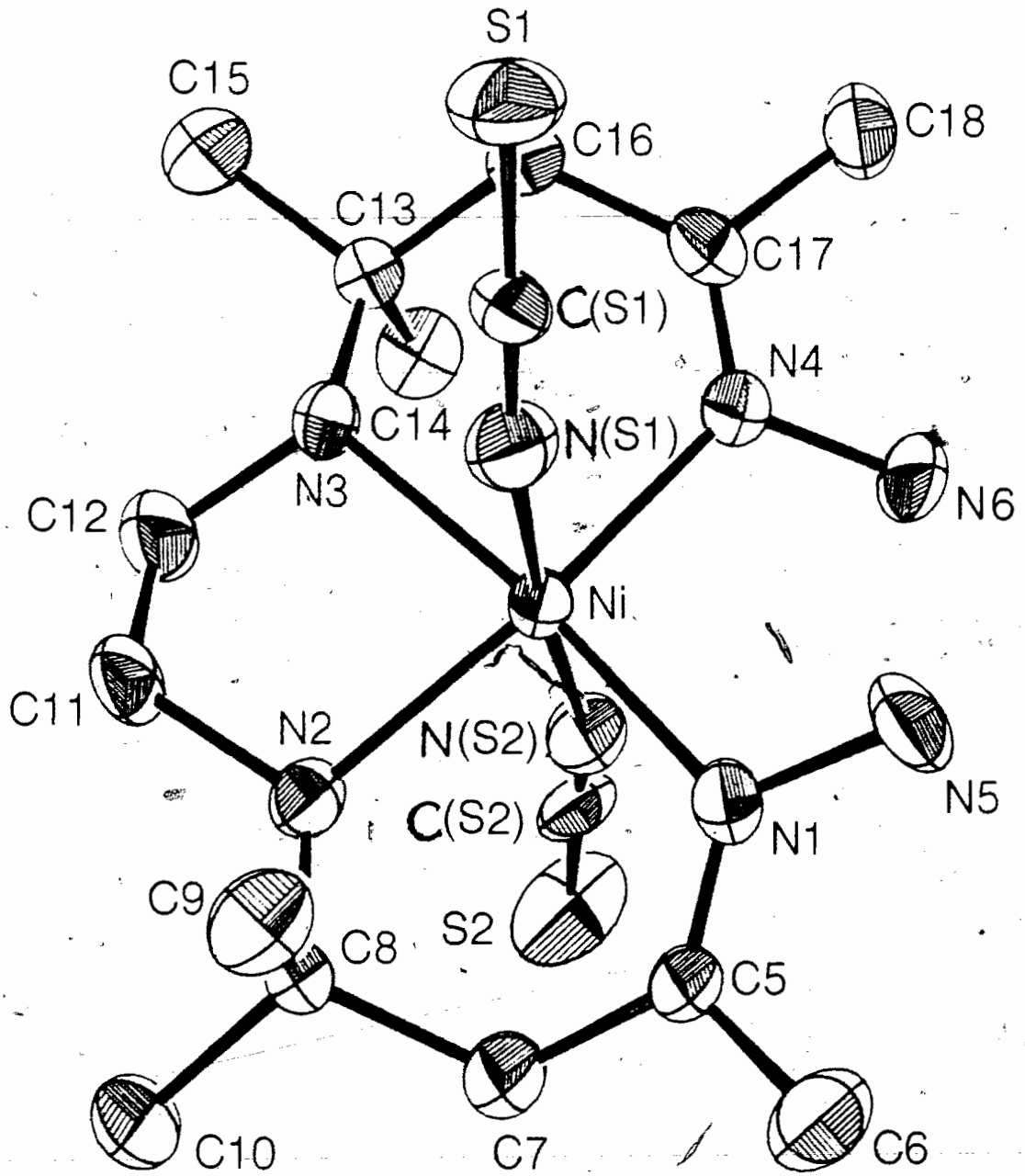
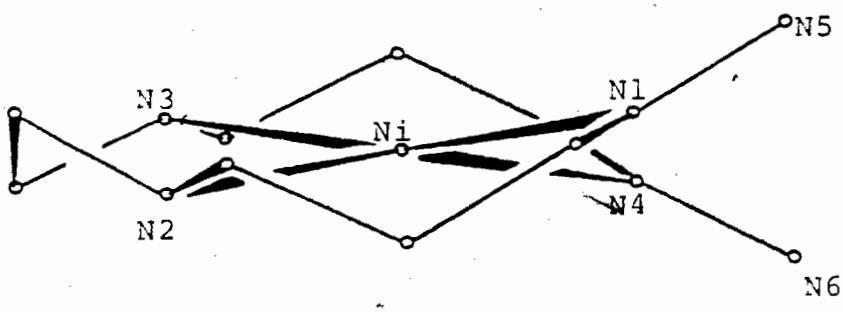


Figure 3.1

Perspective View of $Ni(L0)(NCS)_2$

Figure 3.2,

Displacements of Atoms from the 'NiN1N2N3N4' Plane in $Ni(L0)(NCS)_2$



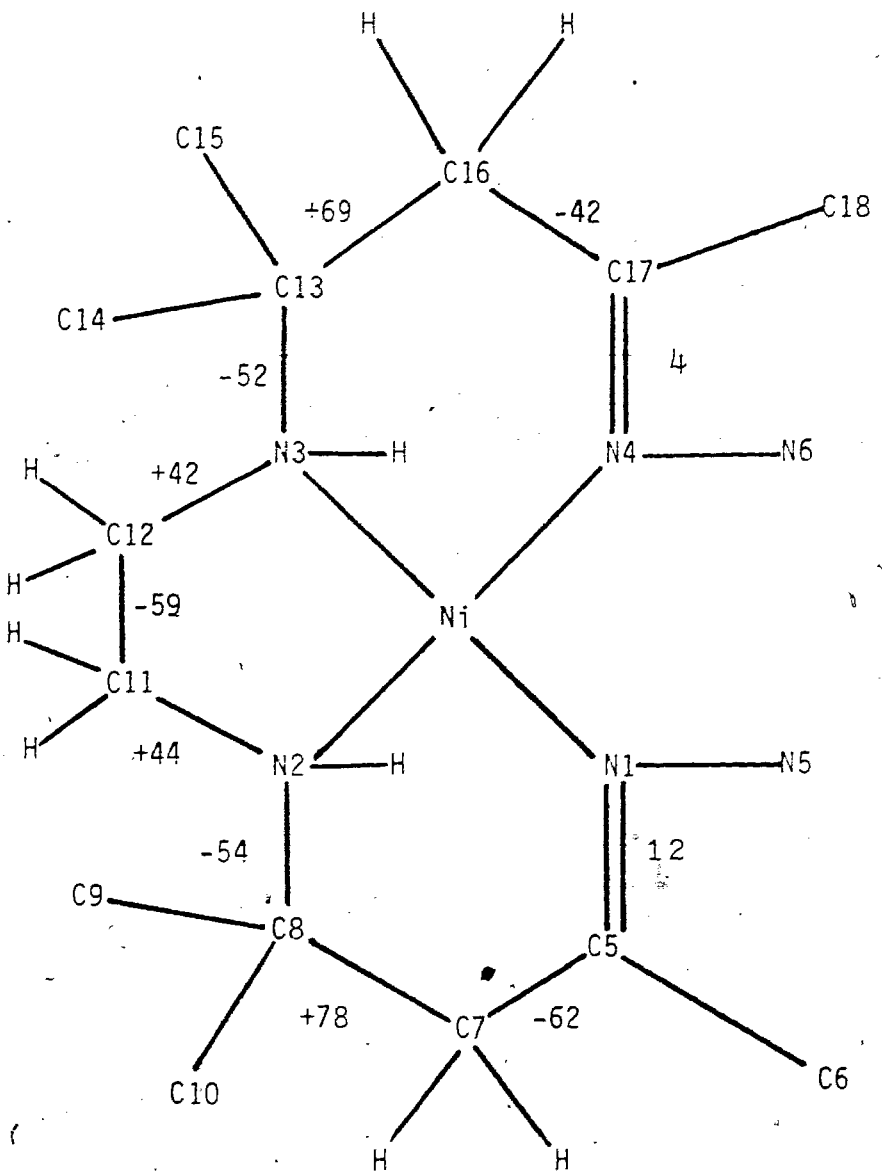


Figure 3.3

Torsion Angles in $Ni(L0)(NCS)_2$ (deg)

Table 3.5

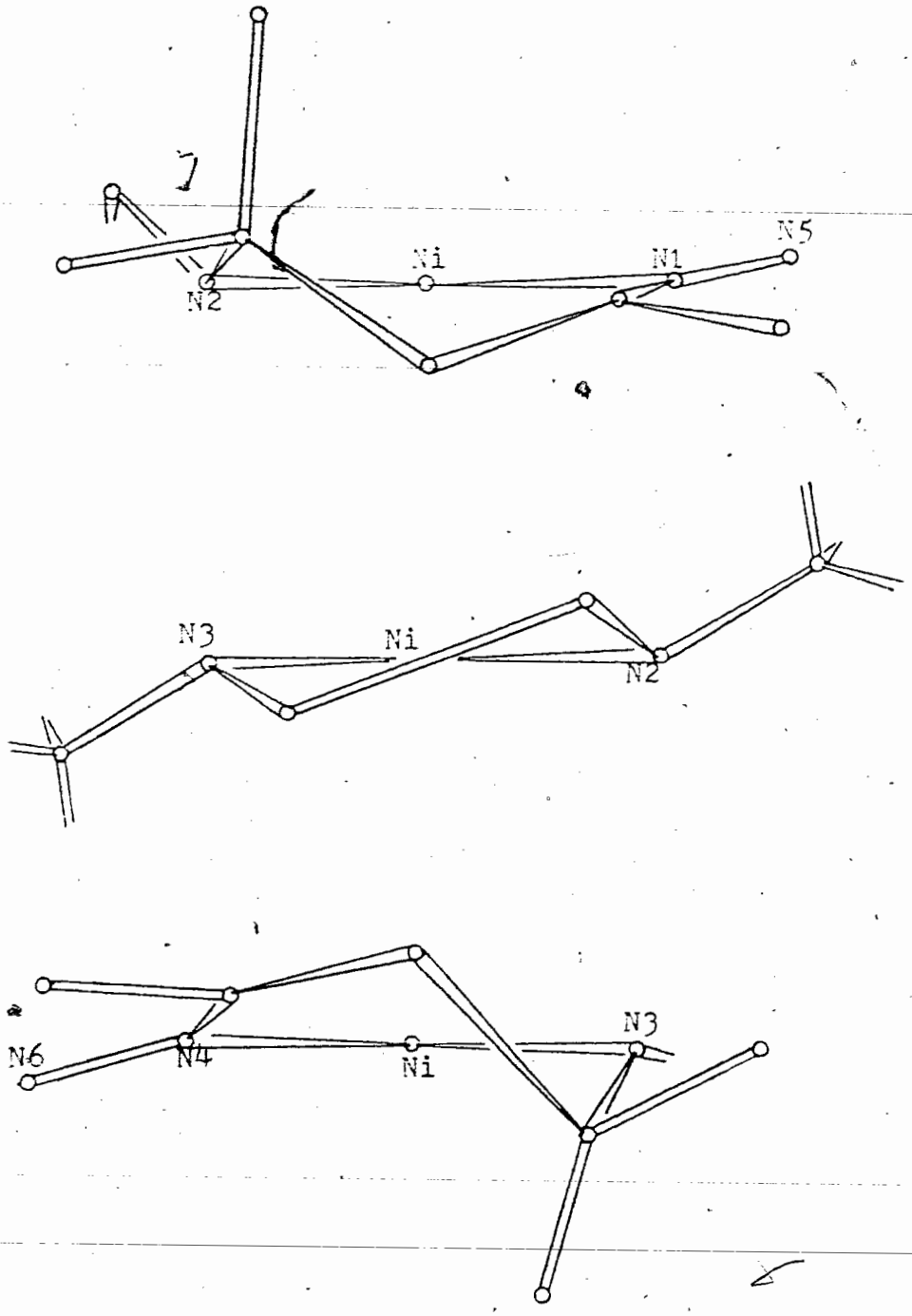
Least Squares Mean Planes Calculated for $Ni(LO)(NCS)_2 \cdot H_2O$

Atoms in Plane	Coefficients of equation of plane†				Displacements (Å)
	X	Y	Z	p	
Ni, N1, N2, N3, N4 $\chi^2 = 4376$	-5.85	-.235	-.776	-2.804	Ni(-.01), N1(.20), N2(-.023), N3(.24), N4(-.19), N5(.78), N6 (-.66), C5(.08), C7(-.51), C8(.14), C11(.31), C12 (-.19), C13(-.10), C16 (.65), C17(.16).
Ni, N1, N2	-.544	-.369	-.754	-2.723	C5(-.1), C6(.24), C7(-.56), C8(.33), C9(1.79), C10(.10), C11(-.72), N5(.40)
Ni, N2, N3	-.453	-.187	-.872	-3.313	C8(.61), C11(.40), C12(-.33), C12(-.58)
Ni, N3, N4	-.617	-.089	-.782	-2.800	C12(-.61), C13(-.33), C14(-1.78), C15(0.0), C16(.60), C17(.31), C18(.36), N6(-.26).

† The orthogonal system of axes (X, Y, Z) has X along the $\underline{a}$ axis, Y in the $\underline{a}\,\underline{b}$ plane, and Z along the c^* axis. χ^2 for a plane $\underline{\ell}X + \underline{m}Y + \underline{n}Z - p = 0$ for the N atoms is given by $\Sigma_{i=1}^{i=N}(Pi^2/\sigma^2(Pi))$, where $\sigma^2(Pi) = \underline{\ell}^2\sigma^2(Xi) + \underline{m}^2\sigma^2(Yi) + \underline{n}^2\sigma^2(Zi)$, and Pi is the distance of atom i from the plane.

Figure 3.4

Projections of Chelate Ring Conformations in $Ni(LO)(NCS)_2$



3iii. $Ni(L0)NO_2(ClO_4)$

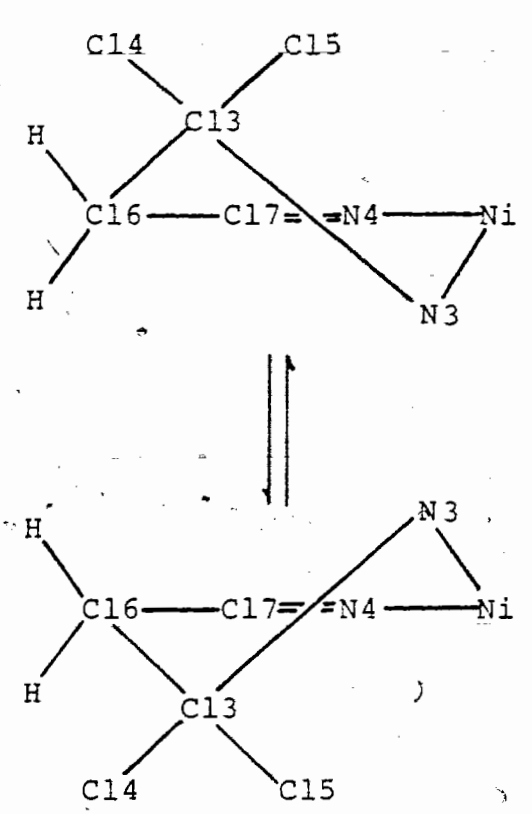
This structure was undertaken after that of $Ni(L0)(NCS)_2$ in a reattempt to determine the identity of L1. Again, however, elimination and/or hydrolysis of L1 had occurred to give a complex of the starting dihydrazone, L0. The incorrect assignment of ligand formulation was again avoidable to some extent, since the analytical data (section Aiii) agree more closely (especially the % Ni) with calculated figures including L0 rather than L1. Also, there is the concurrence of the i.r. spectrum for $Ni(L0)NO_2(ClO_4)$ (figure A.4) with that for $Ni(L0)(NCS)_2 \cdot H_2O$ (figure A.3) in the 1500 → 1700 cm^{-1} region, including the absence of a band assignable as $\nu(C=O)$. This band, which is also absent in $Ni(L0)(ClO_4)_2$ (figure A.2), appears at 1685 cm^{-1} in $Ni(L1)(ClO_4)_2$. Despite this incorrect assignment, the information to be obtained from this compound was deemed useful, and the structure determination was completed.

A perspective view of the cation is shown in figure 3.5. Cations and anions within the unit cell are well separated and afford no significant interactions. The nickel ion is coordinated with roughly octahedral geometry to the two oxygen atoms of the nitrite ligand, and to the nitrogen atoms of the tetradentate ligand L0. The major distortion from regular octahedral coordination arises from the extremely short bite of the bidentate nitrite ion (2.096(5)Å). The ligand L0 can be considered to fold along the N2NiN4 direction so that N1, N2, and N4 occupy three of the equatorial positions of the

octahedron, with N3 in one axial position. The Ni-N bond lengths average 2.08(1)Å (with no one length significantly different from the mean); this is somewhat shorter than the average for the corresponding Ni-N lengths in $Ni(L0)(NCS)_2$ (2.136(9)Å).

The NNiN angles correspond reasonably closely to those in $Ni(L0)(NCS)_2$, despite the different ligand configuration. The N2NiN3 angle formed by the five-membered chelate ring is 83.0(1) deg, the six-membered rings give 92.5(1) deg and 93.8(1) deg, and the N1NiN4 angle is 94.8(2) deg. The latter parameter shows the largest difference from its corresponding value in $Ni(L0)(NCS)_2$ of 100.5(3) deg, and reflects a somewhat more even distribution of bond angles among the coordination sites of L0.

The ligand conformation is analysed in figures 3.6 (torsion angles) and 3.7 (sketches of chelate rings based on deviations of ligand atoms from planes defined by the metal atom and corresponding donor atoms: the planes used to general these diagrams are given in table 3.6). The disordered ring formed by NiN3C13C16C17N4 is shown in its two half-occupied positions. The disorder causes very little disturbance to the donor atoms N3 and N4, as reflected by their unexceptional thermal motion parameters (table 2.8). The two conformations of this chelate approximate the two possible half-chair conformers of cyclohexene, which are interconvertible via chair inversion[5]:



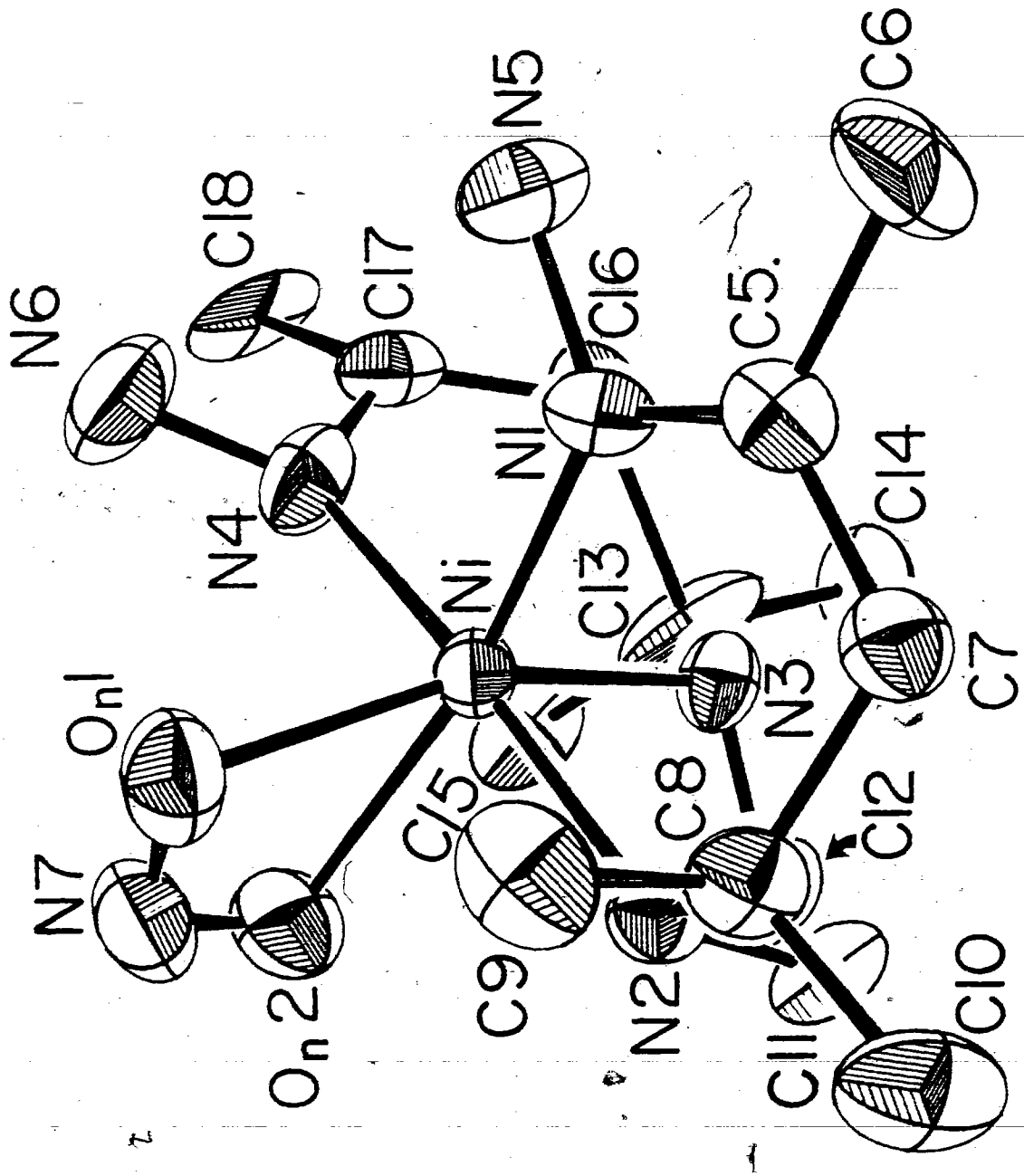
This interconversion can be readily simulated using suitable scale models, and this indicates that two alternative positions of the $-NH_2$ group at N6 would also be expected. Although the motion indicated by the thermal motion parameters is somewhat larger than those for N5, it is not sufficient to imply disorder to the extent apparent from the models. However, allowing for the rigidity of the NiN3N4 moiety and some twisting of the double bond at C17=N4, a concurrence of the structural data with the model systems is possible. The large least-squares estimated errors in the bond distances and angles in this disordered chelate do not permit further analysis. In the NiN1C5C7C8N2 ring, some bond angle strain is evident at C7 (C5C7C8 = 120.5(4) deg).

The five-membered chelate ring formed by NiN2C11C12N3 exhibits some bond torsional strain along N2-C11, and the conformation adopted bears most relation to the envelope conformer of cyclopentane (compare figures 3.6 and 4.1). This appears to be the major source of strain in the tetradentate ligand as a result of its folded configuration. As in the planar L0 complex in 3ii, the N-racemic (RR and SS) isomer mixture is found in the crystal.

The nitrite ligand has Ni-O_n and respective O_n-N_n bonds of 2.171(3), 1.246(6) and 2.132(4), 1.276(6)Å. The ligand can therefore be considered to be asymmetric, the shorter Ni-O length occurring <u>trans</u> to N3.

Figure 3.5

Perspective View of $Ni(L0)NO_2^+$



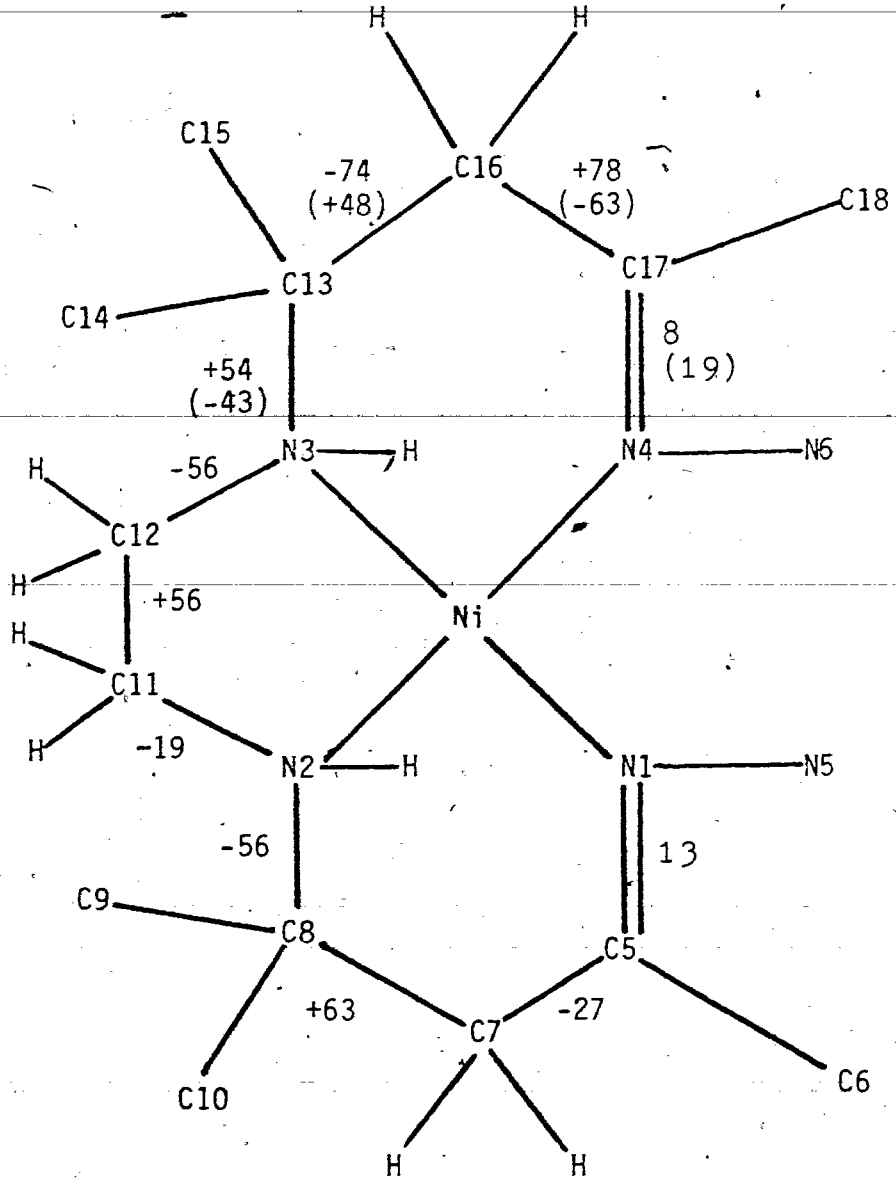


Figure 3.6

Torsion Angles in $Ni(LO)NO_2^+$ (deg)

Figure 3.7 Projections of Chelate Ring Conformations in $Ni(LO)NO_2^+$

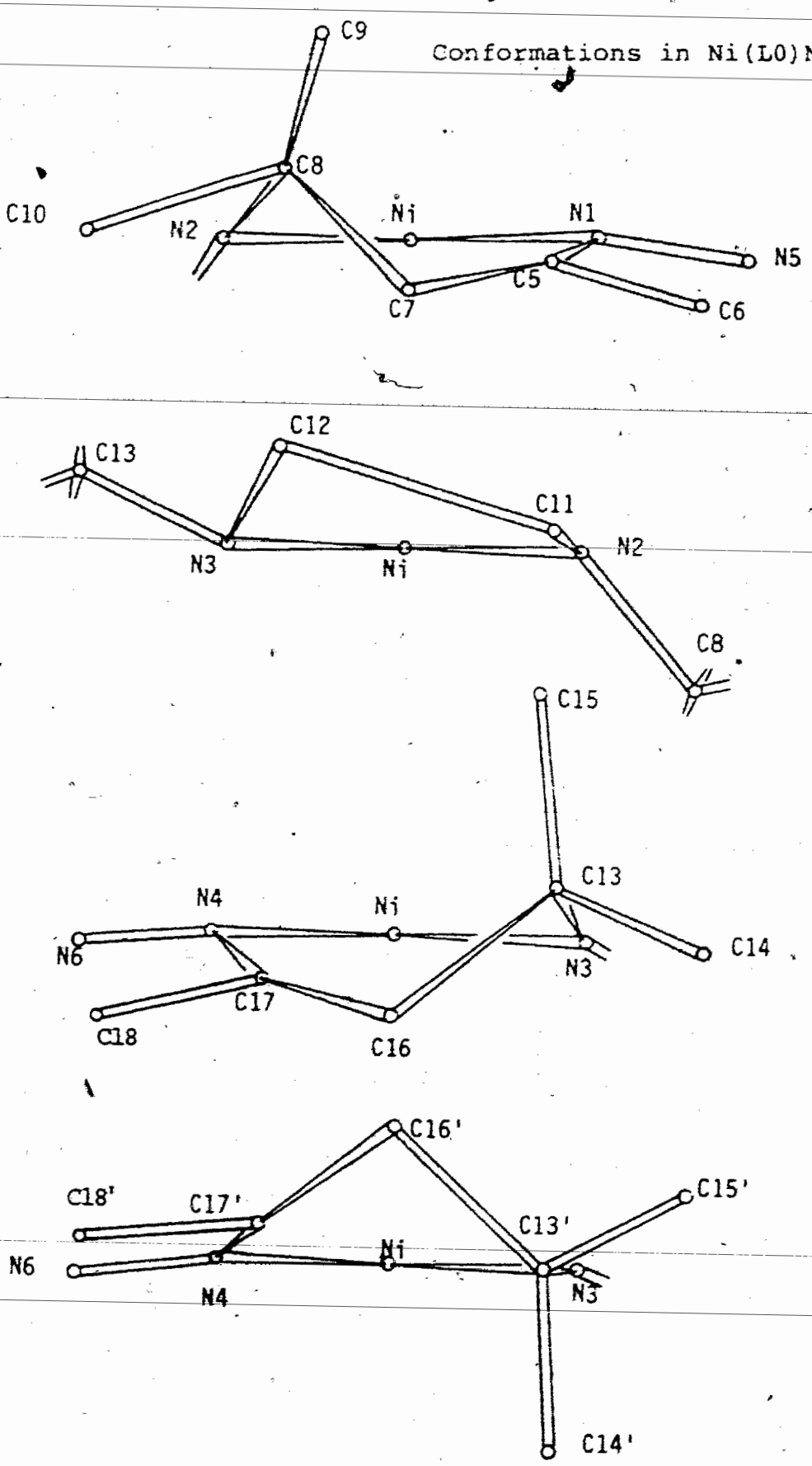


Table 3.6

Equations of the Planes Calculated for $Ni(L0)NO_2^+$

Atoms in the plane	Coefficients of the equation of the plane X	Y	Z	p	Displacements from the plane (Å)
Ni, N1, N2	.263	-.756	-.599	-2.066	N5(-.04),C5(-.19), C6(-.44),C7(-.24), C8(.54),C9(2.00), C10(.34)
Ni, N2, N3	.882	.472	-.003	2.279	C8(-1.17),C11(.23), C12(.84),C13(.56)
Ni, N3, N4	-.904	-.416	-.102	-2.483	C13(.42),C13(.08), C14(-.06),C14'(-1.37), C15(1.81),C15'(.57), C16(-.64),C16'(1.04) C17(-.40),C17'(.36), C18(-.65),C18'(.133)

The orthogonal system of axes (X,Y,Z) has X along the a axis, Y in the ab plane, and Z along the c^* axis.

3iv $\underline{Ni(L2)H_2O(ClO_4)_2 \cdot 3H_2O}$

Packing within the unit cell of this structure is illustrated by means of a projection along the a axis of the unit cell in figure 3.8. As can be seen, an extensive hydrogen-bonding network connects the anions, cations and water molecules of crystallisation. A diagram showing the dimensions of the contacts used to elucidate this network is given in figure 3.9.

A perspective view of the cation is shown in figure 3.10. Of primary importance is the identity of the ligand L2, wherein one carbonyl oxygen of the diketone is seen to have condensed with a hydrazone $-NH_2$ group to give the imine N5=C1, while the condensation of the other oxygen with hydrazone has been arrested at the carbinolamine intermediate. Such intermediates have in some instances been characterised,[41] but are generally considered to be rather short-lived and it is clear in the present case that the species is stabilised by coordination of the -OH to the nickel ion, and by the hydrogen bonding system. Further implications of this result will be discussed in section 3vii of this chapter.

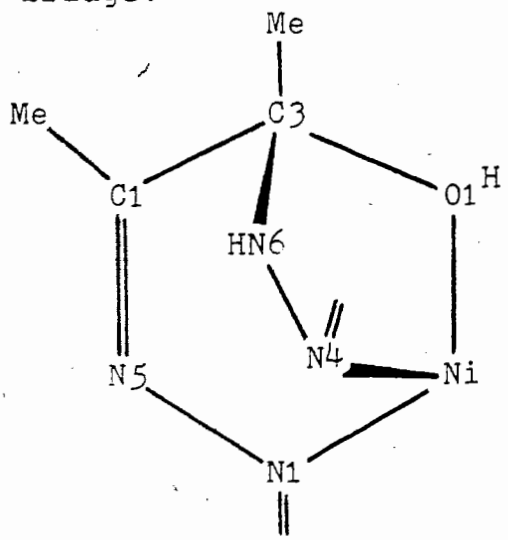
The roughly octahedral coordination geometry about the nickel comprises the carbinolamine oxygen (O1) which is <u>cis</u> to a coordinated water molecule (O2), and four nitrogen atoms of the macrocycle in the remaining positions. The major sources of distortion from regular octahedral geometry arise from the opening of the N1NiN4 angle (100.2(2) deg) at the expense of the N2NiN3 angle of 83.9(2) deg and the N2NiO2 angle of 83.7(2) deg, and also from the Ni-O1 bond which leans towards the

seven-membered chelate ring whence it arises (N1Ni01 = 74.9(2) deg and N4Ni01 = 77.7(2) deg). The Ni-N bond lengths (mean 2.07(2) Å) are not exceptional. The mean is close to the corresponding value for $Ni(L0)NO_2^+$, and perhaps the only systematic feature that can identified is that Ni-N trans to N (2.104(6) and 2.085(6)Å) are longer than those trans to oxygen (2.053(6) and 2.070(6)Å).

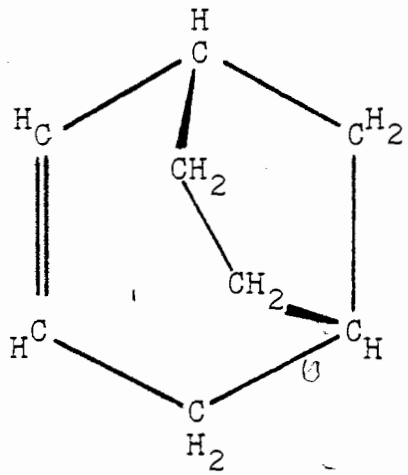
As with the L0 complexes already described, the geometries at the two asymmetric nitrogen donors, N2 and N3, give rise to a racemic mixture of RR and SS enantiomers in the crystal. The conformations of the six and five membered rings match those in $Ni(L0)NO_2^+$, which has the same ligand configuration: NiN1C5C7C8N2 and NiN3C13C16C17N4 - half-chair (cyclohexene) and NiN2C11C12N3 - a strained system, corresponding to an envelope cyclopentane conformer[5], and with torsion angles (-18, +48, -51 deg) which follow closely those in the corresponding chelate ring in $Ni(L0)NO_2^+$ (-19, +48, -56 deg). These ring conformations are analysed as before using torsion angles (figure 3.11) and as deviations from planes calculated for the NiN_2 moieties (figure 3.12). Bond angle strain is again evident in the six-membered chelates (C5C7C8 = 116.8(6) deg and C13C16C17 = 120.0 deg).

The conformation of the chelate system containing the imine and carbinolamine condensation intermediate can be considered as three parts: the five-membered envelope(cyclopentane) NiO1C3N6N4, the six-membered chair (cyclohexene) NiO1C3-C1N5N1, and the seven-membered boat (cycloheptane) NiN1N5C1C3N6-

N4. Alternatively, and perhaps more concisely, it approximates a cycloheptane boat, constrained to this unstable conformation by the C3O1Ni bridge:



Finally, some comparison with the analogous polycyclic hydrocarbon should be possible i.e. bis-cyclo{3.2.1}oct-2-ene:



This compound is known, although no structural data is available. Probably the most closely related structure is that of the antibiotic viomycidine[42] which adopts a similar conformation to the chelate in L2.

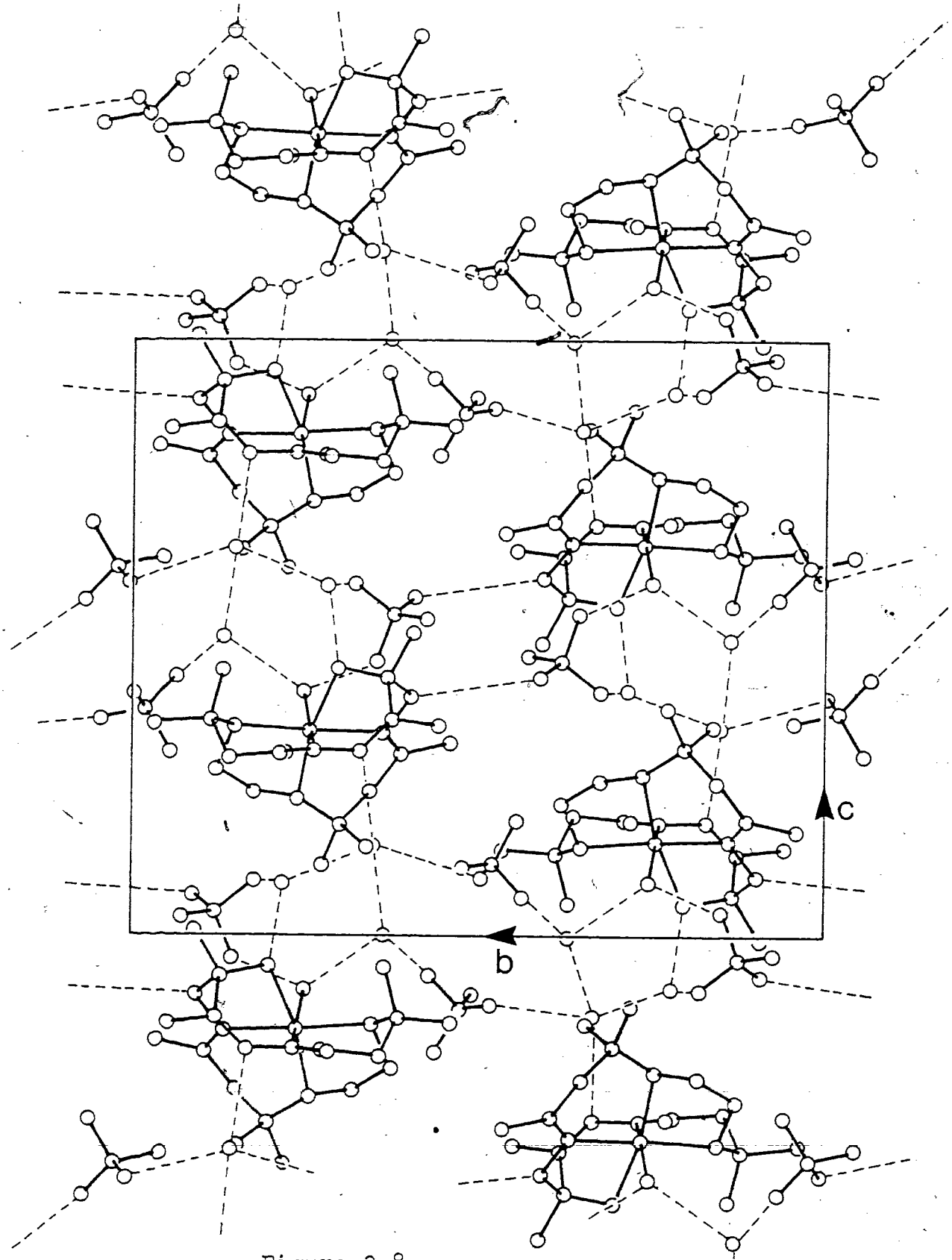


Figure 3.8

Packing Diagram of $Ni(L2)H_2O(ClO_4)_2 \cdot 3H_2O$

Figure 3.9

Hydrogen Bonding in $Ni(L2)H_2O(ClO_4)\cdot 3H_2O$

(distances in Å)

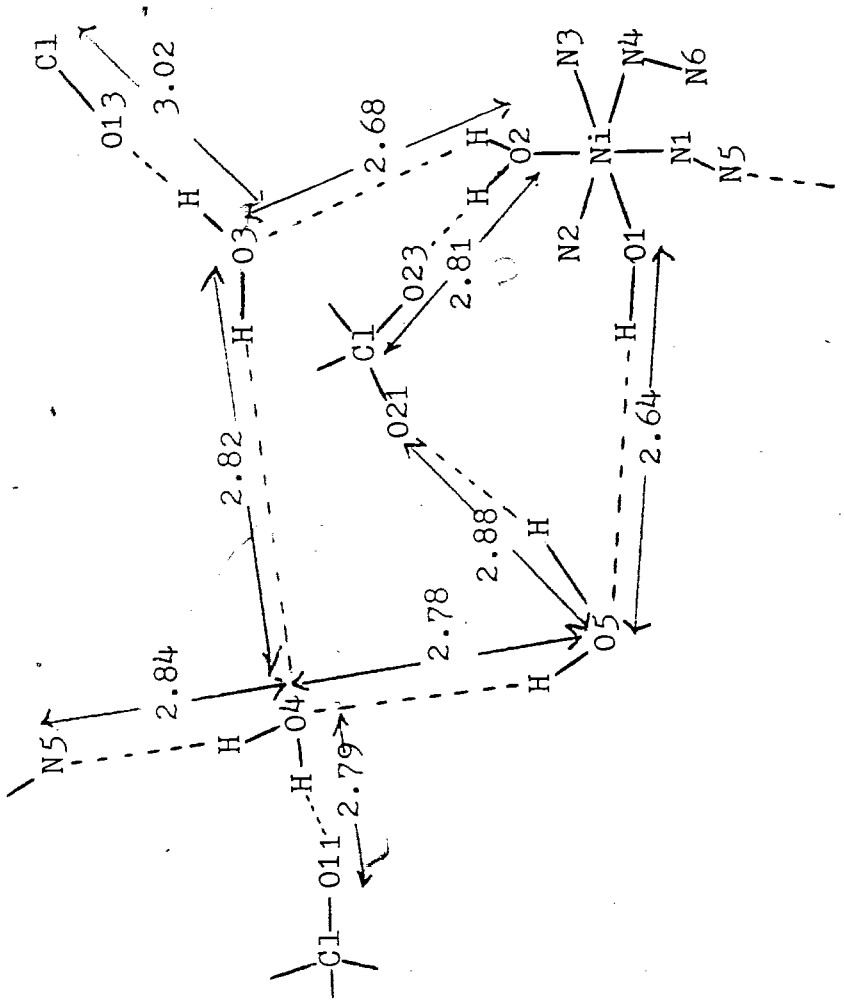
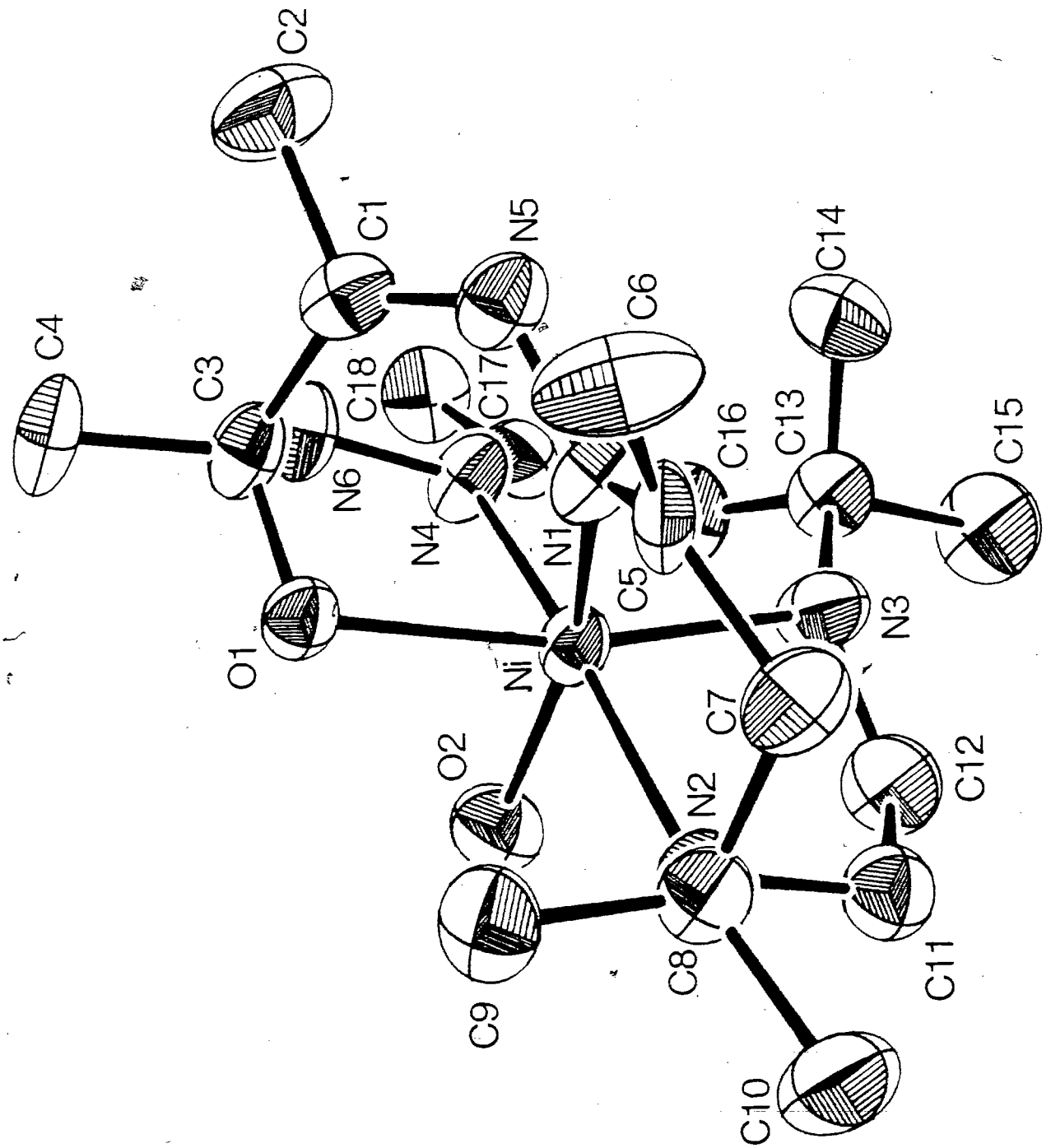


Figure 3.10

Perspective View of $Ni(L2)H_2O^{2+}$



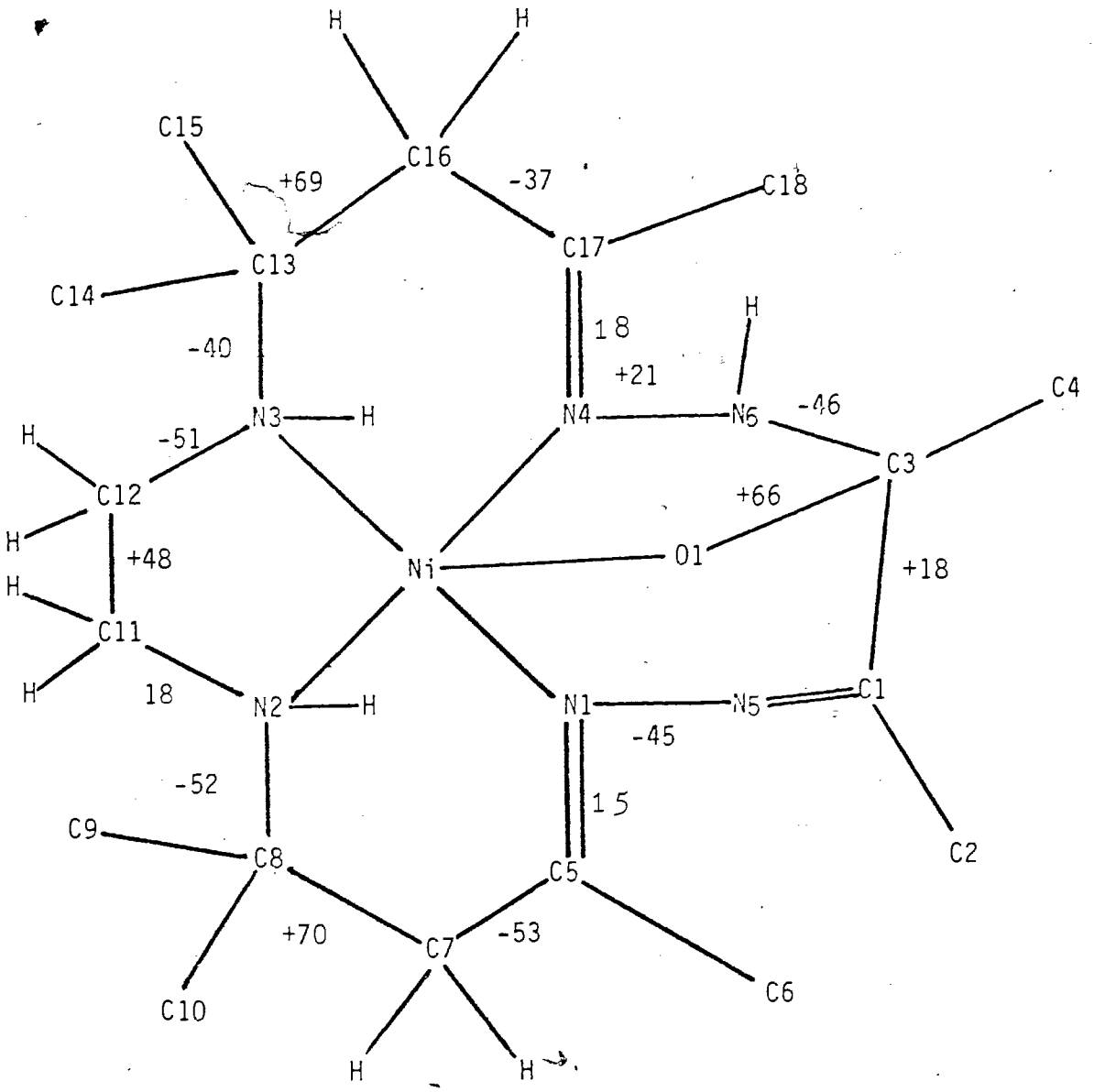


Figure 3.11

Torsion Angles in $Ni(L2)H_2O^{2+}$ (deg)

Figure 3.12

Projections of Chelate Ring Conformations in $Ni(L2)H_2O^{2+}$

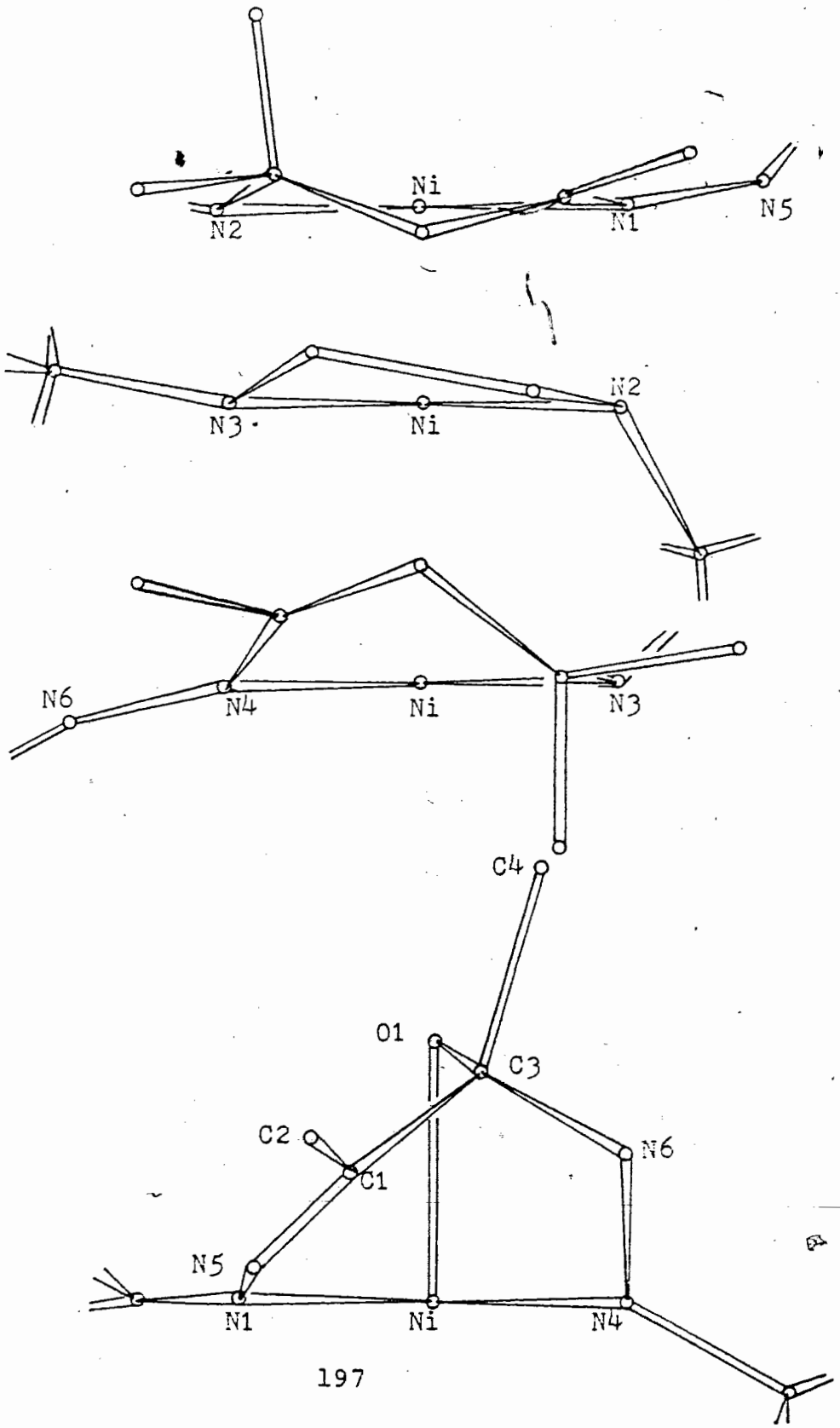


Table 3.7

Equations of the Planes Calculated for $Ni(L2)H_2O^{2+}$

Atoms in the plane	Coefficients of the equation of the plane X	Y	Z	p^+	Displacements from the plane (Å)
Ni,N1,N2	.255	-.065	-.965	-2.499	N5(.22),C5(.049), C6(.50),C7(-.27), C8(.48),C9(1.96), C10(.24),C11(-1.38)
Ni,N2,N3	-.918	-.007	-.397	-2.369	C8(-1.14),C11(.21), C12(.75),C13(.30)
Ni,N3,N4	-.882	.208	-.422	-1.387	C12(.99),C13(.01),C C14(.43),C15(-1.45), C16(.90),C17(.54), C18(.85),N6(-.27)
Ni.N1,N4	.253	-.085	-.964	-2.544	C5(.03),N5(.25) C1(1.09),C2(1.21), C2(1.21),C3(1.93), C4(3.32),01(2.00), N6(1.18),C17(-.78)

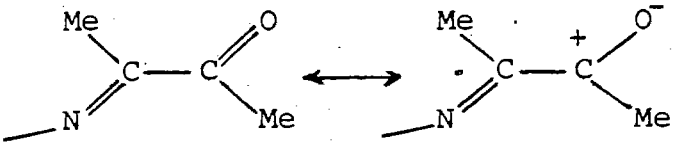
The orthogonal system of axes (X,Y,Z) has X along the a axis, Y in the ab plane, and Z along the c^* axis.

3v. $Ni(L3)NO_2(ClO_4).\frac{1}{2}H_2O$

Cations and anions in the unit cell are linked by the half-occupied water molecule of crystallisation, as described in section 2iv(e). A perspective view of the metal complex cation is shown in figure 3.13. The nitrite ligand is symmetrically bidentate, with the four donors of the ligand L3 disposed among the remaining coordination sites about the metal ion in a configuration similar to that found in $Ni(L0)NO_2^+$. Furthermore, the nickel-nitrogen bond lengths follow the same pattern as those in $Ni(LO)NO_2^+$ and $Ni(L2)H_2O^{2+}$, with the two longest bond lengths (Ni-N2, 2.115(6)Å and Ni-N4, 2.098(6)Å) occurring for trans-related donors, and somewhat shorter Ni-N distances (Ni-N1 = 2.095(6)Å, and Ni-N3 = 2.051(6)Å) trans to nitrite oxygen atoms.

Again, the identity of the ligand L3 is of foremost importance: it is a tautomer of L2, with the imine linkage intact at N5=C1, but instead of a carbinolamine about C3, a free carbonyl species is observed (consistent with the i.r. - figure A.8), with unreacted hydrazone at N4-N6H_2. Surprisingly, there is no suggestion of interaction of the carbonyl oxygen with the water molecule of crystallisation, and considerable thermal motion is evident in O1. The refined bond length of 1.07(2)Å, when corrected for thermal motion (O1 considered to ride on C3) becomes a more chemically reasonable 1.22(2)Å. The torsion angle about C1-C3 of -4 deg indicates the near planarity of the N5C1C2C3O1C4 atoms. Such an arrangement is found for other

compounds containing double-bonded groups connected by a C-C single bond e.g. 1,3-butadiene, acrolein, and 2,3-butanedione[43,44]. The positioning of the double bonds trans- to one another can be ascribed to at least four effects in this case: the relief of steric repulsions between the methyl groups at C2 and C4; some conjugation, demonstrated in resonance language as



Furthermore, repulsions between the dipoles of the C=O and C=N bonds is minimised in the trans- arrangement[44], and the interaction of methyl hydrogen atoms at C4 with the water molecule of crystallisation may also determine this geometry. Again, the relevance of this ligand structure to the overall reaction sequence will be discussed in section 3vi.

The remainder of the ligand forms the two six-membered half-chair (cyclohexene) chelate rings NiN1C5C7C8N2, and NiN3C13C16C17N4, and the five-membered envelope (cyclopentane) ring NiN2C11C12N3. An analysis of the ligand conformation is given in figure 3.14 (torsion angles) and figure 3.5 (displacements from NiN_2 planes). No positions of extraordinary strain are evident, although bond angle strain is observed at C7 (C5C7C8 = 121.0(7) deg) and C16 (C13C16C17 = 119.6(7)).

Interestingly, this combination of chelate conformations completes a series for the cis NiN_4O_2 systems. In Ni(LO)-NO_2^+, one half-chair conformer at NiN1N2 is coupled with a disordered pair at NiN3N4, and a strained five-membered ring at

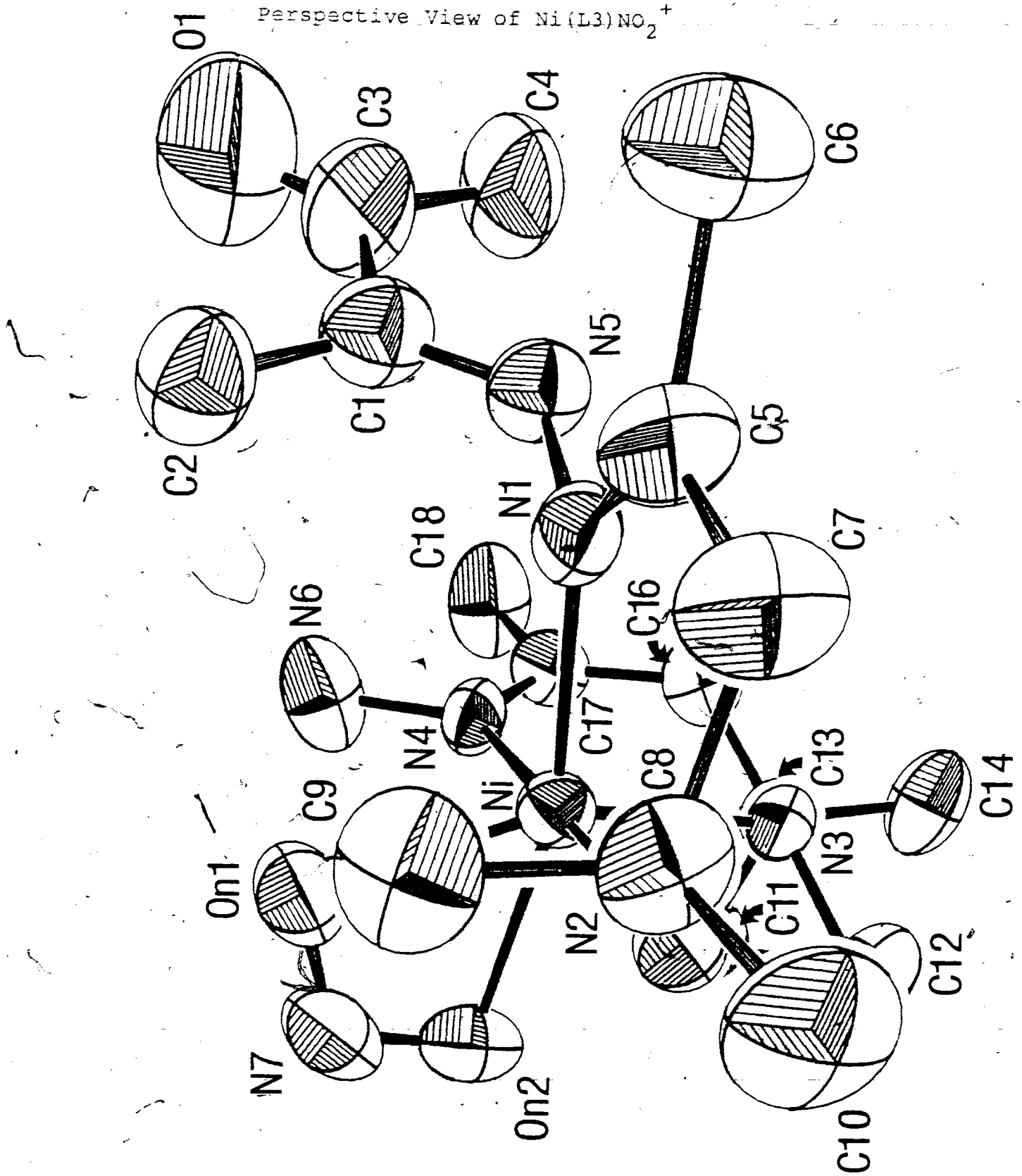
NiN2N3. In $Ni(L2)H_2O^{2+}$, the two six-membered rings are roughly two-fold related (corresponding to one combination of the rings in $Ni(L0)NO_2^+$ - compare figures 3.7 and 3.12), and again with a similar, five-membered ring at NiN2N3. In $Ni(L3)NO_2^+$, the two half-chair six-membered conformers are roughly mirror-related (corresponding to the other combination of the rings in $Ni(L0)NO_2^+$), again with a rather strained, envelope conformer of a five-membered ring. If this were to demonstrate one aspect of this series, it would be the extremely flexible nature of the tetradentate ligand.

As with the other ligands in this series, the chiral centres at N2 and N3 in each cation adopt an RR or SS conformation to give a racemic mixture in the crystal.

The nitrite ligand is bonded asymmetrically, in a manner similar to that in $Ni(L0)NO_2^+$. Respective Ni-O_n and O_n-N_n distances are 2.144(6), 1.31(1) and 2.183(6), 1.25(1) Å, with the shorter Ni-O_n length trans- to N3. The inter-donor atom bite is 2.13(1)Å.

Figure 3.13

Perspective View of $Ni(L3)NO_2^+$



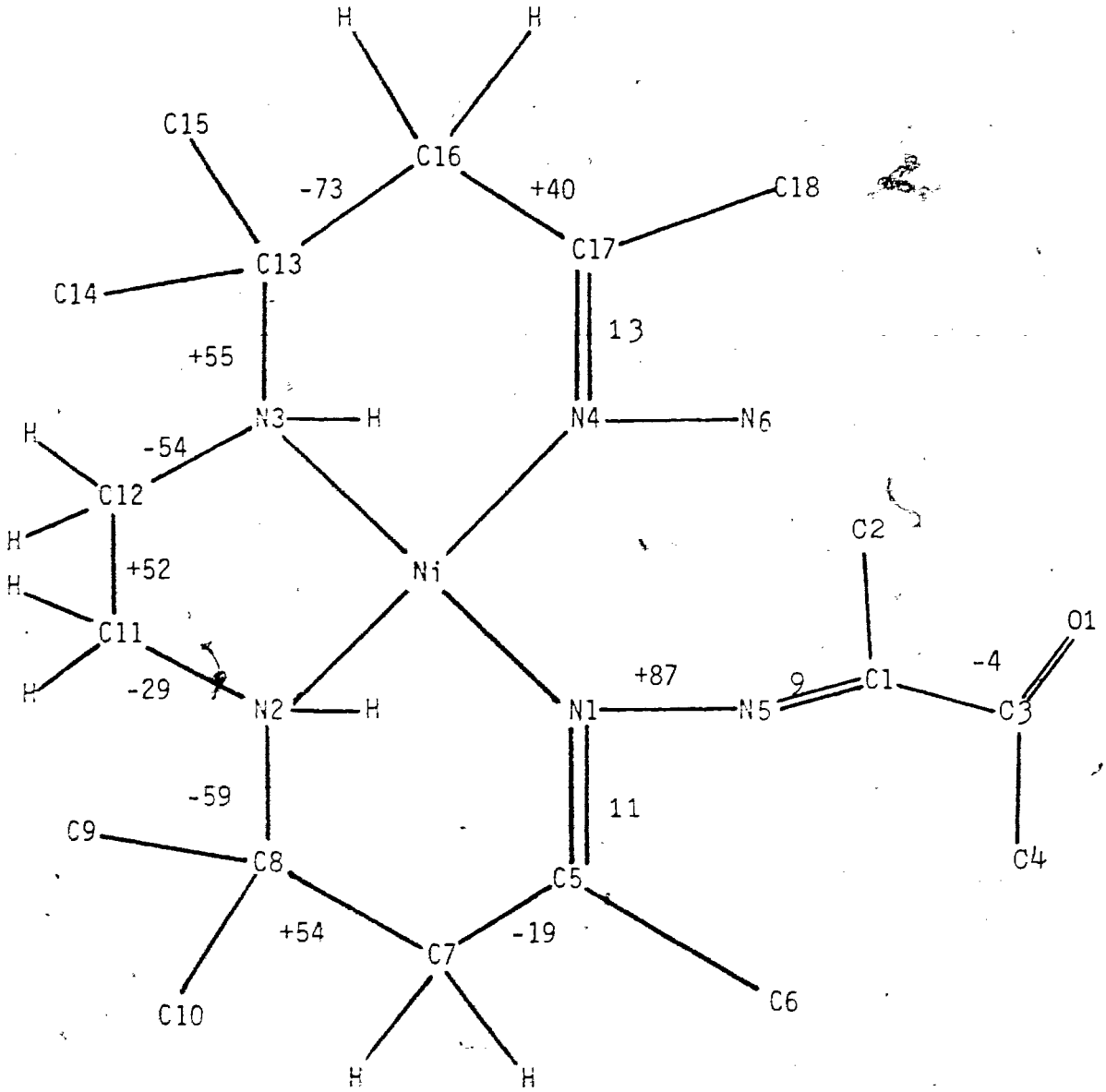


Figure 3.14

Torsion Angles in $Ni(L3)NO_2^+$ (deg)

Figure 3.15

Projections of Chelate Ring Conformations in $Ni(L3)NO_2^+$

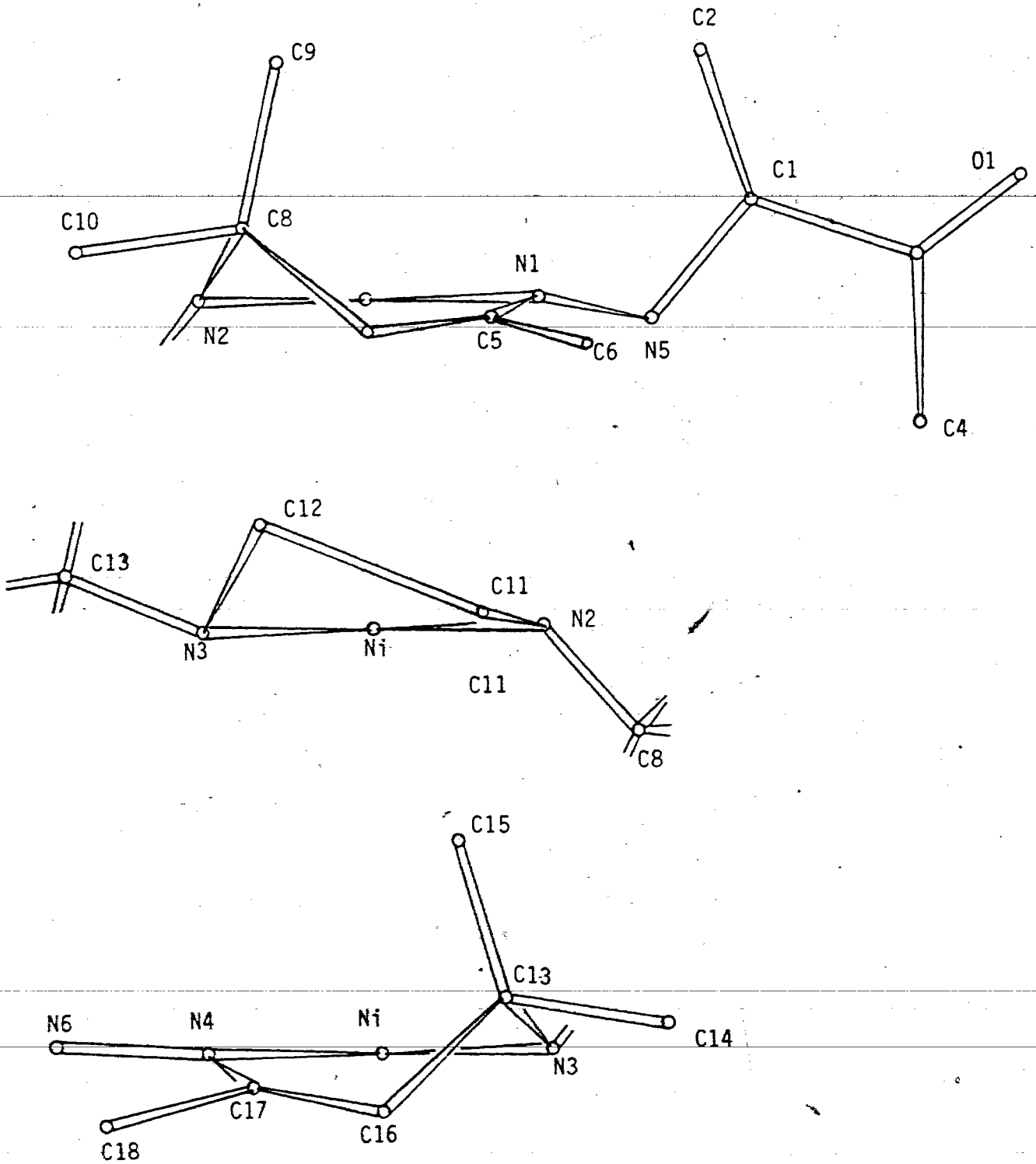


Table 3.8

Equations of the Planes Calculated for $Ni(L3)NO_2^+$

Atoms in the plane	Coefficients of the equation of the plane X	Y	Z	p	Displacements from the plane (Å)
Ni,N1,N2	.662	.281	-.695	.976	N5(-.23),C1(.78), C2(2.21),C3(.38), C4(-1.07),O1(1.15), C5(-.07),C6(-.26), C7(-.15),C8(.66), C9(.54),C10(2.13)
Ni,N2,N3	-.090	-.968	-.234	-2.527	C8(-.99),C11(.03) C12(.74),C13(.48)
Ni,N3,N4	-.128	-.958	-.258	-2.608	C13(.42),C14(1.88), C15(.09),C16(-.49), C17(-.27),C18(-.47), N6(.08)

The orthogonal system of axes (X,Y,Z) has X along the a axis, Y in the ab plane, and Z along the c^* axis.

3vi. $Ni(L4)(ClO_4)_2$

The final product of the condensation reaction crystallises as the simple perchlorate salt; $Ni(L4)^{2+}$ cations contain approximately square planar coordinated metal ions, and there is no suggestion of axial interactions (3.5A) between cations or from perchlorate anions. A perspective view of the cation is given in figure 3.16. The Ni-N bond lengths (table 3.1) are all equal within experimental error, and the mean (1.907(3)Å) is considerably shorter than that of the other complexes, as expected from the lower coordination number. As with the other complexes in this series, there is no differentiation between Ni-N(imine) and Ni-N(amine) bonds. As already stated, the coordination geometry is roughly square planar, the distortions from regular geometry being of two kinds. The relaxation of the N1NiN4 angle (94.2(2) deg) - the angle subtended by the seven-membered chelate, contrasts the N2NiN3 angle of 88.1(2) deg, corresponding to a five-membered chelate. This difference is smaller than that found for the other complexes in this series. Furthermore, there is a tetrahedral distortion of the donor atoms as expressed by the angle of twist between the planes N1NiN4 and N2NiN3 of 22.3 deg. This distortion is evident from the plot of the displacements of the ligand atoms from the least squares mean plane through atoms NiN1N2N3N4 (figure 3.17). The twisting is not a great deal larger than that seen in L0 (16.7 deg) as determined in $Ni(L0)(NCS)_2$ (figure 3.2). Thus, it would appear on this basis, that the formation of the

seven-membered chelate upon condensation of the diketone with L0 causes little change in the coordination properties of the tetradentate ligand. One reason for this can be found by closer inspection of the seven-membered tetra-aza ring NiN1N5C1C3N6N4 which is considerably twisted such that the C1-C3 bond lies ∿ 70 deg to the NiN1N4 plane. Comparisons with alicyclic, seven-membered systems are even more tenuous here since no conformational data are available on 1,3-cycloheptadiene systems. However, the closest cycloheptane conformer is the twist boat (figure 1.1). Torsion angles describing the conformation of this and the other rings in this structure are given in figure 3.18, and diagrams of each ring based on the NiN_2 planes in figure 3.19. The torsion angles about the C1-C3 bond (+69 deg) indicates little torsional strain or steric interactions between the methyl groups at C3 and C4. The displacements of the atoms N5 and N6 (where the condensation took place) from the NiN1N2N3N4 plane (+1.16A and -1.19A respectively) are of the same order as the corresponding values in $Ni(L0)(NCS)_2$ (+0.78A and -0.66A). Again, it would appear that the condensation has caused little rearrangement of the ligand.

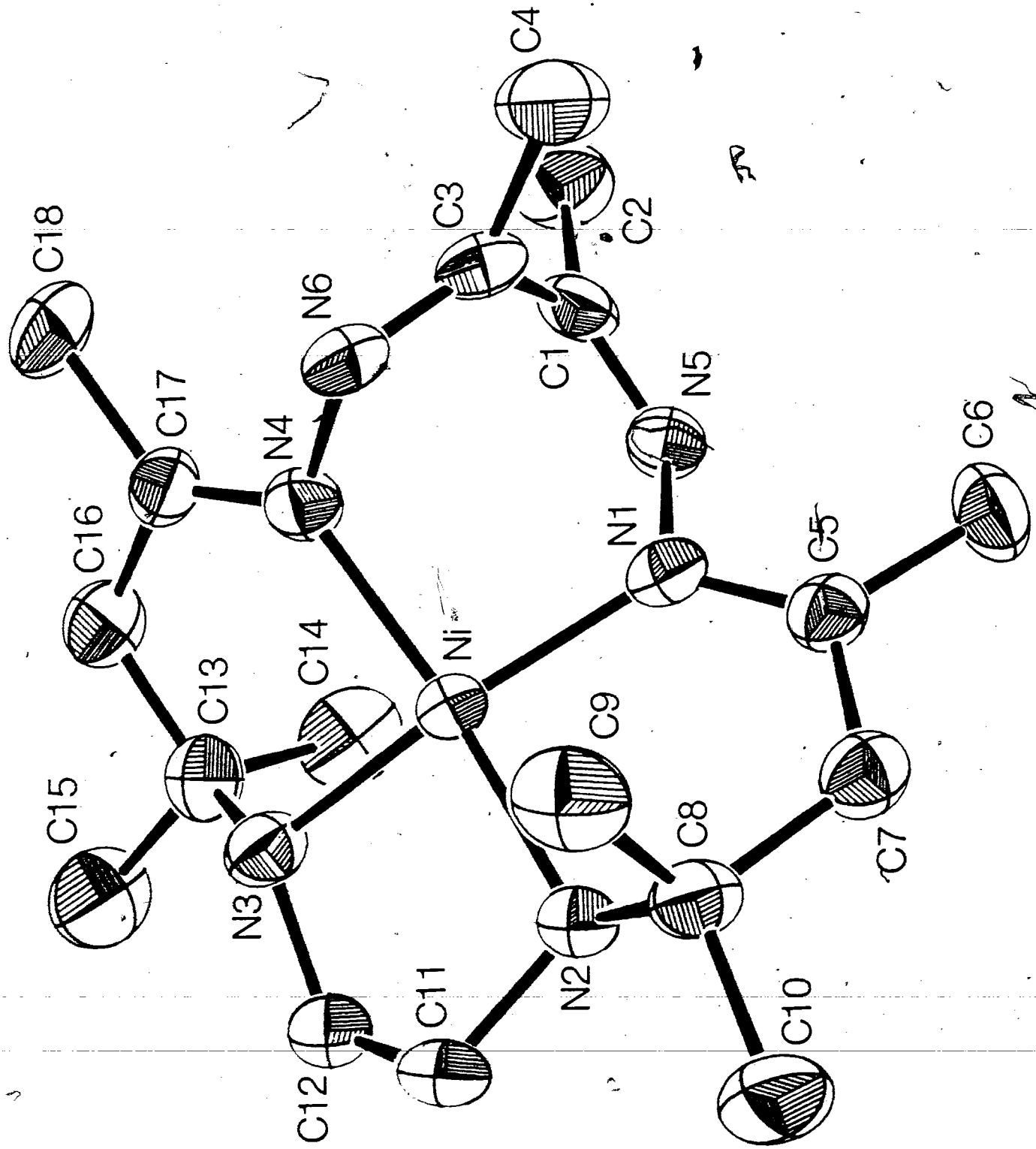
The complex has an approximate, non-crystallographic two-fold axis of symmetry which bisects the C11-C12 and C1-C3 bonds. The five-membered chelate ring NiN2C11C12N3 adopts a strain-free half-chair (cyclopentane) conformation. The six-membered chelates, however, are found to have rather obscure conformations, most closely related to the 1,2 diplanar, or 'sofa' conformer.[5] The relative instability of this system is shown by the torsion angles at C5-C7 and C17-C18 (both +3 deg),

and is supported by calculations on cyclohexene [5] which find this conformer to be approximately 5 kJ mole^{-1} less stable than the half-chair. Interestingly, however, the sofa is stabilised to within 1 kJ mole^{-1} of the half-chair if some twisting (5 deg) of the double bonds (at C5=N1 and C17=N4 in this case) is introduced in to the calculation.[5]

The twisting of double bonds as a result of intra-annular strain has been identified as the major source of chirality and high dipole moment in trans-octadiene[45,46]. A general discussion of the effects of double bond twisting on electronic spectra is also available[47]. The point is made there that twists of ∿40 deg maintain considerable p-orbital overlap and half the resonance energy of the double bond, and that twists of ∿10-20 deg cost very little in terms of overlap or in resonance energy. Dramatic structural evidence of this effect is found in di-μ-chlorotris(trans-cyclooctadiene) dicopper(II)[48]. This contains three crystallographically-distinct olefin systems with deviations from planarity about the double bonds of 40-45 deg. The corresponding C=C bond of 1.40(6) Å appears long, although because of the large error connected with this parameter, it is not possible to infer loss of double bond character. In the present series of complexes, twists range from 4 - 19 deg. In Ni(L4)$^{2+}$, the values are at the high end of this range, but cannot be identified as the extraordinary source of stabilisation of the sofa conformer.

Figure 3.16

Perspective View of $Ni(L4)^{2+}$



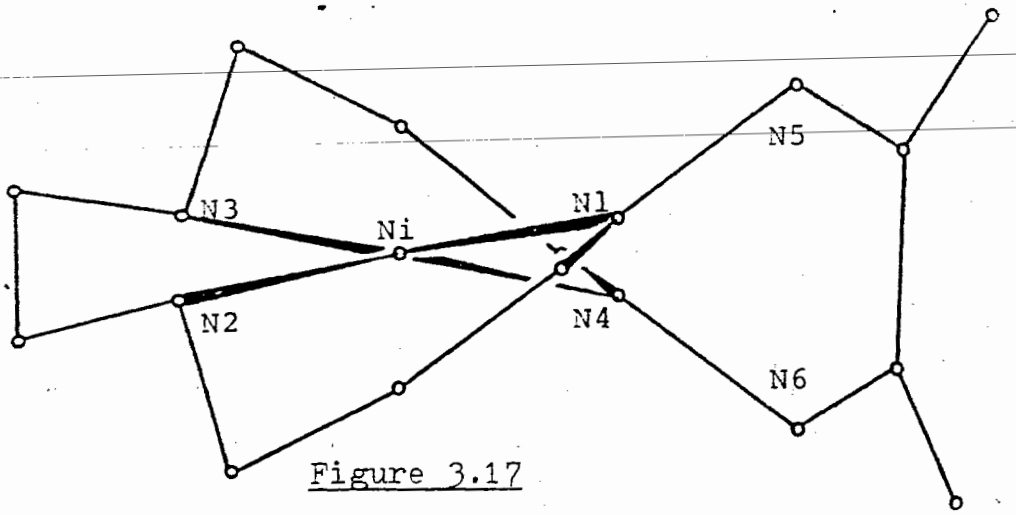


Figure 3.17

Displacements of Atoms from the 'NiN1N2N3N4' Plane in $Ni(L4)^{2+}$

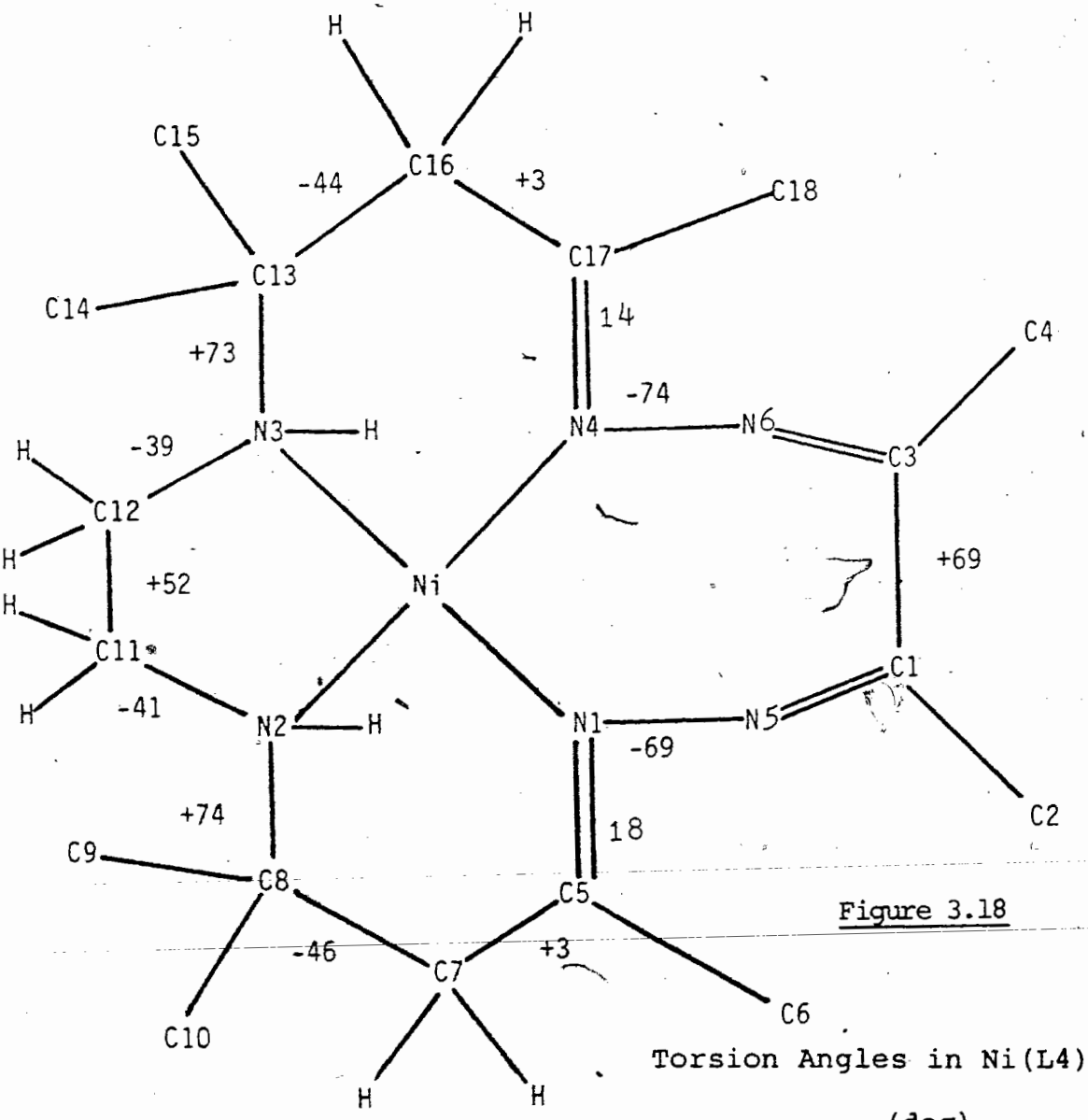


Figure 3.18

Torsion Angles in $Ni(L4)^{2+}$

(deg)

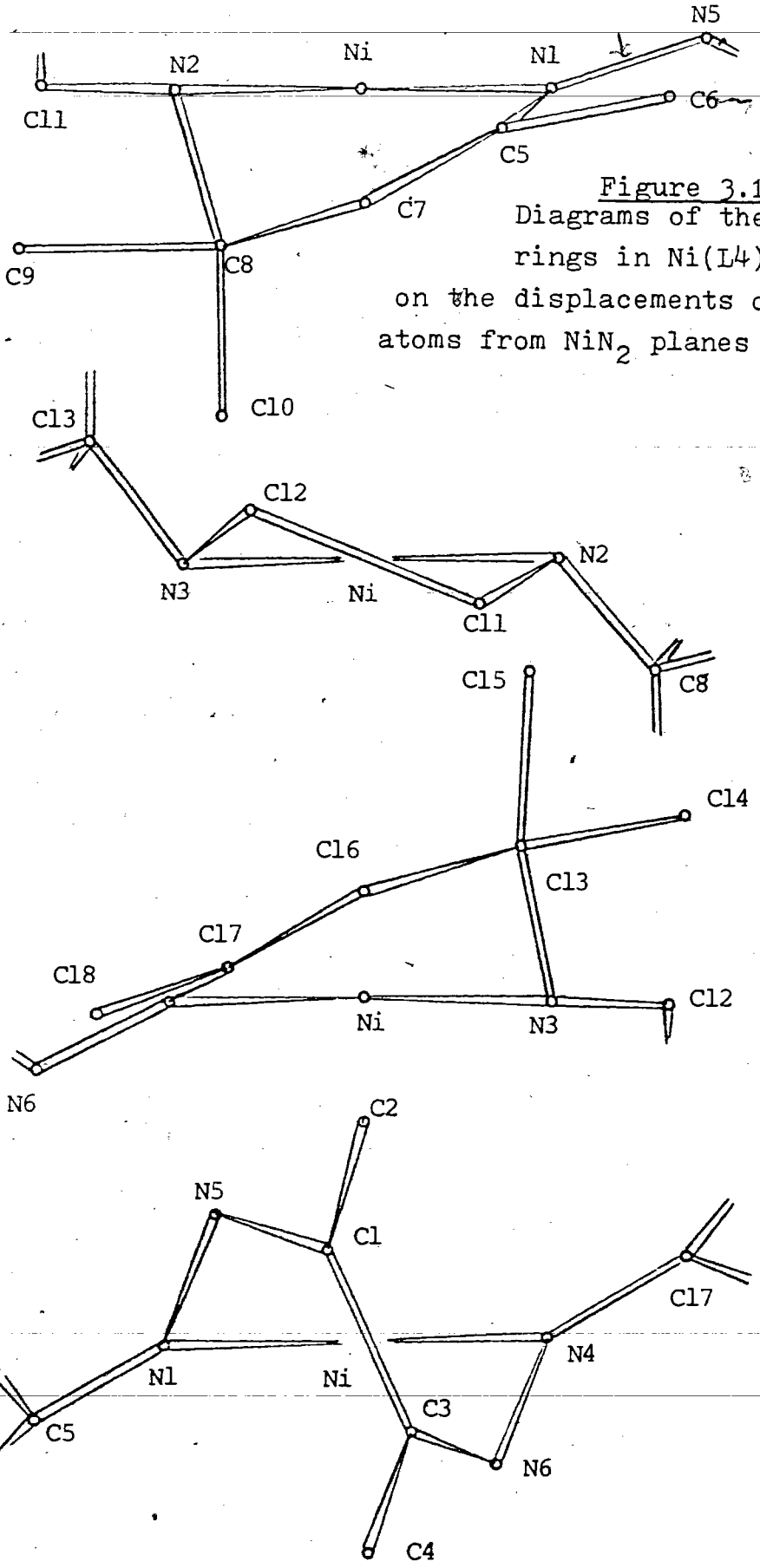


Figure 3.19
Diagrams of the chelate rings in $Ni(L4)^{2+}$ based on the displacements of ligand atoms from NiN_2 planes (table 3.9).

Table 3.9

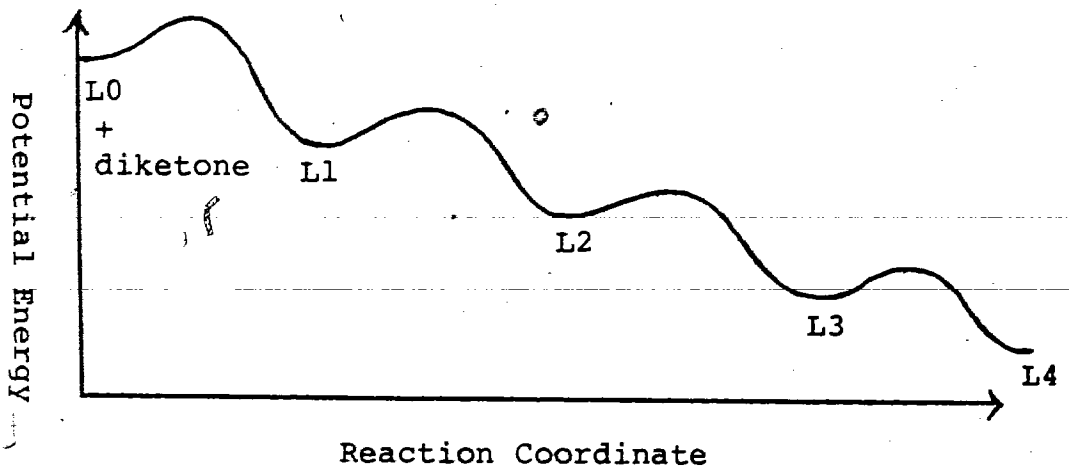
Least Squares Mean Planes Relevant to the Discussion of $Ni(L4)^{2+}$

Atoms in plane	Coefficients of equation of plane†				Displacements (Å)
	X	Y	Z	p	
Ni, N1, N2, N3, N4 χ^2 = 6404	-.995	.790	-.059	-3.207	Ni(0.0), N1(.24), N2(-.30), N3(.25), N4(-.26), N5(1.16), N6(-1.19), C5(-.07), C7(-.89), C8(-1.40), C11(-.50), C12(.46), C13(1.34), C16(.76), C17(-.02).
Ni, N1, N2	.990	-.041	-.138	-3.131	N5(.69),C5(-.28), C6(-.02), C7(-.84), C8(-1.14), C9(-1.41), C10(-.84), C11(.04)
Ni, N2, N3	-.990	-.128	-.063	-3.195	C8(-.89), C11(-.33),C12(.38), C13 (.87)
Ni, N3, N4	-.964	.109	-.242	-3.161	C12(-.04), C13(1.16), C14(2.44), C15(1.37), C16(.80), C17(.24), C18(-.10), N6(-.72)
Ni, N1, N4	0.965	.258	-.047	-3.102	C5(-.54), N5(.98), C1(.68),C2(1.63) C3(-.63), C4(-1.61), N6(-.96), C17 (.47)

† The orthogonal system of axes (X, Y, Z) has X along the $\underline{a}$ axis, Y in the $\underline{a}\,\underline{b}$ plane, and Z along the c^* axis. χ^2 for a plane $\ell X + mY + nZ - p = 0$ for the N atom is given by $\Sigma_{i=1}^{i=N}(Pi^2/\sigma^2(Pi))$, where $\sigma^2(Pi) = \underline{\ell}^2\underline{\sigma}^2(\underline{X}i) + \underline{m}^2\sigma^2(Yi) + \underline{n}^2\sigma^2(Zi)$ and Pi is the distance of atom i from the plane.

3vii. The Reaction Sequence Revisited

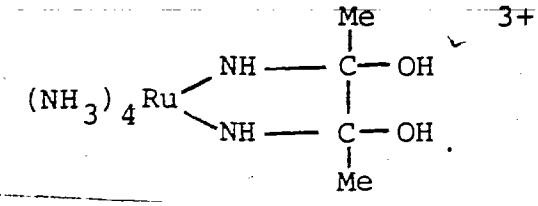
On the basis of the structural results presented in this chapter, together with the conditions under which each complex in the series occurs, and the available analytical and spectral data on these complexes, some reasonable interpretation of the condensation reaction sequence is possible. As stated in the introduction, section 1vi, a study of this kind has some inherent difficulties, not the least of which is the fact that data obtained for thermodynamically stable intermediates is used to generate information concerning the mechanism of the reaction. Some justification for the approach is offered by regarding the isolated complexes as resulting from a fortuitous "quenching" of the solution species to give isolatable products. This assumes that the structures in solution are retained by the eventual crystalline samples, and, as indicated by Professor Curtis, available spectral information suggests that this is the case. Thus, for this discussion, the species $Ni(L1)^{2+}$, $Ni(L2)^{2+}$, $Ni(L3)^{2+}$ could be considered as occurring as the active intermediates in the potential energy/reaction coordinate profile, i.e.,



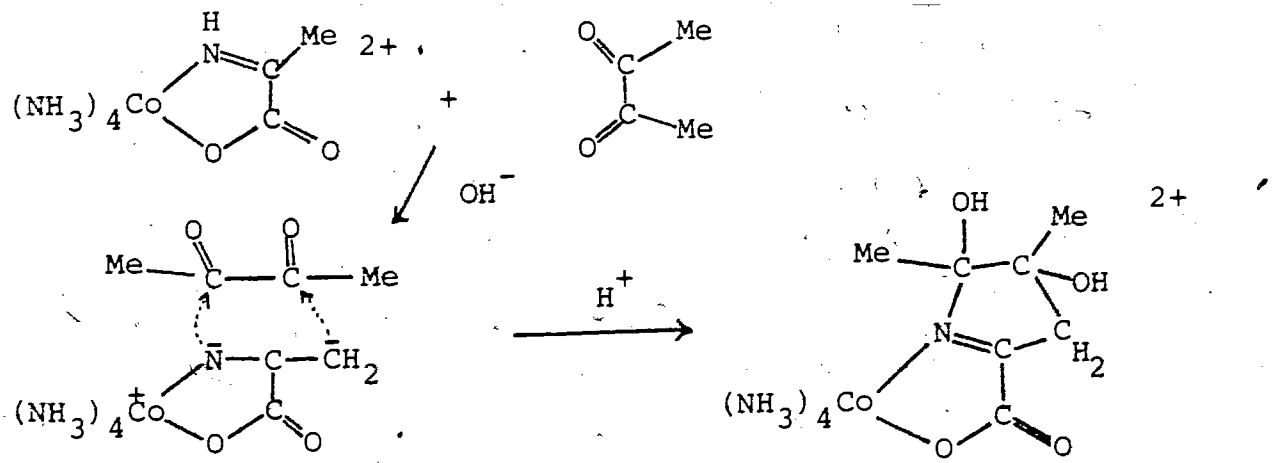
Another factor to be considered is whether the tetradentate ligand structure is retained in the formation of derivatives which provide suitable crystalline samples. For instance, the rapid elimination or hydrolysis of the "L1" ligand to give the starting L0 occurred in the formation of both thiocyanate and nitrite derivatives of L1. This raises two important questions: does an $Ni(L1)^{2+}$ species actually exist, and in the formation of the $Ni(L3)^{2+}$-nitrite derivatives (of which at least two distinct "types", α- and β-, exist) is the structure of L3 retained? For an $Ni(L1)^{2+}$ complex, where incorporation of the 2,3-butanedione into the ligand structure has occurred, there is some clear evidence as to its existence. Calculated analytical figures for such a formulation agree reasonably well with the determined values (section Ai, appendix), and a comparison of the i.r. spectra for $Ni(L0)(ClO_4)_2$ (figure A.2) and $Ni(L1)(ClO_4)_2 \cdot H_2O$ (figure A.1) indicate the appearance of $\nu(C=O)$ at 1685 cm^{-1} in the latter. In the solid state, the perchlorate salt of $Ni(L1)^{2+}$ is stable, but it is clearly quite fragile in solution, either giving L0, or, as apparent from the preparations described in the appendix, L2 or L3, depending on the conditions.

Further structural assignments of L1 are merely speculative: there are precedents for the isolation of a dicarbinolamine species. For instance, in the kinetic study of the condensation of 2,3-butanedione with $Ru(NH_3)_6^{3+}$ (initiated in basic solution by formation of coordinated $-NH_2^-$ nucleophiles) the rate data were explicable in terms of the

rapid formation of the di-carbinolamine[49]:



Second, in the condensation of the same diketone with the complex XII (chapter 1, page 16), a rapid reaction occurred to give, upon acid quenching, an orange, crystalline product, which, upon investigation, was found to contain the 4,5-dihydroxy-4,5-dimethylpyrolidime-2-carboxylate ligand[50]:

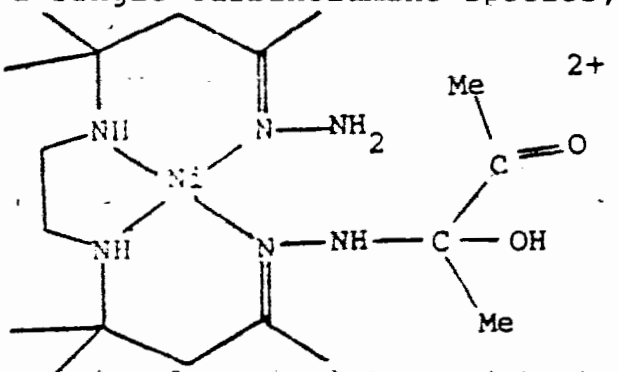


The initial step is assumed to be the addition of the deprotonated imine nitrogen to C=O, followed by degradation of the imine methyl to generate the carbanion which then completes the cyclization by addition to the other C=O. An interesting feature of this reaction is the stereospecificity of the orientation of the methyl and hydroxy groups in the product. The occurence of a cis- configuration is attributed to the bent hydrogen bonding assumed from the short O...O contact of 2.583(8) Å. If the H-bond were initiated before addition to the second C=O centre, then a specific direction could be

imposed on that step to yield the observed geometry of the two carbinol units.

In the present case, the instability of the proposed dicarbinolamine species is not surprising: it is likely that the seven-membered ring (which, presumably, is puckered to at least the same extent as found in $Ni(L4)^{2+}$) will not allow the same stablizing hydrogen-bonding, although, as seen in $Ni(L2)(H_2O)^{2+}$, stabilization via OH bonding to the nickel is a possibility. It could be argued, in fact, that formation of adducts of $Ni(L1)^{2+}$ (in lieu of suitable crystals of the simple complex) destroys any such Ni-hydroxy interaction, rendering the complex open to rapid elimination of the starting diketone.

A more likely structure for the L1 ligand, however, would be a non-cyclic species, incorporating a free carbonyl group, and a single carbinolamine species, i.e.,



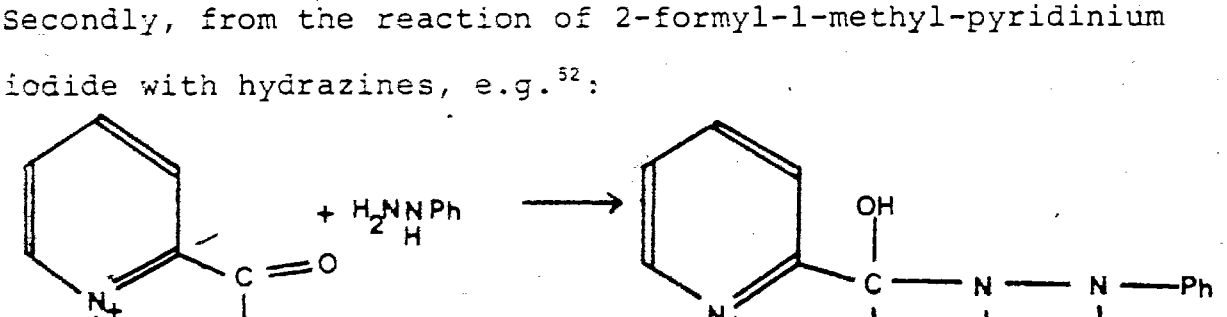
This structure is also consistent with the i.r. (figure A.1) which shows $\nu(C=O)$ at 1685 cm^{-1} and $\nu(N-H)(NH_2)$ at 3405 cm^{-1} (3400 cm^{-1} in $Ni(L0)(ClO_4)_2$). This non-cyclic structure allows also for the instability of L1 in solution, and also makes sense in terms of the products that can be obtained from L1 under various conditions, i.e. the non-cyclic L3, and the cyclic L2 and L4. Furthermore, it is also in accord with the known structure in solution of the

2,3-butanedione which has a trans arrangement of the carbonyl oxygen atoms. Thus the initial incorporation of the diketone into the L0 ligand is more likely to occur by sequential, rather than concerted, nucleophilic attack of the L0 hydrazone group on the carbonyl carbons of the diketone.

The isolation of carbinolamine intermediates is not common. Some examples where isolation has been possible are, firstly, the production of the condensation of chloral hydrate with thiosemicarbazide[51]:

$$Cl_3CCH(OH)_2 + NH_2NHCSNH_2 \longrightarrow Cl_3C\overset{\overset{OH}{|}}{C}(H)-N(H)-N(H)-\overset{\overset{S}{\|}}{C}-NH_2$$

Secondly, from the reaction of 2-formyl-1-methyl-pyridinium iodide with hydrazines, e.g.[52]:



The isolation and structural determination of the carbinolamine L2 in $Ni(L2)H_2O^{2+}$ is particularly fortuitous therefore, and a somewhat rare event considering their abundance as proposed intermediates in all manner of additions to C=O groups[53].

As already stated, in interpreting this structure of $Ni(L3)(NO_2)ClO_4 \cdot \frac{1}{2}H_2O$, the question of whether the structure of the ligand in the simple perchlorate ($Ni(L3)(ClO_4)_2$) is retained in the nitrite derivative must be considered in this instance, since there appears to be more than one derivative.

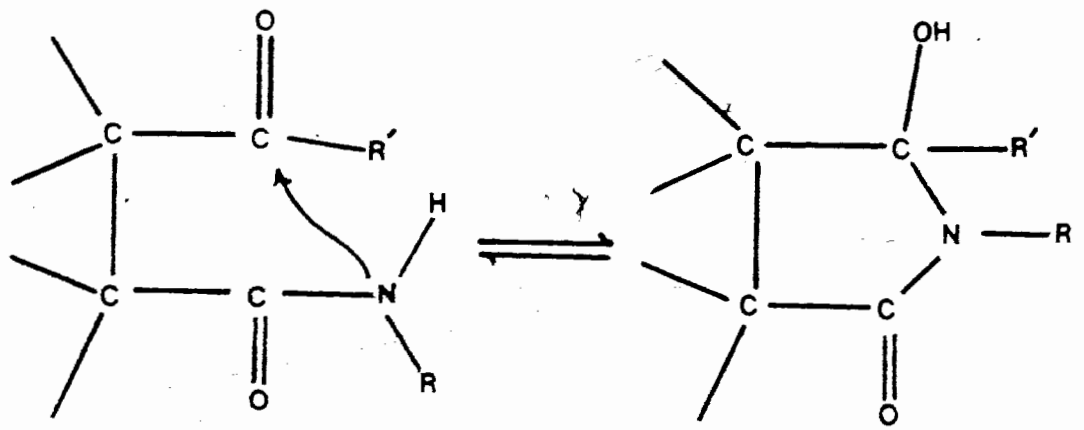
The conditions under which these complexes occur are given in the appendix (sections Avi and Aii). The analytical data indicate that the assignment of the same ligand formulation in $Ni(L3)(ClO_4)_2$ and α-$Ni(L3)NO_2(ClO_4)$ as that found in the crystallographic study of β-$Ni(L3)NO_2ClO_4 \cdot \frac{1}{2}H_2O$ is reasonable. Furthermore, the occurrence in the i.r. of $Ni(L3)(ClO_4)_2$ (at 1717 cm^{-1}; figure A.8) of a strong, sharp band attributable to $\nu(C=O)$ indicates that L3 is the same in each case (although the absence of any bands near 3400 cm^{-1} ($\nu(N-H)$ of $-NH_2$) in $Ni(L3)(ClO_4)_2$ does not support this conclusion). The α-derivative (a lavender compound) is formed immediately from the addition of sodium nitrite to a solution of $Ni(L3)(ClO_4)_2$. A solution of the α-derivative is then converted over a period of days to a dark blue solution of the β-derivative. The i.r. of the α-derivative (figure A.7) does not show any band assignable at $\nu(C=O)$, nor any band near 3400 cm^{-1} assignable as $\nu(N-H)(-NH_2)$. Also, the u.v./visible spectrum of the α- and β-derivatives differ markedly (sections Avi and Avii), although the NO_2^- ion is considered to be bidentate in each case.

On the basis of this incomplete set of analytical and spectral data, therefore, it is tentatively proposed that the L3 structure determined in β-$Ni(L3)NO_2(ClO_4) \cdot \frac{1}{2}H_2O$ is the same as in $Ni(L3)(ClO_4)_2$, and that the α-$Ni(L3)NO_2(ClO_4)_2$ derivative contains the same ligand formulation, but with some tautomeric and/or configurational difference. There is also the possibility of the α-derivative being a product of

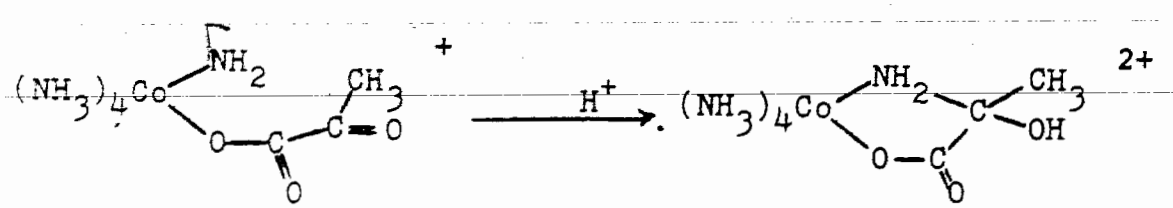
hydrolysis (i.e., L1) which then reacts further upon standing to re-form L3, although the absence of any indication of ν(C=O) does not support this.

Again, such discussion (on the basis of the absence of one peak in the i.r.) are tenuous: participation in strong hydrogen bonding by the carbonyl oxygen could shift the ν(C=O) frequency such that it becomes marked.

L3 (as determined for β-Ni(L3)$NO_2(ClO_4)\cdot\frac{1}{2}H_2O$) and also assigned for Ni(L3)$(ClO_4)_2$) is tautomeric with L2, and this may be compared with other cases of organic ring-closure tautomerisms. The most common of these is in the ring and chain isomers of the carbohydrates[54], although a better analogy to the present system is found in the amides of γ-keto acids[55], i.e.,

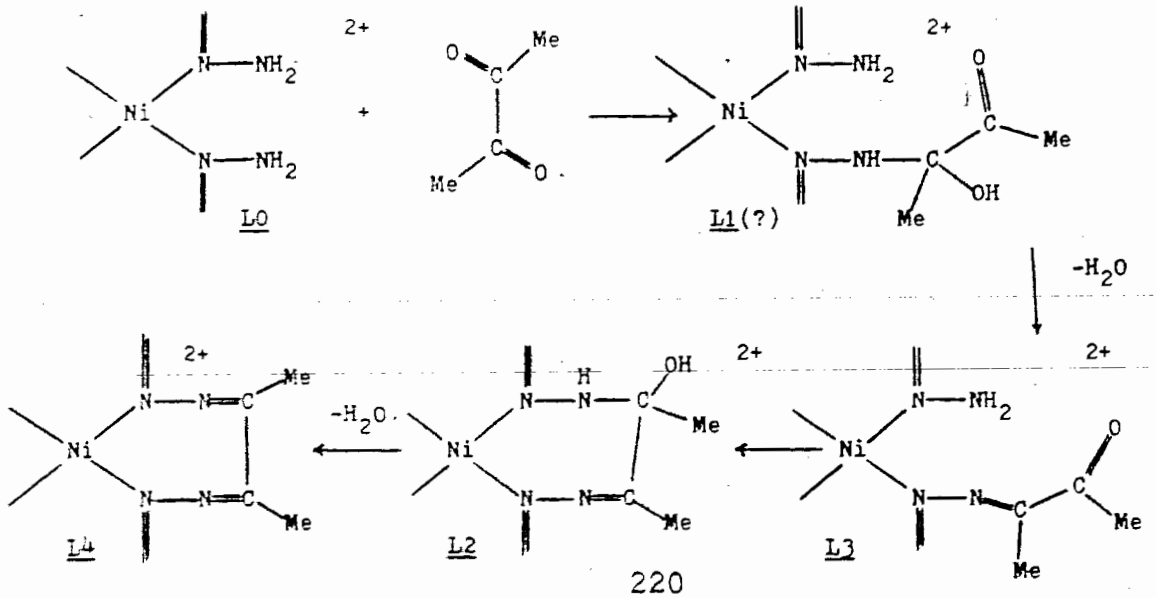


Interestingly, the L3 → L2 process also mimics the amide/pyruvate condensation[27] considered in 1v, page 16:



Investigations of the factors affecting the ease of ring closure reveal that cyclic formation is dependent on the degree of substitution[56] (this being related to the matching of the bond angle external to two substituents in the chain to that in the ring), to the east of rotation about single bonds[57] (which is restricted by increased substitution, thus favouring ring closure), and to the degree of unsaturation[58]. In the present system, of course, isolation of the individual tautomers does not permit much in the way of interpretation of stability relationships: isolation of a particular form may merely indicate it is the less soluble. A proper study would involve methods which do not themselves disturb the equilibrium, i.e., spectroscopy.

The foregoing structural, spectral, and analytical evidence, together with the preparative details for each of the complexes investigated, suggest a reasonable sequence for the condensation of 2,3-butanedione with the dihydrazone L0 to give the macrocycle L4 (figure 3.20).



This scheme is not only consistent with the available structural, spectral, and preparative data, it also makes reasonable chemical sense in the sequential nature of the condensation steps to form the cyclic system, i.e., nucleophilic attack at one carbonyl carbon, followed by elimination of a water molecule to give the imine species, and then cyclisation via nucleophilic attack at the second carbonyl carbon, with final elimination of a second water molecule to give the seven-membered diimine chelate in L4.

Further investigations of this reaction can be envisaged. Structurally, the confirmation of the L1 and L3 formulations should be possible, either by persistence in obtaining crystals of the simple perchlorates of $Ni(L1)^{2+}$ and $Ni(L3)^{2+}$, or by the synthesis of further derivatives where the ligand structure can be clearly seen to be unchanged.

As already stated, the interpretation into a mechanism of structural results obtained by the fortuitous quenching of solution species to give crystalline products involves several important assumptions, and the proposal can only be verified by the application of all possible spectroscopic methods. Further investigations of, for instance, the formation of $Ni(L2)^{2+}$ from $Ni(L1)^{2+}$ in aqueous solution, as opposed to $Ni(L3)^{2+}$ in non-aqueous solution, the $Ni(L2)^{2+}/Ni(L3)^{2+}$ tautomerism, and the kinetics of the condensation reaction require full spectroscopic tracking. It is hoped that the crystallographic work presented here provides something of a foundation for any such studies.

Chapter 4

Magnetic Exchange Interaction in a Carbonate-Bridged Copper(II) Dimer

4i. Introduction

Efforts directed at fully understanding the correlation between the magnetic and structural aspects of polynuclear, transition metal cluster complexes have increased a great deal in recent years. Attention has been focussed on interactions between paramagnetic clusters containing two or more centres, since these yield results which are simpler to interpret both qualitatively and quantitatively. The intensive interest can be attributed to several important potential applications: insight into the nature of overlap reactions between orbitals, especially when these may extend over relatively long distances (and which may have some special relevance to mechanisms of electron transfer processes); results which may be of importance to research into magnetic materials; in the case of copper(II) clusters, there is a relation to the so-called "type III" active sites in blue copper proteins, which are considered to comprise some kind of spin-paired Cu(II) dimer; and for its own sake, an understanding of magnetic/structural relationships is necessary to extend the use of magnetic susceptibility data for predicting the structures of co-ordination complexes. Although inorganic magnetochemistry has been widely used as a structural tool, the magnetic interactions to be discussed here themselves require detailed structural data for their correct interpretation.

Copper(II) complexes have an important place in the study of magnetic exchange: the phenomenon was first recognised

in copper(II) acetate hydrate[59], a system that has recieved by far the most experimental and theoretical attention, although interpretation of its magnetic behavior, especially in relation to that of other copper(II) carboxylate clusters, is still a matter of debate[60]. Copper(II) has a d^9 configuration, with one unpaired electron, and since theories of magnetic susceptibility are relatively simple for such systems, it also makes the study of divalent copper clusters more attractive. Large numbers of stable complexes have been synthesized[61], and have yielded to the sort of systematic structural investigation which is necessary to establish useful structure/magnetism correlations.

Magnetic interactions[62] can be roughly classified as ferromagnetic (where spins on neighboring paramagnetic metal ions align parallel to one another) and antiferromagnetic (where the spins align anti-parallel to one another). Antiferromagnetism (the concern of this work) is further classified according to the strength of the interaction: strong antiferromagnetism causes complete spin-pairing and the complex shows diamagnetic magnetic behavior. Frequently, in complexes where metal atoms are bridged by simple or polyatomic anions, weaker antiferromagnetic interaction gives low-lying excited states of different spins which can be populated at thermal energies. These latter interactions (often referred to as superexchange) occur over large distances (3 to 5 Å). The size and type of magnetic interaction for any system will depend on a variety of factors: the electron configurations of the metal ions, the distance between them, the electronic nature of the bridging and terminal ligands, and the detailed geometry of the cluster.

4ii. Applicable Theory[62]

Curie's law for paramagnetic substances is simply expressed as

$$\chi_m = \frac{C}{T}$$

where χ_m is the molar susceptibility, properly corrected for diamagnetism and temperature-independent paramagnetism, C is the Curie constant, and T is the absolute temperature. Ferromagnetic and antiferromagnetic behavior is easily recognised from χ_m versus T plots. In particular, antiferromagnetics give a maximum in χ_m at a characteristic temperature T_N, the Neel temperature. Above T_N, thermal energies randomise interactions which pair spins, leading to a χ_m/T relationship similar to that predicted by Curie's law. Below T_N, however, the interactions aligning the opposing spins dominate to give decreasing χ_m with decreasing T.

The mechanism(s) by which unpaired electron spins couple, and the precise factors which control the size and type of the interaction in a polynuclear cluster are not clearly understood despite the fact that theoretical foundations were laid fifty years ago in the Heisenberg, Dirac and Van-Vleck (HDVV) model[63,64] Although it contains many assumptions, the HDVV model works very well for a large number of magnetically-condensed systems. It is based on the spin-spin coupling having its origin in the quantum mechanical exchange effect, and for two atoms, i and j, of the total spins $\underline{S}_i = \Sigma \underline{s}_i$ and $\underline{S}_j = \Sigma \underline{s}_j$ ($\underline{s}_i$ and $\underline{s}_j$ are the spin angular momentum operators of the unpaired electrons), the exchange Hamiltonian is

$$\underline{H}_{ex} = -2J_{ij}\underline{S}_i\underline{S}_j .$$

J, the exchange integral is >0 for ferromagnetism and <0 for antiferromagnetism. From this, an expression can be derived for the magnetic susceptibility as a function of various parameters, including the g (gyromagnetic ratio) values for the metal ions involved, the exchange integral J, and absolute temperature, T. Analysis of susceptibility data then involves fitting the experimental χ_m/T curves to the theoretical expression, using J and g as parameters[60]. The simplest such theoretical expression is applicable to two interacting Cu(II) (spin ½) systems, and was first applied by Bleaney and Bowers[59] to copper acetate hydrate, and has since been applied to many Cu(II) dimers. Some recent developments in theory[64] aim to interpret the values and signs of the exchange integral, J, in terms of the orbital structure of the bridging unit[65-67], and some of the qualitative assumptions and arguments involved are relevant to the present work, and are worth summarising here.

When two metal ions are chemically bonded to a common set of closed-shell atoms, any unpaired electrons from the d orbitals on the metals will delocalise through extended molecular orbitals on to the bridge. The nature of the interaction between the unpaired electrons associated with the two metal centres is determined by the symmetry of the atomic orbitals in which these electrons reside. If the unpaired electron from one metal has some probability of being in an orbital which has some (say) p character on a given bridging atom, and an extended orbital with an unpaired electron from the other metal ion overlaps with this same p orbital, then exchange between these electrons will cause a splitting of spin

states such that the lowest energy configuration of the electron spins is when they are aligned antiparallel. This, again, is antiferromagnetic interaction, and it can be alternatively considered as weak bonding between the two metal ions propagated by the bridging ligand. Ferromagnetic interaction, on the other hand, will occur when there is no direct overlapping of orbitals containing the two unpaired metal d electrons which are in molecular orbitals which are orthogonal to each other, and the lowest energy configurations of the two spins will occur when they are parallel.

The simplest example of a bridging system where these two mechanisms may be illustrated is where two metal atoms are bridged by a single atom, M-X-M. If the bridging atom is positioned such that M-X-M is 180°, the metal d-orbitals in which the unpaired electrons are located will overlap the same bridging atom orbital, say the py. This will lead to bonding and antiferromagnetic coupling. Experimental confirmation lies in the structure of $(NH_3)_5Cr\text{-}O\text{-}Cr(NH_3)_5^{2+}$ [68] which has a Cr-O-Cr angle of 180 degrees, and is diamagnetic as a result of strong antiferromagnetic superexchange. The acid derivative of this cation, $(NH_3)_5Cr\text{-}OH\text{-}Cr(NH_3)_5^{3+}$ with a Cr-O-Cr angle of 166 degrees shows much weaker coupling ($J = -16\ cm^{-1}$)[68].

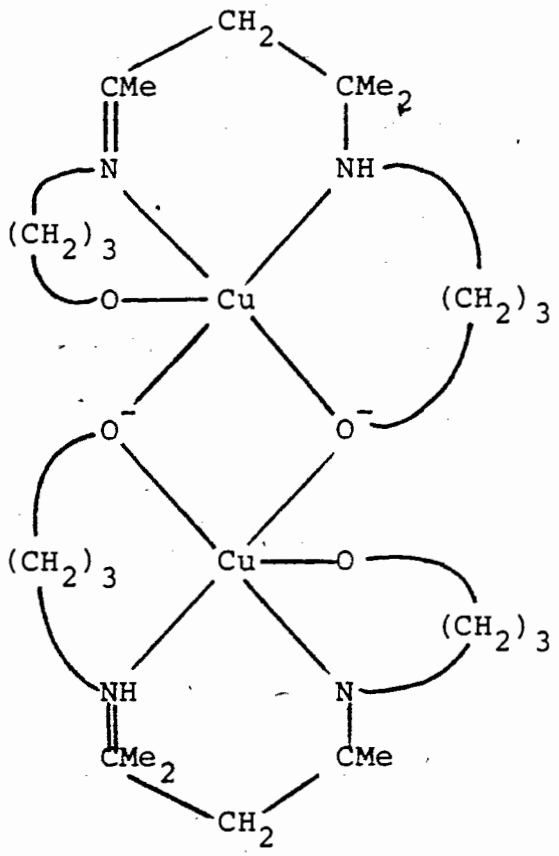
If the MXM angle equals 90 degrees, however, then the same metal d orbitals would overlap with orthogonal (say, px and py) orbitals, and ferromagnetic coupling would result. In the case of polyatomic bridging anions, the symmetries and energies of their molecular orbitals, and their overlap with

metal ion d orbitals is of concern. The resultant magnetic behavior will be the sum of the antiferromagnetic and ferromagnetic contributions from these various interactions.

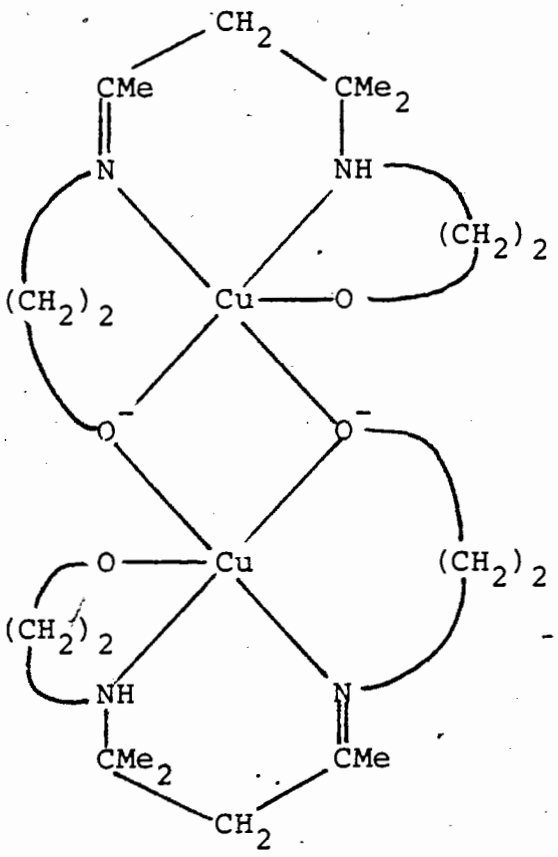
Efforts in the general field of interpreting magnetic exchange interactions can be recognised in two main areas. In systematically combining structural and magnetic data, Hodgson[68] has shown that dimers containing the Cu<O>Cu bridging unit show some interesting correlations. For example, the most ferromagnetic interaction ($2J = +172\ cm^{-1}$) was found for $[Cu(bipy)(OH)]_2(NO_3)_2$, where bipy is 2,2'-bipyridine, with a bridge (CuOCu) angle of 95.6(1) degrees. The largest bridge angle (104.1(2) degrees) occurs for the compound which exhibits the most antiferromagnetic interaction ($2J = -509\ cm^{-1}$) $[Cu(tmen)(OH)]_2Br_2$, where tmen is N,N,N',N'-tetramethylethylenediamine. A similar, though less well-defined trend has been noted in chloro-bridged dimers[69], and in a series of oxo-bridged Cu(II) dimers[70], the size of 2J has been correlated with the degree of distortion of the Cu(II) coordination geometries. Less success has been obtained in attempting similar correlations for carboxylate-bridged dimers[60], except to confirm the insensitivity of 2J to the short (2.56 - 2.88 Å) Cu-Cu distance (i.e., any direct Cu-Cu bonding is not the predominant route for superexchange), and that further investigations are still needed to firmly establish the factors which determine 2J in these complexes.

This point is well illustrated by a recent communication which gives the structures of two Cu(II) oxygen-bridged dimers. These dramatically show how fairly subtle

changes in the geometry of a complex can radically affect magnetic behavior[71]. Complex I has a CuOCu angle of 102.7(3) degrees, a Cu-Cu distance of 3.045(5)Å, while the distance of the copper atom from the square pyramidal basal plane is 0.08 Å, and is diamagnetic in the range 100°K to 300°K. Complex II has corresponding parameters of 98.2 degrees, 2.929(1) Å, and 0.19 Å, and exhibits the magnetic behavior of the monomer, with normal Curie-Weiss temperature dependence[71].



I



II

The other area which can be recognised is the application of molecular orbital theory to interpreting various modes of superexchange. As always, these studies rely heavily on the experimental correlations illustrated above, and future theoretical developments will only be improved or modified (or rejected) after much additional structural and magnetic data become available.

Early theoretical interpretations of superexchange were based on ideas developed for infinite solid lattices [65]. More recently, reports of studies have appeared which seek to extend such analyses to cases involving polyatomic bridging species [72-74]. In particular, an interesting paper by Hoffmann et al [74] establishes a connection between antiferromagnetically-coupled metal centres, and the well-established phenomenon of through-bond or through-space coupling of lone pairs or π electron systems in organic molecules [75].

4iii. Biological Role of Copper[76,77]

Although the understanding of the biological role of copper has escalated in recent years, there is still much speculation as to the exact nature of the coordination site of copper in each of the three types of active sites that have been delineated in copper proteins and enzymes[76]. As for other biologically important transition metals, copper is a required constituent in numerous essential proteins and enzymes which act as oxygen-carriers (hemocyanin), copper transport and hemoglobin formation (ceruloplasmin), oxidases (ascorbic acid

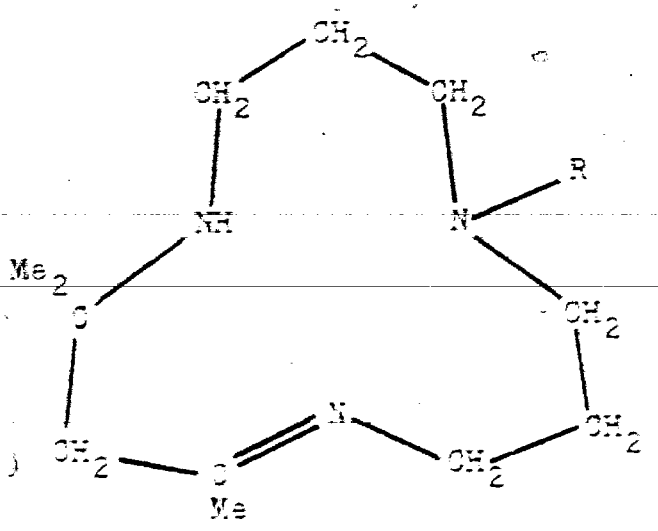
oxidase and cytochrome oxidase), photosynthesis (plastocyanin), and skin pigment formation (tyrosinase).

Of the three types of copper site so far observed, "type III" is the least understood, and the present work may have some bearing on it. This site is characterized by the following properties[76]: a redox potential greater than 0.5 V; diamagnetic properties when oxidised at room temperature; no detectable EPR signal in oxidised or reduced forms at 77 degress K; a near-uv absorption band of moderate intensity. On these bases, the proposed site contains some kind of spin-paired copper(II) dimer. The nature of any of the ligands is unknown.

4iv. Origin of $\{Cu(L2)\}_2CO_3.(ClO_4)_2$

The syntheses described in this section were performed in the laboratory of Professor N.F. Curtis, Victoria University, N.Z.

Condensation reactions of coordinated polyamines with ketones to give cyclic ligands have been described in detail elsewhere in this thesis (section 1v). Reaction of the polyamine bis (4-aza-heptane-1,7-diamine) coordinated to Ni(II) or Au(II) with acetone yields complexes of the macrocyclic ligand III[78].



III

L1, R = H

L2, R = Me

The macrocyclic system was proposed from the properties of the complexes, and confirmed by X-ray crystal analysis of NiL1$(NCS)_2$[79]. The macrocycles were also found to form a number of dinuclear compounds with five coordinate copper(II) and nickel(II), with di-μ-chloro, di-μ-hydroxo, μ-oxalate, μ-carbonate, and other bridging groups. Several of these dimers exhibit spin-pairing via exchange interaction, and the μ-carbonate $[Cu(L2)]_2CO_3 \cdot (ClO_4)_2$ is completely spin-paired, showing only a small, residual, temperature-independent magnetism over the range 100 - 300 deg K. This represents a case where antiferromagnetic superexchange is large enough to cause complete spin-pairing at all temperatures. Examples of such behavior are very rare for Cu(II) dimers[71, 80-82] and a complete structural characterization is clearly desirable in order to establish the exact geometrical conditions which give rise to such unusual magnetic behavior.

4v. Experimental

A sample of $[Cu(L2)]_2CO_3 \cdot (ClO_4)_2$ was kindly supplied by Professor Neil Curtis (Victoria University of Wellington, New Zealand), and large, dark green, elongated plates were grown by slow evaporation of a 1:1 dimethylformamide(DMF)/isopropanol solvent mixture. A fragment of approximate dimensions 0.6 x 0.1 x 0.2 mm was selected and mounted for the purpose of photographic investigation, with the needle axis approximately coincident with the spindle axis of the cameras. Cu radiation (λ = 1.5418 Å) was used to obtain Weissenberg photographs of the hk0 and hk1 layers, together with precession photographs of the 0k1, 1k1, h0l and h1l

layers which established orthorhombic Laue symmetry, with systematic absences $hkl, h+k+l = 2n+1$; $h0l$, $h = 2n+1$; $0kl$, $k = 2n+1$, consistent with the space groups Iba2 and Ibam (the former was indicated by the structure analysis).

Accurate cell dimensions were determined from counter measurement of 12 of the strongest reflections having $2\theta > 25$ deg using a Picker FACS-1 computer-controlled, four-circle diffractometer (MoK_α radiation, $\lambda = 0.70926$ Å)

Crystal data: $Cu_2Cl_2O_{12}N_7C_{30}H_{59}$; formula weight 907.8; space group Iba2; cell dimensions, a = 16.19(1) Å, b = 16.67(1) Å, c = 15.43(I) Å, V = 4164 $Å^3$; measured density (flotation) = 1.35(2) g mL^{-1}, Z = 4, calculated density = 1.34 g mL^{-1}, $\mu(MoK\alpha)$ = 7.0 cm^{-1}, T = 22(± 1) deg C.

Intensity data for the unique set of reflections with $2\theta < 50$ deg were collected using a θ-2θ scan of base width of 1.5 deg (increased to allow for dispersion), at a scan speed of 2 deg min^{-1} using graphite monochromatized Mo-Kα radiation, $\lambda_{\alpha 1}$ = 0.70926 Å. Background counts were made at each scan limit. Two reflections used as standards were measured after every 100 reflections in order to monitor instrumental stability and crystal alignment; their variation was ± 4% over the entire data collection. Measured intensities were corrected for Lorentz and polarization effects; absorption was neglected since it was estimated to introduce a maximum error of ± 1.5% in I, the net count. 1895 reflections were measured, of which 1230 were considered as observed, (i.e., greater than $2.3\sigma_I$, where $\sigma_I = [TC + (t_s/t_B)^2 (B_1 + B_2)$

+ $(kI)^2]^{1/2}$; TC is the total count, B_1 and B_2 are background counts at either end of the scan range, t_s is the scan time, t_b is the total background count time, k is a constant set to 0.03, and I is the net count).

4vi. Structural Determination

The positions of the unique copper and chlorine atoms were determined from a three-dimensional Patterson synthesis based on all the observed data, and these were refined together with a scale factor to give a residual, R = 0.447 where $R = \Sigma(|F_o| - |F_c|) / \Sigma|F_o|$. A Fourier synthesis on F_o with phases from F_c gave the positions of the light atoms coordinated to the copper, and the perchlorate oxygen atoms. Several cycles of full-matrix least-squares refinement and subsequent electron density difference maps gave the positions of all other light atoms in the macrocycle and the complete carbonate anion. With R = 0.085, it was clear that the perchlorate anion was disordered (large oxygen atom anisotropic thermal motion parameters) and that two of these atoms could be better described as "split atoms" (O11, O12 and O13, O14) each assigned an occupancy of 0.5. Furthermore, an array of small but significant peaks on, or close to, the two-fold axis of symmetry were observed in the electron density difference map. Careful inspection of the angles and distances around these peaks revealed a satisfactory picture of a dimethylformamide solvent molecule of crystallization disordered about the two-fold axis,

the nitrogen and oxygen atoms lying on the axis, and the carbon atom of one of the methyl groups being best described as two split atoms (C14, C14'). Hydrogen atom positions were also determined from the electron density difference maps or, in the case of some methyl hydrogens, were calculated. Subsequent refinement of the positions of the non-hydrogen atoms, all of which were assigned anisotropic thermal motion parameters (except for the DMF solvent molecule atoms and the split perchlorate oxygen atoms) gave a final R of 0.052 (227 variables). The only outstanding features were found in a final electron density difference map near the metal ion and the perchlorate anion (0.2 ± 0.07 electrons $\AA^{-3}$). In the early stages of the refinement, unit weights were used; in the later stages, weights = $(1/\sigma_F^2)$ were used, where $\sigma_F = \sigma_I / (L_p(2Fo))$.

Atomic positional coordinates are listed in table 4.1, and thermal motion parameters in table 4.2. A listing of observed and calculated structure factors (x10) ca be found in table 4.3. Atomic scattering factors used in this determination were taken from reference 35, with corrections for anomalous scattering for the copper and chlorine atoms.

Table 4.1

Fractional Atomic Coordinates: $(\{Cu(L2)\}_2CO_3)(ClO_4)_2 \cdot DMF$ X 10^4 (X 10^5 for Cu).

Least-squares estimates errors are given in parentheses.

Atom	x	y	z
Cu	9407(6)	8142(5)	5813
O1	0	0	542(7)
O2	519(4)	460(3)	1759(4)
N1	1232(5)	1930(5)	890(4)
N2	2123(4)	171(4)	587(7)
N3	984(5)	1015(4)	- 670(5)
C1	624(6)	2469(6)	425(5)
C2	809(6)	2448(7)	- 553(6)
C3	914(6)	1681(6)	-1035(5)
C4	1133(6)	275(6)	-1157(5)
C5	2000(7)	- 22(7)	-1050(2)
C6	2189(8)	- 382(8)	- 207(7)
C7	2786(5)	777(6)	558(11)
C8	2674(6)	1475(7)	1146(7)
C9	2132(8)	2097(7)	795(7)
C10	- 242(6)	2183(5)	640(9)
C12	756(8)	3333(6)	734(11)
C31	953(7)	1819(6)	-1988(7)
C(N2)	2182(8)	- 309(9)	1356(10)
C	0	0	1398(8)

Table 4.1 (continued)

Atom	x	y	z
Perchlorate Anion:			
Cl	1643(2)	2643(3)	3324(2)
Cl1	1426(21)	1935(19)	3028(2)
O12 *	1048(11)	2375(11)	2881(11)
O13 *	1894(15)	3383(14)	2840(18)
O14 *	2114(15)	3056(16)	2716(17)
O15	1396(10)	3079(10)	3991(10)
O16	2269(13)	2190(10)	3607(16)
DMF			
N	0	5000	3051(15)
O	0	5000	4483(29)
C13	726(23)	5141(24)	2645(27)
C14*	- 75(29)	560(29)	321(35)
C14*	- 16(30)	415(29)	300(35)
C15	502(27)	5061(30)	3848(34)

* Split atoms, each assigned an occupancy of 0.5.

Table 4.1 (continued)

Calculated Hydrogen Atom Fractional Coordinates
($x10^4$)

	x	y	z
H(N1)	1187	2008	1509
H2(1)	1303	2762	-630
H2(2)	348	2729	-822
H4(1)	1012	375	-1772
H4(2)	738	-142	-967
H5(1)	2345	445	-1133
H5(2)	2099	-408	-1487
H6(1)	1831	-819	-119
H6(2)	2757	-551	-237
H7(1)	2831	964	-18
H7(2)	3288	450	731
H8(1)	3222	1696	1239
H8(2)	2457	1281	1683
H9(1)	2248	2603	1087
H9(2)	2243	2172	178
H10(1)	-336	2141	1339
H10(2)	-635	2559	385
H10(3)	-330	1662	367
H12(1)	1322	3440	614
H12(2)	395	3701	391
H12(3)	611	3404	1334
HN2(1)	1911	-798	1285
HN2(2)	2767	-419	1434
HN2(3)	1964	-6	1813
HC31(1)	500	2294	-2200
HC31(2)	746	1314	-2300
HC31(3)	1475	1934	-2205

Table 4.1 (continued)

DMF Molecule	x	y	z
H(C131)	622	5163	2142
H(C132)	908	5772	2775
H(C133)	391	5506	1959
H(C141)	875	4375	2500
H(C142)	1131	4639	3440
H(C143)	510	3921	3317
H(C14'1)	-460	3840	3000
H(C14'2)	-701	6177	3210
H(C14'3)	-1325	5453	3160
H(C15)	322	4588	4222

Table 4.2

Thermal Motion Parameters: $(\{Cu(L2)\}_2CO_3)(ClO_4)_2 \cdot DMF$

$X\ 10^3$ ($X\ 10^4$ for Cu) $Å^2$

Anisotropic Parameters

Atom	U11	U22	U33	U12	U13	U23
Cu	568(5)	589(5)	316(4)	-140(5)	12(9)	12(8)
O1	58(5)	56(4)	41(5)	- 21(4)	0	0
O2	67(4)	70(4)	30(3)	- 22(4)	0(3)	6(3)
N1	76(5)	84(6)	30(4)	- 23(5)	- 6(4)	1(4)
N2	9(4)	81(5)	43(4)	5(4)	0(7)	22(7)
N3	55(5)	69(6)	37(4)	- 1(4)	- 3(4)	- 1(4)
C1	81(7)	68(6)	33(7)	- 1(5)	6(5)	14(5)
C2	64(7)	100(8)	50(6)	- 15(6)	- 6(5)	33(6)
C3	56(6)	66(6)	35(5)	5(5)	- 7(5)	2(5)
C4	91(9)	87(8)	28(5)	- 17(6)	9(5)	- 15(5)
C5	98(9)	102(8)	49(6)	13(8)	16(7)	- 3(6)
C6	112(10)	72(9)	38(7)	22(8)	24(7)	0(6)
C7	55(5)	117(7)	60(6)	3(6)	- 18(9)	- 2(9)
C8	40(7)	140(12)	60(7)	- 9(7)	- 18(5)	33(7)
C9	89(8)	107(8)	59(9)	- 66(7)	- 2(7)	- 5(6)
C10	77(7)	82(6)	71(7)	24(5)	14(9)	33(8)
C12	179(12)	66(6)	110(12)	- 9(7)	32(13)	- 22(9)
C31	60(6)	84(7)	74(7)	0(6)	17(6)	35(6)
C(N2)	76(10)	104(14)	113(12)	30(10)	26(9)	20(10)
C	80(11)	46(8)	29(8)	4(8)	0	0
O13	260(5)	285(17)	139(10)	-114(14)	43(11)	-115(12)
O14	280(2)	241(18)	415(29)	- 98(15)	-254(23)	122(18)

Table 4.2 (continued)

Atom	U
O11	189(12)
O11'	132(9)
O12	86(5)
O12'	122(8)
N	114(4)
O	153(14)
C13	174(15)
C14	129(21)
C14'	127(23)
C15	208(19)

Table 4.3

Structure Factor Listing: $(\{Cu(L2)\}_2CO_3)(ClO_4)_2 \cdot DMF$

(x 10)

Unobserved reflections are denoted by an asterisk.

L	FO	FC	ALPHA
H=	0, K=	0	
2	1363	1370	1
4	2528	2650	115
6	1189	1151	148
8	1415	1496	164
10	753	777	220
12	670	693	266
14	471	465	274
16	304	305	353
18	342	343	12
H=	0, K=	2	
0	121	20	97
4	723	742	278
6	661	638	98
8	402	409	103
10	541	562	239
12	484	481	239
14	186	203	112
16	296	316	148
18	129	118	28
H=	0, K=	4	
0	1806	1737	359
2	829	805	261
4	401	384	176
6	460	446	353
8	26*	50	226
10	119	104	98
12	77	78	1
14	147	170	176
16	157	173	136
18	11*	37	257
H=	0, K=	6	
0	413	423	186
2	776	715	205
4	747	783	243
6	430	467	275
8	835	857	13
10	671	679	0
12	123	139	107
14	328	329	120
16	226	237	151
H=	0, K=	8	
0	242	196	185
2	491	537	262
4	338	351	264
6	295	297	145
8	196	190	353
10	340	339	99
12	176	193	101
14	95	73	156
16	124	115	145
H=	0, K=	10	
0	208	238	2
2	251	249	26
4	272	264	90
6	391	386	162
8	201	217	156
10	86	70	214
12	178	174	269
14	135	129	345
H=	0, K=	12	
0	549	566	2
2	378	387	26
4	464	481	88
6	413	425	136
8	340	349	156
10	273	275	190
12	266	270	239
14	190	200	114
H=	0, K=	14	
0	83	80	10
2	237	254	58
4	241	239	88
6	202	205	129
8	95	130	162
10	118	125	198
12	148	137	259
H=	0, K=	16	
0	40*	58	185
2	56*	72	208
4	44*	25	307
6	27*	70	141
8	35*	36	211
10	42*	55	255
H=	0, K=	18	
0	94	102	187
2	157	127	226
4	135	137	260
6	127	98	309
H=	1, K=	19	
0	89*	69	187
2	104	63	222
4	100	102	261
H=	1, K=	18	
7	41*	10	341
5	34*	39	256
3	24*	34	235
1	86	35	181
H=	1, K=	17	
0	83*	80	186
2	125	95	220
4	129	101	273
6	101	93	308
8	105	84	26
H=	1, K=	16	
9	102	83	220
7	106	99	342
5	144	122	115
3	154	174	242
1	150	143	215
H=	1, K=	15	
0	44*	21	8
2	97	115	254
4	111	112	96
6	34*	31	80
8	58*	43	235
10	82*	57	181
H=	1, K=	14	
11	15*	75	216
9	78*	107	355
7	61*	87	146
5	129	143	280
3	61*	86	227
1	139	138	180
H=	1, K=	13	
0	172	182	5
2	309	314	223
4	250	248	83
6	286	280	134
8	165	163	148
10	179	176	202
12	174	171	246

L	FO	FC	ALPHA
H= 1, K= 12			
13	11*	43	265
11	10*	44	97
9	73*	57	156
7	32*	82	331
5	73*	60	27
3	32*	48	141
1	20*	33	110
H= 1, K= 11			
0	329	306	3
2	284	308	26
4	334	342	96
6	265	256	138
8	213	221	174
10	176	164	178
12	210	203	257
14	148	153	298
H= 1, K= 10			
15	140	116	131
13	106	114	267
11	209	219	233
9	27*	61	195
7	205	207	140
5	121	117	129
3	255	256	63
1	254	262	20
H= 1, K= 9			
0	53*	21	349
2	284	296	224
4	90	102	92
6	235	223	177
8	8*	17	257
10	81	79	162
12	33*	45	187
14	120	107	1
16	11*	35	212
H= 1, K= 8			
15	81*	78	140
13	210	208	300
11	79	62	238
9	321	334	185
7	220	206	198
5	214	219	94
3	408	392	227
1	460	467	21
H= 1, K= 7			
0	752	760	182
2	755	713	234
4	574	559	260
6	394	406	144
8	491	485	359
10	353	367	228
12	179	157	254
14	187	161	144
16	197	191	146
H= 1, K= 6			
17	61*	67	222
15	83*	79	103
13	27*	36	141
11	150	133	149
9	178	159	18
7	298	304	329
5	417	403	105
3	262	268	112
1	142	157	164
H= 1, K= 5			
0	229	212	188
2	316	411	175
4	223	192	215
6	305	316	147
8	424	441	5
10	342	329	6
12	153	137	93
14	226	227	120
16	172	179	157
H= 1, K= 4			
17	173	179	174
15	221	228	145
13	118	135	92
11	333	319	219
9	541	552	8
7	621	587	130
5	734	726	277
3	482	472	208
1	398	371	249
H= 1, K= 3			
0	4*	29	4
2	509	477	250
4	318	314	199
6	371	412	63
8	71	82	51
10	196	162	207
12	9*	85	259
14	103	103	240
16	49*	60	358
18	11*	51	11
H= 1, K= 2			
17	150	163	184
15	135	126	143
13	144	158	95
11	187	203	251
9	285	275	6
7	707	703	335
5	619	621	132
3	725	720	280
1	1162	1183	180
H= 1, K= 1			
0	1447	1285	1
2	1251	1251	228
4	440	475	133
6	746	799	117
8	685	685	152
10	505	514	225
12	366	370	257
14	226	237	110
16	260	249	340
18	206	186	19
H= 2, K= 0			
0	120	73	12
2	400	336	50
4	399	418	349
6	493	485	129
8	715	751	147
10	287	321	206
12	143	148	204
14	69*	67	21
16	170	162	147
18	44*	62	30
H= 2, K= 1			
17	71*	88	140
15	198	181	175
13	70*	33	144
11	349	355	245
9	294	285	30
7	769	795	335
5	613	621	352
3	1088	1045	210

L	FO	FC	ALPHA
H=	2, K=	1	
1	1374	1310	232
H=	2, K=	2	
0	374	471	1
2	970	948	207
4	372	327	139
6	241	233	339
8	188	224	206
10	70	72	144
12	191	165	28
14	66*	13	267
16	10*	58	29
18	11*	47	220
H=	2, K=	3	
17	303	295	191
15	264	266	129
13	439	421	107
11	287	307	60
9	710	696	3
7	668	641	146
5	856	842	272
3	589	562	306
1	1007	1000	160
H=	2, K=	4	
0	169	173	183
2	392	353	95
4	277	322	132
6	226	249	266
8	150	143	78
10	8*	38	223
12	180	200	131
14	86	106	105
16	40*	47	266
H=	2, K=	5	
17	164	176	159
15	157	173	153
13	98	97	16
11	330	338	224
9	276	263	21
7	534	556	304
5	227	208	147
3	456	485	207
1	595	593	245
H=	2, K=	6	
0	220	230	183
2	421	387	246
4	149	164	229
6	318	318	335
8	217	214	141
10	176	183	229
12	119	114	214
14	106	71	115
16	97	117	140
H=	2, K=	7	
17	91*	89	134
15	176	170	147
13	73*	95	269
11	255	261	182
9	208	212	158
7	255	265	154
5	133	133	218
3	550	556	1
1	230	231	55
H=	2, K=	8	
0	32*	65	352
2	73	105	146
4	171	193	357
6	177	198	250
8	99	84	13
10	77	51	136
12	117	89	157
14	82*	68	220
16	49*	26	134
H=	2, K=	9	
15	175	166	138
13	248	244	301
11	143	177	247
9	354	350	196
7	346	359	188
5	462	472	106
3	567	561	83
1	504	508	17
H=	2, K=	10	
0	95	139	2
2	81	71	5
4	143	148	106
6	101	107	269
8	9*	98	267
10	107	101	139
12	64*	81	253
14	82*	105	131
H=	2, K=	11	
15	125	95	303
13	122	144	259
11	197	186	229
9	163	168	176
7	243	242	139
5	163	192	109
3	275	280	225
1	253	266	218
H=	2, K=	12	
0	261	273	2
2	240	232	29
4	186	183	78
6	100	138	171
8	110	88	177
12	123	125	244
14	76*	75	141
H=	2, K=	13	
13	11*	63	247
11	88*	91	58
9	103	76	348
7	173	178	339
5	104	137	136
3	118	106	218
1	198	209	180
H=	2, K=	14	
0	9*	57	4
2	68*	76	56
4	97	77	82
6	60*	13	143
8	10*	25	247
10	10*	66	196
12	80*	73	268
H=	2, K=	15	
11	152	131	52
9	118	128	23
7	151	149	145
5	227	210	112
3	167	195	242
1	178	172	204
H=	2, K=	16	
0	14*	12	345
2	37*	14	97

L	FO	FC	ALPHA
4	33*	23	300
6	40*	74	309
8	44*	30	7
10	11*	24	96
H=	2, K=	17	
9	70*	74	14
7	87*	69	353
5	112	110	277
1	110	99	207
7	87*	69	353
5	112	110	277
3	137	141	247
1	110	99	207
H=	2, K=	18	
0	23*	11	333
2	11*	24	175
4	11*	41	237
6	11*	43	299
H=	2, K=	19	
3	25*	25	79
1	50*	33	221
H=	3, K=	19	
0	61*	46	2
2	103	52	249
4	11*	26	106
H=	3, K=	18	
7	11*	20	331
5	11*	41	109
3	11*	36	252
1	66*	5	180
H=	3, K=	17	
0	73*	57	1
2	25*	40	249
4	37*	34	132
6	45*	9	213
8	55*	15	219
H=	3, K=	16	
9	121	103	24
7	137	107	345
5	160	166	110
3	193	189	250
1	126	120	222
H=	3, K=	15	
0	39*	19	188
2	60*	19	222
4	87	55	275
6	22*	21	255
8	59*	51	217
10	11*	13	192
H=	3, K=	14	
11	137	103	218
9	101	98	358
7	162	156	138
5	177	178	305
3	109	114	221
1	151	163	192
H=	3, K=	13	
0	71*	51	355
2	48*	14	216
4	51*	62	131
6	99	88	307
8	76*	75	112
10	27*	53	95
12	11*	25	11
H=	3, K=	12	
13	39*	36	301
11	28*	43	174
9	94	85	202
7	74*	74	85
5	106	100	249
3	58*	86	225
1	18*	57	132
H=	3, K=	11	
0	187	210	181
2	8*	66	227
4	107	108	301
6	68*	26	250
8	130	153	15
10	9*	15	198
12	82*	78	179
14	11*	38	0
H=	3, K=	10	
15	169	151	141
13	203	200	274
11	265	274	246
9	240	244	188
7	424	443	155
5	435	425	110
3	462	468	245
1	382	377	19
H=	3, K=	9	
0	7*	9	28
2	102	98	226
4	179	201	94
6	26*	58	357
8	96	105	239
10	137	118	137
12	97	87	282
14	69*	73	107
16	11*	33	256
H=	3, K=	8	
15	207	207	148
13	207	211	297
11	191	192	188
9	430	436	182
7	443	444	174
5	524	553	119
3	583	591	60
1	486	479	22
H=	3, K=	7	
0	94	114	177
2	357	382	253
4	134	145	251
6	166	151	190
8	64*	56	143
10	79	98	237
12	84	63	182
14	68*	111	0
16	24*	40	305
H=	3, K=	6	
17	88*	36	118
15	10*	79	18
13	9*	87	351
11	111	108	158
9	69	40	114
7	273	252	174
5	95	103	153
3	374	393	13
1	347	351	203
H=	3, K=	5	

L	FO	FC	ALPHA
H= 3, K= 5			
0	56	22	23
2	64	98	125
4	138	156	63
6	70	100	28
8	159	130	157
10	248	246	145
12	60*	54	105
14	155	133	107
16	11*	63	352
H= 3, K= 4			
17	246	237	174
15	295	290	135
13	262	263	100
11	405	400	229
9	559	576	19
7	471	478	146
5	261	257	280
3	793	834	251
1	1227	1176	216
H= 3, K= 3			
0	608	656	180
2	573	605	92
4	75	61	20
6	49*	60	0
8	133	98	226
10	51*	44	214
12	92	116	55
14	114	105	225
16	50*	32	229
H= 3, K= 2			
17	175	182	176
15	205	197	140
13	261	256	97
11	364	350	251
9	476	494	5
7	602	572	142
5	441	459	114
3	106	114	254
1	982	986	168
H= 3, K= 1			
0	664	750	180
2	478	555	120
4	154	114	331
6	236	237	358
8	56*	79	58
10	92	96	114
12	139	149	249
14	54*	26	151
16	37*	38	216
18	11*	27	182
H= 4, K= 0			
0	581	452	184
2	882	767	92
4	484	532	111
6	622	593	145
8	527	514	359
10	118	129	227
12	141	171	110
14	52*	72	136
16	45*	117	208
H= 4, K= 1			
17	146	135	184
15	64*	101	249
13	200	201	82
11	56*	79	358
9	416	395	345
7	264	275	352
5	291	304	260
3	431	430	340
1	1445	1422	153
H= 4, K= 2			
0	871	886	359
2	405	392	241
4	149	169	237
6	521	562	304
8	70	52	221
10	198	182	54
12	122	114	26
14	62*	67	162
16	149	140	168
H= 4, K= 3			
17	149	150	167
15	308	283	143
13	158	141	103
11	456	472	248
9	284	289	219
7	640	649	138
5	299	300	145
3	904	923	239
1	1109	1119	237
H= 4, K= 4			
0	624	605	1
2	715	711	216
4	199	143	256
6	380	380	144
8	314	329	148
10	252	258	221
12	246	239	253
14	154	171	142
16	109	122	332
H= 4, K= 5			
17	121	120	169
15	82*	109	250
13	154	132	81
11	67*	71	356
9	502	496	7
7	122	90	235
5	317	312	236
3	119	104	227
1	589	570	186
H= 4, K= 6			
0	765	738	2
2	515	539	220
4	466	427	257
6	193	188	144
8	464	477	175
10	453	454	178
12	201	197	246
14	296	295	300
16	174	179	337
H= 4, K= 7			
15	67*	72	330
13	165	157	114
11	177	184	147
9	393	394	174
7	195	199	191
5	448	441	103
3	347	333	14
1	297	287	353
H= 4, K= 8			
0	487	513	1
2	424	405	51
4	396	397	107
6	318	303	146
8	207	205	159
10	109	109	241
12	222	214	254

L	FO	FC	ALPHA
14	74*	72	296
16	58*	66	343
H=	4, K=	9	
15	182	185	338
13	169	163	106
11	248	257	244
9	148	153	185
7	417	402	153
5	331	339	116
3	452	454	58
1	247	253	217
H=	4, K=	10	
0	67*	28	193
2	135	145	233
4	34*	63	51
6	88	82	22
8	109	70	216
10	23*	56	166
12	10*	53	185
14	11*	2	109
H=	4, K=	11	
13	93	117	274
11	92	128	220
9	215	214	188
7	183	189	153
5	287	295	104
3	280	264	252
1	327	333	15
H=	4, K=	12	
0	263	271	183
2	224	221	218
4	175	185	263
6	211	200	133
8	162	171	0
10	161	167	55
12	93	105	86
14	97	102	121
H=	4, K=	13	
13	70*	56	96
11	10*	65	30
9	63*	84	356
7	132	108	351
5	119	126	301
3	87	88	244
1	207	199	173
H=	4, K=	14	
0	9*	21	148
2	75*	109	241
4	119	94	234
6	84	67	274
8	83*	60	25
10	76*	68	217
12	11*	55	105
H=	4, K=	15	
11	55*	70	52
9	60*	42	7
7	76*	89	332
5	134	123	301
3	142	124	241
1	68*	70	219
H=	4, K=	16	
0	48*	39	3
2	22*	16	342
4	10*	21	183
6	38*	43	110
8	41*	44	119
10	40*	31	171
H=	4, K=	17	
7	67*	38	351
5	65*	79	281
3	71*	81	244
1	54*	34	199
H=	4, K=	18	
0	111	106	4
2	95	101	55
4	59*	92	97
6	116	78	125
H=	4, K=	19	
3	43*	41	61
1	68*	62	28
H=	5, K=	19	
0	128	129	4
2	81*	100	52
H=	5, K=	18	
5	11*	12	136
3	50*	26	159
1	49*	23	222
H=	5, K=	17	
0	107	106	5
2	107	131	52
4	62*	91	104
6	102	114	124
8	92	65	172
H=	5, K=	16	
9	11*	25	228
7	34*	45	249
5	29*	58	110
3	61*	51	247
1	10*	25	161
H=	5, K=	15	
0	41*	38	354
2	69*	105	250
4	90	86	248
6	10*	7	140
8	69*	79	254
10	29*	46	249
H=	5, K=	14	
11	39*	49	19
9	10*	17	260
7	47*	65	329
5	72*	65	137
3	76*	110	206
1	52*	40	227
H=	5, K=	13	
0	211	201	186
2	217	211	221
4	219	226	254
6	136	151	132
8	193	179	357
10	147	141	28
12	109	127	254
H=	5, K=	12	
13	86*	62	117
11	29*	5	340
9	90	84	6
7	53*	52	57
5	119	105	251

L	FO	FC	ALPHA
H=	5, K=	12	
3	52*	32	112
1	76*	62	97
H=	5, K=	11	
0	359	371	183
2	272	269	213
4	278	272	261
6	215	219	329
8	229	247	7
10	187	179	229
12	132	143	88
14	142	123	134
H=	5, K=	10	
15	11*	16	271
13	101	113	275
11	54*	33	240
9	88	83	167
7	9*	46	297
5	126	109	81
3	78	58	152
1	162	157	145
H=	5, K=	9	
0	215	183	1
2	164	188	246
4	217	215	114
6	240	236	114
8	91	111	94
10	83	111	250
12	146	150	244
14	11*	66	270
H=	5, K=	8	
15	75*	74	356
13	10*	26	281
11	147	159	217
9	9*	42	341
7	112	107	131
5	87	71	145
3	313	311	24
1	71	79	221
H=	5, K=	7	
0	743	723	2
2	670	663	229
4	591	621	85
6	519	535	127
8	515	518	162
10	399	389	201
12	322	323	254
14	255	240	298
16	201	193	340
H=	5, K=	6	
15	54*	32	122
13	120	132	279
11	42*	28	254
9	59*	21	12
7	222	231	106
5	229	229	134
3	57*	92	140
1	291	329	143
H=	5, K=	5	
0	939	917	2
2	1224	1178	218
4	531	570	96
6	782	824	125
8	555	529	171
10	562	556	200
12	345	343	257
14	350	356	303
16	227	225	339
H=	5, K=	4	
17	104	73	189
15	76*	34	50
13	45*	51	125
11	98	102	141
9	345	319	17
7	194	195	137
5	297	299	276
3	253	267	145
1	472	465	199
H=	5, K=	3	
0	797	747	359
2	77	157	158
4	112	137	97
6	258	243	241
8	172	177	83
10	42*	62	30
12	96	81	245
14	44*	69	256
16	46*	30	205
H=	5, K=	2	
17	58*	69	176
15	93	94	112
13	9*	33	15
11	84	66	223
9	105	102	7
7	209	192	306
5	79	68	124
1	275	251	250
H=	5, K=	1	
0	758	817	182
2	318	315	179
4	605	587	259
6	571	553	330
8	573	615	349
H=	6, K=	2	
12	243	249	140
14	197	207	98
16	92	86	179
H=	6, K=	3	
17	19*	59	342
15	138	123	135
13	178	177	269
11	199	203	205
9	148	152	165
7	250	234	174
5	326	313	112
3	407	403	224
1	574	541	356
H=	6, K=	4	
0	718	753	1
2	236	240	12
4	592	566	119
6	263	227	128
8	339	367	193
10	211	199	164
12	230	216	113
14	193	208	107
16	98	88	22
H=	6, K=	5	
15	97	79	4
13	180	177	271
11	164	154	226
9	46*	56	206
7	8*	20	359
5	276	267	128

L	FO	FC	ALPHA
3	174	196	345
1	158	152	352
H=	6, K=	6	
0	521	537	3
2	828	809	219
4	479	462	54
6	570	545	143
8	525	545	157
10	466	456	207
12	310	307	226
14	233	208	139
16	244	241	333
H=	6, K=	7	
15	49*	59	148
13	10*	63	173
11	69*	53	188
9	187	202	6
7	137	117	308
5	63*	54	278
3	51*	86	93
1	98	124	280
H=	6, K=	8	
0	490	496	2
2	129	148	226
4	500	452	106
6	230	222	96
8	223	239	188
10	106	152	212
12	210	216	281
14	130	144	110
H=	6, K=	9	
15	112	98	134
13	67*	56	129
11	72*	116	223
9	241	222	11
7	288	295	330
5	213	205	274
3	339	351	249
1	280	284	210
H=	6, K=	10	
0	66*	28	206
2	8*	51	191
4	174	179	273
6	82	100	306
8	180	177	212
10	58*	72	4
12	99	87	160
14	64*	84	143
H=	6, K=	11	
13	39*	89	107
11	70*	53	254
9	107	106	11
7	119	112	351
5	156	160	276
3	149	156	251
1	53*	80	217
H=	6, K=	12	
0	283	252	184
2	330	319	215
4	249	255	259
6	318	327	144
8	245	249	341
10	166	166	216
12	163	172	63
H=	6, K=	13	
11	92	56	358
9	56*	12	28
7	10*	21	340
5	9*	48	275
3	102	96	219
1	28*	37	309
H=	6, K=	14	
0	49*	33	341
2	99	92	248
4	153	130	268
6	66*	101	114
8	55*	59	50
10	80*	64	26
H=	6, K=	15	
9	54*	55	181
7	94	97	115
5	20*	42	116
3	87	48	251
1	123	94	224
H=	6, K=	16	
0	73*	101	3
2	45*	71	222
4	76*	46	142
6	10*	57	122
8	33*	26	151
H=	6, K=	17	
7	75*	40	149
5	63*	49	105
3	32*	62	111
1	67*	53	224
H=	6, K=	18	
0	159	140	4
2	113	136	52
4	108	120	87
H=	7, K=	18	
3	76*	28	250
1	53*	30	227
H=	7, K=	17	
0	105	87	4
2	126	124	59
4	86*	75	94
6	78*	59	144
H=	7, K=	16	
7	89*	99	151
5	144	135	97
3	143	159	82
1	162	153	211
H=	7, K=	15	
0	103	101	0
2	10*	15	213
4	10*	15	184
6	10*	16	352
8	11*	18	145
10	88*	32	172
H=	7, K=	14	
11	69*	91	237
9	85*	78	194
7	130	146	127
5	104	97	136
3	30*	65	213
1	148	138	212
H=	7, K=	13	

L	FO	FC	ALPHA
H= 7, K= 13			
0	97	70	188
2	52*	54	132
4	152	125	270
6	98	111	308
8	80*	74	357
10	56*	41	351
12	37*	21	107
H= 7, K= 12			
13	11*	47	101
11	121	74	15
9	10*	36	60
7	36*	35	249
5	9*	47	134
3	115	116	215
1	107	104	102
H= 7, K= 11			
0	8*	19	218
2	121	127	202
4	104	108	256
6	203	202	147
8	127	115	146
10	10*	58	57
12	103	117	53
H= 7, K= 10			
13	164	166	95
11	189	158	251
9	197	203	3
7	232	222	344
5	270	262	272
3	296	308	261
1	323	319	191
H= 7, K= 9			
0	153	155	181
2	92	104	103
4	137	134	103
6	63*	45	1
8	121	119	217
10	63*	81	113
12	42*	55	211
14	11*	12	149
H= 7, K= 8			
15	138	173	141
13	154	138	140
11	149	151	52
9	317	319	16
7	319	323	337
5	151	159	300
3	367	385	229
1	420	452	225
H= 7, K= 7			
0	344	349	2
2	208	212	52
4	269	279	113
6	110	118	104
8	181	174	198
10	150	145	177
12	110	75	105
14	97	93	114
H= 7, K= 6			
15	98	47	228
13	48*	51	252
11	101	119	237
9	71*	59	309
7	101	86	149
5	271	277	133
3	185	169	222
1	49*	57	354
H= 7, K= 5			
0	9*	18	246
2	424	435	78
4	244	288	60
6	261	255	160
8	135	132	161
10	249	223	214
12	79*	102	226
14	124	123	334
16	107	97	342
H= 7, K= 4			
15	152	173	332
13	228	241	278
11	277	278	213
9	343	327	186
7	334	336	162
5	452	473	101
3	406	419	54
1	343	352	346
H= 7, K= 3			
0	239	260	179
2	325	306	264
4	52*	46	197
6	64*	157	83
8	45*	60	61
10	137	114	110
12	39*	27	274
14	22*	19	3
16	19*	54	92
H= 7, K= 2			
17	121	133	0
15	183	183	332
13	211	210	271
11	264	273	232
9	264	261	181
7	479	480	159
5	617	602	134
3	481	469	58
1	839	848	12
H= 7, K= 1			
2	269	274	180
0	668	701	181
4	105	86	337
6	230	209	111
8	307	316	348
10	159	196	52
12	203	179	92
14	110	127	97
16	113	105	146
H= 8, K= 0			
0	86	44	181
2	97	108	28
4	198	183	143
6	172	191	215
8	152	146	137
10	74*	70	348
12	57*	51	242
14	104	121	24
16	29*	35	226
H= 8, K= 1			
15	89	60	356
13	215	214	111
11	68*	91	274
9	429	419	181
7	327	330	188
5	488	494	107
3	210	198	101
1	681	709	350

L	FO	FC	ALPHA
H= 8, K= 2			
0	91	141	1
2	201	221	136
4	204	192	59
6	7*	9	11
8	70	70	157
10	188	189	139
12	110	106	225
14	76*	51	105
16	11*	38	49
H= 8, K= 3			
15	253	257	333
13	164	172	276
11	407	397	227
9	221	213	189
7	620	640	140
5	404	408	128
3	509	536	222
1	308	315	214
H= 8, K= 4			
0	104	110	179
2	88	61	87
4	66	101	228
6	64*	75	231
8	68*	67	213
10	96	70	277
12	78*	77	240
14	73*	85	5
16	11*	13	217
H= 8, K= 5			
15	96	85	336
13	158	162	111
11	87	109	178
9	336	340	195
7	208	203	194
5	464	457	110
3	324	323	253
1	345	350	12
H= 8, K= 6			
0	275	283	0
2	84	111	14
4	135	131	127
6	95	100	348
8	74*	76	220
10	109	110	128
12	10*	26	227
14	45*	52	191
H= 8, K= 7			
15	112	89	118
13	100	120	137
11	104	98	139
9	289	285	14
7	71*	80	248
5	25*	10	244
3	80	68	227
1	261	248	203
H= 8, K= 8			
0	144	131	182
2	133	119	135
4	132	163	103
6	100	113	303
8	87	100	221
10	9*	31	309
12	40*	36	143
14	69*	24	20
H= 8, K= 9			
13	142	151	90
11	222	206	249
9	175	171	4
7	295	287	341
5	224	237	298
3	389	380	250
1	422	426	209
H= 8, K= 10			
0	224	220	359
2	69*	14	118
4	77	33	153
6	93	77	331
8	78*	93	189
10	10*	54	143
12	75*	51	28
H= 8, K= 11			
13	84*	87	97
11	110	95	218
9	123	83	23
7	9*	55	131
5	103	100	103
3	92	86	237
1	84	109	194
H= 8, K= 12			
0	67*	38	181
2	71*	91	116
4	93	60	274
6	21*	40	113
8	49*	26	88
10	27*	36	105
12	49*	1	300
H= 8, K= 13			
11	11*	50	232
9	64*	73	190
7	130	101	145
5	48*	67	127
3	9*	8	59
1	138	132	357
H= 8, K= 14			
0	104	111	1
2	10*	72	245
4	50*	57	89
6	10*	30	53
8	78*	76	173
10	97	74	176
H= 8, K= 15			
9	134	146	201
7	158	163	147
5	168	171	106
3	191	196	248
1	202	200	211
H= 8, K= 16			
0	18*	37	4
2	91	79	256
4	95	41	102
6	11*	37	168
H= 8, K= 17			
5	64*	64	85
3	62*	82	247
1	111	77	219
H= 8, K= 18			
0	11*	8	4
H= 9, K= 17			

L	FO	FC	ALPHA
H= 9, K= 17			
0	11*	16	189
2	11*	45	223
H= 9, K= 16			
5	98	100	94
3	142	118	251
1	83*	104	217
H= 9, K= 15			
0	10*	12	19
2	71*	118	249
4	50*	49	87
6	96	68	121
8	11*	41	155
H= 9, K= 14			
9	117	102	196
7	139	152	152
5	110	118	123
3	116	135	61
1	165	185	27
H= 9, K= 13			
0	135	142	4
2	106	88	251
4	125	121	89
6	96	109	102
8	138	143	161
10	109	107	199
H= 9, K= 12			
11	11*	17	135
9	34*	35	145
7	10*	24	333
5	51*	60	345
3	34*	41	211
1	29*	28	109
H= 9, K= 11			
0	117	115	3
2	201	201	244
4	32*	41	152
6	144	130	140
8	134	121	142
10	96	69	229
12	29*	26	232
H= 9, K= 10			
13	135	124	78
11	137	113	226
9	114	102	348
7	120	126	137
5	166	168	272
3	118	109	268
1	152	154	166
H= 9, K= 9			
0	161	138	358
2	50*	38	180
4	54*	80	201
6	56*	61	348
8	9*	61	174
10	10*	56	121
12	10*	62	24
H= 9, K= 8			
13	102	98	98
11	159	155	226
9	209	210	12
7	257	262	342
5	229	239	130
3	317	314	238
1	377	377	214
H= 9, K= 7			
0	254	254	184
2	96	117	200
4	319	291	282
6	108	117	344
8	209	234	218
10	68*	43	214
12	77*	79	126
14	47*	54	131
H= 9, K= 6			
15	62*	47	348
13	23*	17	204
11	52*	48	234
9	9*	17	105
7	65*	49	153
5	79	50	81
3	131	125	247
1	21*	47	98
H= 9, K= 5			
0	210	199	356
2	42*	48	200
4	162	181	150
6	125	90	340
8	120	133	334
10	103	104	9
12	29*	51	132
14	91	81	147
H= 9, K= 4			
15	91*	123	144
13	178	166	111
11	121	145	220
9	299	301	197
7	217	227	162
5	390	409	114
3	381	375	59
1	401	389	215
H= 9, K= 3			
0	68	31	2
2	198	195	223
4	39*	46	83
6	99	112	137
8	133	157	25
10	94	93	184
12	134	146	215
14	100	100	104
16	27*	35	145
H= 9, K= 2			
15	159	161	145
13	176	172	275
11	269	254	232
9	271	272	172
7	442	460	150
5	343	338	98
3	348	374	56
1	446	418	356
H= 9, K= 1			
0	577	551	1
2	397	402	17
4	348	376	107
6	346	352	141
8	166	173	166
10	203	191	205
12	262	271	255
14	171	163	131
16	91*	98	13
H= 10, K= 0			

L	FO	FC	ALPHA
0	778	798	2
2	526	539	20
4	488	457	85
6	621	632	159
8	370	386	154
10	290	286	232
12	391	374	244
14	180	190	143

H= 10, K= 1

L	FO	FC	ALPHA
15	94	108	132
13	70*	71	205
11	189	193	208
9	25*	27	131
7	243	228	125
5	78	94	188
3	168	198	22
1	226	197	29

H= 10, K= 2

L	FO	FC	ALPHA
0	461	511	2
2	333	333	11
4	406	407	99
6	286	260	110
8	193	180	182
10	264	273	172
12	193	209	246
14	197	190	281

H= 10, K= 3

L	FO	FC	ALPHA
15	29*	53	271
13	138	144	110
11	33*	36	146
9	163	164	193
7	79	77	225
5	218	228	94
3	242	236	102
1	233	238	13

H= 10, K= 4

L	FO	FC	ALPHA
0	123	115	186
2	92	52	159
4	78	104	248
6	138	133	263
8	185	169	3
10	108	120	354
12	10*	56	183
14	60*	78	107

H= 10, K= 5

L	FO	FC	ALPHA
15	65*	65	333
13	10*	16	88
11	129	125	217
9	97	75	204
7	116	124	139
5	39*	51	298
3	237	216	21
1	140	155	256

H= 10, K= 6

L	FO	FC	ALPHA
0	187	213	186
2	453	435	228
4	245	250	254
6	284	287	332
8	277	264	5
10	204	217	211
12	145	112	78
14	154	156	144

H= 10, K= 7

L	FO	FC	ALPHA
13	11*	24	114
11	101	112	50
9	116	89	226
7	203	210	335
5	157	171	144
3	204	221	219
1	189	167	227

H= 10, K= 8

L	FO	FC	ALPHA
0	140	125	187
2	124	144	220
4	242	247	264
6	136	137	302
8	95	83	17
10	102	90	22
12	112	92	245

H= 10, K= 9

L	FO	FC	ALPHA
13	124	115	95
11	76*	69	224
9	114	123	350
7	121	105	303
5	215	215	268
3	82	55	277
1	120	101	129

H= 10, K= 10

L	FO	FC	ALPHA
0	240	234	1
2	149	162	53
4	93	68	114
6	65*	103	119
8	121	139	159
10	79*	87	192
12	46*	22	278

H= 10, K= 11

L	FO	FC	ALPHA
11	53*	49	246
9	62*	23	154
7	86	99	332
5	77*	105	341
3	46*	82	208
1	75*	80	215

H= 10, K= 12

L	FO	FC	ALPHA
0	275	293	3
2	120	153	229
4	178	158	91
6	173	163	126
8	193	210	156
10	137	119	221

H= 10, K= 13

L	FO	FC	ALPHA
9	11*	46	186
7	99	82	152
5	10*	22	151
3	73*	80	229
1	111	96	216

H= 10, K= 14

L	FO	FC	ALPHA
0	138	113	5
2	179	184	58
4	138	124	87
6	139	136	116
8	129	91	165

H= 10, K= 15

L	FO	FC	ALPHA
7	49*	30	165
5	87	73	110
3	30*	75	90
1	31*	68	214

H= 10, K= 16

L	FO	FC	ALPHA
0	36*	19	186
2	68*	42	208
4	11*	9	309

H= 11, K= 16

L	FO	FC	ALPHA
H= 11, K= 16			
1	63*	59	194
H= 11, K= 15			
0	11*	3	24
2	56*	44	89
4	11*	32	63
H= 11, K= 14			
7	44*	27	272
5	21*	25	249
3	51*	34	147
1	51*	19	295
H= 11, K= 13			
0	235	234	3
2	213	231	51
4	167	149	102
6	146	157	131
8	145	112	176
H= 11, K= 12			
9	11*	26	226
7	97	56	120
5	70*	13	134
3	87	75	213
1	46*	85	105
H= 11, K= 11			
0	250	241	3
2	175	163	227
4	127	123	84
6	156	136	113
8	176	177	152
10	117	122	219
H= 11, K= 10			
11	29*	4	253
9	122	100	174
7	10*	46	187
5	72*	85	245
3	108	92	114
1	97	109	358
H= 11, K= 9			
0	47*	43	358
2	9*	39	81
4	64*	60	259
6	30*	29	142
8	66*	46	214
10	10*	39	184
12	54*	75	228
H= 11, K= 8			
13	11*	34	251
11	10*	7	175
9	20*	30	280
7	9*	19	160
5	96	101	249
3	60*	61	21
1	127	129	86
H= 11, K= 7			
0	251	251	185
2	218	230	208
4	296	276	255
6	229	218	132
8	253	255	357
10	201	197	20
12	136	142	78
H= 11, K= 6			
13	11*	8	265
11	49*	65	252
9	36*	72	131
7	91	79	148
5	129	117	147
3	97	118	235
1	50*	58	260
H= 11, K= 5			
0	391	398	183
2	420	456	224
4	305	307	264
6	287	289	143
8	290	283	5
10	222	222	217
12	123	128	85
14	126	129	132
H= 11, K= 4			
13	110	90	92
11	62*	64	12
9	109	114	337
7	42*	95	309
5	159	157	281
3	8*	57	199
1	103	107	157
H= 11, K= 3			
0	123	158	179
2	86	115	246
4	111	114	249
6	44*	93	114
8	34*	49	265
10	62*	69	206
12	14*	6	279
14	11*	49	30
H= 11, K= 2			
13	26*	25	186
11	29*	51	255
9	73*	55	224
7	131	128	340
5	101	112	131
3	110	99	224
1	104	95	178
H= 11, K= 1			
0	431	423	3
2	394	403	28
4	377	393	95
6	407	406	139
8	273	273	165
10	219	216	193
12	229	220	242
14	184	173	301
H= 12, K= 0			
0	277	284	4
2	124	116	131
4	284	269	88
6	51*	54	123
8	228	243	184
10	210	209	156
12	122	119	259
14	146	138	298
H= 12, K= 1			
13	47*	56	98
11	10*	18	252
9	73*	45	12
7	53*	43	28
5	124	137	137
3	34*	41	331
1	131	138	178

L	FO	FC	ALPHA
H= 12, K= 2			
0	75	61	173
2	284	275	62
4	153	160	56
6	212	212	162
8	54*	51	127
10	103	94	249
12	51*	49	224
14	88*	89	4
H= 12, K= 3			
13	149	135	93
11	170	183	226
9	190	189	359
7	270	295	341
5	241	254	296
3	331	339	237
1	358	373	196
H= 12, K= 4			
0	95	113	183
2	259	230	233
4	40*	37	309
6	249	238	147
8	120	103	105
10	146	136	95
12	106	101	62
H= 12, K= 5			
13	95	106	126
11	108	105	52
9	109	116	214
7	70*	75	146
5	165	168	110
3	124	140	226
1	112	89	207
H= 12, K= 6			
0	274	270	183
2	144	151	196
4	228	227	276
6	158	165	304
8	202	214	21
10	143	154	12
12	30*	74	106
H= 12, K= 7			
11	11*	2	181
9	93	115	211
7	106	100	153
5	79	56	158
3	41*	66	213
1	107	112	247
H= 12, K= 8			
0	92	79	356
2	72*	49	201
4	48*	56	234
6	108	124	136
8	42*	81	267
10	10*	44	128
12	121	90	54
H= 12, K= 9			
11	101	90	241
9	189	189	177
7	194	201	154
5	138	169	88
3	165	160	256
1	193	193	8
H= 12, K= 10			
0	52*	53	7
2	112	116	249
4	50*	45	211
6	10*	34	102
8	100	88	141
10	38*	65	221
H= 12, K= 11			
9	98	77	214
7	142	124	140
5	102	126	117
3	127	138	64
1	99	119	50
H= 12, K= 12			
0	247	252	2
2	149	141	227
4	116	128	107
6	79*	92	138
8	126	113	185
H= 12, K= 13			
7	19*	22	297
5	11*	39	60
3	43*	27	100
1	10*	12	217
H= 12, K= 14			
0	11*	14	12
2	24*	56	78
4	24*	23	254
6	11*	13	249
H= 12, K= 15			
3	11*	71	267
1	80*	89	207
H= 13, K= 14			
3	11*	49	272
1	93	81	199
H= 13, K= 13			
0	11*	18	179
2	54*	24	49
4	11*	23	282
6	11*	25	141
H= 13, K= 12			
7	50*	15	146
5	78*	51	99
3	59*	44	253
1	10*	31	222
H= 13, K= 11			
0	128	111	2
H= 13, K= 12			
5	78*	51	99
3	59*	44	253
1	10*	31	222
H= 13, K= 11			
0	128	111	2
2	62*	52	256
4	63*	92	109
6	11*	30	92
8	64*	54	192
H= 13, K= 10			
9	113	121	198
7	208	194	144
5	182	184	109

L	FO	FC	ALPHA
H= 13, K= 10			
3	185	188	251
1	207	198	24
H= 13, K= 9			
0	10*	16	10
2	136	141	246
4	47*	11	16
6	62*	40	131
8	10*	45	129
10	79*	56	208
H= 13, K= 8			
11	25*	57	243
9	187	181	187
7	135	161	155
5	90	122	102
3	127	115	58
1	146	151	211
H= 13, K= 7			
0	98	96	359
2	49*	24	148
4	45*	53	104
6	75*	49	3
8	35*	55	197
10	64*	38	182
H= 13, K= 6			
11	11*	20	12
9	38*	57	226
7	84	75	134
5	9*	22	176
3	9*	28	93
1	41*	68	51
H= 13, K= 5			
0	56*	78	184
2	9*	37	83
4	114	101	108
6	73*	40	277
8	63*	59	223
10	10*	8	105
12	75*	29	115
H= 13, K= 4			
13	110	126	122
11	152	134	220
9	184	188	30
7	196	182	349
5	243	249	304
3	278	295	238
1	274	273	206
H= 13, K= 3			
0	40*	46	358
2	135	114	257
8	88	67	274
10	10*	68	110
12	21*	19	213
H= 13, K= 2			
13	147	134	90
11	148	145	229
9	155	144	349
7	197	192	338
5	166	177	305
3	165	148	242
1	262	266	185
H= 13, K= 1			
0	24*	47	176
2	89	66	50
4	60*	68	29
6	53*	24	90
8	42*	38	121
10	82	62	177
12	11*	39	252
H= 14, K= 0			
0	50*	23	204
2	17*	62	49
4	72*	58	307
6	53*	31	279
8	59*	64	358
10	10*	14	169
12	10*	31	135
H= 14, K= 1			
11	131	116	59
9	10*	42	306
7	176	175	142
5	38*	35	19
3	111	117	173
1	23*	41	181
H= 14, K= 2			
0	9*	46	353
2	34*	57	189
4	9*	31	104
6	89	101	138
8	71*	18	215
10	26*	54	253
12	35*	31	277
H= 14, K= 3			
11	87	105	219
9	209	202	9
7	176	162	347
5	300	289	103
3	216	225	255
1	259	254	184
H= 14, K= 4			
0	107	120	0
2	108	126	214
4	9*	16	279
6	54*	60	170
8	98	61	141
10	10*	65	187
12	50*	42	212
H= 14, K= 5			
11	100	73	7
9	10*	12	3
7	64*	71	15
5	110	85	351
3	145	147	217
1	108	100	255
H= 14, K= 6			
0	148	162	2
2	67*	74	60
4	112	108	101
6	75*	58	144
8	90	107	180
10	70*	57	203
H= 14, K= 7			
9	78*	85	201
7	79*	87	147
5	10*	41	195
3	89	88	219
1	164	155	56
H= 14, K= 8			

L	FO	FC	ALPHA
0	111	102	3
2	148	135	228
4	30*	56	86
6	80*	97	131
8	77*	83	148
10	72*	74	215
H=	14, K=	9	
9	134	123	187
7	141	116	146
5	139	152	100
3	143	155	85
1	185	200	17
H=	14, K=	10	
0	10*	51	1
2	10*	30	164
4	79*	69	103
6	54*	34	60
8	11*	18	158
H=	14, K=	11	
7	11*	70	144
5	10*	51	124
3	67*	56	59
1	76*	74	22
H=	14, K=	12	
0	46*	45	186
2	10*	9	329
4	36*	46	107
H=	14, K=	13	
3	11*	36	260
1	39*	63	193
H=	15, K=	12	
3	51*	39	237
1	41*	28	242
H=	15, K=	11	
0	88	104	184
2	10*	35	220
4	33*	72	279
H=	15, K=	10	
5	18*	37	128
3	68*	55	57
1	46*	72	212
H=	15, K=	9	
0	82*	72	3
2	33*	11	21
4	34*	81	99
6	10*	60	93
H=	15, K=	8	
7	74*	39	149
5	73*	70	88
3	34*	75	98
1	145	127	15
H=	15, K=	7	
0	173	172	4
2	176	182	228
4	113	121	96
6	127	144	136
8	120	102	162
H=	15, K=	6	
9	10*	28	108
7	92	37	88
5	10*	38	238
3	10*	14	251
1	77*	84	61
H=	15, K=	5	
0	171	167	4
2	159	153	221
4	120	102	101
6	117	128	134
8	115	131	174
10	42*	92	196
H=	15, K=	4	
9	56*	67	14
7	101	95	340
5	116	124	297
3	163	168	227
1	94	90	233
H=	15, K=	3	
0	23*	42	357
2	53*	48	281
4	10*	21	114
6	45*	46	111
8	84*	66	117
10	11*	22	246
H=	15, K=	2	
11	38*	62	226
9	84*	81	359
7	135	118	337
5	133	140	108
3	96	117	239
1	131	124	177
H=	15, K=	1	
0	158	142	185
2	115	98	197
4	121	118	252
6	129	117	133
8	114	136	349
10	126	98	212
H=	16, K=	0	
0	282	309	183
2	182	165	204
4	200	214	274
6	153	166	140
8	181	180	358
10	126	122	25
H=	16, K=	1	
9	40*	13	332
7	68*	53	91
5	10*	7	299
3	10*	34	333
1	86	49	148
H=	16, K=	2	
0	46*	47	189
2	155	181	228
4	81*	86	246
6	119	100	144
8	88	64	352
10	68*	76	25
H=	16, K=	3	
9	11*	51	176
7	10*	16	264
5	68*	32	338
3	10*	60	221
1	26*	63	137

L	FO	FC	ALPHA
H= 16, K= 4			
0	89	106	3
2	80*	107	218
4	75*	51	82
6	101	109	139
8	104	91	146
H= 16, K= 5			
9	42*	33	344
7	64*	50	93
5	67*	50	196
3	10*	34	90
1	67*	82	249
H= 16, K= 6			
0	209	192	4
2	164	164	224
4	150	143	94
6	137	132	129
8	156	139	184
H= 16, K= 7			
7	62*	16	222
5	11*	45	62
3	10*	43	156
1	10*	58	340
H= 16, K= 8			
0	118	123	3
2	105	85	224
4	94	105	82
6	89	84	123
H= 16, K= 9			
5	11*	4	208
3	11*	25	341
1	11*	41	144
H= 16, K= 10			
0	11*	58	184
2	24*	50	224
4	58*	54	253
H= 17, K= 9			
0	27*	5	350
2	11*	24	228
H= 17, K= 8			
3	78*	38	261
1	93	64	186
H= 17, K= 7			
0	55*	70	6
2	117	104	227
4	93	80	254
H= 17, K= 6			
5	37*	67	78
3	11*	45	115
1	10*	40	355
H= 17, K= 5			
0	122	109	5
2	81*	106	52
4	88	87	99
6	42*	74	123
H= 17, K= 4			
7	102	111	138

L	FO	FC	ALPHA
5	75*	75	123
3	81*	87	52
1	133	108	219
H= 17, K= 3			
0	53*	63	0
2	48*	20	83
4	36*	32	208
6	11*	14	209
8	11*	40	79
H= 17, K= 2			
7	105	93	163
5	67*	84	113
3	69*	69	77
1	93	121	10
H= 17, K= 1			
0	127	132	184
2	148	113	215
4	88*	113	274
6	87*	110	337
8	97	81	357

L	FO	FC	ALPHA
H= 18, K= 0			
0	11*	45	355
2	34*	34	158
4	11*	31	150
6	64*	63	346
H= 18, K= 1			
5	61*	48	141
3	47*	48	90
1	11*	75	17
H= 18, K= 2			
0	11*	28	355
2	11*	38	51
4	63*	48	271
6	64*	17	200
H= 18, K= 3			
5	69*	95	118
3	116	98	247
1	131	139	20
H= 18, K= 4			

L	FO	FC	ALPHA
0	61*	84	2
2	29*	18	91
4	65*	62	102
H= 18, K= 5			
3	72*	74	60
1	86*	58	226
H= 18, K= 6			
0	56*	23	8
2	87*	77	56
H= 19, K= 3			
0	65*	39	2
H= 19, K= 2			
1	72*	76	6
H= 19, K= 1			
0	95	76	1
2	55*	51	62

Table 4.4

Bond Distances and Angles: $(\{Cu(L2)\}_2CO_3)(ClO_4)_2 \cdot DMF$.

Distances (Å)		Angles (Deg.)	
Cu - N1	1.978(8)	N1 Cu N2	104.5(0.3)
Cu - N2	2.195(7)	N1 Cu N3	93.9(0.3)
Cu - N3	1.961(7)	N1 Cu O1	144.2(0.3)
Cu - O1	2.041(1)	N1 Cu O2	98.0(0.3)
Cu - O2	2.028(5)	N2 Cu N3	93.2(0.3)
N1 - C1	1.51(1)	N2 Cu O1	109.0(0.2)
N1 - C9	1.49(1)	N2 Cu O2	98.5(0.3)
N2 - C6	1.54(1)	N3 Cu O1	96.4(0.4)
N2 - C7	1.48(1)	N3 Cu O2	160.7(0.3)
N2 - C(N2)	1.43(1)	O1 Cu O2	65.3(0.3)
N3 - C3	1.25(1)	Cu N1 C1	106.8(0.5)
N3 - C4	1.47(1)	Cu N1 C9	112.7(0.5)
C1 - C10	1.52(1)	Cu N2 C(N2)	109.5(0.5)
C1 - C12	1.53(1)	Cu N2 C6	110.5(0.5)
C1 - C2	1.54(1)	Cu N2 C7	107.4(0.5)
C2 - C3	1.49(1)	Cu N3 C3	126.3(0.5)
C3 - C31	1.49(1)	Cu N3 C4	111.5(0.5)
C4 - C5	1.50(1)	Cu O1 C	88.3(0.5)
C5 - C6	1.47(1)	Cu O2 C	90.3(0.4)
C7 - C8	1.49(1)	Cu O1 Cu	176.6(0.2)
C8 - C9	1.46(1)	N1 C1 C10	108.1(0.7)
C - O1	1.32(1)	N1 C1 C12	108.6(0.8)
C - O2	1.27(1)	N1 C1 C2	108.9(0.9)
N - C13	1.35(4)	C2 C1 C10	112.8(0.9)
N - C14	1.59(5)	C2 C1 C12	107.4(0.9)
N - C14'	1.48(4)	C10 C1 C12	110.9(0.9)
N - C15	1.49(4)	C1 C2 C3	122.1(0.8)
C15 - O	1.28(4)	C2 C3 C31	125.3(0.9)
mean C1 - O	1.35	C2 C3 N3	125.3(0.9)

Table 4.4 (continued)

Angles (Deg.)	
C31 C3 N3	111.4(0.8)
C3 N3 C4	122.1(0.8)
N3 C4 C5	112.1(0.8)
C4 C5 C6	115.4(0.9)
C5 C6 N2	116.6(0.9)
C6 N2 C7	109.7(0.9)
C6 N2 C(N2)	108.8(0.7)
C(N2) N2 C7	111(1)
N2 C7 C8	115.4(0.9)
C7 C8 C9	113.7(0.9)
C8 C9 N1	114.7(0.8)
O1 C O2	116.1(0.6)
O2 C O2'	127(1)
C13 N C14	128(2)
C13 N C14'	107(6)
C13 N C15	94(2)
C14 N C15	104(2)
C14' N C15	102(2)
N C15 O	115(2)
mean O Cl O	109

4vii Discussion

Description of the Structure

The unit cell comprises four discrete L2-Cu-CO_3-Cu-L2 dimeric cations, eight perchlorate anions, and four DMF molecules of solvation, all well separated and affording no unusually short interionic or intermolecular contacts. A complete list of bond lengths and angles is given in table 4.4, a perspective view of the dimer, showing the labelling employed, is given in figure 4.1, and a view of the macrocyclic ligand in figure 4.2.

The co-ordination sphere of each copper atom contains the three nitrogen atoms of the macrocycle and two oxygen atoms of the bridging carbonate anion. The two halves of the dimer are related by a crystallographic two-fold axis of symmetry which passes through one oxygen (O1) and the carbon atom (C) of the carbonate bridge.

The five co-ordinate geometry about each copper atom can be estimated by inspection of the angles subtended at the central atom by the metal-ligand bonds. The 'best' square pyramid has basal angles XCuX in the cyclic sequence X = O1, O2, N1, N3 of 65.3, 98.0, 93.9 and 96.4 deg, with apex-base angles N2CuX in the same sequence of 109.0, 98.5, 105.6 and 93.2 deg. The 'best' trigonal bipyramid on the other hand has basal angles XCuX in the sequence X = O1, N2 and N3 of 109.0, 104.5 and 144.2 deg, with apex-base angles (N3CuX) of 96.4, 93.2 and 93.9 deg, and O2CuX of 65.3, 98.5

Figure 4.1

Perspective View of the $\{Cu(L2)\}_2CO_3^{2+}$ Cation

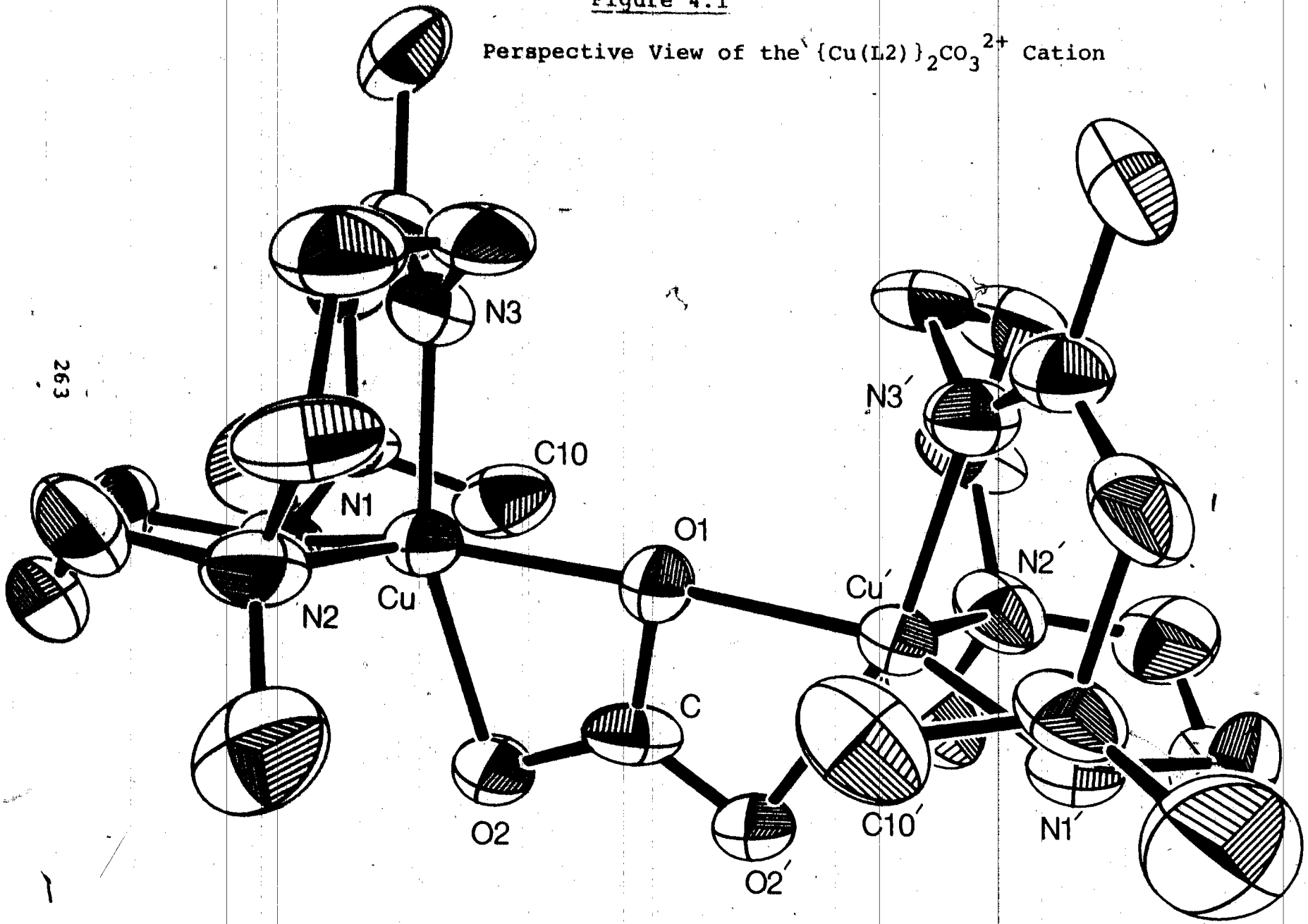
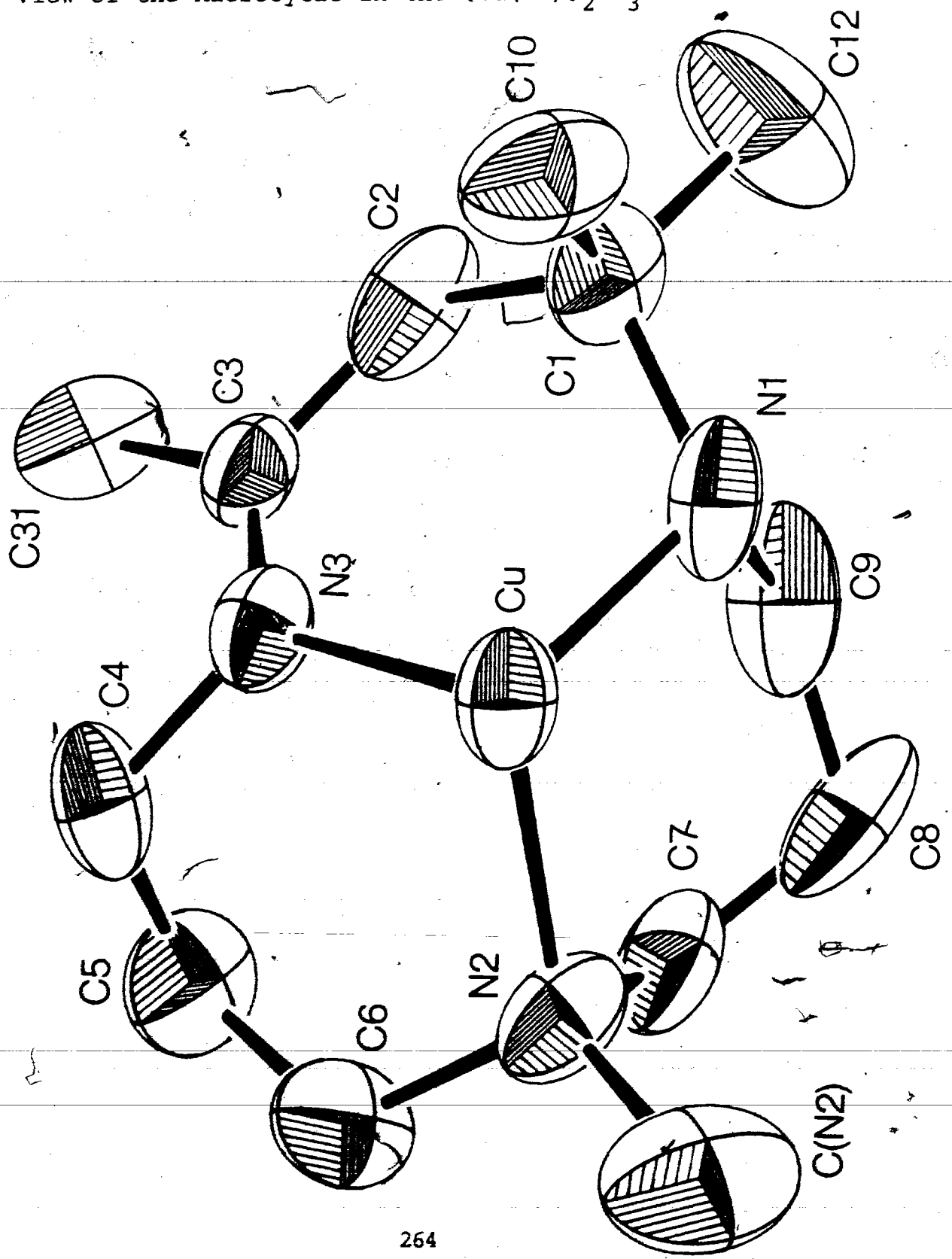


Figure 4.2

View of the Macrocycle in the $\{Cu(L2)\}_2CO_3^{2+}$ Cation



and 98.0 deg. Clearly, the choice is a difficult one and not important since either requires considerably irregularity; the square pyramid is adopted, therefore, with N2 axial. Furthermore, as a consequence of the conformation adopted by the triazamacrocycle L2, there is a lone contact (2.95(2) Å) from the metal atom to a ligand methyl carbon atom (C10). Very similar structural behavior occurs in $Ni(L1)(NCS)_2$[79], where the Ni... methyl carbon distance is 2.92 Å. Indeed, the entire ligand configuration and conformation in both complexes is very similar. A useful method of analysing and displaying the ligand conformation involves regarding each chelate section separately in terms of the displacements of ligand atoms from the plane formed by the central atom and the respective donor atoms. These planes are listed in table 4.5 and illustrated schematically in figure 4.3. If compared to a similar analysis reported for $Ni(L1)(NCS)_2$[79], the close resemblance is apparent. The two saturated chelate rings adopt chair conformations, while the conformation of the imine chelate ring is determined by the planarity of the imine group.

The question has been raised[79] as to whether the adopted conformation of the triazamacrocycle in these complexes is accidental or not; i.e., does the ligand determine the square pyramidal geometry by this preferred conformation placing C10 in the vacant octahedral site, or is the conformation of the ligand the result of a preferred square pyramid? The fact that, despite a change in metal ion, crystal packing

Table 4.5

Calculated Mean Planes: $(\{Cu(L2)\}_2CO_3)(ClO_4)_2 \cdot DMF$

Atoms Defining the Plane	Equation of the Plane† l	m	n	p	Displacements from the Plane Å
Cu, N1, N3	.970	-.244	-.007	-1.139	C4(.54), C3(-.38), C31(-.36), C2(-.85), C1(-1.17), C10(-2.41), C12(-1.31), C9(1.35)
Cu, N2, N3	-.481	-.860	-.167	2.051	C3(-.81), C4(1.07), C5(.79), C6(.95), C7(-1.38), C(N2)(.44)
Cu, N1, N2	.125	.216	-.968	+.385	C6(1.00), C(N2)(-1.31), C7(.40), C8(-.25), C9(.39), C1(.77)

† These are the coefficients of planes given by

$$lX + mY + nZ + p = 0,$$

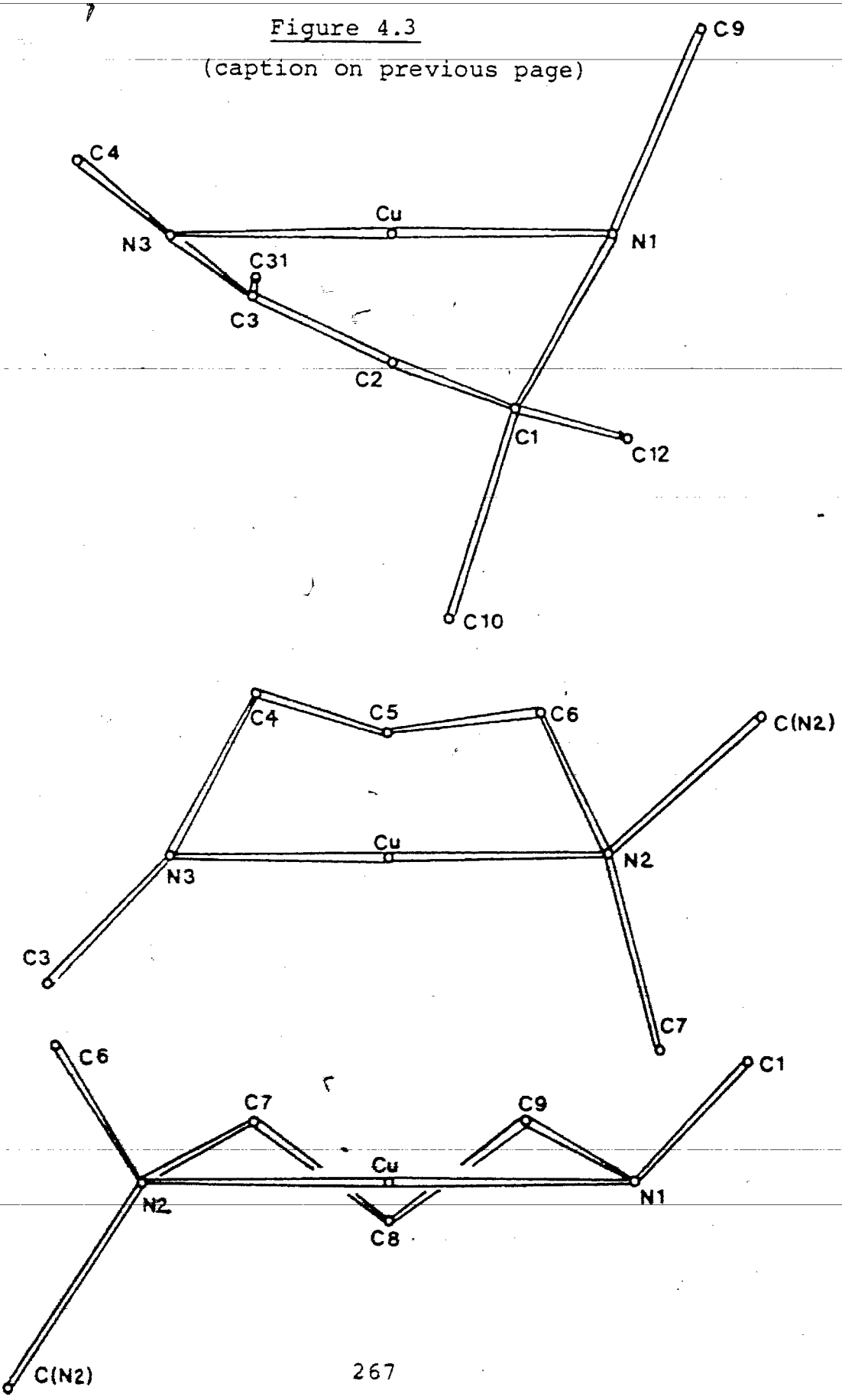
where the orthogonal system of axes, X, Y, Z has X along the a axis, Y in the a b plane, and Z along the c* axis.

Figure 4.3 (OVERLEAF)

Projections of the Chelate Ring Conformations in $\{Cu(L2)\}_2CO_3^{2+}$

Figure 4.3

(caption on previous page)

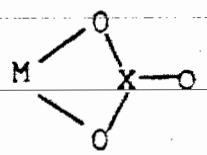


environment, and substitution of one hydrogen atom (in L1) for a methyl group (in L2), similar metal co-ordination and ligand conformation are found, emphasises the earlier conclusion[79] that the twelve ring macrocycles have co-ordination properties similar to larger triazamacrocycles as a consequence of general stereochemical interactions by the methyl groups (C10 and C12), rather than any stabilization caused by their specific siting.

A survey of Ni(II) triazamacrocyles[84] shows that those with less than 12 ring members tend to form six-coordinate complexes, while those with more than 12 ring members form five-coordinate complexes. The change in coordination number with ring size can be attributed to the steric crowding caused by the increased number of methylene groups.

Ligands L1 and L2 (12 ring members) appear to have coordination properties similar to the larger macrocycles, and this may be a consequence of the general stereochemical effect of the methyl groups, and not any stabilisation caused by any specific siting of them.

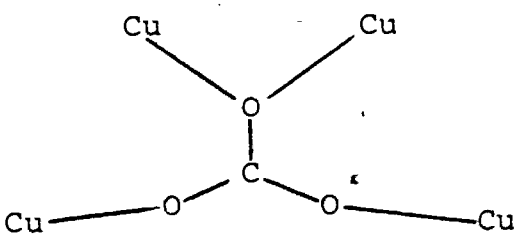
Previous structural studies[85-93] have shown various possible bonding modes for carbonate and nitrate ligands. The predominant bridging mode approximates



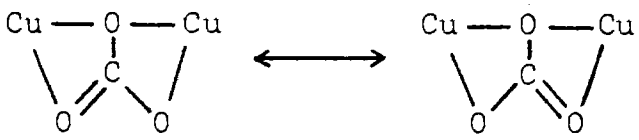
X = N, C

and is found for carbonate in complex dimers of a variety

of metal ions: $Cu(NH_3)_2CO_3$[87], $Co(NH_3)_4CO_3Br$[90], $Pt(PPh_3)CO_3$[91], $(Mo(CO)(PMe_2Ph)_3CO_3)_2$[92] and $Rh_2(CO_3)(PPh_3)_5 \cdot C_6H_6$[93]. The mode of bridging of the carbonate ion in the present complex is completely novel; it acts (within experimental error) as a symmetrical bidentate ligand to both copper atoms, with Cu-O1 = 2.041(1) Å, Cu-O2 = 2.028(5) Å, CuO1Cu = 176.6(0.2) deg and O1CuO2 = 54.3(0.3) deg. A structure somewhat related to it is that of malachite, $Cu(OH)_2CO_3$,[88] where one of the carbonate oxygen atoms interacts with two Cu(II) ions, with CuOCu non-linear, and where the other two oxygen atoms interact with separate Cu(II) ions in sites of a different type, i.e.



The range of C-O bond lengths in these complexes is 1.245(3)[85] Å to 1.36(2)[87] Å, the distance in each case depending largely on the interaction with the metal ion, which is affected in some cases by the other ligands in the coordination sphere. Where bond lengths are accurate enough to show it, the C-O length decreases as the metal oxygen interaction decreases; e.g., in $Cu(NH_3)_2CO_3$[87], the Cu-O and respective C-O distances are 2.303(2), 1.245(3); 1.989(2), 1.299(3); and 1.936(2), 1.307(3) Å. In $[Cu(L2)]_2CO_3^{2+}$, these distances are 2.028(1), 1.27(1) (C-O2) and 2.041(5), 1.32(1)Å (C-O1), and could be considered to reflect a certain stabilisation of two of three possible resonance forms:



The C-O lengths in free carbonate as found in calcite are 1.294(4) Å.[94] The copper oxygen distances lie to the high end of a range of Cu(II)-oxygen lengths of 1.88 to 2.04 Å found in carbonato-, carboxylato-, and β-diketonato complexes[87].

In all structurally characterised, bridging carbonato complexes, the bridging anion is essentially planar (exactly planar in the present case), and it is observed that, when bound as a bidentate ligand, the four-membered ring formation causes the OCO angle to decrease from 120 deg to an average of 116 deg[93] (116.1(0.6) deg for $\{Cu(L2)\}_2CO_3^{2+}$.

Exchange Interaction

The points remaining for discussion are clear. $\{Cu(L2)\}_2CO_3(ClO_4)$.DMSO exhibits a novel mode of bridging for the carbonate anion, and it also displays magnetic behavior (diamagnetism as a result of very effective superexchange) which is rare.

Since the MOM = 180 deg arrangement is already established as one that gives strong antiferromagnetic coupling, a simple interpretation, similar to that given in section 4ii, is immediately possible by recognising the nearly linear CuOlCu (176.6(0.2)deg) geometry in $\{Cu(L2)\}_2CO_3^{2+}$. Indeed, this may be the essential aspect of the adopted geometry which leads to diamagnetism. However, such an interpretation would ignore the fact that the CO_3^{2-} bridge is bonded in a symmetrical, bidentate manner to each Cu(II) ion, which implies that any delocalisation of metal d electron density would occur through extended m.o.s on the carbonate anion rather than only via atomic orbitals on Ol. If this is the case, then the geometry and electronic structure (particularly the shapes and symmetries of the carbonate m.o.s) must be considered in more detail.

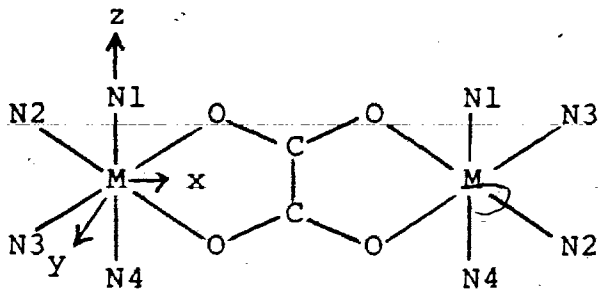
At least four studies have been described which endeavour to interpret the antiferromagnetism in copper (II) complexes by considering superexchange via bridging polyatomic anion m.o.s.[72-74,35] Two of these[72,35] deal only with carboxylate- bridged dimers, and, in agreement with a conclusion drawn from structural/magnetic correlations, establish that, although the

Cu ions are held in reasonable proximity (2.5 - 2.8 A), the Cu-Cu bond that is suggested by this arrangement is not primarily responsible for the observed antiferromagnetism. Rather, it is the overlap of metal d orbitals containing the unpaired electron density with either carboxylate oxygen lone pairs or the delocalised π electron system on the O····C····O moiety, which is important for the exchange interaction.

More relevant to the present case are the similar studies reported for metal centres symmetrically-bridged by oxalate and squarate anions.[73,74] One approach[74] uses the difference in energy ($\varepsilon_i - \varepsilon_j$) between the two highest-occupied dimer m.o.s (as calculated by an extended Huckel method) as an indication of the extent and type of interaction. When $\varepsilon_i = \varepsilon_j$, complete ferromagnetism occurs, and as $\varepsilon_i - \varepsilon_j$ increases, antiferromagnetism becomes dominant. The diamagnetism exhibited by $\{Cu(L2)\}_2CO_3^{2+}$ implies a very large $\varepsilon_i/\varepsilon_j$ splitting (>700 cm^{-1}). Furthermore, the calculations give support to two important considerations (already put forward qualitatively[73]) which contribute to the $\varepsilon_i - \varepsilon_j$ value. The exact geometry about the metal ion, which determines the orbital which accomodates the unpaired spin, and the geometry of the bridging ligand i.e. whether or not it is symmetrically bonded to the metal ions. The latter point is explicable on simple symmetry considerations. If the bridge is symmetric in its interaction with the two metal ions, the unpaired electrons on both metals will be delocalised into the same bridge m.o., and only antiferromagnetic coupling can result. Distortions from symmetrical bridging will allow some overlap on to orthogonal

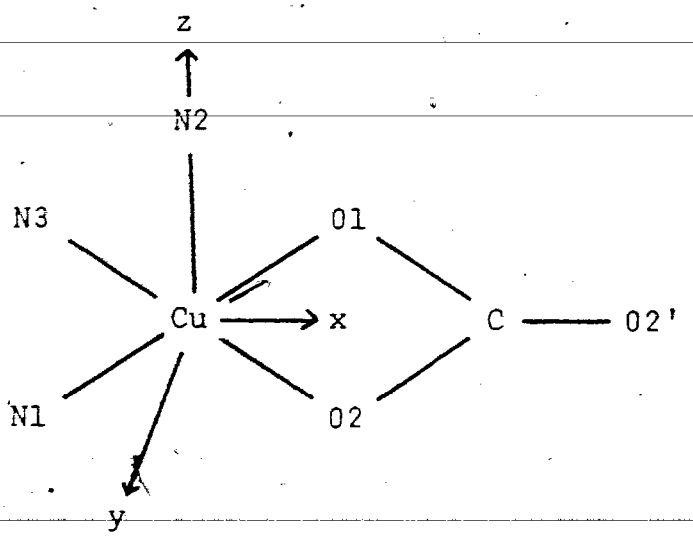
bridge m.o.s, and ferromagnetic behavior will become important.

These points are illustrated by comparing the structures of $Ni\{(en)\}_2(C_2O_4)^{2+}$ and $Cu\{(dien)\}_2(C_2O_4)^{2+}$ (en = diethylenediamine, dien = di-(2-aminoethyl) amine)[96]. Both cations contain six-coordinate metal ions, bridged by oxalate. The nickel compound exhibits antiferromagnetic behaviour (J= -17 cm^{-1}), whereas the copper complex exhibits none. If the following cartesian coordinates are assigned:



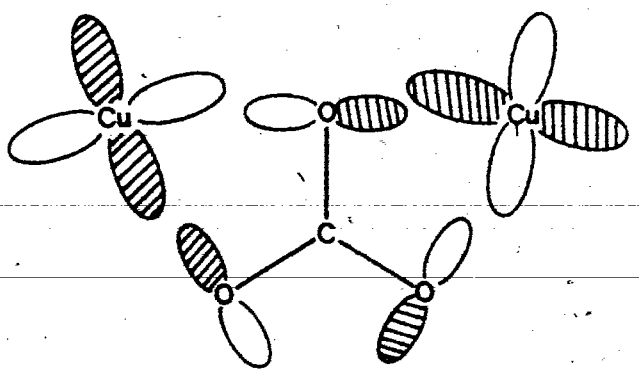
the stronger ligand field of the N-donors causes splitting of the metal e_g orbitals, with the d_{xy} being lower in energy. For Ni(II), therefore, unpaired electrons occupy the d_{xy} and d_{z^2} orbitals, and it can be seen intuitively, and is confirmed by calculation[74], that the overlap of the d_{xy} orbital with oxalate m.o.s is larger than that of the d_{z^2} orbital. The geometry about the Cu(II) ion is considerably distorted from octahedral, with N3 replaced by a long contact to an oxygen atom (water). The lack of exchange is thus explained by the spin density lying in the d_{z^2} orbital, and also by the fact that the oxalate anion is not symmetrically bridging (Cu-O1 = 2.230(6)A, and Cu-O2 = 1.965(6)A)[96].

The title compound can now be considered using a similar coordinate system:



Assuming square pyramidal geometry with N2 apical and N3. N1, O1 and O2 basal, the d_{xy} orbital will be higher in energy than the d_{z^2}, and will contain the unpaired spin density. The highest occupied carbonate m.o.s are non-bonding and almost entirely located on the oxygen atoms.[97,98] They correspond (in a localised bond picture) to the oxygen atom lone pairs.

Using the guidelines thus established, and recognising the geometry of the dimer, it is not a difficult task to sketch the metal d_{xy} and the carbonate a_2'' π(non-bonding) orbitals which, upon overlap, provide an effective route for strong exchange interaction:



It would be interesting to see if calculations of the type which were successful for the oxalate and squarate systems, are able to not only support the above assignment, but also to give some quantitative interpretation of the observed diamagnetism resulting from exchange interaction. Furthermore, the question as to whether consideration of the linear CuOlCu system is sufficient to account for the diamagnetism, or whether symmetrical bridging via the entire carbonate anion is the essential structural parameter, will require further theoretical inspection.

Chapter 5

Factors Affecting the Shape of High Coordinate Complexes

i Introduction

Metal complexes which exhibit a coordination number of seven or more are no longer regarded simply as structural oddities. Early reviews[99-101] set the stage for a rapid increase in the synthesis and full structural characterization of over 200 such species. The state of the art now includes a detailed analysis of the shape characteristics of any complex, replacing the previous emphasis on bond lengths and angles. As a result of this (predominantly crystallographic) data, information is now available to be able to readily observe possible reaction pathways between various polytopes.[102-104] In order to do this, a consistent method of quantitatively describing the geometry of any complex is required. Although in original publications this is far from the case, recent reviews have gone a long way in carefully analysing data using a coherent approach.[105,106] Furthermore, these analyses provide a way of estimating the accuracy of the predictions of high coordinate geometry which result from calculations based on the minimization of inter-donor atom repulsion.

ii Molecular Geometry

In describing the geometry of complexes of low coordination number (2-6), a list of bond lengths and angles usually suffices to distinguish the molecular geometry. For

high coordination complexes, this is inadequate, and among the procedures suggested to describe more complicated geometries, two are worthy of some discussion. Both depend on the differences between the observed molecular geometry and corresponding ideal polyhedra. This not only helps to keep the description within the realms of the average chemist's intuition, it is also of direct chemical interest, because the ideal geometries often lie at calculated energy minima, and distortions from them are thus indicative of special electronic or steric features of the molecule.

The first procedure is based on work by Dollase[107] where the root mean square difference between the coordinates observed in a coordination sphere and those of an ideal polyhedron is minimized by the method of least squares, by varying the orientation of the coordination and (where appropriate) the shape of the ideal polyhedron within the limits of the ideal symmetry. The merit of this procedure is that the distortion from any particular symmetry is given by one value Δ where

$$\Delta = \sum_{i=1}^{i=n} d_i^{\,2}/n$$

where n is the number of atoms around the coordination sphere, and d_i is the distance between comparable points in the observed and ideal polyhedra. A computer program has been developed by Drew[104] which automatically fits a set of coordinates to all the ideal polyhedra for that particular coordination number, and so it can be seen whether a structure can be adequately described in terms of one polyhedron or two (or three), and thus whether

its structure is on the reaction pathway from one polyhedron to another. The biggest disadvantage to this procedure is that it requires a non-trivial computer program to calculate the r.m.s. separation.

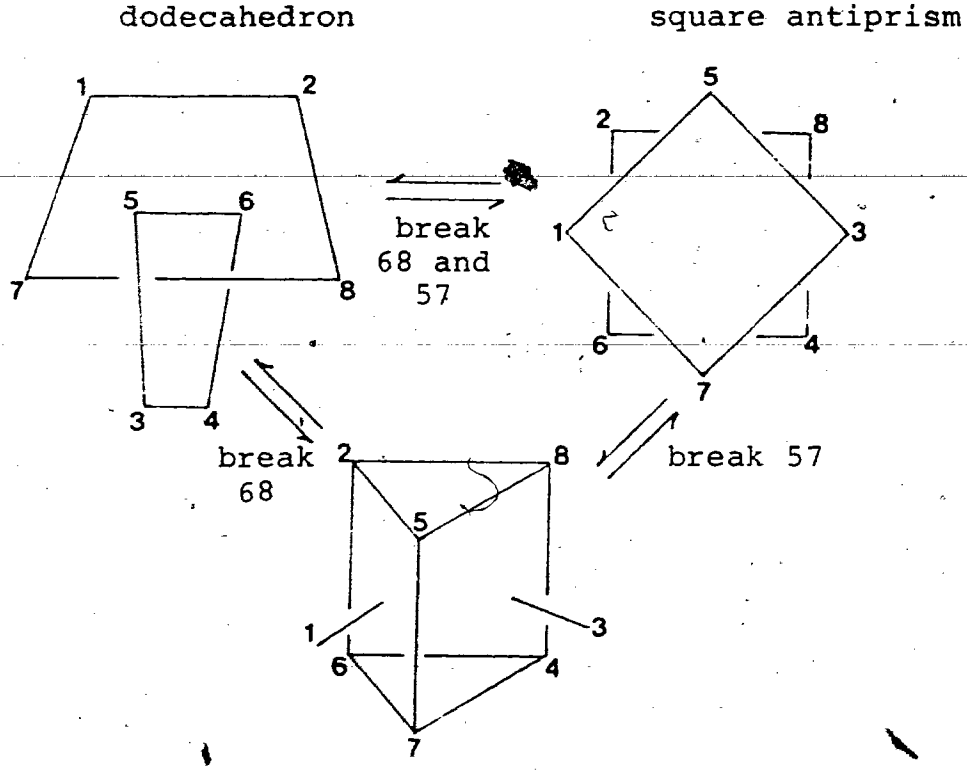
The second method is based on a suggestion by Porai-Koshits and Aslanov,[108] and applied more generally to high coordination by Muetterties and Guggenberger.[103,109] In this method, a numerical estimation of shape is obtained from comparison of the dihedral angles (δ) formed by the normals to adjacent polytopal faces to those calculated for the appropriate ideal polyhedra. These angles have been shown to be most useful in analysing and discussing eight coordination[104] and less useful for other coordination numbers since several sets of angles can be chosen, each set being characteristic of a different polyhedron. This analysis has the advantage of being readily calculable from meanplane data, and for polyhedra of the dodecahedral class (the concern of this chapter), there is no ambiguity in the choice of the δ angles.

iii Eight Coordination

The original description of eight coordination polyhedra by Hoard and Silverton[110] has needed little change over the years. The two most commonly observed polyhedra are the dodecahedron and the square antiprism. Another polyhedron commonly used to describe intermediate geometries (and which is relevant to the present work) is the bicapped trigonal prism (figure 5.1).

Figure 5.1

Eight Coordinate Polyhedra



δ and ϕ angles describing the polyhedra above (from ref 108)

δ angles	Values (deg)		
	dodecahedron	square antiprism	bicapped trigonal prism
1(57)3	29.5	0.0	21.8
1(67)4	29.5	0.0	0.0
2(58)3	29.5	52.4	48.2
2(68)4	29.5	52.4	48.2
ϕ	0.0	24.5	14.1

Dodecahedron (symmetry $\bar{4}2m$)

The dodecahedron contains two types of ligand site, called A and B (figure 5.1). The A sites (1, 2, 3, 4) form an elongated tetrahedron, and the B sites (5, 6, 7, 8) form a flattened one. Alternatively, sites 1, 2, 5, 7 and 8, and 3, 4, 5 and 6 form interlocking trapezoids which lie in mutually orthogonal mirror planes. δ angles are calculated over the edges joining the B sites, and are equal to 29.5 deg for the ideal, regular dodecahedron, although the only requirement from the $\bar{4}2m$ symmetry is that all four are identical. A further pair of angles (Ψ) which assess the planarity of the trapezoids have also been found useful. These are the angles between planes of atoms 7, 8, (1, 2), and 1, 2, (7, 8), and between plans 5, 6, (3, 4), and 3, 4, (5, 6), where (n, m) signifies the midpoint of the edge between atoms n and m. For the ideal, regular polyhedron these Ψ angles are both equal to 0.0 deg.

Square Antiprism (symmetry $\bar{8}2m$)

The square antiprism contains only one type of ligand site (figure 5.1). δ angles are calculated over two diagonals of the squares and over two edges which connect the squares. For the ideal, regular polyhedron, these angles are 0.0, 0.0, 52.4, and 52.4 deg, although the $\bar{8}2m$ symmetry requires only that the first two are zero and the second two are non-zero and equal.

Bicapped Trigonal Prism (symmetry ?)

Discussion of the shape parameters which adequately describe the so-called bicapped trigonal prism is somewhat more complicated. If it is to be considered equivalent to a tricapped trigonal prism with one capping atom removed, the δ angles are 0.0, 21.8, 48.2, and 48.2 deg, and the Ψ angles are both 14.1 deg. However, this assumes that the $\bar{6}$m2 symmetry of the tricapped trigonal prism has been preserved, which is unjustified, since the removal of one capping atom allows the unique quadrilateral face to contract, with the result that only mm2 symmetry is maintained. It is with this latter model only that agreement with real geometries is found. It should be noted that all square antiprisms also fit this model, but the the two can be distinguished by the two smallest δ angles (= 0.0 and 0.0 deg for the square antiprism, and 0 - 15 and 20 - 30 deg for the bicapped trigonal prism).

Reaction Pathways

To proceed from the dodecahedron to the square antiprism, atoms 1, 7, 3, 5 become one square face, and atoms 2, 8, 4, 6 the other, this pathway maintaining 222 symmetry. To proceed from the dodecahedron to the bicapped trigonal prism, two atoms in the A sites (in this case 1 and 3) become the capping atoms in the bicapped trigonal prism, and the 68 edge is broken. The pathway maintains two-fold symmetry. To proceed from the square antiprism to the bicapped trigonal prism, one of the square faces becomes slightly puckered, and

an edge is formed (57) across the diagonal of the face, thus maintaining mm2 symmetry. Clearly, there is only a small difference between the bicapped trigonal prism and a midpoint on the 222 pathway from the dodecahedron to the square antiprism (figure 5.1). Whether the bicapped trigonal prism is a distinct geometry, or is just part of a broad pathway from the dodecahedron to the square antiprism is discussed further along with the results of the work described in this chapter.

One further complication is the fact that the dodecahedron can be distorted to two different square antiprisms depending on whether the 17 and 53, or 17 and 46 edges become one of the squares. Similarly, the square antiprism can be distorted towards four different dodecahedra depending on which edge is bisected (12, 25, 58, or 83). This is particularly important in considering tetrakis (bidentate) systems since different choices lead to different isomers, though, as an inspection of the available data will show, surprisingly few such isomers actually occur.

iv Existing Theory of High Coordination

A simple and successful method of predicting the shapes of molecules of coordination numbers two through six is VSEPR where the number and type of electron pairs is assumed to determine the geometry, i.e., bonding forces are considered to dominate.[111] As the coordination number increases, non-bonding repulsions between electron clouds on adjacent donor atoms become more important, until at coordination numbers

of eight or more, a predictive theory based solely on inter-donor atom repulsion is necessary. Such a theory has been applied with most success by Kepert,[112,113] and since the results presented in this chapter will be closely compared to the predicted geometry, some theoretical background is pertinent.

The stereochemical arrangement of any number of ligand donor atoms surrounding a central atom is obtained by minimization of the total repulsion energy U obtained by summing over all donor atom - donor atom interactions u_{ij}. u_{ij} is assumed to be purely repulsive, and inversely proportional to some power n of the distance d_{ij} between two donor atoms i and j. If all metal-donor atom distances are equal (i.e., all donor atoms lie on the surface of a sphere, radius r), the results can be expressed in the form:

$$U = \sum_{ij} u_{ij} = \sum_{ij} a_n d_{ij}^{-n} = a_n X r^{-n} \qquad (i>j)$$

where a_n is a proportionality constant, and X the repulsion energy coefficient, which is a function of n and the geometry of the polyhedron. The nature of the central atom is considered to play no part in determining the stereochemistry; its sole purpose is to hold the donor atoms onto the surface of the sphere.

The most appropriate value of n in the repulsion law cannot be known exactly. Fortunately, the geometry corresponding to each minimum on the potential energy surface does not usually depend very much on the assumed value of n. In those few cases where the calculated geometry does depend

on n, the best agreement with experiment is obtained for n=6 to 10.

It is assumed that each bonded bidentate ligand is sufficiently rigid that interaction between its donor atoms can be considered to be constant, and this interaction is therefore omitted when summing over all the donor atom - donor atom interactions. Each bidentate ligand is imagined as being of fixed "normalized bite" b: the distance between the donor atoms of the chelate divided by the metal to donor atom distance. Predicted and experimentally determined stereochemistries are found to be very dependent on b.

The method of calculation involves the above energy expressions coupled with elementary trigonometry. Each donor atom is considered as being on the surface of a sphere of unit radius, its position being given by its spherical coordinates ϕ_i and θ_i. Three such coordinates are sufficient to specify the position of both ends of any bidentate ligand, as the fourth can be calculated from the other three and b. Three angular coordinates can be fixed when defining the coordinate axes. The distance d_{ij} between any two donor atoms i and j is then given by:

$$d_{ij}^2 = 2 - 2\cos\phi_i\cos\phi_j - 2\sin\phi_i\sin\phi_j\cos(\theta_i - \theta_j)$$

The calculation technique is simply to allow all angular coordinates to systematically vary until a minimum in the repulsion energy is reached.

The simplicity of this theory enables its use for structurally complicated molecules. The ability to predict

new structures and rationalize known structures as a function of the normalized bite of the bidentate ligands is the important advance offered by this approach. These successes cannot at present be achieved using theories which are "metal-centered" (e.g., valence bond, crystal field, ligand field, and molecular orbital).

iv Metal Tropolonates

The tropolonate ligand (T) has been shown to form high coordinate complexes with a wide varity of metals. Previous structural studies have shown it to be a compact, planar ligand with a fairly constant inter-donor atom separation.[114-117] This chapter describes the crystal and molecular structure of tetrakis(tropolonato) zirconium(IV), whose geometry is compared with that of the similarly coordinated scandium(III),[115] hafnium(IV),[117] and niobium(V)[116] complexes. The variations in geometry amongst this series are correlated with change in metal ion, metal-donor atom distance, and the normalized bite, b. The relation of these results to the aspects of high coordination previously mentioned is also considered.

v Experimental

$Zr(C_7H_5O_2)_4 \cdot (CHCl_3)_{2.5}$ was prepared according to the method described by Muetterties and Wright.[91] Zirconium tetrachloride (0.25 g, 0.001 mole) was dissolved in chloroform (20 mL) and added with stirring to a solution of tropolone

(0.6 g, 0.0045 mole) in chloroform (10 mL). A further 10 mL of chloroform was added to this mixture, which was then refluxed for 15 minutes. Slow evaporation of the resulting brown solution gave rust-coloured crystals, which became yellow and amorphous when stored in the absence of chloroform. Rapid loss of chloroform of crystallization and the accompanying loss of crystalline character made accurate thermogravimetric analysis impossible, and the mounting for investigation of a single crystal very difficult. Finally a crystal of approximate dimensions 0.9 x 0.13 x 0.06 mm was sealed in an atmosphere of chloroform in a Lindemann glass capillary tube, and mounted along the needle axis. Copper radiation (λ = 1.5418 Å) was used in a preliminary photographic investigation which established triclinic Laue symmetry, with the a axis approximately coincident with the needle axis of the crystal. Accurate cell dimensions were determined from counter measurement of 12 of the strongest reflections have $2\theta > 20$ deg using a Picker FACS-a computer controlled four circle diffractometer (MoKα radiation, λ = 0.70926 Å), with a take-off angle of 1.0 deg.

Crystal Data: $Zr(C_7H_5O_2)_4 \cdot (CHCl_3)_{2.5}$, formula weight 844.3, crystallizes in the triclinic space group $P\bar{1}$; a = 11.714(3) A, b = 15.163(4) A, c = 10.317(3) A, α = 91.74 deg, β = 73.9(3) deg, γ = 100.94(2) deg, V = 1683.3 A^3, d_m = 1.60 g mL g mL^{-1} (by flotation), Z = 2, d_c = 1.67 g mL^{-1}, μ(Mo Kα) = 9.23 cm^{-1}, t = 22(±1) deg C.

Reflections for the unique set of data were

collected in two shells using a scintillation detector with pulse height analysis, with a symmetric θ-2θ scan at a speed of 2 deg/min. For data where $\sin\theta<0.2164$, a scan base width of 1.5 deg was used, with background counts of 10 s made at both scan limits; for data where $0.2164<\sin\theta<0.3826$, a scan base of 0.9 deg was used, with background counts of 4 s. After each 70 reflections, two standard reflections were measured; their variation was ±5% over the entire data collection. The measured intensities were corrected for Lorentz and polarization effects; absorption was neglected since it was estimated to produce an extreme error of ±6% in I, the net count. A total of 4527 reflections were measured, of which 2774 were classed as observed (i.e., greater than $2.3\sigma_I$, where $\sigma_I = [T_c + (t_s/t_b)^2(B_1 + B_2) + (kI)^2]^{\frac{1}{2}}$ where T_c is the total count, t_s is the scan time, t_b is the total background count time, B_1 and B_2 are the background counts at either end of the scan range, k is a constant set to 0.03, and I is the net count).

vi Structure Determination and Refinement

A three-dimensional Patterson synthesis based on all the data gave the position of the zirconium atom; refinement of these atomic parameters and two scale factors (for the inner and outer shells of data) gave R = 0.439, where $R = \sum(|F_o| - |F_c|)/\sum|F_o|$. A Fourier synthesis gave the positions of the eight oxygen atoms, and the three chlorine atoms of one molecule of chloroform. Several cycles of

refinement and subsequent electron density difference maps gave the positions of a further molecule of chloroform and all the tropolonate carbon atoms. With all these atoms assigned anisotropic thermal motion parameters, full matrix least square refinement gave an R of 0.101, though it was clear that one tropolonate ligand (ligand 3) was irregular. The seven carbon atoms and one oxygen atom had very large thermal motion components in a direction approximately perpendicular to the general plane of the ring, suggesting that the ring was disordered between two alternative positions. Furthermore, there were some large peaks in the electron density difference map which were close to this ring. The disorder in ligand 3 was accommodated by arranging the seven carbon atoms and one oxygen atom (O(5)) in two positions, each with half occupancy. Upon continuing the refinement, with alternate occupancy factors and isotropic thermal motion parameters, this model behaved well, with refined occupancy factors remaining at 0.5. The peaks thus far unaccounted for in the difference map suggested another molecule of chloroform. However, since this molecule was extremely close to a centre of symmetry, and since, in either position, it had close contact with one position of ligand 3, it was assigned an occupancy factor of 0.25. A list of the short contacts which led to this model is given in table 5.1, and the resulting packing within the unit cell is illustrated in figure 5.2. Two further ramifications of the presence of the partially occupied, disordered molecule of chloroform should be mentioned. When the molecule is

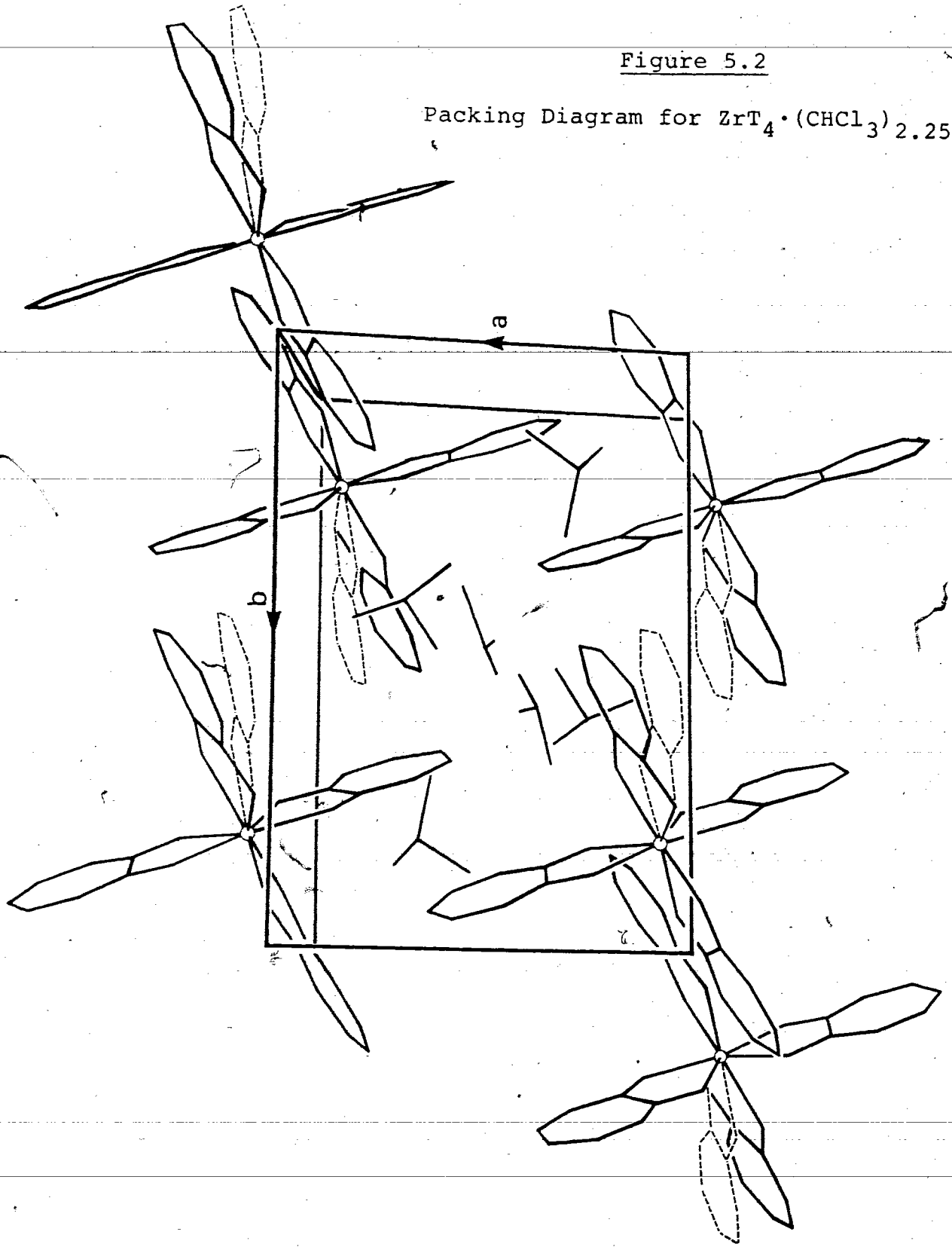
Table 5.1

Shortest Intermolecular Contacts in Crystalline $ZrT_4(CHCl_3)_{2.25}$ (Å)

H(32)-Cl(8)	2.49
H(33)-C(3)	2.34
H(33)-Cl(8)	1.79
H(33)-Cl(9)	2.72
H(33)-H(3)	1.52
H(34)-Cl(9)	2.33
C(31)-Cl(7)	2.59
C(32)-Cl(7)	2.56
C(32)-Cl(8)	2.56
C(33)-Cl(7)	2.62
C(33)-Cl(8)	2.03
C(33)-Cl(8*)	2.83
C(33)-Cl(9)	2.89
C(33)-C(3)	2.92
C(34)-C(3)	2.58
C(35)-Cl(7)	2.97
C(36)_Cl(7)	2.90
C(37)-Cl(7)	2.79
H(35')-Cl(3')	2.40
H(46)-H(3)	2.18
H(45)-Cl(7)	2.50
H(46)-Cl(7)	2.70
C(46)-H(3)	2.70

Figure 5.2

Packing Diagram for $ZrT_4 \cdot (CHCl_3)_{2.25}$



present, ligand 3 is bent away to relieve any short intermolecular contacts that occur. The alternative position adopted by the ligand creates several short contacts with another chloroform molecule of crystallization, notably with the chlorine atom labelled Cl(3), with subsequent disorder imparted to this molecule (table 5.1). The disorder is manifested in the large chlorine atom thermal motion parameters; in particular, the extreme motion exhibited by chlorine atom Cl(3) in one direction (z) implied two alternative positions. This model was adopted (each Cl(3) position being assigned an occupancy of 0.5), and behaved well during further refinement. Some minor disorder is also imparted to ligand 4, which is apparent from the rather high thermal motion parameters for the carbon atoms of this ring (see table 5.3). All hydrogen atom positions were calculated. Full matrix, least squares refinement of all the non-hydrogen atomic parameters, with all atoms assigned anisotropic thermal motion parameters except the carbon atoms of ligand 3, oxygen atom O(5), and chloroform carbon atoms, gave a final R of 0.075.

Constant unit weights were used in the early stages of r refinement; in the final stages, weights = $1/\sigma(F)^2$ where $\sigma(F) = \sigma_I/(Lp)(2F_0)$ were used. A table of the measured and calculated structure factors (x10) is given in table 5.4. Atomic positional coordinates are listed in table 5.3, and thermal motion parameters are shown in table 5.4.A perspective view of the ZrT_4 molecule, showing labelling and the disorder in ligand 3, is given in figure 5.3.

Table 5.2

Fractional Atomic Coordinates: $ZrT_4(CHCl_3)_{2.25}$
(x 10^4, x 10^5 for Zr)

Atom Type	x	y	z
Zr	-22056(8)	18206(7)	7586(11)
Cl(1)	4221(3)	3422(2)	3829(4)
Cl(2)	6211(3)	4830(3)	3399(4)
Cl(3)	4788(23)	4305(18)	1509(26)
Cl(3')	5362(24)	4475(15)	1270(21)
Cl(4)	709(4)	1362(3)	-4078(4)
Cl(5)	2106(3)	1451(3)	-2197(4)
Cl(6)	1610(4)	3063(3)	-3096(5)
Cl(7)	-20(17)	3356(12)	3778(16)
Cl(8)	-505(17)	5020(15)	4726(26)
Cl(9)	1675(25)	4625(20)	4539(40)
O(1)	-1137(5)	830(4)	-236(6)
O(2)	-3376(5)	611(4)	364(6)
O(3)	-1796(6)	1258(4)	2436(7)
O(4)	-3711(6)	1735(5)	2570(9)
O(5)	-2027(13)	3089(10)	1859(16)
O(5')	-1846(13)	3279(10)	1160(16)
O(6)	-1272(5)	2398(5)	382(7)
O(7)	-3634(6)	2384(5)	1248(9)
O(8)	-1670(6)	2245(5)	-1346(8)
C(11)	-1625(8)	87(7)	-708(10)
C(12)	-1905(7)	-492(7)	-1395(10)
C(13)	-1213(8)	-1266(7)	2036(11)
C(14)	-2345(8)	-1693(7)	2140(11)
C(15)	-3458(7)	-1446(7)	1541(11)
C(16)	-3708(7)	-739(7)	-756(10)
C(17)	-2944(8)	-37(7)	-362(10)

Table 5.2 (continued)

Atom Type	x	y	z
C(21)	-2539(9)	1108(7)	3601(13)
C(22)	-2281(9)	720(8)	4652(14)
C(23)	-2928(11)	479(8)	5960(13)
C(24)	-4090(12)	602(8)	6603(11)
C(25)	-4854(10)	960(9)	6106(15)
C(26)	-4698(9)	1293(8)	4851(13)
C(27)	-3687(9)	1396(7)	3689(13)
C(31)	-956(18)	3576(14)	1856(22)
C(32)	-835(20)	4388(16)	2501(23)
C(33)	210(26)	4973(18)	2565(29)
C(34)	1407(27)	4841(20)	2114(30)
C(35)	1854(21)	4199(17)	1338(27)
C(36)	1276(22)	3457(16)	930(27)
C(37)	-11(23)	3131(18)	1112(27)
C(31')	-736(19)	3737(14)	914(23)
C(32')	-547(19)	4641(15)	1197(22)
C(33')	514(22)	5262(15)	1103(24)
C(34')	1662(21)	5118(16)	711(24)
C(35')	2058(18)	4360(15)	245(23)
C(36')	1438(19)	3496(15)	157(24)
C(37')	168(21)	3210(16)	483(26)
C(41)	-3535(16)	2620(7)	-1972(15)
C(42)	-4517(11)	2888(6)	-1248(15)
C(43)	-4589(19)	3193(12)	-2455(24)
C(44)	-3803(27)	3334(16)	-3684(28)
C(45)	-2632(23)	3135(12)	-4043(18)
C(46)	-2043(12)	2790(9)	-3245(20)
C(47)	-2396(12)	2532(8)	-1894(16)
C(1)	5504(10)	3982(8)	2619(12)
C(2)	1096(10)	1936(8)	-2723(11)
C(3)	270	4246	4744

Table 5.2 (continued)

Atom Type	x	y	z
H(12)	-65	-3308	-143
H(13)	-563	-1564	-2480
H(14)	-2367	-2213	-2696
H(15)	-4145	-1833	-1716
H(16)	-4556	-726	-415
H(22)	-1481	588	4416
H(23)	-2519	190	6468
H(24)	-4364	409	7537
H(25)	-5617	979	6741
H(26)	-5386	1489	4727
H(32)	-1580	4574	2966
H(33)	105	5534	3023
H(34)	2009	5299	2363
H(35)	2730	4288	1019
H(36)	1788	3064	426
H(32')	-1275	4889	1504
H(33')	435	5866	1377
H(34')	2284	5623	764
H(35')	2929	4435	-119
H(36')	1923	3045	-169
H(42)	-5232	2857	-515
H(43)	-5356	3340	-2426
H(44)	-4044	3592	-4391
H(45)	-2179	3256	-4976
H(46)	-1240	2711	-3725
H(1)	6044	3574	2254
H(2)	338	1896	-1954
H(3)	-24	3991	5627

Table 5.3

Thermal Motion Parameters: $ZrT_4(CHCl_3)_{2.25}$

($\times 10^3$, $\times 10^4$ for Zr $Å^2$)

a) Anistropic Atoms

Atom Type	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Zr	210(6)	489(8)	734(9)	84(5)	102(5)	91(6)
Cl(1)	85(3)	113(3)	185(4)	0(2)	30(3)	48(3)
Cl(2)	127(3)	145(4)	122(3)	-41(3)	-26(3)	-32(3)
Cl(3)	270(19)	158(12)	255(25)	51(12)	-215(20)	-60(14)
Cl(3')	417(32)	172(17)	79(8)	161(19)	86(14)	3(9)
Cl(4)	177(4)	155(4)	136(4)	54(3)	-43(3)	-26(3)
Cl(5)	83(3)	189(4)	190(4)	67(3)	-20(3)	10(3)
Cl(6)	136(4)	108(4)	237(5)	-5(3)	1(3)	40(3)
Cl(7)	197(19)	166(17)	189(13)	64(15)	215(12)	-19(11)
Cl(8)	114(19)	138(16)	246(27)	29(17)	-22(18)	-42(16)
Cl(9)	193(26)	241(31)	491(53)	-66(24)	-197(34)	165(33)
O(1)	21(4)	62(5)	78(6)	7(4)	-8(4)	-12(4)
O(2)	19(3)	53(5)	77(5)	7(3)	-12(3)	-10(4)
O(3)	33(4)	75(5)	56(5)	5(4)	-3(4)	-3(4)
O(4)	48(5)	84(6)	93(7)	34(4)	-35(5)	-31(5)
O(6)	39(4)	56(5)	97(6)	6(4)	-15(4)	-12(5)
O(7)	33(4)	62(5)	110(7)	12(4)	-27(5)	8(5)
O(8)	44(5)	83(6)	107(7)	15(4)	-29(5)	5(5)
C(11)	26(6)	41(7)	57(7)	5(5)	-13(5)	-3(6)
C(12)	16(5)	56(7)	73(8)	9(5)	-4(5)	-9(6)
C(13)	24(6)	71(9)	84(9)	17(6)	-2(6)	-10(7)
C(14)	35(6)	57(8)	91(9)	12(6)	-19(6)	-28(7)
C(15)	33(6)	58(8)	91(9)	4(6)	-27(6)	-20(7)
C(16)	18(5)	53(7)	78(9)	3(5)	-10(5)	-28(7)
C(17)	37(6)	47(7)	55(8)	27(6)	-10(5)	-4(6)

Table 5.3 (cont'd)

Atom Type	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
C(21)	31(6)	51(7)	61(9)	4(6)	-15(6)	-12(6)
C(22)	47(7)	86(10)	63(10)	24(7)	-9(7)	-7(8)
C(23)	71(9)	90(10)	71(10)	22(8)	-19(8)	-1(8)
C(24)	67(9)	78(9)	61(9)	16(8)	11(7)	1(7)
C(25)	44(8)	93(11)	91(12)	23(7)	14(8)	-15(9)
C(26)	32(7)	77(9)	78(10)	14(6)	-3(7)	-18(8)
C(27)	32(7)	59(8)	73(10)	15(6)	-12(7)	-20(7)
C(41)	76(10)	34(7)	101(12)	9(7)	-52(10)	-1(7)
C(42)	73(1)	72(9)	121(13)	28(7)	-58(9)	-15(8)
C(43)	155(20)	76(13)	212(24)	44(13)	-138(19)	-13(16)
C(44)	243(37)	110(16)	206(30)	-22(20)	-186(31)	31(19)
C(45)	231(25)	98(14)	89(14)	-17(16)	-94(18)	16(10)
C(46)	98(11)	87(11)	94(13)	-4(9)	-30(10)	7(10)
C(47)	63(10)	56(9)	86(12)	3(7)	-23(9)	-8(8)

b) Isotropic Atoms†

Atom Type	U	Atom Type	U
O(5)	54(5)	$3C_1'$	49(6)
O(5')	53(5)	$3C_2'$	63(6)
C(31)	44(6)	$3C_3'$	76(7)
C(32)	70(7)	$3C_4'$	76(7)
C(33)	103(9)	$3C_5'$	59(6)
C(34)	114(10)	$3C_6'$	51(7)
C(35)	74(7)	$3C_7'$	44(7)
C(36)	65(8)	C_1	84(4)
C(37)	60(9)	C_2	88(4)
		C_3	89

† Tropolonato hydrogen atoms were assigned temperature factors of U = 0.063 Å^2 and chloroform hydrogen atoms were assigned temperature factors of U = 0.089 Å^2.

Table 5.4

Structure Factor Listing: $ZrT_4(CHCl_3)_{2.25}$
(x 10)

Unobserved reflections are indicated by an asterisk.

L	FO	FC
H= 0, K= 0		
1	989	1028
2	48*	18
3	465	455
4	447	-460
5	8*	-51
6	308	-332
7	268	-285
8	54*	20
9	85*	-42
10	15*	-22
H= 0, K= 1		
10	50*	63
9	88*	-85
8	13*	30
7	103	-132
6	417	-417
5	178	-160
4	133	-129
3	503	-529
2	415	-421
1	114	108
0	445	427
H= 0, K= 2		
0	601	-572
1	355	-367
2	223	-208
3	98	96
4	419	-454
5	311	-310
6	253	234
7	12*	31
8	238	243
9	115	91
10	15*	41
H= 0, K= 3		
10	15*	21
9	107	-91
8	66*	98
7	222	238
6	427	482
5	432	447
4	27*	-47
3	444	445
2	54*	-103
1	1250	-1199
0	834	-812

L	FO	FC
H= 0, K= 4		
0	383	-378
1	1521	1491
2	426	437
3	358	365
4	472	478
5	173	-136
6	255	234
7	53*	-1
8	184	-179
9	52*	-37
10	44*	-56
H= 0, K= 5		
10	106*	-96
9	142	-156
8	219	-247
7	179	-170
6	169	-183
5	291	-282
4	243	261
3	76*	-61
2	356	352
1	1192	1213
0	615	-622
H= 0, K= 6		
0	844	843
1	287	-301
2	379	-372
3	320	-299
4	427	-453
5	405	-412
6	351	-367
7	218	-225
8	112	-100
9	26*	58
10	53*	54
H= 0, K= 7		
9	90*	76
8	146	114
7	68*	91
6	116	-89
5	12*	13
4	174	-176
3	823	-845
2	900	-879
1	421	-407
0	33*	9

L	FO	FC
H= 0, K= 8		
0	388	-408
1	233	-260
2	403	-405
3	105	128
4	142	137
5	132	149
6	242	261
7	56*	55
8	15*	47
9	16*	20
H= 0, K= 9		
8	81*	34
7	52*	31
6	88*	91
5	376	393
4	12*	36
3	270	283
2	347	386
1	171	-177
0	57*	-76
H= 0, K= 10		
0	12*	-57
1	110	152
2	132	122
3	247	250
4	240	239
5	14*	4
6	85*	-67
7	134	-110
8	151	-147
H= 0, K= 11		
7	126	-156
6	192	-170
5	116	-103
4	14*	8
3	202	225
2	255	247
1	399	388
0	74*	61
H= 0, K= 12		
0	230	203
1	129	91
2	14*	80
3	14*	-39
4	77*	-54

L	FO	FC
5	66*	-79
6	81*	-109
7	32*	-9
H= 0, K= 13		
6	16*	52
5	15*	-1
4	81*	-46
3	107	-99
2	74*	-30
1	96*	-63
0	14*	-56
H= 0, K= 14		
0	140	-114
1	15*	-57
2	15*	-21
3	79*	54
4	113	68
5	83*	74
H= 0, K= 15		
4	112*	116
3	169	149
2	214	192
1	15*	52
0	22*	34
H= 0, K= 16		
0	202	182
1	171	188
H= 1, K= 15		
0	186	-211
1	151	-102
2	105	-83
3	50*	5
H= 1, K= 14		
5	55*	3
4	95*	-108
3	230	-213
2	152	-135
1	181	-197
0	99*	-113
H= 1, K= 13		
0	225	191

L	FO	FC
1	91*	105
2	25*	-34
3	122	-132
4	224	-229
5	144	-175
6	120	-118
H=	1, K=	12
7	127	-128
6	181	-185
5	222	-177
4	38*	-23
3	70*	-47
2	158	158
1	114	122
0	100*	106
H=	1, K=	11
0	46*	21
1	29*	57
2	170	140
3	213	204
4	104	111
5	59*	43
6	44*	-42
7	137	-111
8	94*	-73
H=	1, K=	10
8	16*	23
7	15*	3
6	97	51
5	43*	-6
4	13*	15
3	113	134
2	70*	-102
1	63*	-72
0	233	-217
H=	1, K=	9
0	106	-112
1	84*	-120
2	521	-535
3	12*	31
4	153	-143
5	224	-248
6	88*	81
7	14*	5
8	57*	31
9	16*	77
H=	1, K=	8
9	95*	62
8	51*	36
7	59*	-76
6	178	196
5	132	-128
4	351	-356
3	362	-352
2	513	-496
1	155	-142
0	72*	-50
H=	1, K=	7
0	247	264
1	63*	88
2	189	-172
3	173	153
4	342	-343
5	174	-194
6	274	-281
7	325	-339
8	171	-157
9	15*	-23
H=	1, K=	6
10	16*	-10
9	170	-144
8	224	-232
7	138	-178
6	274	-273
5	12*	10
4	288	279
3	274	-263
2	840	850
1	912	908
0	542	537
H=	1, K=	5
0	497	495
1	266	-258
2	869	854
3	381	394
4	256	276
5	451	451
6	238	243
7	68*	-36
8	119	-107
9	102*	-124
10	39*	-58
H=	1, K=	4
10	16*	10
9	104	-50
8	160	152
7	356	383
6	399	423
5	427	423
4	480	473
3	334	-336
2	492	-493
1	1728	-1682
0	48*	16
H=	1, K=	3
0	608	-623
1	1120	-1072
2	438	430
3	7*	46
4	276	-276
5	362	-371
6	118	146
7	164	174
8	229	216
9	101*	105
10	53*	29
H=	1, K=	2
10	15*	23
9	67*	49
8	13*	88
7	39*	-50
6	301	-324
5	371	-394
4	269	-281
3	180	186
2	459	453
1	52*	54
0	212	209
H=	1, K=	1
0	1257	1204
1	1137	1056
2	307	-314
3	144	137
4	633	-659
5	8*	37
6	203	-208
7	223	-228
8	26*	-26
9	65*	21
10	101	-71
H=	1, K=	0
10	15*	-73
9	75*	-44
8	273	-249
7	72*	-46
6	143	-158
5	431	432
4	714	735
3	388	-399
2	92	94
1	1035	1035
0	104	119
H=	2, K=	0
1	211	-194
2	311	-311
3	164	146
4	372	-378
5	186	172
6	153	176
7	141	132
8	162	197
9	122	-102
10	110	-77
11	16*	-73
H=	2, K=	1
11	97*	-87
10	30*	-33
9	124	-119
8	291	-272
7	45*	-62
6	219	206
5	258	272
4	163	169
3	197	190
2	567	552
0	1609	-1535
H=	2, K=	2
0	474	438
1	904	864
2	318	-307
3	178	181
4	113	-121
5	379	-366
6	63*	15
7	218	-214
8	85*	-91
9	14*	18
10	60*	-53

L	FO	FC
H=	2, K=	3
10	57*	43
9	90*	77
8	85*	-96
7	137	-142
6	130	-188
5	515	-524
4	183	209
3	90	82
2	1146	-1155
1	1548	1465
0	390	381
H=	2, K=	4
0	154	-158
1	694	-654
2	84	-61
3	758	-760
4	76*	-93
5	9*	-5
6	231	-205
7	63*	101
8	167	172
9	260	246
10	15*	51
H=	2, K=	5
10	22*	11
9	122	75
8	27*	63
7	352	373
6	277	273
5	233	211
4	445	436
3	220	-233
2	957	-957
1	999	-986
0	510	-512
H=	2, K=	6
0	75*	-56
1	514	-487
2	192	222
3	338	332
4	60*	-55
5	312	308
6	193	181
7	76*	85
8	67*	83
9	15*	-7
10	73*	9
H=	2, K=	7
9	115	-86
8	77*	-89
7	73*	80
6	154	-121
5	131	127
4	97	110
3	232	-218
2	1132	1133
1	456	451
0	263	-252
H=	2, K=	8
0	148	154
1	114	-92
2	526	542
3	216	208
4	80*	-85
5	136	-116
6	122	-88
7	190	-201
8	100	-65
9	35*	15
H=	2, K=	9
9	100*	71
8	30*	84
7	14*	-56
6	126	-146
5	195	-191
4	207	-204
3	426	-421
2	540	-551
1	63*	-66
0	107	98
H=	2, K=	10
1	331	-316
2	396	-392
3	421	-420
4	53*	-9
5	88*	-20
6	55*	41
7	120	132
8	135	152
H=	2, K=	11
7	144	139
6	137	151
5	25*	69
4	119	114
3	50*	81
2	13*	12
1	13*	-19
0	310	-274
H=	2, K=	12
0	117	74
1	94*	-64
2	119	95
3	433	463
4	176	162
5	167	163
6	90*	94
7	95*	-58
H=	2, K=	13
6	105*	-128
5	43*	-72
4	60*	-33
3	107	96
2	244	249
1	266	229
0	176	144
H=	2, K=	14
0	184	173
1	40*	79
2	55*	-31
3	149	-134
4	215	-220
H=	2, K=	15
2	69*	-80
1	16*	-68
0	47*	32
H=	3, K=	14
4	113	47
3	98*	69
2	31*	41
1	118	77
0	134	144
H=	3, K=	13
0	15*	9
1	144	121
2	133	124
3	237	235
4	145	168
5	68*	49
H=	3, K=	12
6	120	112
5	112	79
4	219	199
3	86*	-103
2	14*	38
1	73*	-25
0	162	-159
H=	3, K=	11
0	47*	-121
1	210	-224
2	160	-155
3	471	-480
4	243	-235
5	32*	-41
6	15*	35
7	105*	109
H=	3, K=	10
8	16*	-9
7	26*	-59
6	114	-139
5	278	-287
4	14*	-40
3	260	-274
2	179	-172
1	63*	71
0	157	-172
H=	3, K=	9
0	143	150
1	148	157
2	386	385
3	138	130
4	13*	17
5	13*	-36
6	234	-204
7	215	-210
8	118	-133
H=	3, K=	8
9	57*	-83
8	15*	-47
7	37*	46
6	96	82

L	FO	FC
5	87*	83
4	214	200
3	605	568
2	261	268
1	223	233
0	206	227
H=	3, K=	7
0	570	-565
1	318	-317
2	240	-246
3	481	468
4	124	121
5	265	272
6	349	328
7	118	100
8	118	116
9	15*	25
H=	3, K=	6
10	16*	3
9	86*	68
8	28*	93
7	326	290
6	226	211
5	81*	105
4	58*	-16
3	196	-196
2	889	-853
1	596	-616
0	440	-420
H=	3, K=	5
0	414	409
1	40*	-43
2	8*	-23
3	222	-224
4	404	-406
5	11*	-24
6	161	-150
7	18*	-40
8	167	179
9	147	178
10	81*	55
H=	3, K=	4
10	56*	46
9	83*	71
8	146	-127
7	66*	-86
6	12*	-54
5	373	-378
4	106	112
3	8*	-17
2	54*	-9
1	715	708
0	351	348
H=	3, K=	3
0	195	210
1	593	577
2	931	911
3	157	-138
4	248	238
5	159	153
6	281	-269
7	150	-165
8	81*	-103
9	43*	-103
10	15*	-12
H=	3, K=	2
10	122	-49
9	60*	-89
8	212	-203
7	115	-89
6	283	294
5	303	291
4	522	524
3	582	572
2	610	-592
1	415	-388
0	45*	13
H=	3, K=	1
0	540	-526
1	380	-378
2	442	-420
3	79*	107
4	70*	-57
5	229	227
6	292	316
7	173	161
8	242	200
9	60*	-56
10	84*	-61
11	28*	-26
H=	3, K=	0
11	80*	37
10	98*	80
9	14*	35
8	194	222
7	42*	80
6	84*	46
5	209	221
4	342	-329
3	140	122
2	236	-222
1	509	-473
0	960	-869
H=	4, K=	0
0	131	-112
1	33*	-27
2	234	-227
3	289	-285
4	233	-255
5	356	-345
6	159	-153
7	87*	-84
8	47*	18
9	14*	-10
10	97*	81
11	66*	16
H=	4, K=	1
11	16*	58
10	101*	112
9	98*	84
8	102	104
7	163	-132
6	193	204
5	8*	39
4	286	-281
3	120	-118
2	532	-526
1	944	-880
0	154	-170
H=	4, K=	2
0	1015	-993
1	119	-117
2	172	-166
3	393	-376
4	359	340
5	105	135
6	251	273
7	285	286
8	186	-203
9	75*	43
10	15*	-32
H=	4, K=	3
10	137	-119
9	133	-108
8	125	-108
7	25*	34
6	393	376
5	369	362
4	404	410
3	281	289
2	84	76
1	341	345
0	98	-135
H=	4, K=	4
0	222	231
1	442	462
2	1101	1087
3	475	471
4	187	189
5	422	424
6	261	-284
7	89*	-82
8	137	-134
9	194	-204
10	34*	-25
H=	4, K=	5
10	16*	2
9	53*	-41
8	206	-187
7	99	-104
6	165	-170
5	220	-213
4	9*	3
3	104	107
2	393	376
1	697	643
0	562	555
H=	4, K=	6
0	9*	31
1	52*	-2
2	96	-83
3	196	-186
4	195	-193
5	74*	-33
6	255	-231
7	75*	-113
8	68*	24
9	88*	46
10	112	79
H=	4, K=	3

L	FO	FC
H=	4, K=	7
9	147	131
8	152	150
7	139	98
6	67*	77
5	77*	58
4	93	-67
3	12*	4
2	387	-422
1	459	-481
0	52*	87
H=	4, K=	8
0	383	-387
1	192	-191
2	30*	-62
3	220	209
4	322	315
5	137	117
6	138	137
7	139	126
8	125	100
9	16*	-30
H=	4, K=	9
8	15*	-33
7	71*	-37
6	89*	101
5	24*	-67
4	98	80
3	312	343
2	172	187
1	401	390
0	91*	74
H=	4, K=	10
0	214	219
1	92*	53
2	289	335
3	127	137
4	167	-225
5	20*	-19
6	186	-176
7	178	-162
8	90*	-83
H=	4, K=	11
7	104*	-55
6	57*	-78
5	260	-240
4	313	-286
3	210	-205
2	144	-130
1	14*	50
0	14*	51
H=	4, K=	12
0	15*	-37
1	155	-152
2	273	-294
3	329	-341
4	186	-207
5	55*	45
6	35*	45
H=	4, K=	13
5	163	82
4	16*	14
3	124	-120
2	91*	-147
1	238	-214
0	148	-143
H=	4, K=	14
0	141	-121
1	16*	-54
2	48*	18
H=	5, K=	13
0	35*	-18
1	121	-113
2	126	-110
3	176	-160
H=	5, K=	12
5	45*	-83
4	38*	-72
3	15*	36
2	53*	79
1	89*	92
0	154	190
H=	5, K=	11
0	97*	139
1	142	122
2	146	164
3	216	214
4	109*	108
5	43*	63
6	94*	-59
H=	5, K=	10
7	16*	29
6	180	180
5	68*	115
4	250	240
3	150	145
2	14*	39
1	74*	58
0	14*	-50
H=	5, K=	9
0	266	-297
1	70*	26
2	228	209
3	106	-106
4	103	124
5	284	279
6	192	214
7	226	240
8	48*	69
H=	5, K=	8
9	134	108
8	190	191
7	191	209
6	199	189
5	19*	21
4	80*	-82
3	13*	35
2	354	-355
1	29*	-37
0	118	-124
H=	5, K=	7
0	83*	55
1	12*	70
2	163	-171
3	288	-263
4	78*	-87
5	229	-230
6	174	-159
7	101	92
8	72*	90
9	106*	108
H=	5, K=	6
9	108	-61
8	15*	-42
7	168	-156
6	281	-233
5	198	-166
4	229	-229
3	344	334
2	252	285
1	29*	26
0	362	393
H=	5, K=	5
0	16*	11
1	395	403
2	299	291
3	242	254
4	396	368
5	133	163
6	254	-262
7	233	-255
8	110	-46
9	45*	-99
10	42*	-24
H=	5, K=	4
10	90*	-31
9	36*	-8
8	14*	-83
7	98	56
5	307	318
4	468	456
3	169	149
2	49*	-39
1	274	-298
0	9*	-7
H=	5, K=	3
0	431	-454
1	700	-729
2	45*	91
3	691	-646
4	136	-111
5	12*	44
6	197	169
7	238	228
8	89*	133
9	93*	94
10	16*	26
H=	5, K=	2
10	99*	72
9	112	91
8	51*	-27

L	FO	FC
7	108	-87
6	112	113
5	366	-369
4	727	-690
3	600	-562
2	272	-276
1	558	-548
0	651	-645
H=	5, K=	1
0	46*	23
1	307	340
2	254	-217
3	590	-582
4	170	-189
5	889	-899
6	399	-401
7	13*	-58
8	221	-223
9	14*	-50
10	15*	22
H=	5, K=	0
11	36*	8
10	147	-132
9	105	-83
8	222	-230
7	400	-386
6	244	-242
5	53*	-101
4	66*	27
3	829	823
2	463	459
1	204	181
0	1002	961
H=	6, K=	0
0	71*	-63
1	878	857
2	404	380
3	443	418
4	409	408
5	227	228
6	357	373
7	103	126
8	98	39
9	71*	-38
10	106*	-77
H=	6, K=	1
10	67*	-79
9	113	-118
8	224	-172
7	326	-305
6	63*	-80
5	124	98
4	198	204
3	558	545
2	399	395
1	740	728
0	454	480
H=	6, K=	2
0	138	123
1	98	85
2	44*	21
3	9*	17
4	85	-41
5	496	-448
6	462	-475
7	137	-105
8	196	-192
9	64*	-85
10	16*	12
H=	6, K=	3
10	50*	54
9	142	114
8	14*	67
7	53*	-62
6	118	-123
5	332	-298
4	508	-483
3	304	-306
2	281	-287
1	366	-392
0	178	-177
H=	6, K=	4
0	154	-176
1	346	-384
2	422	-429
3	91	-85
4	127	-140
5	12*	-11
6	132	97
7	225	181
8	145	131
9	175	159
10	57*	50
H=	6, K=	5
9	15*	-5
8	15*	23
7	122	80
6	129	213
5	321	321
4	196	183
2	257	268
3	57*	129
1	285	-284
0	252	-256
H=	6, K=	6
0	13*	-15
1	436	487
2	423	408
3	245	249
4	311	310
5	26*	-12
6	48*	-48
7	184	-131
8	75	-129
9	93*	-144
H=	6, K=	7
9	92*	-100
8	15*	-51
7	225	-206
6	69*	-39
5	164	-179
4	257	-250
3	13*	22
2	152	167
1	176	192
0	416	435
H=	6, K=	8
0	89*	96
1	13*	94
2	13*	8
3	202	-210
4	14*	55
5	80*	-90
6	142	-126
7	15*	-10
8	75*	-46
H=	6, K=	9
7	15*	23
6	50*	50
5	70*	-76
4	85*	-83
3	52*	-87
2	14*	-66
1	14*	-6
0	109	100
H=	6, K=	10
2	174	-154
0	129	-129
1	116	-149
3	38*	-57
4	15*	34
5	132	153
6	135	111
7	99*	125
H=	6, K=	11
6	62*	58
5	154	127
4	172	193
3	189	198
2	101*	108
1	81*	-63
0	158	-130
H=	6, K=	12
0	16*	69
1	198	222
2	150	152
3	154	161
4	108*	112
H=	7, K=	11
0	137	-144
1	139	-144
2	147	-154
3	41*	-84
4	50*	44
H=	7, K=	10
6	16*	-72
5	88*	-133
4	97*	-151
3	263	-280
2	123	-164
1	88*	-99
0	59*	95
H=	7, K=	9
0	293	320

L	FO	FC
H=	7, K=	9
1	108*	141
2	41*	24
3	15*	-78
4	138	-126
5	257	-237
6	207	-224
7	104*	-123
H=	7, K=	8
7	219	-227
6	73*	-82
5	15*	24
4	14*	5
3	91*	92
2	210	196
1	219	284
0	133	201
H=	7, K=	7
0	66*	-77
1	314	347
2	191	221
3	14*	18
4	161	165
5	87*	98
6	50*	27
7	15*	-61
8	173	-172
H=	7, K=	6
9	99*	-75
8	63*	18
7	103	66
6	116	119
5	212	176
4	72*	-116
3	235	271
2	87*	117
1	125	-131
0	19*	-67
H=	7, K=	5
0	137	-155
1	161	-137
2	321	-375
3	75*	-60
4	212	-207
5	134	-147
6	170	161
7	138	130
8	58*	79
9	93*	94
H=	7, K=	4
9	51*	-24
8	68*	87
7	54*	69
6	251	-214
5	252	-241
4	467	-439
3	473	-442
2	139	-135
1	95*	-105
0	176	187
H=	7, K=	3
0	672	675
1	373	361
2	67*	40
3	385	340
4	107	98
5	302	-274
6	473	-443
7	238	-216
8	90*	-78
9	15*	-34
10	35*	1
H=	7, K=	2
10	16*	-46
9	67*	-66
8	170	-175
7	215	-225
6	152	-141
5	205	223
4	586	543
3	362	346
2	364	383
1	350	363
0	210	236
H=	7, K=	1
0	261	-292
1	202	192
2	397	359
3	94	72
4	362	358
5	188	178
6	151	160
7	250	235
8	40*	60
9	75*	71
10	52*	-19
H=	7, K=	0
10	58*	63
9	15*	36
8	148	126
7	227	245
6	302	310
5	295	280
4	88	-49
3	86	-63
2	165	-150
1	478	-448
0	691	-626
H=	8, K=	0
0	122	101
1	169	-168
2	167	-174
3	260	-268
4	252	-244
5	304	-293
6	70*	-83
7	116	-75
8	59*	71
9	111	93
10	140	110
H=	8, K=	1
10	42*	7
9	48*	48
8	191	179
7	138	133
6	117	113
5	44*	17
4	212	-195
3	400	-378
2	404	-368
1	318	-337
0	260	-246
H=	8, K=	2
0	106	-95
1	442	-434
2	265	-216
3	33*	-7
4	60*	26
5	154	177
6	112	119
7	165	154
8	119	108
9	72*	47
H=	8, K=	3
9	15*	-30
8	109	-97
7	109	-83
6	161	-149
5	170	171
4	242	212
3	31*	26
2	297	303
1	195	214
0	114	-114
H=	8, K=	4
0	56*	114
1	207	280
2	13*	30
3	90*	110
4	90*	-77
5	219	-222
6	185	-174
7	162	-169
8	141	-131
9	90*	-27
H=	8, K=	5
8	51*	47
7	15*	38
6	123	-130
5	203	-211
4	359	-382
3	282	-319
2	79*	-92
1	91*	-93
0	106	108
H=	8, K=	6
0	123	-139
1	282	-293
2	442	-479
3	295	-326
4	203	-192
5	269	-268
6	75*	-4
7	85*	105
8	22*	93
H=	8, K=	7

L	FO	FC
7	140	153
6	146	161
5	15*	38
4	76*	-54
3	81*	-46
2	141	-170
1	187	-223
0	259	-282

H= 8, K= 8

L	FO	FC
0	15*	3
1	15*	-12
2	90*	117
3	182	185
4	176	177
5	223	273
6	185	191
7	61*	63

H= 8, K= 9

L	FO	FC
5	78*	70
4	97*	77
3	90*	112
2	212	214
1	149	158
0	113*	148

H= 8, K= 10

L	FO	FC
0	159	174
1	126	146
2	31*	-55
3	78*	-17
4	77*	-124

H= 9, K= 9

L	FO	FC
2	50*	18
3	176	198

H= 9, K= 8

L	FO	FC
5	16*	31
4	66*	50
3	86*	-124
2	235	-217
1	172	-202
0	256	-264

H= 9, K= 7

L	FO	FC
0	114	-112
1	205	-258
2	240	-324
3	248	-308
4	185	-212
5	93*	-127
6	16*	-59

H= 9, K= 6

L	FO	FC
7	16*	-60
6	180	-173
5	183	-164
4	161	-194
3	198	-250
2	169	-186
1	72*	75
0	96*	103

H= 9, K= 5

L	FO	FC
0	235	250
1	325	351
2	267	260
3	148	137
4	45*	39
5	36*	-55
6	88*	-61
7	126	-143
8	124	-120

H= 9, K= 4

L	FO	FC
8	16*	23
7	78*	62
6	15*	46
5	261	251
4	208	200
3	161	183
2	281	352
1	14*	3
0	118	-155

H= 9, K= 3

L	FO	FC
0	223	-238
1	299	-313
2	82*	-92
3	36*	63
4	14*	8
5	142	142
6	232	249
7	139	126
8	145	157

H= 9, K= 2

L	FO	FC
9	47*	74
8	146	159
7	179	167
6	216	208
5	56*	23
4	19*	-9
3	301	-289
2	221	-233
1	164	-190
0	216	-199

H= 9, K= 1

L	FO	FC
0	306	320
1	13*	48
2	67*	28
3	279	-236
4	203	-180
5	108	-98
6	83*	-69
7	59*	-32
8	110	124
9	112*	153

H= 9, K= 0

L	FO	FC
9	62*	60
8	15*	-85
7	94*	-85
6	132	-103
5	149	-126
4	155	170
3	43*	55
2	75*	-79
1	353	352
0	339	358

H= 10, K= 0

L	FO	FC
1	46*	45
2	337	346
3	402	381
4	245	251
5	168	167
6	14*	-37
7	59*	-19
8	96*	-95

H= 10, K= 1

L	FO	FC
8	170	-157
7	15*	-24
6	99*	-84
5	89*	-92
4	150	108
3	116	184
2	247	225
1	330	337
0	84*	132

H= 10, K= 2

L	FO	FC
0	178	181
1	275	272
2	118	94
3	61*	5
4	311	-309
5	171	-141
6	66*	-43
7	15*	14
8	16*	49

H= 10, K= 3

L	FO	FC
7	141	158
6	157	172
5	53*	-5
4	187	-196
3	281	-263
2	85*	-134
1	14*	-11
0	15*	-66

H= 10, K= 4

L	FO	FC
0	156	-140
1	148	-157
2	135	-149
3	141	137
4	224	212
5	224	210
6	273	291
7	191	140

H= 10, K= 5

L	FO	FC
6	124	128
5	184	209
4	204	253
3	184	215
2	21*	94
1	91*	70
0	115	106

H= 10, K= 6

L	FO	FC
0	184	229
1	78*	123
2	172	217

L	FO	FC
H=	10, K=	6
3	131	103
4	103*	106
5	16*	69
H=	10, K=	7
4	97*	-57
3	83*	-83
2	16*	42
1	93*	76
H=	11, K=	5
2	65*	-120
3	16*	-10
H=	11, K=	4
5	16*	3
4	114*	-129
3	107*	-149
2	163	-207
1	138	-125
H=	11, K=	3
0	84*	117
1	85*	-3
2	95*	-88
3	214	-241
4	261	-270
5	202	-181
6	135	-101
H=	11, K=	2
6	175	-175
5	101*	-110
4	15*	-1
3	15*	23
2	185	191
1	96*	122
0	149	169
H=	11, K=	1
0	82*	71
1	42*	37
2	250	291
3	246	231
4	132	131
5	146	118
6	48*	-46
7	59*	-65
H=	11, K=	0
7	115	114
6	98*	71
5	47*	72
4	101	58
3	15*	38
2	15*	-5
1	15*	-10
0	130	-109
H=	12, K=	0
1	150	-180
2	224	-251
3	276	-270
4	210	-201
5	27*	1
H=	12, K=	1
5	187	191
4	159	146
3	52*	54
2	50*	-102
1	81*	-73
H=	12, K=	2
3	272	298
H=	11, K=	-7
-1	47*	-21
H=	11, K=	-6
-2	90*	-78
-1	249	-295
H=	11, K=	-5
-1	245	-245
-2	159	-180
H=	11, K=	-4
-2	35*	-93
-1	67*	76
H=	11, K=	-3
-1	278	301
-2	119	130
H=	11, K=	-2
-2	120*	172
-1	137	166
H=	11, K=	-1
-1	93*	-60
-2	16*	-44
H=	11, K=	0
-2	175	-214
-1	191	-183
H=	10, K=	0
-1	87*	28
-2	236	-271
-3	245	-260
H=	10, K=	-1
-4	97*	-75
-3	265	-277
-2	362	-389
-1	267	-290
H=	10, K=	-2
-1	136	-117
-2	200	-203
-3	74*	4
-4	139	151
H=	10, K=	-3
-4	90*	141
-3	219	231
-2	154	112
-1	45*	49
H=	10, K=	-4
-1	83*	-29
-2	136	133
-3	174	151
-4	16*	-26
H=	10, K=	-5
-3	15*	-61
-2	92*	-47
-1	95*	-68
H=	10, K=	-6
-1	112	-73
-2	233	-225
-3	76*	-130
H=	10, K=	-7
-3	16*	-47
-2	112	-134
-1	139	-120
H=	10, K=	-8
-1	111	62
-2	15*	40
-3	102*	107
H=	10, K=	-9
-2	241	241
-1	270	266
H=	10, K=	-10
-1	216	171
H=	9, K=	-12
-1	16*	14
H=	9, K=	-11
-1	149	148
-2	102	85
H=	9, K=	-10
-3	156	174
-2	65*	46
-1	56*	93
H=	9, K=	-9
-1	156	-119
-2	34*	-67
-3	35*	35
H=	9, K=	-8
-4	115*	-123
-3	179	-161
-2	278	-265

L	FO	FC
-1	247	-262
H=	9, K=	-7
-1	14*	-66
-2	252	-258
-3	309	-346
-4	254	-294
H=	9, K=	-6
-4	231	-252
-3	157	-140
-2	14*	10
-1	14*	-35
H=	9, K=	-5
-1	178	-156
-2	107	23
-3	267	230
-4	15*	-11
-5	105*	-123
H=	9, K=	-4
-5	16*	50
-4	160	187
-3	262	274
-2	58*	113
-1	87*	-104
H=	9, K=	-3
-1	228	-220
-2	103	-20
-3	50*	52
-4	149	184
-5	96*	116
H=	9, K=	-2
-5	105	65
-4	15*	7
-3	293	-270
-2	315	-340
-1	227	-222
H=	9, K=	-1
-1	123	94
-2	156	-164
-3	337	-347
-4	69*	-137
-5	96*	-124
H=	9, K=	0
-5	16*	-5
-4	91*	-22
-3	114	-91
-2	347	326
-1	338	370
H=	8, K=	0
-1	274	268
-2	233	266
-3	394	392
-4	225	209
-5	182	218
-6	71*	93
H=	8, K=	-1
-6	92*	-98
-5	15*	-31
-4	32*	16
-3	182	198
-2	318	316
-1	221	204
H=	8, K=	-2
-1	143	-142
-2	177	142
-4	20*	-94
-5	138	-128
-6	50*	-79
H=	8, K=	-3
-6	87*	50
-5	15*	-21
-4	14*	-6
-3	162	-207
-2	37*	-51
-1	281	-248
H=	8, K=	-4
-1	252	-236
-2	180	-179
-3	86*	-21
-4	191	171
-5	145	164
-6	125	181
H=	8, K=	-5
-6	100*	106
-5	188	186
-4	402	371
-3	80*	92
-2	13*	18
-1	198	167
H=	8, K=	-6
-1	401	421
-2	98*	113
-3	267	274
-4	198	222
-5	61*	32
H=	8, K=	-7
-5	134	-141
-4	117	-143
-3	79*	16
-2	104	62
-1	103	68
H=	8, K=	-8
-1	158	-110
-2	96	-79
-3	159	-176
-4	248	-215
-5	150	-147
H=	8, K=	-9
-4	114	-81
-3	113	-95
-2	14*	-60
-1	342	-327
H=	8, K=	-10
-1	277	-256
-2	15*	67
-3	56*	49
-4	16*	112
H=	8, K=	-11
-3	27*	107
-2	95*	136
-1	119	72
H=	8, K=	-12
-1	254	272
-2	102*	106
-3	109	92
H=	8, K=	-13
-2	16*	-18
-1	16*	61
H=	7, K=	-14
-2	94*	75
-1	227	186
H=	7, K=	-13
-1	157	194
-2	211	181
-3	45*	32
H=	7, K=	-12
-4	125	109
-3	55*	89
-2	221	206
-1	130	129
H=	7, K=	-11
-1	90*	-72
-2	78*	16
-3	79*	85
-4	44*	55
H=	7, K=	-10
-5	87*	-59
-3	176	-118
-2	229	-186
-1	100	-85
H=	7, K=	-9
-1	103	-47
-2	171	-185
-3	90*	-126
-4	199	-195
-5	190	-207
H=	7, K=	-8
-6	61*	-121
-5	222	-262
-4	14*	24
-3	184	162
-2	68*	117
-1	433	416

L	FO	FC
H=	7, K=	-7
-1	374	381
-2	460	426
-3	389	366
-4	374	349
-5	29*	-19
-6	15*	-14
H=	7, K=	-6
-6	150	164
-5	292	291
-4	320	337
-3	231	231
-2	382	367
-1	136	104
H=	7, K=	-5
-1	231	-252
-2	144	-144
-3	102	-62
-4	14*	74
-5	226	219
-6	160	178
H=	7, K=	-4
-7	39*	42
-6	70*	-55
-5	14*	5
-4	116	-136
-3	348	-346
-2	231	-219
-1	99	-128
H=	7, K=	-3
-1	35*	31
-2	190	190
-3	123	93
-4	226	-249
-5	14*	-40
-6	121	-108
-7	80*	-44
H=	7, K=	-2
-7	63*	-99
-6	15*	-56
-5	58*	13
-4	83*	137
-3	426	403
-2	243	232
-2	243	232
-1	513	491
H=	7, K=	-1
-1	12*	-2
-2	265	267
-3	389	425
-4	247	250
-5	92*	130
-6	15*	75
-7	72*	-23
H=	7, K=	0
-7	69*	88
-6	73*	122
-5	68*	81
-4	141	124
-3	195	214
-2	55*	-152
-1	381	-391
H=	6, K=	0
-1	317	-320
-2	239	-249
-3	326	-344
-4	102	-82
-5	170	-189
-6	136	-129
-7	30*	78
H=	6, K=	-1
-7	98	96
-6	79*	11
-5	13*	14
-4	146	171
-3	142	-115
-2	292	-309
-1	463	-459
H=	6, K=	-2
-1	165	-155
-2	591	560
-3	289	264
-4	185	226
-5	241	257
-7	56*	-55
H=	6, K=	-3
-7	124	-145
-6	83*	-62
-5	13*	5
-4	193	172
-3	348	326
-2	402	390
-1	781	783
H=	6, K=	-4
-1	614	617
-2	125	112
-3	95	63
-4	386	-388
-5	255	-244
-6	237	-264
-7	238	-230
H=	6, K=	-5
-7	15*	-50
-6	156	-169
-5	204	-197
-4	564	-537
-3	303	-278
-2	98	-124
-1	50*	-45
H=	6, K=	-6
-1	529	-494
-2	351	-346
-3	93*	-109
-4	217	-218
-5	14*	13
-6	70*	75
-7	64*	84
H=	6, K=	-7
-7	44*	103
-6	137	134
-5	237	225
-4	186	181
-3	159	136
-2	83*	-40
H=	6, K=	-8
-1	72*	99
-2	325	316
-3	13*	73
-4	271	238
-5	116	94
-6	76*	-90
H=	6, K=	-9
-6	146	-175
-5	191	-185
-4	77*	22
-3	14*	-85
-2	112	119
-1	149	140
H=	6, K=	-10
-1	117	-103
-2	201	-243
-3	262	-241
-4	165	-185
-5	223	-222
-6	124	-118
H=	6, K=	-11
-5	98*	-103
-4	130	-134
-3	132	-105
-2	131	-123
-1	226	-181
H=	6, K=	-12
-1	108	-43
-2	14*	-22
-3	76*	60
-4	74*	-53
H=	6, K=	-13
-4	124	83
-3	187	179
-2	45*	14
-1	15*	7
H=	6, K=	-14
-1	228	227
-2	86*	114
-3	57*	74
H=	6, K=	-15
-1	223	183
H=	5, K=	-15
-1	82*	29
-2	137	103

L	FO	FC
H=	5, K= -14	
-3	84*	89
-2	40*	-60
-1	105	-118
H=	5, K= -13	
-1	254	-233
-2	246	-238
-3	171	-166
-4	71*	26
H=	5, K= -12	
-5	143	-132
-4	217	-208
-3	240	-290
-2	260	-237
-1	140	-138
H=	5, K= -11	
-1	65*	8
-2	14*	-28
-3	199	-185
-4	240	-227
-5	138	-172
-6	109*	-123
H=	5, K= -10	
-6	199	-208
-5	90*	-106
-4	125	-124
-3	85*	-50
-2	343	340
-1	328	303
H=	5, K= -9	
-1	104	67
-2	403	393
-3	293	315
-4	14*	31
-5	186	186
-6	15*	-44
-7	16*	12
H=	5, K= -8	
-7	90*	110
-6	108	114
-5	165	181
-4	229	230
-3	93*	96
-2	202	-179
-1	251	-244
H=	5, K= -7	
-1	392	-378
-2	426	-418
-3	281	-282
-4	87*	67
-5	127	139
-6	14*	58
-7	104	97
H=	5, K= -6	
-8	16*	69
-7	45*	-64
-6	66*	-82
-5	200	-223
-4	270	-279
-3	225	-251
-2	453	-421
-1	188	181
H=	5, K= -5	
-1	643	658
-2	387	390
-3	38*	52
-4	113	-130
-5	221	-220
-6	55*	-98
-7	140	-127
-8	89*	-89
H=	5, K= -4	
-8	134	-137
-7	15*	16
-6	75*	-20
-5	46*	-21
-4	207	205
-3	210	227
-2	636	641
-1	673	661
H=	5, K= -3	
-1	107	-125
-2	411	420
-3	473	444
-4	133	145
-5	224	222
-6	144	160
-7	116	146
-8	15*	-22
H=	5, K= -2	
-8	15*	103
-7	215	213
-6	138	127
-5	117	-95
-4	121	119
-3	46*	-4
-2	397	-407
-1	612	-603
H=	5, K= -1	
-1	413	-389
-2	366	-359
-3	757	-790
-4	228	-209
-5	132	-132
-6	151	-176
-7	14*	28
-8	97*	87
H=	5, K= 0	
-8	46*	-3
-7	182	-181
-6	116	-127
-5	296	-350
-4	197	-203
-3	270	-273
-2	627	-602
-1	340	326
H=	4, K= 0	
-1	256	271
-2	660	659
-3	430	-417
-4	91	101
-5	115	90
-6	213	-224
-7	139	-172
-8	167	-121
-9	67*	-75
H=	4, K= -1	
-9	16*	18
-8	68*	-28
-7	153	-178
-6	119	-118
-5	269	-284
-4	566	-596
-3	440	-440
-2	17*	86
-1	91	60
H=	4, K= -2	
-1	383	-365
-2	178	-183
-3	413	-403
-4	497	-534
-5	270	-255
-6	122	-120
-7	63*	47
-8	207	226
-9	61*	81
H=	4, K= -3	
-9	16*	26
-8	175	208
-7	134	117
-6	128	125
-5	76*	71
-4	42*	11
-3	86*	51
-2	456	-459
-1	674	-699
H=	4, K= -4	
-1	153	-144
-2	230	-227
-3	315	314
-4	242	263
-5	218	214
-6	204	240
-7	14*	60
-8	70*	73
-9	42*	-54
H=	4, K= -5	
-8	54*	-111
-7	113	-115
-6	169	145
-5	110	109
-4	180	187
-3	562	584
-2	120	-110
-1	8*	23
H=	4, K= -6	
-1	725	716

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	4, K=	-6	-5	105	92	-1	189	157	-1	145	174
			-4	34*	41	-2	167	173			
-2	520	557	-3	312	282	-3	60*	-28	H=	3, K=	-7
-3	142	133	-2	169	183	-4	94*	-117			
-4	179	177	-1	87*	144	-5	135	-138	-1	172	188
-5	213	-213							-2	839	896
-6	122	-152	H=	4, K=	-12	H=	3, K=	-12	-3	125	107
-7	72*	-94							-4	220	-202
-8	15*	-69	-1	108	78	-6	16*	-4	-5	183	-159
			-2	14*	12	-5	21*	2	-6	131	-158
H=	4, K=	-7	-3	84*	-60	-4	218	241	-7	14*	-9
			-4	69*	-71	-3	468	442	-8	71*	-76
-8	56*	-13	-5	80*	-75	-2	207	188			
-7	64*	-30	-6	185	-154	-1	272	256	H=	3, K=	-6
-6	20*	-8									
-5	261	-260	H=	4, K=	-13	H=	3, K=	-11	-9	110*	-128
-4	204	-184							-8	26*	48
-3	244	-248	-5	90*	-99	-1	88*	-96	-7	37*	5
-2	74*	48	-4	98*	-125	-2	238	-213	-6	132	112
-1	703	737	-3	194	-223	-3	190	196	-5	27*	-35
			-2	282	-264	-4	358	340	-4	105	107
H=	4, K=	-8	-1	14*	-44	-5	229	234	-3	154	188
						-6	156	172	-2	91	83
-1	290	-300	H=	4, K=	-14	-7	16*	35	-1	90	97
-2	213	-219									
-3	336	-306	-1	247	-248	H=	3, K=	-10	H=	3, K=	-5
-4	34*	-72	-2	132	-169						
-5	13*	-1	-3	167	-155	-7	85*	110	-1	583	-576
-6	47*	79	-4	22*	-11	-6	164	190	-2	732	-717
-7	141	139				-5	196	204	-3	253	-252
-8	153	144	H=	4, K=	-15	-4	78*	-29	-4	358	401
						-3	155	-159	-5	52*	64
H=	4, K=	-9	-3	74*	97	-2	199	-245	-6	76*	101
			-2	16*	88	-1	316	-304	-7	67*	56
-7	174	213	-1	15*	-17				-8	21*	29
-6	216	220				H=	3, K=	-9	-9	16*	-51
-5	121	109	H=	3, K=	-16						
-4	102	93				-1	198	-227	H=	3, K=	-4
-3	13*	5	-1	88*	-34	-2	506	-505			
-2	50*	-33				-3	254	-255	-9	38*	78
-1	182	-145	H=	3, K=	-15	-4	203	-191	-8	157	189
						-5	93*	106	-7	33*	8
H=	4, K=	-10	-1	132	-134	-6	14*	68	-6	80*	-72
			-2	124	-96	-7	54*	29	-5	87	83
-1	144	116	-3	54*	-91	-8	65*	58	-3	396	-413
-2	144	103							-2	479	-481
-3	156	155	H=	3, K=	-14	H=	3, K=	-8	-1	825	-853
-4	91*	127									
-5	216	216	-4	113*	-173	-8	27*	-19	H=	3, K=	-3
-6	124	151	-3	196	-203	-7	46*	-49			
-7	16*	54	-2	153	-137	-6	55*	-5	-1	598	599
			-1	148	-166	-5	220	-199	-2	219	-235
H=	4, K=	-11				-4	365	-349	-3	481	-458
			H=	3, K=	-13	-3	244	-224	-4	354	-360
-6	15*	-34				-2	95	86	-5	134	-173

L	FO	FC
-6	361	-363
-7	13*	-74
-8	32*	65
-9	122	101
H=	3, K=	-2
-9	15*	-22
-8	157	-166
-7	111	-83
-6	258	-262
-5	277	-285
-4	401	-412
-3	333	-342
-2	340	-333
-1	21*	-35
H=	3, K=	-1
-1	206	209
-2	903	901
-3	324	327
-4	223	-213
-5	85	70
-6	177	-165
-7	13*	-35
-8	252	-280
-9	129	-117
H=	3, K=	0
-9	46*	-58
-8	14*	-89
-7	79*	64
-6	184	196
-5	265	273
-4	172	164
-3	815	807
-2	978	974
-1	6*	-32
H=	2, K=	0
-1	1144	-1107
-2	258	254
-3	227	-225
-4	43*	12
-5	9*	27
-6	203	214
-7	342	352
-8	150	207
-9	114	104
-10	16*	52
H=	2, K=	-1

L	FO	FC
-10	16*	-33
-9	15*	-29
-8	31*	40
-7	131	143
-6	248	260
-5	366	384
-4	378	387
-3	597	608
-2	296	294
-1	1084	-1060
H=	2, K=	-2
-1	976	942
-2	710	-718
-3	513	528
-4	265	270
-5	139	143
-6	79*	77
-7	171	-165
-8	81*	-97
-9	61*	-66
-10	59*	-39
H=	2, K=	-3
-9	15*	-11
-8	64*	-23
-7	210	-216
-6	107	-141
-5	175	178
-4	340	-334
-3	111	108
-2	119	-113
-1	119	-106
H=	2, K=	-4
-1	951	961
-2	216	-221
-3	390	-396
-4	388	-408
-5	478	-480
-6	80*	-140
-7	32*	-20
-8	65*	5
-9	146	135
H=	2, K=	-5
-9	115	129
-8	141	104
-7	65*	96
-6	166	154

L	FO	FC
-5	52*	16
-4	327	-339
-3	310	-334
-2	768	-773
-1	376	-367
H=	2, K=	-6
-1	583	-604
-2	16*	-14
-3	185	-190
-4	463	469
-5	279	263
-6	143	145
-7	257	258
-8	15*	-18
-9	15*	-7
H=	2, K=	-7
-9	80*	-123
-8	103*	-114
-7	146	125
-6	116	109
-5	139	138
-4	344	337
-3	128	134
-2	313	331
-1	172	-146
H=	2, K=	-8
-1	299	303
-2	437	458
-3	270	283
-4	174	159
-5	118	-100
-6	166	-156
-7	14*	-98
-8	140	-151
H=	2, K=	-9
-8	86*	-79
-7	164	-170
-6	219	-230
-5	122	-109
-4	226	-212
-3	12*	-22
-2	286	248
-1	101	-74
H=	2, K=	-10
-1	136	-125

L	FO	FC
-2	289	-277
-4	148	-151
-5	113	-130
-6	82*	-35
-7	15*	-9
-8	67*	29
H=	2, K=	-11
-7	114	103
-6	120	170
-5	112	102
-4	119	-165
-3	165	-170
-2	373	-404
-1	267	-272
H=	2, K=	-12
-1	13*	-26
-2	50*	16
-3	14*	48
-4	240	233
-5	214	210
-6	15*	93
H=	2, K=	-13
-6	73*	-38
-5	89*	-7
-4	129	120
-3	199	170
-2	103	71
-1	148	165
H=	2, K=	-14
-1	82*	13
-2	59*	-4
-3	15*	15
-4	15*	-67
-5	113	-68
H=	2, K=	-15
-4	159	-136
-3	136	-97
-2	100*	-85
-1	128	-108
H=	2, K=	-16
-1	189	-193
H=	1, K=	-16

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	1, K= -16		-3	207	198	-3	288	-292	-6	104	91
			-2	187	198	-4	319	-335	-7	287	315
-1	99*	6	-1	12*	55	-5	571	-591	-8	185	176
						-6	184	-202	-9	112	87
H=	1, K= -15		H=	1, K= -9		-7	45*	-52	-10	46*	45
						-8	14*	-50			
-1	207	209	-1	383	411	-9	37*	36	H=	1, K= 0	
-2	81*	116	-2	116	147	-10	64*	62			
-3	120	102	-3	444	420				-10	85*	124
-4	105	41	-4	206	208	H=	1, K= -4		-9	56*	31
			-5	52*	48				-8	91*	89
H=	1, K= -14		-6	83*	-58	-10	47*	-76	-7	45*	76
			-7	105	-69	-9	131	-150	-6	176	-196
-5	122	78	-8	103*	-96	-8	87*	-95	-5	326	-336
-4	222	249				-7	187	-212	-4	248	-270
-3	155	193	H=	1, K= -8		-6	90	-98	-3	110	-113
-2	182	182				-5	185	-185	-2	253	247
-1	41*	61	-9	16*	-49	-4	8*	-14	-1	46*	-13
			-8	45*	-10	-3	194	195			
H=	1, K= -13		-7	100	90	-2	197	208	H=	1, K= -16	
			-6	109	88	-1	243	260			
-1	142	-156	-5	448	454				0	116	90
-2	64*	50	-4	237	259	H=	1, K= -3		1	120	90
-3	87*	37	-3	11*	4						
-4	138	143	-2	276	273	-1	1636	1672	H=	1, K= -15	
-5	171	172	-1	263	249	-2	231	226			
-6	120	110				-3	644	684	4	146	-106
			H=	1, K= -7		-4	369	363	3	128	-89
H=	1, K= -12					-5	177	203	2	59*	4
			-1	690	-696	-6	385	397	1	15*	38
-7	121	110	-2	307	-321	-7	137	-114	0	156	133
-6	241	220	-3	333	344	-8	113	-106			
-5	15*	82	-4	253	255	-9	62*	-47	H=	1, K= -14	
-4	14*	50	-5	354	375	-10	52*	-43			
-3	105	-89	-6	181	177				0	50*	31
-2	69*	16	-7	211	204	H=	1, K= -2		1	138	-148
-1	72*	-100	-8	71*	69				2	257	-228
			-9	90*	47	-10	16*	-16	3	89*	-108
H=	1, K= -11					-9	77*	-21	4	140	-146
			H=	1, K= -6		-8	129	102	5	63*	-53
-1	56*	-29				-7	153	183			
-2	156	-176	-9	152	130	-6	261	243	H=	1, K= -13	
-3	160	-166	-9	152	130	-5	763	781			
-4	13*	70	-7	13*	38	-4	493	503	6	72*	41
-5	70*	-78	-6	47*	64	-3	395	-422	5	15*	-12
-6	82*	55	-5	48*	13	-2	32*	47	4	96*	-44
-7	57*	77	-4	349	-372	-1	81	-65	3	14*	-37
			-3	510	-530				2	147	-155
H=	1, K= -10		-2	355	-366	H=	1, K= -1		1	225	-207
			-1	558	-592				0	178	-187
-8	59*	-61				-1	506	-504			
-7	134	-114	H=	1, K= -5		-2	1348	-1401	H=	1, K= -12	
-6	131	-124				-3	330	-325			
-5	189	-182	-1	72*	80	-4	8*	-38	0	233	-207
-4	148	-180	-2	311	311	-5	55*	11	1	113	-97

L	FO	FC
2	79*	127
3	45*	100
4	173	132
5	74*	135
6	105	80
7	109	67
H=	1, K=	-11
7	55*	-75
5	14*	26
4	152	129
3	307	290
2	289	308
1	45*	69
0	12*	-39
H=	1, K=	-10
0	427	439
1	411	405
2	176	188
3	92	77
4	84*	24
5	170	-189
6	99	-62
7	95*	-103
8	92*	-102
H=	1, K=	-9
9	16*	12
8	15*	-33
7	69*	-75
6	191	-182
5	143	-130
4	60*	-103
3	382	-400
2	102	100
1	183	183
0	229	227
H=	1, K=	-8
0	177	176
1	157	-182
2	500	-495
3	334	-322
4	296	-273
5	81*	-62
6	103	47
7	52*	10
8	97*	94
9	120	115
H=	1, K=	-7
9	48*	60
8	85*	54
7	73*	-12
6	155	206
5	214	249
4	9*	50
3	198	189
2	450	-441
1	471	-465
0	205	-212
H=	1, K=	-6
0	124	-182
1	517	517
2	87	60
3	252	262
4	129	144
5	171	-195
6	60*	-91
7	42*	-9
8	123	-38
9	98*	-75
10	62*	-35
H=	1, K=	-5
10	92*	-74
9	145	-155
8	62*	-57
7	289	-264
6	174	-127
5	75*	-61
4	200	-198
3	335	337
2	79*	125
1	53*	54
0	526	-516
H=	1, K=	-4
0	199	201
1	422	410
2	89	84
3	124	100
4	306	-301
5	883	-897
6	373	-405
7	154	-169
8	14*	-5
9	46*	-25
10	15*	12
H=	1, K=	-3
10	70*	94
9	41*	41
8	13*	-6
7	80*	121
6	93	-46
5	598	-578
4	839	-900
3	1350	-1362
2	116	-104
1	119	-89
0	105	-75
H=	1, K=	-2
0	802	-787
1	529	-529
2	1129	-1185
3	1320	-1414
4	198	-188
5	254	-264
6	109	-134
7	185	188
8	32*	16
9	145	96
10	127	120
H=	1, K=	-1
10	93*	-63
9	14*	18
8	43*	-42
7	153	179
6	320	337
5	671	710
4	117	148
3	26*	143
2	347	-340
1	731	-763
0	780	-749
H=	2, K=	-1
0	526	-509
1	519	-502
2	777	-761
3	205	217
4	72*	91
5	8*	-14
6	106	107
7	197	222
8	86*	117
9	100*	81
10	146	129
11	16*	10
H=	2, K=	-2
10	146	140
9	103	84
8	55*	79
7	93	58
6	221	-229
5	46*	-45
4	948	-966
3	1402	-1443
2	557	-556
1	1633	-1701
0	842	814
H=	2, K=	-3
0	680	680
1	840	855
2	415	-418
3	279	-278
4	279	-296
5	342	-352
6	330	-301
7	357	-374
8	90*	-144
9	49*	-19
10	15*	-24
H=	2, K=	-4
10	102*	-104
9	100*	-102
8	125	-32
7	143	-114
6	87*	65
5	8*	38
4	359	355
3	165	178
2	66*	-72
1	247	256
0	85	-88
H=	2, K=	-5
0	401	-399
1	135	-144
2	247	256
3	352	357
4	247	247
5	9*	131
6	314	353
7	162	144
8	14*	20

L	FO	FC
H=	2, K=	-5
9	48*	-22
10	54*	-30
H=	2, K=	-6
10	35*	-7
9	59*	87
8	276	273
7	184	209
6	281	293
5	102	65
4	28*	29
3	78*	84
2	370	-387
1	317	-321
0	773	-797
H=	2, K=	-7
0	46*	-26
1	145	-176
2	453	-444
3	233	-229
4	251	-255
5	346	-302
6	22*	2
7	143	89
8	218	225
9	162	144
10	111*	90
H=	2, K=	-8
9	64*	18
8	55*	-10
7	14*	-67
6	233	-229
5	85*	-85
4	277	-298
3	217	-206
2	230	213
1	112	-106
0	583	593
H=	2, K=	-9
0	478	480
1	526	511
2	394	427
3	57*	37
4	53*	-19
5	130	105
6	13*	-27
7	117	-116
8	104	-93
9	32*	-5
H=	2, K=	-10
8	51*	-20
7	55*	28
6	14*	29
5	269	232
4	284	317
3	249	267
2	324	323
1	92	111
0	73*	-85
H=	2, K=	-11
0	231	-261
1	353	-375
2	104	-116
3	13*	14
4	96*	81
5	162	154
6	96*	87
7	165	141
8	16*	45
H=	2, K=	-12
7	73*	99
6	75*	-9
5	59*	-77
4	136	-134
3	126	-132
2	181	-179
1	260	-237
0	281	-288
H=	2, K=	-13
0	27*	1
1	19*	-12
2	201	-157
3	143	-133
4	32*	-102
5	135	-116
6	74*	-70
H=	2, K=	-14
5	35*	-47
4	117	-53
3	15*	-17
2	44*	29
1	95*	37
0	63*	65
H=	2, K=	-15
0	48*	-33
1	40*	42
2	15*	66
3	44*	75
4	63*	69
H=	2, K=	-16
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1	80*	-29
0	106*	-145
H=	3, K=	-16
0	31*	-75
1	86*	-67
2	67*	-43
H=	3, K=	-15
4	16*	37
3	108	105
2	90*	31
1	75*	-39
0	132	-107
H=	3, K=	-14
0	104	-93
1	120	77
2	102	108
3	208	182
4	148	132
5	110	46
H=	3, K=	-13
6	58*	-15
5	15*	-17
4	59*	5
3	81*	101
2	166	155
1	284	280
0	151	190
H=	3, K=	-12
0	278	253
1	13*	-41
2	199	-169
3	170	-165
4	178	-182
5	185	-156
6	15*	-31
7	74*	-40
H=	3, K=	-11
8	84*	41
7	63*	33
6	71*	-57
5	140	-132
4	77*	5
3	320	-291
2	292	-332
1	104	-87
0	133	-134
H=	3, K=	-10
0	309	-334
1	297	-331
2	240	-242
3	88*	-147
4	47*	80
5	217	182
6	103	97
7	133	128
8	113	83
H=	3, K=	-9
9	16*	-28
8	68*	-21
7	92*	83
6	122	122
5	242	265
4	238	254
3	427	478
2	462	478
1	211	-200
0	367	-364
H=	3, K=	-8
0	352	358
1	577	568
2	445	480
3	451	434
4	31*	-17
5	52*	-80
6	82*	67
7	94*	119
8	134	-124
9	15*	-45

L	FO	FC
H=	3, K=	-7
10	16*	54
9	80*	-8
8	20*	-67
7	13*	-62
6	257	-254
5	62*	-87
4	125	-108
3	68*	-66
2	190	151
1	475	481
0	8*	68
H=	3, K=	-6
0	39*	24
1	436	-437
2	240	-247
3	392	-386
4	571	-589
5	164	-189
6	12*	-23
7	96*	165
8	232	239
9	151	132
10	74*	40
H=	3, K=	-5
10	53*	40
9	131	121
8	137	76
7	212	188
6	420	420
5	450	464
4	680	690
3	433	-433
2	542	-560
1	344	-350
0	471	-482
H=	3, K=	-4
0	630	604
1	357	360
2	122	87
3	338	358
4	918	931
5	443	423
6	271	314
7	213	270
8	115	139
9	61*	97
10	15*	21
H=	3, K=	-3
10	85*	-141
9	231	-256
8	136	-145
6	108	84
5	457	479
4	305	303
3	132	-109
2	1143	1207
1	440	-426
0	49*	-29
H=	3, K=	-2
0	873	849
1	472	476
2	326	317
3	453	459
4	257	-252
5	584	-620
6	235	-245
7	244	-214
8	110	-92
9	14*	14
10	80*	14
11	72*	50
H=	3, K=	-1
11	95*	47
10	79*	85
9	58*	-6
8	133	120
7	114	76
6	9*	-67
5	100	-109
4	703	-723
3	308	-315
2	234	-225
1	127	122
H=	4, K=	-1
0	436	407
1	466	-431
2	30*	38
3	254	257
4	254	246
5	376	-364
6	263	-298
7	257	-271
8	162	-178
9	14*	-51
10	47*	-45
11	63*	20
H=	4, K=	-2
11	75*	47
10	125	-120
9	255	-201
8	87*	-61
7	239	216
6	11*	24
5	308	329
4	179	197
3	374	393
2	342	376
1	600	-594
0	323	299
H=	4, K=	-3
0	389	-389
1	749	-751
2	174	-162
3	67*	109
4	334	336
5	268	272
6	113	157
7	251	255
8	49*	32
9	48*	28
10	87*	-68
H=	4, K=	-4
10	47*	14
9	177	193
8	13*	16
7	247	270
6	185	201
5	263	239
4	119	92
3	1109	-1137
2	496	-514
1	44*	47
0	405	-422
H=	4, K=	-5
0	168	169
1	330	319
2	125	-127
3	436	-450
4	563	-568
5	305	-301
6	80*	-59
7	63*	-126
8	55*	-25
9	140	154
10	34*	64
H=	4, K=	-6
10	77*	-40
9	25*	-52
8	158	-156
7	300	-247
6	199	-222
5	186	-223
4	131	-104
3	122	-143
2	92	-90
1	702	717
0	168	172
H=	4, K=	-7
0	471	466
1	675	649
2	476	503
3	365	352
4	50*	83
5	118	-99
6	37*	19
7	127	-93
8	118	-118
9	104*	-88
10	66*	-60
H=	4, K=	-8
9	167	-174
8	45*	-51
7	14*	51
6	81*	135
5	181	154
4	360	390
3	632	734
2	116	90
1	179	-175
0	139	-131
H=	4, K=	-9
0	166	-218
1	443	-475
2	226	-213
3	157	123
4	17*	-63
5	79*	117

L	FO	FC
H=	4, K=	-9
6	105*	135
7	83*	66
8	149	126
9	15*	-13
H=	4, K=	-10
8	72*	84
7	14*	-30
6	123	-139
5	160	-157
4	215	-244
3	224	-221
2	12*	-29
1	12*	-79
0	109	114
H=	4, K=	-11
0	385	353
1	241	271
2	13*	-5
3	133	-188
4	208	-181
5	27*	-54
6	14*	-54
7	71*	-63
8	16*	1
H=	4, K=	-12
7	166	-120
6	15*	-40
5	70*	-27
4	48*	41
3	59*	116
2	127	158
1	293	290
0	129	165
H=	4, K=	-13
0	14*	-20
1	114	121
2	195	207
3	227	209
4	213	229
5	90*	120
6	15*	-2
7	124	-66
H=	4, K=	-14
6	16*	65
5	15*	40
4	15*	80
3	15*	56
2	63*	57
1	14*	-40
0	270	-248
H=	4, K=	-15
0	139	-160
1	207	-176
2	139	-129
3	55*	-92
4	54*	-26
H=	4, K=	-16
2	71*	-10
1	39*	-21
0	16*	82
H=	5, K=	-15
4	172	-155
3	104*	-82
2	116	-95
1	40*	-46
0	149	77
H=	5, K=	-14
0	105*	-145
1	151	-165
2	133	-119
3	127	-145
4	106	-73
5	15*	28
H=	5, K=	-13
6	87*	52
5	15*	26
4	67*	12
3	64*	-64
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1	14*	-13
0	131	-116
H=	5, K=	-12
0	75*	38
1	13*	-14
3	55*	68
2	106	66
4	172	192
5	113	63
6	15*	-19
7	15*	-23
H=	5, K=	-11
8	164	-139
7	125	-119
6	159	-105
5	14*	-55
4	164	105
3	37*	51
2	230	269
1	162	156
0	66*	-45
H=	5, K=	-10
0	217	196
1	119	149
2	82*	1
3	177	-189
4	315	-293
5	205	-221
6	50*	-48
7	29*	-8
8	59*	-32
H=	5, K=	-9
9	87*	88
8	149	106
7	72*	19
6	169	-143
5	178	-244
4	219	-269
3	65*	-74
2	280	-315
1	236	-254
0	99	109
H=	5, K=	-8
0	264	-294
1	168	-172
2	282	-291
3	52*	-103
4	12*	66
5	145	140
6	80*	26
7	56*	82
8	167	164
9	48*	27
H=	5, K=	-7
10	50*	-55
9	121	-113
8	51*	-32
7	13*	-42
6	195	195
5	318	357
4	306	345
3	175	210
2	214	-226
1	108	68
0	187	-186
H=	5, K=	-6
0	621	585
1	203	209
2	269	297
3	176	169
4	39*	-7
5	72*	131
6	154	111
7	13*	30
8	31*	6
9	141	-126
10	128	-82
H=	5, K=	-5
10	15*	20
9	120	-113
8	155	-134
7	61*	-79
6	60*	-86
5	56*	-58
4	135	120
3	53*	39
2	743	741
1	742	739
0	185	189
H=	5, K=	-4
0	86	48
1	210	197
2	519	521
3	44*	-19
4	598	-600
5	311	-314
6	99	-92
7	154	-153
8	13*	-43
9	84*	47
10	120	84

L	FO	FC
H=	5, K=	-3
10	15*	40
9	65*	53
8	40*	17
7	131	133
6	175	196
5	188	173
4	205	-227
3	286	-276
2	573	-578
1	911	-912
0	399	-396
H=	5, K=	-2
0	560	-565
1	373	-374
2	640	-647
3	48*	64
4	487	495
5	432	441
6	35*	4
7	123	123
8	138	145
9	51*	56
10	15*	-44
11	50*	-44
H=	5, K=	-1
11	92*	-42
10	173	-151
9	96*	-74
8	13*	14
7	70*	-63
6	49*	75
5	322	335
4	533	533
3	576	577
2	247	-234
1	459	472
0	346	-335
H=	6, K=	-1
0	632	-601
1	344	-338
2	99	-124
3	190	-207
4	105	116
5	584	622
6	207	268
7	184	184
8	237	273
9	62*	90
10	60*	52
H=	6, K=	-2
10	122	122
9	96	44
8	55*	49
7	82*	89
6	45*	99
5	130	133
4	267	-264
3	496	-502
2	630	-668
1	153	-189
0	85*	-76
H=	6, K=	-3
0	661	649
1	248	250
2	386	382
3	290	280
4	89*	-80
5	253	-269
6	415	-442
7	124	-123
8	30*	30
9	102	57
10	164	153
H=	6, K=	-4
10	15*	20
9	52*	-81
8	109	-102
7	53*	-78
6	237	-257
5	45*	-48
4	198	182
3	567	605
2	744	746
1	329	316
0	683	706
H=	6, K=	-5
0	153	-138
1	75*	-45
2	458	485
3	482	476
4	199	247
5	206	213
6	164	177
7	112	158
8	57*	-18
9	130	-123
10	60*	-77
H=	6, K=	-6
10	78*	-36
9	97*	-26
8	107	-85
7	55*	18
6	291	279
5	197	242
4	386	408
3	56*	-18
2	343	-332
1	81*	-120
0	461	-471
H=	6, K=	-7
0	206	-230
1	214	-206
2	234	-269
3	265	-306
4	127	-139
5	21*	-14
6	139	174
7	65*	25
8	103	64
9	116	81
10	16*	3
H=	6, K=	-8
9	110	116
8	15*	120
7	50*	10
6	13*	-45
5	207	-229
4	159	-176
3	244	-257
2	283	-320
1	135	104
0	213	214
H=	6, K=	-9
0	267	284
1	170	196
2	92*	-105
3	315	-334
4	127	-146
5	141	-141
6	45*	-73
7	67*	-27
8	15*	-62
9	64*	-17
H=	6, K=	-10
8	160	-128
7	153	-115
6	178	-143
5	86*	-80
4	13*	47
3	187	208
2	190	225
1	72*	48
0	195	228
H=	6, K=	-11
0	195	-202
1	264	-221
2	145	153
3	159	157
4	127	121
5	170	165
6	21*	5
7	15*	19
8	35*	-10
H=	6, K=	-12
7	153	125
6	82*	71
5	65*	104
4	67*	-27
3	80*	-63
2	68*	-11
1	159	-185
0	205	-189
H=	6, K=	-13
0	14*	-55
1	183	-149
2	86*	-149
3	131	-112
4	76*	-96
5	94*	2
6	66*	46
H=	6, K=	-14
5	124	-129
4	154	-156
3	84*	-63
2	54*	-58

L	FO	FC
H=	6, K=	-14
1	108	75
0	171	171
H=	6, K=	-15
0	188	185
1	212	209
2	113	79
3	16*	17
H=	7, K=	-15
2	16*	68
1	158	118
H=	7, K=	-14
0	163	166
1	127	139
2	114	75
3	95*	81
4	68*	90
5	81*	-13
H=	7, K=	-13
6	111	-75
5	205	-196
4	56*	-79
3	15*	3
2	55*	34
1	149	167
0	166	146
H=	7, K=	-12
0	76*	28
1	63*	-37
2	114	-137
3	35*	-44
4	109	-87
5	86*	-121
6	15*	4
7	47*	46
H=	7, K=	-11
7	144	117
6	150	149
5	90*	133
4	54*	-11
3	78*	8
2	103	-46
1	237	-231
0	213	-231
H=	7, K=	-10
0	27*	-65
1	13*	60
2	13*	-14
3	112	119
4	84*	96
5	265	227
6	120	144
7	54*	57
8	58*	0
H=	7, K=	-9
9	112	-93
8	170	-156
7	156	-160
6	54*	-87
5	94*	109
4	95	78
3	127	143
2	172	187
1	381	372
H=	2, K=	-10
-3	326	-341
H=	7, K=	-9
0	246	242
H=	7, K=	-8
0	305	311
1	359	383
2	223	205
3	251	-257
4	129	-149
5	60*	-55
6	198	-224
7	87*	-103
8	33*	-94
9	58*	-51
H=	7, K=	-7
9	46*	22
8	88*	-50
7	64*	-57
6	120	-158
5	328	-333
4	196	-228
3	218	-255
2	62*	-65
1	75*	-102
0	95	-17
H=	7, K=	-6
0	205	-201
1	420	-409
2	228	-255
3	225	-277
4	227	-220
5	240	-315
6	87*	-52
7	51*	72
8	124	94
9	137	152
10	122	64
H=	7, K=	-5
10	75*	-54
9	39*	-20
8	73*	-64
7	101	70
6	167	149
5	100	169
4	286	272
3	170	-169
2	155	-164
1	661	-691
0	328	-324
H=	7, K=	-4
0	107	83
1	83*	-44
2	100	71
3	327	331
4	326	356
5	118	122
6	100	83
7	26*	-46
8	14*	-46
9	83*	-93
10	145	-100
H=	7, K=	-3
10	78*	-85
9	80*	-71
8	62*	-18
7	180	-206
6	127	-160
5	76*	-103
4	28*	-40
3	348	383
2	139	145
1	483	473
0	952	882
H=	7, K=	-2
1	190	199
2	151	157
3	193	-206
4	331	-305
5	235	-259
6	375	-373
7	205	-221
8	14*	-29
9	30*	29
10	102*	108
H=	7, K=	-1
10	149	118
9	97*	75
8	70*	16
7	77*	87
6	239	248
5	63*	-101
4	382	-396
3	198	-204
2	297	-315
1	166	-186
0	410	-363
H=	8, K=	-1
0	531	504
1	299	291
2	283	306
3	30*	-6
4	230	-207
5	320	-344
6	243	-251
7	249	-256
8	47*	-66
9	15*	25
10	87*	78
H=	8, K=	-2
10	140	-99
9	67*	-85
8	119	-146
7	226	-205
6	84*	40

L	FO	FC
5	234	-267
4	125	-134
3	330	333
2	443	477
1	384	379
0	62*	-38
H=	8, K=	-3
0	311	-298
1	12*	116
2	419	408
3	68*	113
4	249	282
5	179	145
6	19*	15
7	78*	-38
8	141	-134
9	152	-134
10	108*	-105
H=	8, K=	-4
10	23*	-19
9	16*	9
8	15*	12
7	212	188
6	94*	128
5	280	283
4	266	258
3	61*	-28
2	324	-307
1	267	-249
0	55*	-107
H=	8, K=	-5
0	224	-181
1	456	-443
2	519	-562
3	385	-356
4	81*	-28
5	48*	-85
6	58*	-50
7	162	180
8	140	118
9	193	133
H=	8, K=	-6
9	87*	58
8	15*	13
7	111	-96
6	270	-299
5	176	-154
4	184	-213
3	297	-307
2	277	-258
1	109	-111
0	105	63
H=	8, K=	-7
0	134	151
1	306	317
2	228	194
3	13*	39
4	78*	-68
5	91*	-120
6	218	-221
7	147	-188
8	92*	-111
9	51*	-60
H=	8, K=	-8
9	90*	-52
8	76*	-62
7	117	-75
6	130	95
5	76*	30
4	31*	43
3	288	292
2	132	168
1	224	219
0	44*	-70
H=	8, K=	-9
0	406	-374
1	146	-159
2	14*	-23
3	101*	113
4	121	82
5	255	245
6	282	322
7	101*	99
8	72*	56
H=	8, K=	-10
8	16*	103
7	92*	101
6	121	124
5	15*	43
4	86*	-49
3	29*	-64
2	357	-355
1	345	-352
0	246	-286
H=	8, K=	-11
0	120	77
1	39*	-102
2	276	-302
3	188	-196
4	188	-169
5	166	-172
6	16*	-43
7	109	19
H=	8, K=	-12
6	158	-134
5	156	-145
4	188	-183
3	80*	-131
2	55*	6
1	134	155
0	324	313
H=	8, K=	-13
0	125	126
1	105*	109
2	95*	111
3	73*	63
4	113*	102
5	130	79
H=	8, K=	-14
3	105*	75
2	59*	52
1	75*	-51
0	62*	-100
H=	9, K=	-13
4	147	168
3	89*	64
2	49*	62
1	49*	-92
0	84*	-136
H=	9, K=	-12
0	83*	89
1	102*	102
2	173	159
3	55*	102
4	167	157
5	105*	133
H=	9, K=	-11
6	76*	-83
5	16*	-49
4	115	-94
3	15*	-78
2	134	132
1	158	182
0	288	205
H=	9, K=	-10
0	102*	-57
1	15*	-34
2	119	-113
3	216	-213
4	167	-183
5	237	-219
6	104*	-125
7	93*	37
H=	9, K=	-9
8	159	110
7	118*	137
6	96*	56
5	48*	-15
4	15*	-11
3	15*	-79
2	276	-256
1	402	-390
0	368	-378
H=	9, K=	-8
0	381	-366
1	395	-406
2	128	-175
3	78*	120
4	221	191
5	275	280
6	242	289
7	174	187
8	61*	84
H=	9, K=	-7
8	141	-79
7	16*	-2
6	220	173
5	118	164
4	246	253
3	302	260
2	192	195
1	77*	66

L	FO	FC
H=	9, K=	-7
0	53*	60
H=	9, K=	-6
0	205	227
1	230	216
2	109*	115
3	70*	84
4	79*	-88
5	82*	-75
6	225	-210
7	252	-237
8	130	-100
9	17*	-31
H=	9, K=	-5
9	24*	35
8	109	46
7	220	-206
6	256	-235
5	66*	-41
4	244	-240
3	119	-135
2	71*	-85
1	126	-147
0	166	128
H=	9, K=	-4
0	191	-169
1	24*	-100
2	259	-278
3	225	-189
4	179	-193
5	14*	-26
6	70*	32
7	154	144
8	175	178
9	157	127
H=	9, K=	-3
9	96*	58
8	186	188
7	261	251
6	181	162
5	134	134
4	91*	-67
3	115	-74
2	251	-224
1	143	-140
0	286	-263
H=	9, K=	-2
0	406	-367
1	87*	-40
2	204	205
3	400	384
4	179	176
5	167	151
6	81*	92
7	182	153
8	44*	-8
9	75*	-67
H=	9, K=	-1
9	16*	-27
8	158	-148
7	55*	-24
6	67*	68
5	83*	-78
4	176	182
3	288	270
2	271	299
1	381	363
0	116	87
H=	10, K=	-1
0	15*	-29
1	98*	-112
2	15*	-14
3	267	231
4	316	291
5	208	229
6	57*	42
7	72*	84
8	131	89
H=	10, K=	-2
8	214	207
7	188	214
6	179	147
5	208	195
4	76*	53
3	207	-211
2	451	-436
1	476	-410
0	158	-154
H=	10, K=	-3
0	109	51
1	248	-268
2	302	-316
3	440	-431
4	328	-327
5	15*	-38
6	15*	5
7	52*	-32
8	83*	81
H=	10, K=	-4
8	75*	-66
7	204	-192
6	182	-189
5	194	-184
4	360	-339
3	49*	-10
2	206	198
1	197	211
0	15*	26
H=	10, K=	-5
0	114	-64
1	348	326
2	431	431
3	136	208
4	14*	-36
5	129	-173
6	131	-116
7	64*	-77
8	135	-116
H=	10, K=	-6
8	117	-85
7	35*	96
6	119*	143
5	108*	109
4	109*	134
3	131	168
2	197	211
1	39*	26
0	124	-144
H=	10, K=	-7
0	181	-207
1	127	-159
2	136	-117
3	49*	54
4	267	287
5	167	194
6	158	151
7	131	126
8	16*	78
H=	10, K=	-8
7	79*	51
6	59*	-18
5	74*	8
4	133	150
3	139	-151
2	225	-267
1	258	-265
0	145	-163
H=	10, K=	-9
0	246	273
1	93*	69
2	84*	-44
3	185	-174
4	76*	-86
5	145	-155
6	161	-112
7	98*	-78
H=	10, K=	-10
6	131	-52
5	62*	-27
4	16*	41
3	120	117
2	256	267
1	314	332
0	321	308
H=	10, K=	-11
0	49*	91
1	165	162
2	240	257
3	269	267
4	233	205
5	95*	111
H=	10, K=	-12
3	149	161
2	138	100
1	82*	-31
H=	11, K=	-10
1	103*	69
2	146	97
3	212	217
4	188	187

L	FO	FC
H=	11, K=	-9
5	49*	-13
4	16*	61
3	68*	117
2	124	127
1	219	226
0	227	228
H=	11, K=	-8
0	168	198
1	115*	119
2	103*	81
3	16*	-9
4	87*	-72
5	124	-78
6	111*	-93
H=	11, K=	-7
7	16*	52
6	16*	-29
5	134	-109
4	116	-114
3	114	-119
2	16*	-11
1	152	-143
0	59*	-36
H=	11, K=	-6
0	258	-236
1	203	-194
2	15*	-74
3	78*	-50
4	115	38
5	16*	52
6	141	165
7	159	146
H=	11, K=	-5
7	119	111
6	213	219
5	209	183
4	208	254
3	196	201
2	94*	157
1	15*	16
0	68*	-73
H=	11, K=	-4
0	103*	120
1	323	322
2	434	426
3	332	354
4	224	198
5	15*	-54
6	16*	-51
7	134	-110
H=	11, K=	-3
7	273	-268
6	245	-233
5	244	-262
4	133	-100
3	30*	-8
2	93*	70
1	359	347
0	294	273
H=	11, K=	-2
0	60*	60
1	147	-75
2	381	-375
3	269	-261
4	152	-209
5	185	-156
6	122	-105
7	180	-162
H=	11, K=	-1
7	119	101
6	69*	5
5	15*	-18
4	131	-143
3	308	-331
2	220	-217
1	143	-135
0	170	-168
H=	12, K=	-1
0	17*	50
1	52*	-22
2	205	-160
3	224	-244
4	223	-268
5	226	-239
6	33*	-38
H=	12, K=	-2
6	17*	-128
5	163	-200
4	53*	-49
3	80*	-24
2	177	161
1	176	188
0	213	232
H=	12, K=	-3
0	241	219
1	233	184
2	262	311
3	221	225
4	102*	128
5	16*	20
6	70*	-9
H=	12, K=	-4
6	131	124
5	168	205
4	235	249
3	144	136
2	75*	11
1	40*	-76
0	124	-99
H=	12, K=	-5
0	159	-171
1	244	-248
2	266	-261
3	187	-200
4	16*	-34
5	92*	101
H=	12, K=	-6
5	79*	-138
4	259	-255
3	182	-148
2	69*	-137
1	131	-111
H=	12, K=	-7
1	188	172
2	81*	120
3	84*	36
4	114*	-152
H=	0, K=	1
-10	150	-121
-9	94*	-79
-8	189	-197
-7	140	-156
-6	24*	22
-5	574	572
-4	708	725
-3	695	731
-2	1419	1446
-1	543	528
H=	0, K=	2
-1	469	-481
-2	656	640
-3	47*	-66
-4	408	429
-5	364	346
-6	191	203
-7	136	156
-8	14*	-50
-9	22*	16
-10	118	-131
H=	0, K=	3
-10	77*	32
-9	80*	92
-8	14*	-10
-7	210	167
-6	12*	26
-5	87	-45
-4	238	-255
-3	248	239
-2	555	568
-1	677	650
H=	0, K=	4
-1	212	-219
-2	280	263
-3	89	-37
-4	544	-542
-5	369	-368
-6	151	127
-7	80*	131
-8	15*	3
-9	96*	86
-10	17*	14
H=	0, K=	5
-10	17*	55
-9	35*	16
-8	77*	25
-7	14*	19
-6	303	-312
-5	177	-153

L	FO	FC
H=	0, K=	5
-4	19*	-38
-3	348	-353
-2	51*	93
-1	571	590
H=	0, K=	6
-1	7*	11
-2	85	-99
-3	326	341
-4	105	119
-5	120	82
-6	196	-204
-7	160	-176
-8	73*	-84
-9	82*	-127
H=	0, K=	7
-9	62*	-65
-8	116	-43
-7	15*	-15
-6	27*	-6
-5	55*	57
-4	192	180
H=	0, K=	8
-3	173	-155
-4	122	108
H=	0, K=	7
-3	298	297
-2	155	172
-1	143	162
H=	0, K=	8
-1	434	-436
-2	125	118
-5	281	273
-6	103*	105
-7	50*	7
-8	98*	77
-9	87*	26
H=	0, K=	9
-8	111*	141
-7	130	113
-6	98*	69
-5	59*	10
-4	87*	-48
-3	224	-218
-2	355	-345
-1	78*	-88
H=	0, K=	10
-1	13*	-74
-2	130	-139
-3	74*	-62
-4	94*	-111
-5	282	-245
-6	15*	-71
-7	16*	-23
-8	17*	-4
H=	0, K=	11
-7	135	-114
-6	106*	-97
-5	200	-177
-4	74*	-106
-3	47*	-54
-2	156	138
-1	210	222
H=	0, K=	12
-1	266	292
-2	219	202
-3	173	173
-4	66*	115
-5	16*	30
-6	16*	-27
H=	0, K=	13
-6	17*	61
-5	16*	74
-4	197	167
-3	107*	113
-2	15*	35
-1	15*	57
H=	0, K=	14
-1	187	-161
-2	16*	-23
-3	23*	-36
-4	81*	12
-5	66*	52
H=	0, K=	15
-3	169	-130
-2	133	-127
-1	114	-72
H=	1, K=	15
-1	152	-138
-2	99*	-91
H=	1, K=	14
-4	199	168
-3	118	90
-2	36*	58
-1	47*	14
H=	1, K=	13
-1	117*	140
-2	193	192
-3	189	169
-4	16*	18
-5	17*	0
H=	1, K=	12
-6	44*	-43
-5	85*	-106
-4	95*	-18
-3	15*	-7
-2	41*	69
-1	272	264
H=	1, K=	11
-1	14*	-54
-2	126	-113
-3	131	-126
-4	179	-127
-5	38*	-33
-6	16*	7
-7	24*	-5
H=	1, K=	10
-7	102*	68
-6	122	116
-5	174	155
-4	35*	-7
-3	172	-168
-2	113	-131
-1	350	-353
H=	1, K=	9
-1	82*	-28
-2	74*	6
-3	199	196
-4	252	230
-5	176	179
-6	102*	113
-7	16*	86
-8	57*	57
H=	1, K=	8
-8	85*	-98
-7	53*	-16
-6	119	-148
-5	144	144
-4	295	303
-3	284	300
-2	538	532
-1	135	154
H=	1, K=	7
-1	138	-160
-2	468	440
-3	439	432
-4	91*	-134
-5	13*	-14
-6	207	-214
-7	154	-90
-8	93*	-115
-9	17*	-29
H=	1, K=	6
-9	49*	28
-8	41*	-62
-7	50*	-8
-6	141	-178
-5	251	-251
-4	221	-214
-3	53*	-50
-2	222	-207
-1	179	173
H=	1, K=	5
-1	73*	90
-2	744	-734
-3	220	-208
-4	492	-470
-5	12*	-123
-6	75*	73
-7	49*	52
-8	82*	51
-9	134	135

L	FO	FC
H=	1, K=	4
-9	76*	31
-8	71*	66
-7	77*	20
-6	126	174
-5	229	244
-4	8*	-5
-3	259	-279
-2	219	228
-1	287	281
H=	1, K=	3
-1	234	224
-2	435	-444
-3	628	636
-4	380	389
-5	9*	48
-6	390	367
-7	112	-95
-8	65*	-23
-9	76*	-38
-10	98*	-83
H=	1, K=	2
-10	29*	-70
-9	117*	-103
-8	14*	-18
-7	134	-123
-6	176	-105
-5	9*	31
-4	579	556
-3	341	314
-2	1001	1009
-1	364	335
H=	1, K=	1
-1	358	341
-2	891	862
-3	81	84
-4	217	-219
-5	366	-372
-6	189	-211
-7	48*	-75
-8	104	-83
-9	15*	-48
-10	16*	16
H=	2, K=	1
-10	61*	70
-9	121	74
-8	147	100
-7	141	116
-6	92*	88
-5	180	-182
-4	506	-515
-3	577	-570
-2	177	189
-1	266	-270
H=	2, K=	2
-1	697	668
-2	89	84
-3	449	-448
-4	153	-145
-5	568	-561
-6	165	-192
-7	41*	12
-8	15*	-37
-9	85*	23
H=	2, K=	3
-9	118	-86
-8	15*	-57
-7	256	-289
-6	339	-335
-5	121	125
-4	99	103
-3	45*	89
-2	819	810
-1	336	340
H=	2, K=	4
-1	604	596
-2	222	-201
-3	502	495
-4	535	532
-5	171	192
-6	98*	97
-7	126	-57
-8	15*	3
-9	112	-79
H=	2, K=	5
-9	74*	6
-8	54*	69
-7	15*	18
-6	103	50
-5	144	157
-4	257	251
-3	19*	37
-2	225	-218
-1	164	-168
H=	2, K=	6
-1	824	-803
-2	321	-314
-3	237	-238
-4	329	-330
-5	106	-71
-6	110	127
-7	65*	-28
-8	74*	14
-9	17*	45
H=	2, K=	7
-8	16*	-7
-7	116	-88
-6	134	-140
-5	248	-283
-4	322	-336
-3	344	-350
-2	184	-174
-1	26*	-57
H=	3, K=	7
-1	306	-300
H=	2, K=	8
-1	304	328
-2	132	116
-3	91*	41
-4	154	116
-5	208	-163
-6	137	-117
-7	79*	-89
-8	130	-144
H=	2, K=	9
-7	40*	-5
-6	94*	-17
-5	57*	15
-4	123	117
-3	286	315
-2	319	321
-1	50*	101
H=	2, K=	10
-1	74*	-45
-2	107	-83
-3	116	113
-4	109*	138
-5	134	150
-6	130	67
-7	17*	55
H=	2, K=	11
-6	87*	16
-5	129	99
-4	15*	-4
-3	205	-156
-2	237	-223
-1	158	-146
H=	2, K=	12
-1	185	-204
-2	203	-174
-3	15*	-29
-4	103*	-88
-5	16*	-10
H=	2, K=	13
-4	70*	-97
-3	16*	21
-2	90*	90
-1	173	123
H=	2, K=	14
-1	161	142
-2	146	118
-3	17*	72
H=	2, K=	15
-1	71*	19
H=	3, K=	14
-2	24*	12
-1	128	117
H=	3, K=	13
-1	45*	-51
-2	48*	-88
-3	170	-130
H=	3, K=	12
-5	89	70
-4	111	34
-3	119	-77

L	FO	FC
H=	3, K=	12
-2	197	-189
-1	245	-214
H=	3, K=	11
-2	16*	-114
-3	130	102
-4	127*	160
-5	18*	7
H=	3, K=	10
-6	18*	7
-5	86	15
-4	198	140
-3	87*	108
-2	350	315
-1	15*	82
H=	3, K=	9
-1	222	227
-2	98*	82
-3	72*	55
-4	98*	-117
-5	211	-191
-6	77*	-39
-7	151	-100
H=	3, K=	8
-7	17*	-40
-6	73*	-65
-5	141	-153
-4	274	-259
-3	337	-317
-2	230	-259
-1	174	-171
H=	3, K=	7
-2	304	-315
-3	556	-568
-4	97*	-127
-5	81*	66
-6	102*	78
-7	16*	74
-8	91*	71
H=	3, K=	6
-8	91*	59
-7	88*	74
-6	228	221
-5	392	397
-4	13*	34
-3	108	92
-2	134	131
-1	566	-566
H=	3, K=	5
-1	77*	-79
-2	329	312
-3	775	771
-4	467	415
-5	227	201
-6	111	92
-7	77*	40
-8	87*	-38
H=	3, K=	4
-9	18*	-53
-8	125	-61
-7	208	-168
-6	220	-176
-5	14*	28
-4	436	402
-3	346	344
-2	534	534
-1	451	460
H=	3, K=	3
-1	381	361
-2	418	-405
-3	97	-85
-4	9*	-31
-5	250	-256
-6	148	-151
-7	172	-142
-8	38*	-21
-9	48*	19
H=	3, K=	2
-9	159	121
-8	150	150
-7	80*	91
-6	188	179
-5	14*	-71
-4	263	-256
-3	169	-148
-2	349	-347
-1	421	-418
H=	3, K=	1
-1	1031	985
-2	115	-116
-3	86	-100
-4	568	570
-5	103	86
-6	286	263
-7	376	317
-8	113*	109
-9	143	103
H=	4, K=	1
-9	95*	-8
-8	17*	-57
-7	16*	-25
-6	77*	103
-5	404	352
-4	343	320
-3	688	691
-2	309	291
-1	320	-301
H=	4, K=	2
-1	361	-355
-2	358	-367
-3	9*	58
-4	267	242
-5	202	166
-6	99*	128
-7	269	242
-8	69*	97
H=	4, K=	3
-8	129*	123
-7	187	184
-6	51*	30
-5	62*	3
-4	328	-313
-3	277	-280
-2	575	-551
-1	517	-520
H=	4, K=	4
-1	8*	15
-2	465	-441
-3	56*	-45
-4	107*	-155
-5	235	-216
-6	183	-152
-7	122	33
-8	64*	-19
H=	4, K=	5
-8	92*	-66
-7	141	-108
-6	91*	-110
-5	40*	-89
-4	54*	18
-3	289	283
-2	325	339
-1	466	453
H=	4, K=	6
-1	469	580
-2	505	591
-3	120	123
-4	276	303
-5	145	148
-6	40*	-8
-7	60*	-28
H=	4, K=	7
-7	110*	103
-6	154	189
-5	214	224
-4	170	215
-3	104*	125
-2	118	76
-1	14*	-30
H=	4, K=	8
-1	151	-263
-2	292	-293
-3	139	-178
-4	16*	45
-5	76*	53
-6	117*	119
-7	18*	84
H=	4, K=	9
-6	25*	-24
-5	17*	-50
-4	158	-185
-3	178	-153
-2	97*	-74
-1	233	-262
H=	4, K=	10
-1	158	177
-2	16*	-4

L	FO	FC
-3	105*	41
-4	68*	-49
-5	81*	-74
H=	4, K=	11
-5	18*	-19
-4	43*	5
-3	116*	142
-2	58*	113
-1	16*	43
H=	4, K=	12
-1	17*	-14
-2	17*	30
-3	53*	70
-4	115*	113
H=	4, K=	13
-2	86*	-77
-1	54*	-96
H=	5, K=	13
-1	129	96
H=	5, K=	12
-2	97*	121
-1	118*	149
H=	5, K=	11
-1	69*	-7
-2	64*	-10
-3	138	-137
-4	119*	-175
H=	5, K=	10
-4	83*	-92
-3	105*	-170
-2	124*	-209
-1	82*	-127
H=	5, K=	9
-1	124	-154
-2	187	-194
-3	180	-192
-4	84*	37
-5	24*	98
H=	5, K=	8
-6	35*	68
-5	150	127
-4	85*	71
-3	81*	112
-2	15*	40
-1	182	-231
H=	5, K=	7
-1	327	414
-2	203	204
-3	118*	171
-4	123	142
-5	23*	12
-6	74*	-61
H=	5, K=	6
-7	129	-126
-6	186	-221
-5	65*	-60
-4	84*	-56
-3	14*	18
-2	118	-73
-1	232	276
H=	5, K=	5
-1	310	-372
-2	88*	-97
-3	321	-324
-4	310	-316
-5	15*	-3
-7	17*	31
H=	5, K=	4
-7	41*	75
-6	200	165
-5	108*	-35
-4	300	-251
-3	13*	-87
-2	335	-385
-1	380	-380
H=	5, K=	3
-1	307	-315
-2	198	-167
-3	123	105
-4	14*	-31
-5	88*	50
-6	71*	143
-7	89*	102
-8	91*	93
H=	5, K=	2
-8	49*	-59
-7	130	-117
-6	147	116
-5	90*	104
-4	215	189
-3	351	329
-2	318	308
-1	355	-354
H=	5, K=	1
-1	443	452
-2	129	108
-3	77*	60
-4	197	156
-5	125	-86
-6	107*	-75
-7	273	-262
-8	115	-75
H=	6, K=	1
-7	82*	-63
-6	240	-220
-5	274	-230
-4	98*	-157
-3	125	-79
-2	40*	25
-1	76*	45
H=	6, K=	2
-1	417	419
-2	239	236
-3	76*	57
-4	134	97
-5	15*	34
-6	182	-172
-7	136	-159
H=	6, K=	3
-7	17*	-54
-6	28*	30
-5	38*	44
-4	255	236
-3	206	170
-2	131	97
-1	327	346
H=	6, K=	4
-1	122	-180
-2	180	170
-3	51*	43
-4	15*	108
-5	239	204
-6	211	192
-7	68*	23
H=	6, K=	5
-6	243	231
-5	89*	28
-4	138	-82
-3	204	-204
-2	236	-259
-1	153	-159
H=	6, K=	6
-1	136	-184
-2	194	-211
-3	236	-252
-4	49*	-55
-5	113*	-137
-6	41*	3
H=	6, K=	7
-5	194	-219
-4	134	-107
-3	76*	78
-2	41*	-56
-1	62*	4
H=	6, K=	8
-1	166	229
-2	180	192
-3	106*	140
-4	16*	-2
-5	76*	-51
H=	6, K=	9
-4	102*	85
-3	32*	106
-2	67*	38
-1	114*	160
H=	6, K=	10
-1	83*	-103
-2	16*	-115

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	6, K=	10	-1	139	171	-4	83*	107	-5	112	-67
						-3	112	111	-6	112	42
-3	17*	-35	H=	7, K=	7	-2	251	264			
						-1	373	379	H=	8, K=	1
H=	6, K=	11	-1	119	-134						
			-2	51*	-49	H=	7, K=	3	-6	143	134
-2	114*	-172	-3	55*	-86				-5	227	211
-1	60*	-140	-4	72*	-98	-1	71*	78	-4	216	191
						-2	125	137	-3	15*	62
H=	6, K=	12	H=	7, K=	6	-3	54*	-42	-2	70*	-93
						-4	177	-165	-1	81*	-40
-1	77*	67	-5	108*	71	-5	16*	-29			
			-4	63*	36	-6	170	-150	H=	8, K=	2
H=	7, K=	10	-3	44*	35						
			-2	102*	-65	H=	7, K=	2	-1	164	-214
-2	139	116	-1	96*	-154				-2	514	-491
-1	151	171				-6	84*	-93	-3	124	-127
			H=	7, K=	5	-5	183	-118	-4	128	-114
H=	7, K=	9				-4	117	-139	-5	17*	47
			-1	74*	4	-3	397	-381			
-1	200	274	-2	245	265	-2	267	-273	H=	8, K=	3
-2	198	226	-3	84*	56	-1	108	82			
-3	17*	127	-4	155	86				-5	146	-168
			-5	203	155	H=	7, K=	1	-4	186	-228
H=	7, K=	8							-3	229	-221
			H=	7, K=	4	-1	341	-312	-2	241	-263
-4	114	35				-2	492	-446	-1	14*	-36
-3	16*	-22	-6	17*	-62	-3	256	-233			
-2	60*	61	-5	16*	97	-4	189	-170			

L	FO	FC
H=	8, K=	4
-1	15*	68
-2	97*	84
-3	16*	-37
-4	98*	-61
-5	138	-132
H=	8, K=	5
-4	156	134
-3	134	164
-2	119*	174
-1	181	234
H=	8, K=	6
-1	66*	-103
-2	55*	72
-3	138	158
-4	103*	112
H=	8, K=	7
-3	67*	-121
-2	67*	-110
-1	225	-251

L	FO	FC
H=	8, K=	8
-1	122*	-147
-2	111*	-159
H=	8, K=	9
-1	122*	118
H=	9, K=	7
-1	89*	55
H=	9, K=	6
-2	98*	140
-1	145	248
H=	9, K=	5
-1	71*	166
-2	100*	-95
-3	17*	-53
H=	9, K=	4
-3	155	-193
-2	314	-319

L	FO	FC
-1	173	-186
H=	9, K=	3
-1	361	-422
-2	151	-178
-3	16*	-46
-4	17*	-66
H=	9, K=	2
-4	132	184
-3	142	181
-2	115	89
-1	120*	-141
H=	9, K=	1
-1	271	247
-2	328	326
-3	298	255
-4	161	137
H=	10, K=	1
-3	17*	-55
-2	180	172
-1	214	193

L	FO	FC
H=	10, K=	2
-1	149	171
-2	319	310
-3	110*	153
H=	10, K=	3
-2	165	155
-1	16*	-38
H=	10, K=	4
-1	169	-212
-2	136	-132
H=	10, K=	5
-1	128	-146
H=	11, K=	2
-1	192	225
H=	11, K=	1
-1	108*	-45

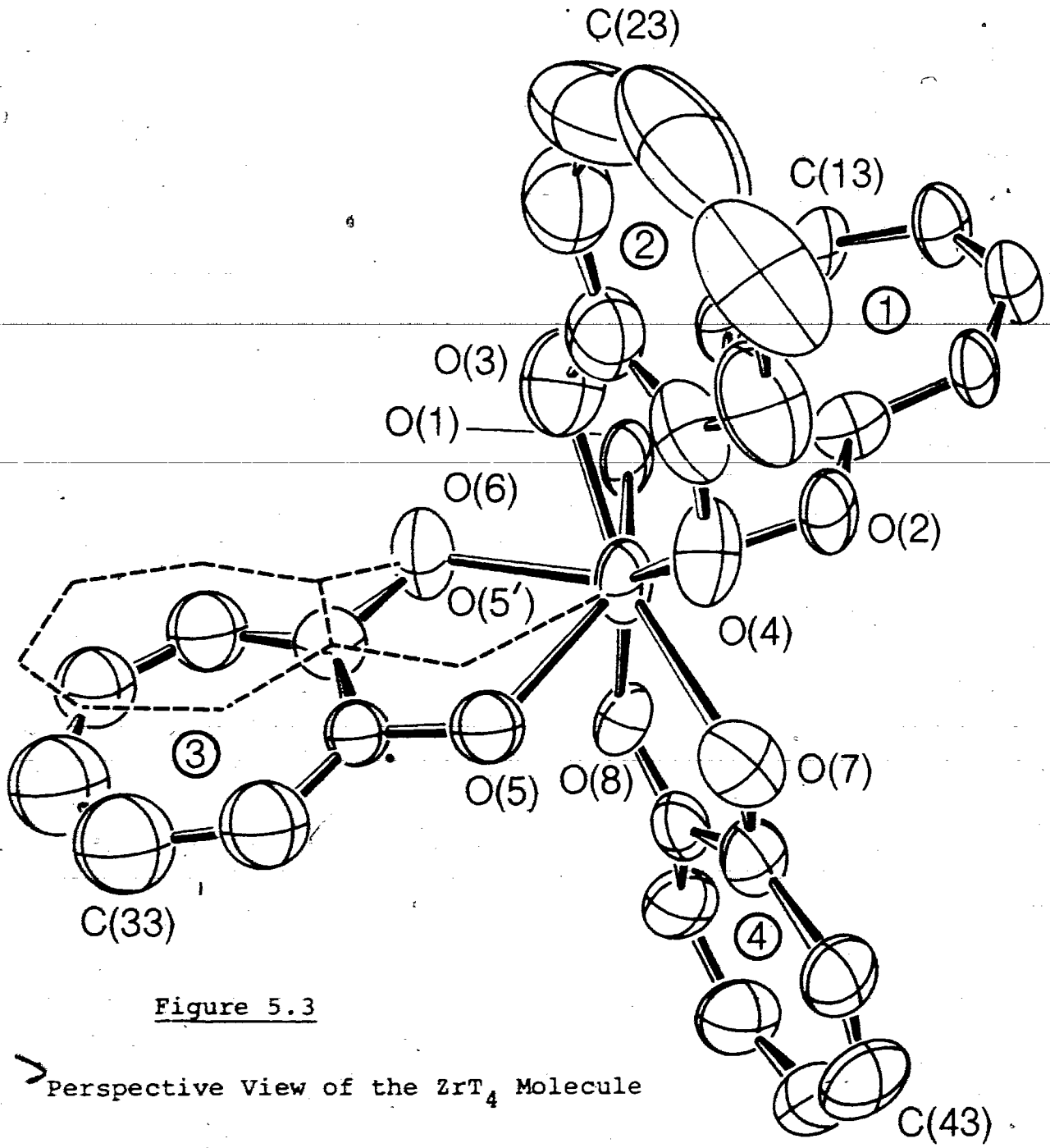


Figure 5.3

Perspective View of the ZrT_4 Molecule

5 vii Discussion

The 'ZrO_8' Polyhedron

A view of the polyhedron described by the eight oxygen atoms of the coordination sphere is given in figure 5.4. Bond lengths and angles within this polyhedron are listed in table 5.5.

The procedure described by Porai-Koshits and Aslanov is used to describe the coordination polyhedron. (In this discussion, the position adopted by ligand 3 when the nearby chloroform is present is ignored; the atomic coordinates of oxygen atom O(5) are used, rather than those of O(5)'). The four values of δ required are the angles formed by normals to the triangular faces which intersect along the edges connecting the vertices O(5), O(2), O(8), and O(3). Also, the angles Ψ which indicate the planarity of the intersecting trapezoids O(1), O(2), O(5), O(6), and O(3), O(4), O(7), O(8) have been calculated according to the method outlined in section ii. These parameters are given in table 5.6, along with similarly determined values for MO_8 polyhedra in $HScT_4$,[115] HfT_4,[117] $NbT_4(H_3O{\cdot}Cl_3)_{\frac{1}{2}}$[116] and ideal polyhedra of the dodecahedral class. A comparison of these values suggests that the ZrO_8 polyedron is best described as a dodecahedron, distorted slightly towards a bicapped trigonal prism. What information does this offer in relation to predictive theory and reaction pathways?

Calculations similar to those described in section iv have been performed for complexes of the type M(bidentate)$_4$

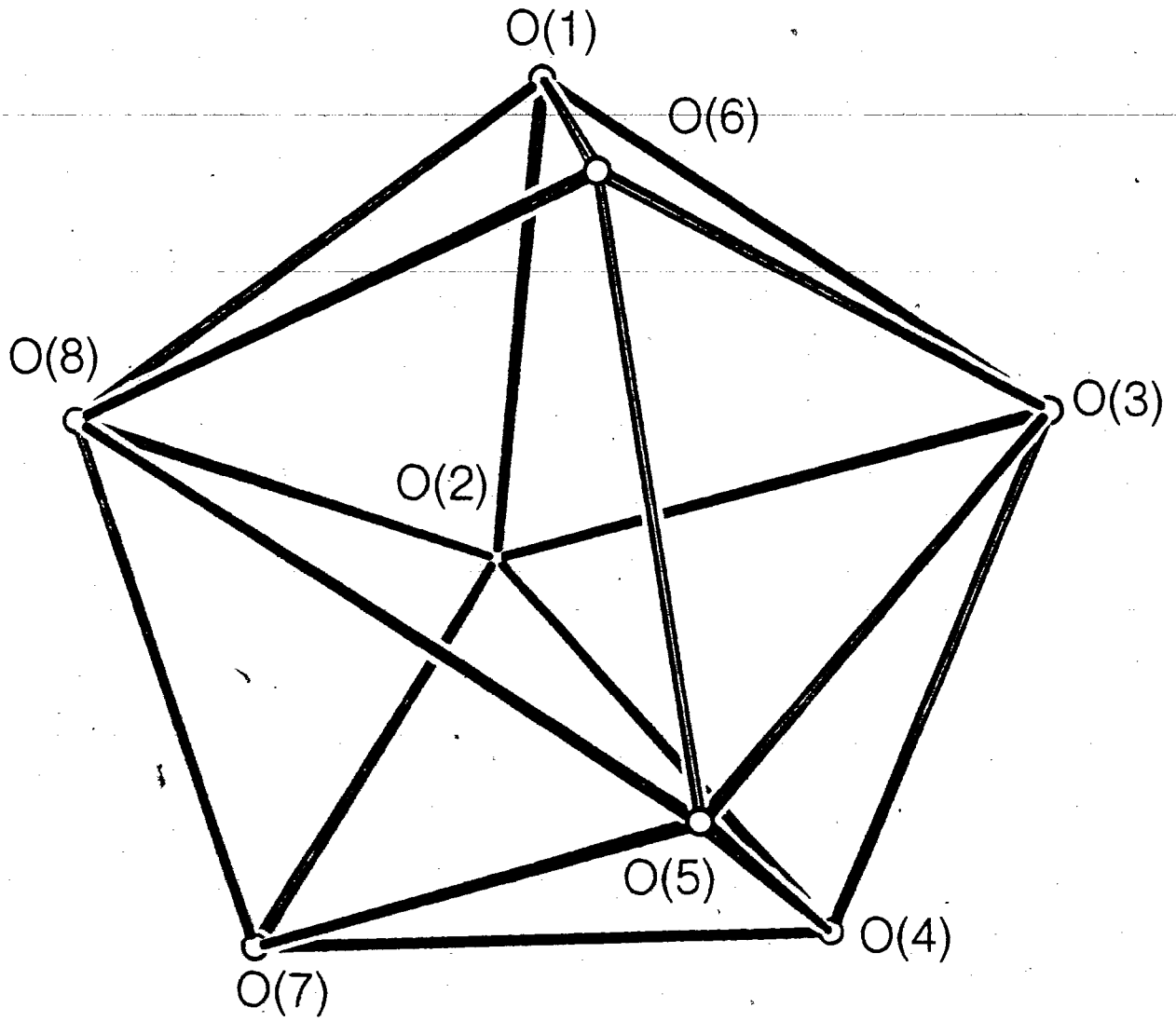


Figure 5.4

Perspective View of the 'ZrO_8' Polyhedron

Table 5.5

Bond Lengths and Angles in the 'ZrO_8' Polyhedron

Bond Lengths (Å)				Angles (°)	
Zr-O(1)	2.188(6)			O_1ZrO_2	69.4(2)
Zr-O(2)	2.172(6)			O_3ZrO_4	69.0(3)
Zr-O(3)	2.161(7)			O_5ZrO_6	71.5(5)
Zr-O(4)	2.172(8)			$O_5'ZrO_6$	66.6(5)
Zr-O(5)	2.197(6)			O_7ZrO_8	68.8(3)
Zr-O(5')	2.220(14)			O_1ZrO_3	78.2(2)
Zr-O(6)	2.208(14)			O_1ZrO_6	70.7(2)
Zr-O(7)	2.206(7)			O_1ZrO_8	77.1(3)
Zr-O(8)	2.168(8)			O_2ZrO_3	95.9(2)
O(1)-O(2)	2.480(7)	O_4-O_7	2.589(12)	O_2ZrO_4	79.8(2)
O(3)-O(4)	2.457(9)	O_5-O_7	2.882(17)	O_2ZrO_7	78.6(2)
O(5)-O(6)	2.574(15)	O_5'-O_7	2.655(16)	O_2ZrO_8	91.6(3)
O(5')-O(6)	2.425(15)	O_5-O_8	3.452(17)	O_3ZrO_5	84.4(5)
O(7)-O(8)	2.471(10)	O_5'-O_8	2.961(16)	O_3ZrO_5'	101.4(6)
O(1)-O(3)	2.743(9)	O_6-O_8	2.713(10)	O_3ZrO_6	78.6(3)
O(1)-O(6)	2.538(9)	O_5-O_5'	0.743(18)	O_4ZrO_5	70.5(5)
O(1)-O(8)	2.713(10)			O_4ZrO_5'	85.4(5)
O(2)-O(3)	3.218(8)			O_4ZrO_7	72.5(3)
O(2)-O(4)	2.786(9)			O_5ZrO_7	81.5(5)
O(2)-O(7)	2.772(9)			$O_5'ZrO_7$	73.7(5)
O(2)-O(8)	3.111(9)			O_5ZrO_8	104.2(5)
O(3)-O(5)	2.936(16)			$O_5'ZrO_8$	84.9(5)
O(3)-O(5')	3.390(16)			O_6ZrO_8	76.9(3)
O(3)-O(6)	2.759(10)			O_5ZrO_5'	19.3(5)
O(4)-O(5)	2.529(17)				
O(4)-O(5')	2.979(18)				

TABLE 5.6

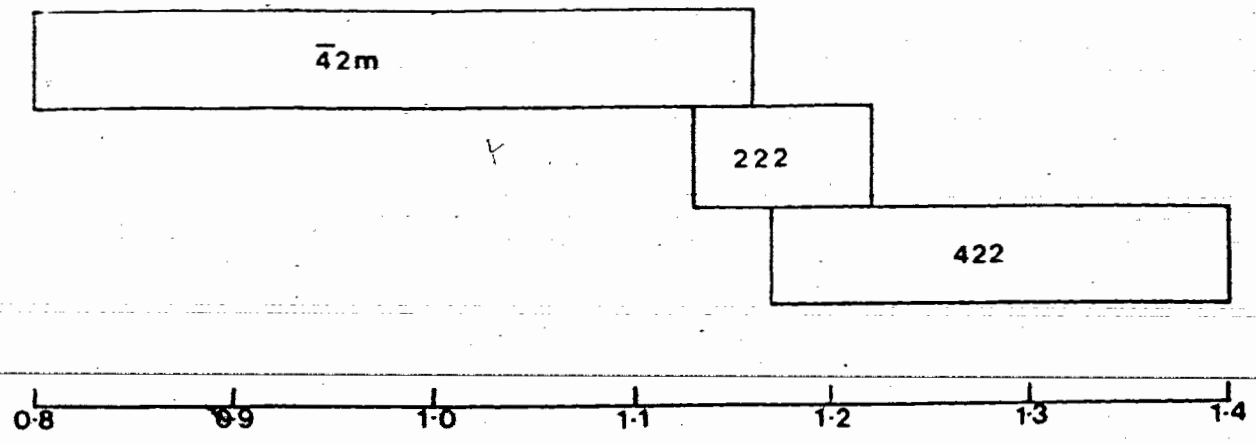
δ and ϕ Values for Regular Polyhedra of the Dodecahedral Class and for Metal Tetrakis-(tropolonato) Complexes

	δ, deg.				ϕ, deg.	
Dodecahedron	29.5	29.5	29.5	29.5	0	0
Bicapped Trigonal Prism	0	21.7	48.2	48.2	16.1	16.1
Square Antiprism	0	0	52.5	52.5	24.5	24.5
ScT_4^-	13.4	29.0	42.3	43.0	10.8	10.8
ZrT_4	22.9	31.8	32.4	40.1	6.6	1.9
NbT_4^+	19.4	21.0	42.9	45.1	11.5	13.9
HfT_4	29.1	29.4	33.9	38.3	3.6	4.0

by Blight and Kepert,[118] and they indicate that at low values of the normalized bite, b, the most stable geometry corresponds to a dodecahedron of overall symmetry $\bar{4}2m$. As the value of b increases (1.14 - 1.23), two geometries of equal stability corresponding to the $\bar{4}2m$ dodecahedron and the 222 square antiprism are obtained. At large normalized bites, 1.17 - 1.40, the most stable geometry corresponds to an 422 square antiprism, where the ligands span the edges connecting the square faces. Two areas of uncertainty occur where a choice of two possible isomers exists: b = 1.13 - 1.17 ($\bar{4}2m$ dodecahedron or 222 square antiprism) and b = 1.17 - 1.22 (222 square antiprism or 422 square antiprism). The range of existence of the isomers as a function of b is shown in figure 5.5, together with drawings of the particular tetrakis (bidentate) isomers that occur in the discussion. Also, a diagram of the generalized eight coordination indicating the angular coordinates used in these calculations is given in figure 5.6.

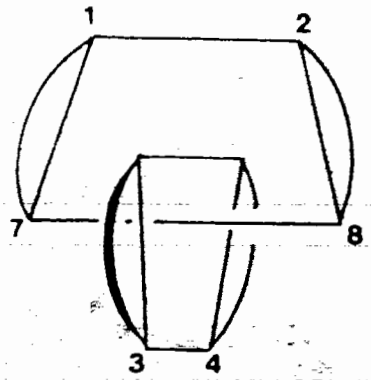
The most useful method of displaying the theoretical results described above is in terms of a projection of the potential energy surface on to the θ_A - θ_B plane, since this most clearly separates the different ideal geometries.[112] The potential energy surface for M(bidentate)$_4$ complexes where b = 1.15 and n = 6 is shown in figure 5.7. The centre of the surface at θ_A - θ_B = 45 deg corresponds to the dodecahedron. Distortion of this polyhedron by decreasing θ_A and increasing θ_B (or vice versa) along the potential energy valley gives the 222 square antiprism at θ_A = 35 deg and θ_B = 53 deg. Also seen

Figure 5.5

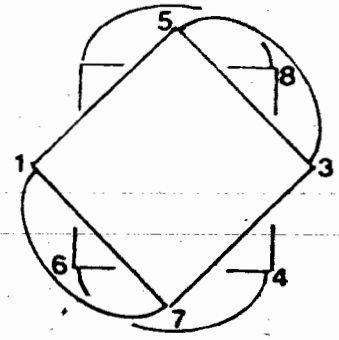


b, the normalised bite (as defined in text)

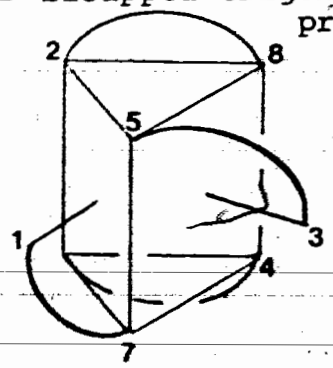
$\bar{4}2m$ dodecahedron



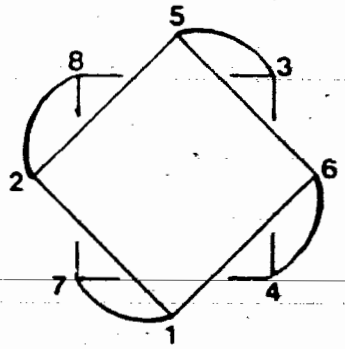
222 square antiprism



mm2 bicapped trigonal prism



$\bar{4}22$ square antiprism



Range of Existence of the Tetrakis-(bidentate) Isomers

Figure 5.6

Generalized Eight Coordination-Angular Parameters

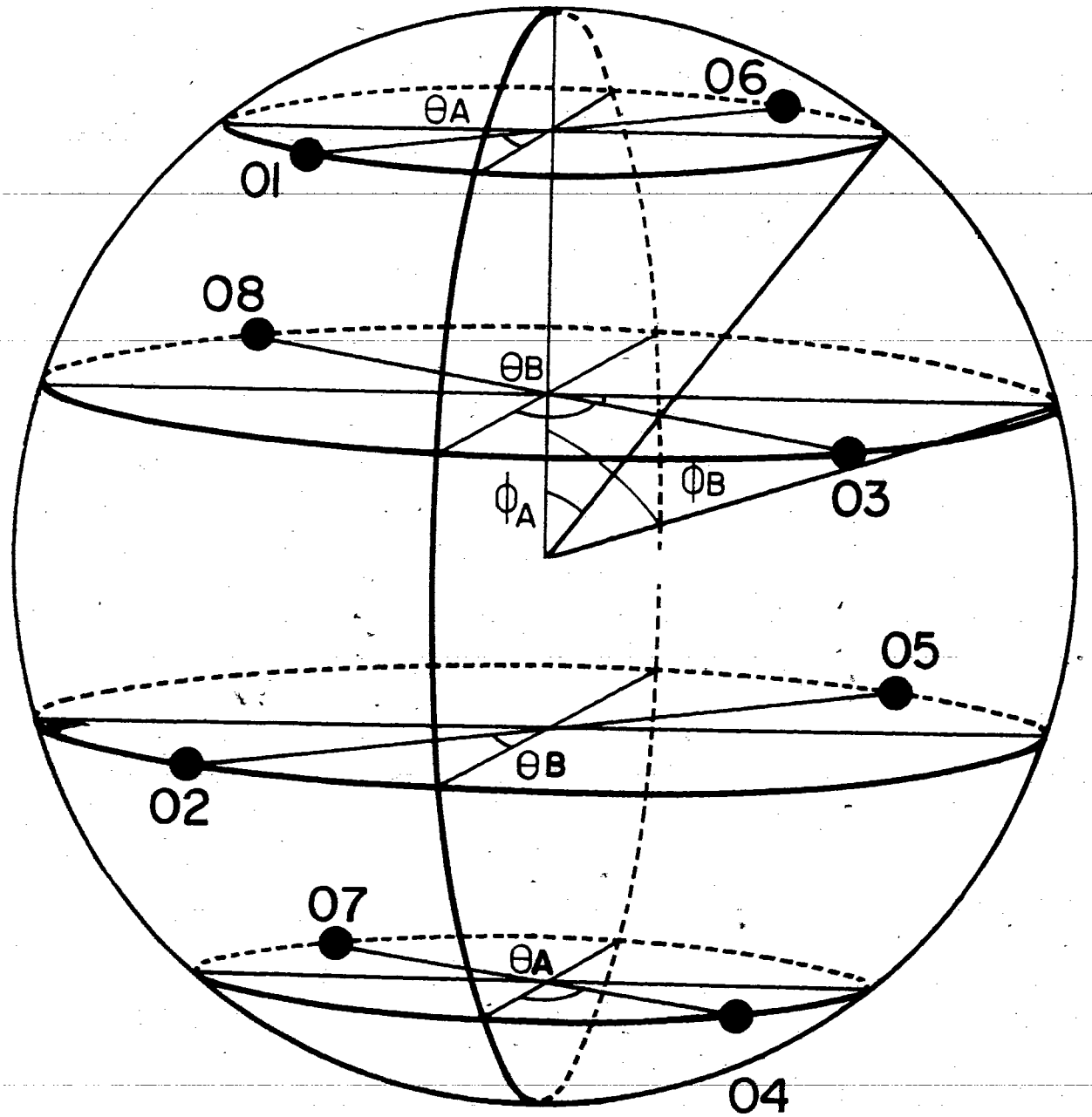
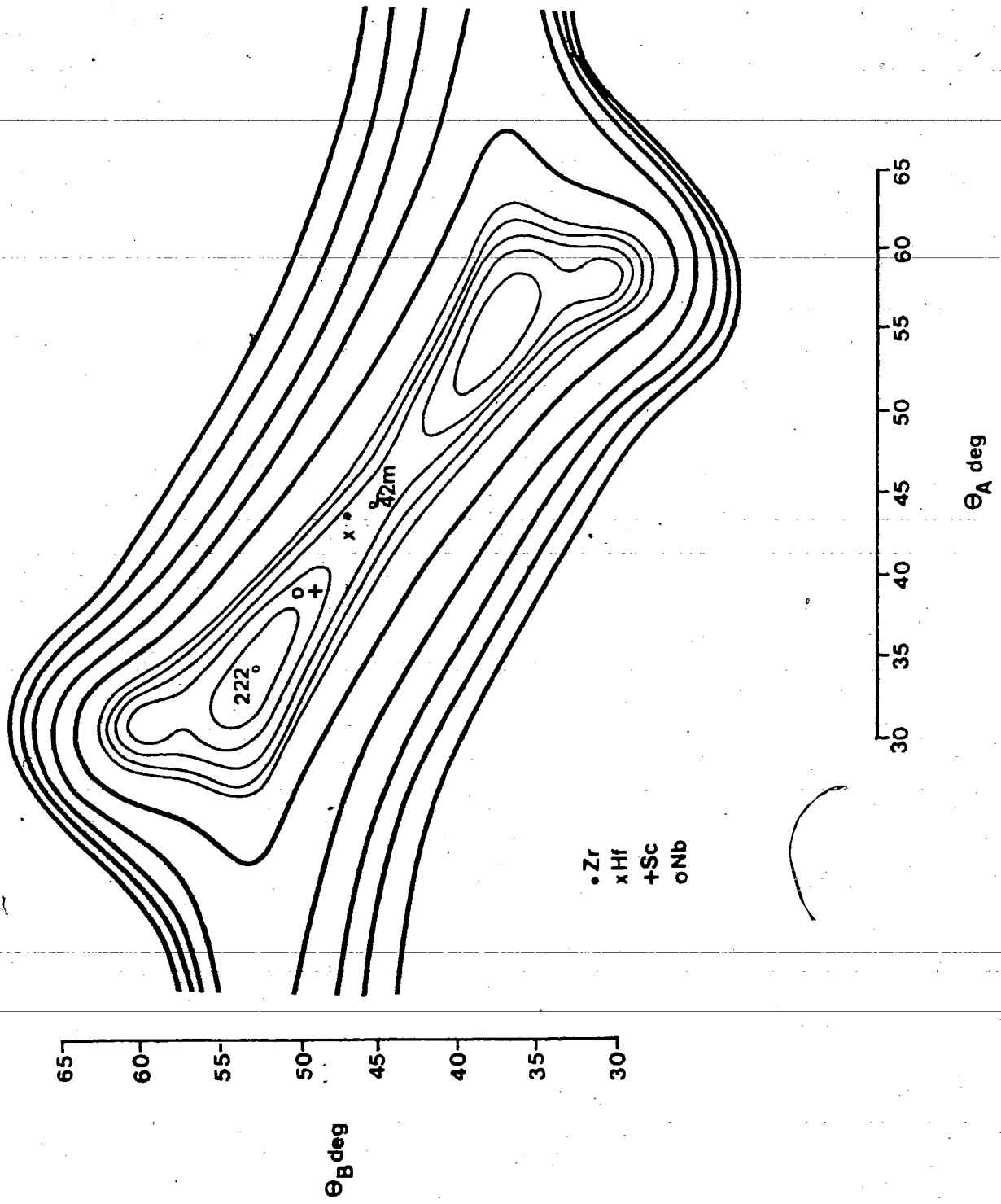


Figure 5.7

The Relationship Between Predicted and Observed Geometries in Tetrakis(bidentate) Complexes



on this surface is the emergence of a third minimum, corresponding to the 422 square antiprism, at lower θ_A and higher θ_B values. This latter minimum becomes distinct when b = 1.7. Further distortion (θ_A = 26 deg and θ_B = 65 deg) gives the $\bar{8}2m$ square antiprism. Also shown in the figure are the positions of the M(tropolonate)$_4$ complexes (M = Sc, Hf, Zr, and Nb) in terms of their determined θ_A and θ_B values. It can be seen that all four complexes lie in the predicted shallow potential valley, and the relative distortions from ideal dodecahedral geometry are seen. There appears to be no obvious correlation between the extent of distortion from any one geometry as a function of the metal (or metal to donor atom distance), or with the charge on the complexes. Table 5.7, however, gives the complete list of angles which describe the ideal and determined polyhedra occurring in figure 5.5. This indicates that the experimental values of ϕ_A are lower, and ϕ_B higher, consistently than those for ideal geometries. The origin of this difference can be ascribed to a certain degree to the overall longer ($\sim$1%) M - O_A bonds (O_A = O_1, O_6, O_4, O_7) over the M - O_B bond lengths (O_B = O_2, O_3, O_5, O_8). The lengthening of the M - O_A distance would clearly allow a small decrease in ϕ_A, and a consequent increase in ϕ_B. Simple geometric considerations show that, if say the O_A....O_B interligand distance is fixed, a lengthening in the M - O_A bonds of $\sim$1% leads to a similar decrease in ϕ_A of $\sim$1%. The fact that observed values of ϕ_A are smaller by factors of 4 to 9% than calculated values (table 5.7), means that the major source of the difference in these angular parameters is the shortening of

Table 5.7

Angular Parameters which Define the Observed and Predicted Geometries of the Tetrakis-(tropolonato) Complexes

	b	deg				Å	Å	
		ϕ_A	ϕ_B	θ_A	θ_B	$O_A \cdots O_A$	$M - O_A$	$\frac{O_A \cdots O_A}{M - O_A}$
$\bar{4}2m$ dodecahedron	1.15	39.2	67.7	45.0	45.0			1.264
222 square antiprism	1.15	37.5	72.9	33.4	52.5			1.217
ScT_4^-	1.13	36.3	74.5	37.8	48.3	2.632	2.215	1.188
ZrT_4	1.145	35.8	74.4	44.3	47.9	2.563	2.193	1.168
HfT_4	1.143	36.0	74.4	43.0	48.9	2.575	2.182	1.176
NbT_4^+	1.16	35.7	73.7	37.8	49.7	2.438	2.088	1.169

the $O_A....O_B$ contacts in the tropolonato complexes. A comparison of $O_A....O_B/M-O_A$ ratios for calculated and observed geometries takes into account the longer $M - O_A$ bonds in these complexes, and shows decreases of 3 to 12% in the ratios, implying similar decreases in the lengths of the $O_A....O_B$ contacts relative to those calculated using the repulsion model (table 5.7).

An inspection of high coordinate chelate complexes shows[116], as observed for the tropolonates above, that the shortest, non-imposed interligand contact within the coordination sphere always occurs between approximately coplanar ligands. The only exceptions occur where the isomer adopted does not allow any such mutual arrangement of ligands, or where the bite of the ligand is very small, although there are nitrate and other four-ring chelate complexes that do follow this pattern. It has been stated previously[116], and is reiterated here, that there appears to be a definite correlation between the length of the non-imposed contact between two ligands (with O or S donors) in a high coordinate complex, and their mutual orientation. It has also been suggested[116] that the interaction of overlapping lone pairs of electrons on the adjacent donor atoms with empty d orbitals on the central metal could act against the Coulombic repulsion forces. Thus, although a theory based only on repulsive forces predicts with reasonable success the geometry of these complexes, inclusion of some attractive component, where applicable, appears to be necessary to predict the finer details of the shape.

A recent report gives some interesting results which are relevant to the above proposal.[119] The crystal and molecular structures of $Ti(Et_2mtc)_4$ and $Zr(Et_2mtc)_4$ (Et_2mtc = N,N-diethylmonothiocarbamate) show two important effects. Firstly, the oxygen and sulphur donor atoms do not sort into A and B positions in the dodecahedral geometry, but partially sort so that two sulphur atoms are in the A sites and two are in the B sites; in this way all four sulphur atoms are located on one side of the structure, and the four oxygen atoms on the other. This preference for sulphur and oxygen to be <u>trans</u> to one another to reduce the competition for available metal π-electrons is also seen and discussed for $Ru(DMSO)_6^{2+}$ in Chapter 6 of this text.

Secondly, in the Ti compound, the S....S and O....O contacts between adjacent coplanar ligands are surprisingly short (S....S = 3.212(3), and O....O = 2.491(6) A). Since the other S....S contacts in the coordination sphere (3.327(2) - 3.367(2) A) are also short, it appeared that the novel isomer was stabilized by weak attractive S....S interactions, similar to those suggested for the stabilization of <u>cis</u> - monothio-β-diketonate complexes,[120] and trigonal prismatic dithiolene complexes.[121] It was to test this hypothesis that the structure of the Zr compound was determined, where the larger metal - donor atom distance would establish the importance of the S....S interactions. The result was that the same stereoisomer was obtained, with now the only short interligand contacts occuring between atoms at the A sites where adjacent

ligands are approximately coplanar (S....S = 3.396(2), O....O = 2.608(5) A). An approximately equal opening of the structure occurred on the oxygen and sulphur "sides" of the coordination sphere as a result of the increased metal - ligand bond lengths. This indicates (1) that, save the contacts between coplanar ligands, the S....S contacts do not appear to be important in determining the geometry, and (2) that the geometry of both complexes is determined by the trans influence of the sulphur atoms.[119]

To this point in the discussion, the tetrakis(tropolonate) metal complexes have been described in two different ways. According to the potential valley generated by Blight and Kepert's calculations,[118] the geometries lie somewhere between those of an ideal dodecahedron of overall symmetry $\bar{4}2m$, and a square antiprism of symmetry 222. This implies, from the point of view of reaction pathways, that they lie on the '222' pathway from the $\bar{4}2m$ dodecahedron to the 422 square antiprism (figure 5.1). The other description, based on the criteria proposed by Porai-Koshits and Aslanov,[108] is that these complexes are dodecahedral (symmetry $\bar{4}2m$), distorted towards a bicapped trigonal prism (symmetry mm2), which reduces to only 2-fold point symmetry when the bidentate ligands are considered, i.e. the structures lie on the '2-fold' reaction pathway between the dodecahedron and the bicapped trigonal prism as shown in figure 5.1. Is the bicapped trigonal prism a distinct geometry, or simply a part of the single broad pathway from the dodecahedron to the square antiprism? From an inspection of

all eight coordinate structures whose geometries can be considered as in some way distorted dodecahedra, two categories emerge.[104] The majority have δ values which include 2 equivalent but large angles, and 2 equivalent but small angles. These two small values represent the simultaneous flattening of 2 edges to form the square faces of square antiprism, and these structures would therefore be considered to be on the '222' pathway. The other group (including the tetrakis(tropolonates)) have 2 non-equivalent small values, indicating only one square face being formed, and so can be said to lie on the '2-fold' pathway from a dodecahedron to a bicapped trigonal prism. Why only one square face is being formed is not clear, but it does appear to be a well-established effect. It would appear that, in terms of a reaction pathway, there is a separate geometry, usually referred to as a bicapped trigonal prism,[104] although this is a misnomer, since the implied three-fold symmetry has been completely lost. From the point of view of the predictive calculations of Kepert,[113] however, this geometry cannot be distinguished within the shallow minimum of potential energy which connects the dodecahedron with the square antiprism.

The Tropolonate Ligands and Chloroform Molecules

Bond lengths and angles within the tropolonate ligands are given in table 5.8, and include values for both positions of ligand 3. The dimensions do not differ significantly from those obtained in previous structural studies on metal tropolonates.[114,117] The seven-membered rings are very nearly

planar in each ligand, with slight twisting of the carbon skeleton relative to the plane formed by the metal and oxygen atoms, the angle of twist ranging from 1.05 deg (ligand 3) to 9.33 deg (ligand 1).

Carbon - chlorine bond lengths within the chloroform molecules of crystallization average 1.17A and the Cl-C-CL angles average 111 deg.

Table 5.8

Bond Lengths and Angles in the Tropolonato Ligands

a) Bond Lengths (Å)

Bond Type	Ligand 1(O_1,O_2)	2(O_3,O_4)	3(O_5,O_6)	3'(O_5',O_6)	4(O_7,O_8)
O(1)-C(1)	1.307(9)	1.27(1)	1.33(2)	1.31(2)	1.29(1)
O(2)-C(7)	1.310(9)	1.29(1)	1.36(3)	1.25(2)	1.29(1)
C(1)-C(7)	1.46(1)	1.47(1)	1.43(3)	1.41(3)	1.44(1)
C(1)-C(2)	1.38(1)	1.38(1)	1.38(3)	1.38(3)	1.39(1)
C(2)-C(3)	1.37(1)	1.37(1)	1.38(3)	1.39(3)	1.37(2)
C(3)-C(4)	1.39(1)	1.38(1)	1.40(3)	1.35(3)	1.34(3)
C(4)-C(5)	1.40(1)	1.35(1)	1.33(3)	1.35(3)	1.41(3)
C(5)-C(6)	1.35(1)	1.36(1)	1.32(3)	1.39(3)	1.38(2)
C(6)-C(7)	1.38(1)	1.42(1)	1.45(3)	1.41(3)	1.39(2)

b) Bond Angles (deg)

Angle Type	Ligand 1(O_1,O_2)	2(O_3,O_4)	3(O_5,O_6)	3'(O_5',O_6)	4(O_7,O_8)
C(7)C(1)C(2)	128(1)	124(1)	127(2)	126(2)	129(1)
C(1)C(2)C(3)	129(1)	133(1)	129(2)	131(2)	128(2)
C(2)C(3)C(4)	129(1)	126(1)	128(2)	127(2)	133(2)
C(3)C(4)C(5)	127(1)	128(1)	129(3)	128(2)	125(3)
C(4)C(5)C(6)	129(1)	130(1)	129(3)	131(2)	129(2)
C(5)C(6)C(7)	131(1)	131(1)	130(2)	126(2)	132(2)
C(6)C(7)C(1)	126(1)	125(1)	125(2)	128(2)	124(1)
O(1)C(1)C(7)	113(1)	113(1)	110(2)	114(2)	113(1)
O(2)C(7)C(1)	113(1)	113(1)	120(2)	112(2)	114(1)
O(1)C(1)C(2)	120(1)	123(1)	123(2)	119(2)	118(1)
O(2)C(7)C(6)	121(1)	122(1)	114(2)	120(2)	121(1)

Chapter 6

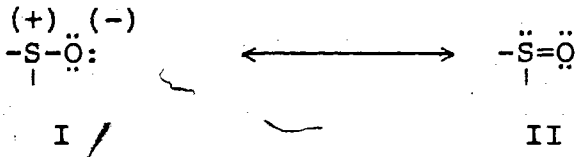
The Crystal and Molecular Structure of the Hexakis (dimethylsulphoxide) ruthenium(II) Cation

6 i. Introduction

The initial motivation for studying ruthenium/dimethylsulphoxide sytems (Professor B. R. James *et al*, University of British Columbia) was to extend the range of ruthenium complexes which act as homogeneous catalysts, predominantly for hydrogenation reactions. Among those already known in this respect are complexes with simple halides, and nitrogen, phosphine, and arsine ligands.[122]

Sulphoxide ligands have special interest in that bonding to the metal may occur via the sulphur or oxygen atoms. Because these two modes of bonding impart different electronic and steric properties to the complex,[123] an appreciation of their effect is essential for an evaluation of such compounds as potential catalysts. Previous structural and spectral studies[124,125] have shown that bonding occurs exclusively via the oxygen atom in complexes of "class a" metals,[16] and, in the absence of extraordinary steric influences resulting from bulky alkyl groups in the ligand,[126,127] bonding generally occurs via the sulphur atom in complexes of "class b" metals. The only exception is found in the square planar cis - $Pd(DMSO)_4^{2+}$ and cis - $Pt(DMSO)_4^{2+}$, which have 2S- and 2O- bonded ligands.[125] Ruthenium is considered to lie on the border of the "class a"/"class b" classification, and so the type of bonding to be found is not easy to predict, and i.r. and n.m.r. data can lead to ambiguity. The S-O

stretching frequency has been of great importance in the study of the complexes of DMSO. The sulphur-oxygen bond has considerable double bond character, which in simple Lewis notation approximates :[123]



I II

Bonding of the metal ion to the oxygen atom stabliizes I, lowering the bond order of the S-O bond, and decreases ν(S-O); bonding to sulphur stabilizes II and increases the S-O bond order, and ν(S-O). Unfortunately, ν(S-O) varies with the nature of the solvent and with concentration, and its use in determining the existence and/or ratio of S-bonded to O-bonded ligands can be limited. Proton n.m.r. is somewhat more useful, since a shift of ~1 p.p.m. downfield from that of free DMSO is observed for the methyl hydrogens of S-bonded ligands. O-bonded ligands show considerably less variation from the free value of τ = 7.40[128]. As a tool for determining the number of each type of ligand, however, problems arise from exchange of ligands with (especially O-bonded) solvents.[129]

One further interest in sulphoxide ligands (not pursued further in this text) lies in the pyramidal geometry about the sulphur atom. $R_1R_2S{=}O$ ligands will exhibit chirality at the sulphur, and the possibility of catalytic asymmetric hydrogenation is suggested.[124]

6 ii. Homogeneous Catalysis[122,130]

The rapid escalation in research into an understanding of homogeneous catalysis over the past 20 years can be attributed to several factors. It has followed closely the many advances made in transition metal and organometallic chemistry which have provided methods of preparation of a wide variety of metal complexes, together with methods for elucidating their electronic and molecular structures. The specificity towards reaction of particular substrates, the ability to function under mild conditions, and their relative ease of study over heterogeneous systems have made homogeneous catalysis an attractive field of research. Industrial application of these studies is already widespread (e.g., the Wacker, Oxo, and some Ziegler-Natta processes, and methanol carbonylation).

Halpern[130] has identified two themes which contribute to an understanding of homogeneous catalysis: the elucidation of the catalytic mechanism (via kinetic studies), and the dependence of the catalytic mechanism on the structure and electron configuration of the catalyst. Studies relating to the first theme have been numerous and successful in resolving many reactions into component steps so that, for instance, in homogeneous hydrogenation, the elementary step involving the reaction of H_2 is recognisable. More limited progress has been made in the second theme; for instance, understanding how the reactivity toward H_2 depends on the electron configuration of the catalyst. Catalytic activity requires that the catalytic intermediate be labile, and that its thermodynamic stability

lies within narrowly defined limits. The number and nature of the other ligands in the metal complex catalyst is therefore a necessary prerequisite for the understanding of the mechanism.

6'iii. Experimental Section

A $[Ru(DMSO)_6][BF_4]_2$ crystal of approximate dimensions 0.11 x 0.27 x 0.09 mm was mounted along the needle axis for the purpose of data collection. Using copper radiation (λ = 1.541Å), Weissenberg photographs of the reciprocal lattice layers $h0\ell$, $h1\ell$, and precession photographs of the $hk0$ and $0k\ell$ zones were taken which established monoclinic Laue symmetry, with systematic absences consistent with the space group $P2_1/c$. Accurate cell parameters were determined from counter measurement of 12 of the strongest reflections having $2\theta > 30^\circ$, using a Picker FACS-1 computer-controlled, four-circle diffractometer, and Mo Kα radiation ($\lambda\alpha_1$ = 0.70926Å).

The crystal was mounted with the b-axis (corresponding to the needle direction) slightly offset from the ϕ axis of the diffractometer. The crystal has a formula weight 743.5, space group $P2_1/c$: a = 17.833(4)Å, c = 33.800(8)Å, β = 109.68(1)°. V = 5952.0Å^3, d_M = 1.62(2) gcm^{-3} (flotation), Z = 8, d_x = 1.66 g cm^{-3}, μ(Mo Kα) = 9.83 cm^{-1}, T = 21(±1)°C. Reflections for the unique set of data were measured in two sets using a scintillation detector with pulse height analysis and monochromatised radiation (graphite monochromator, λ(Mo Kα) = 0.70926Å). Those reflections for which $\sin\theta < 0.1737$ were measured with a symmetrical θ-2θ scan of 1.2° base width

with 10s background counts made at both scan limits. For reflections where $0.1737 < \sin\theta < 0.3420$, a scan of 0.8° base width was used, with 4s background counts. Two standard reflections were measured after each 100 reflections; their variation was ±3% over the entire data collection. The intensities were corrected for Lorentz and polarisation effects; absorption was neglected since it was estimated to introduce an extreme error of ±8.0% in F. A total of 5569 reflections were measured, of which 3961 were considered to be observed (i.e., greater than $2.3\sigma_{I(net)}$, where $\sigma_{I(net)} = [TC + (\frac{t_s}{t_b})^2(B_1+B_2)+(kI)^2]^{1/2}$, where TC is the total counts, B_1 and B_2 are the background counts, t_s is the scan time, t_b is the total background count time, k is a constant set to 0.03, and I is the net count).

6 iv. Structure Determination and Refinement

Examination of the three-dimensional Patterson function based on data for which $\sin\theta < 0.1737$ gave the positions of the two ruthenium atoms of the unit cell, and ten sulphur atoms. Refinement of the scale and these atomic coordinates gave R = 0.456, where $R = \Sigma(|F_o|-|F_c|)/\Sigma|F_o|$. Several cycles of refinement and subsequent electron density difference maps based on the complete set of observed data gave the positions of all non-hydrogen atoms. A difference Fourier synthesis based on an inner set of data revealed the positions of at least one of the hydrogen atoms of each methyl group. The remaining hydrogen atom positions were then calculated, with a C-H bond

length of $0.076A^2$. Anisotropic thermal parameters were assigned to all non-hydrogen atoms save the boron atoms, and full matrix, least-squares refinement reduced the R-factor to a final value of 0.051. At this stage, comparison of the inter-atomic distances and angles within each cation showed that they adopted very similar configurations and that the pattern of bond lengths and angles in one cation was followed very closely in the other. An inspection of the ruthenium atomic coordinates and thermal motion parameters revealed (i) that the ruthenium atoms are roughly related by the transformation 1/2 + x,y, 1/2 - z, and (ii) that U_{22} is the highest thermal motion parameter for one ruthenium and the lowest for the other. The possibility existed that the refinement had been "locked" by this false symmetry, relating the two cations, in particular with respect to the y-coordinates of the ruthenium atoms. An electron density difference map showing the detail around each metal atom, however, showed no outstanding features, and the refinement was then terminated. The highest peaks in the final difference map (1.0 ± 0.1 electrons/A^3) occurred near the BF_4^- anions. In the early refinement, constant unit weights were used; in the later stages, weights ($= \frac{1}{\sigma^2(F)}$) were given in terms of $\sigma_{(F)} = \sigma_{(I)}/(L_p \cdot 2F_o)$. Atomic scattering factors used were taken from reference 35, and included corrections for anomalous dispersion for ruthenium and sulphur atoms. Final atomic parameters are given in table 6.1, and thermal motion parameters in table 6.2. A structure factor listing is given in table 6.3. Bond lengths and angles are listed in table 6.4.

Table 6.1

Fractional Atomic Coordinates: $Ru(DMSO)_6(BF_4)_2$
($\times 10^4$, $\times 10^5$ for Ru, $\times 10^3$ for B)

Atom type	Cation I			Cation II		
	x	y	z	x	y	z
Ru	222(5)	24213(9)	10204(2)	54688(4)	24582(9)	39651(2)
S1	784(2)	1739(3)	647(1)	5836(2)	713(3)	3689(1)
S2	-953(2)	1096(3)	663(1)	6748(2)	2974(3)	4288(1)
S3	-422(2)	4182(3)	625(1)	5310(2)	1388(3)	4510(1)
S4	1375(2)	697(3)	1655(1)	5084(2)	3179(3)	2987(1)
S5	1072(2)	4793(3)	1598(1)	3486(2)	2367(3)	3660(1)
S6	-301(2)	2803(3)	1886(1)	4541(2)	5108(3)	3858(1)
O1	988(5)	359(8)	710(2)	6304(4)	1021(7)	3414(2)
O2	-1177(4)	1039(8)	203(2)	7287(4)	1977(8)	4530(3)
O3	234(4)	4961(7)	577(2)	4863(4)	160(7)	4394(2)
O4	478(4)	978(6)	1476(2)	5475(4)	3610(6)	3452(2)
O5	1018(4)	3432(6)	1435(2)	4265(4)	2090(6)	3590(2)
O6	-661(4)	2923(6)	1403(2)	5099(4)	4186(6)	4180(2)
C11	1681(6)	2607(12)	773(3)	6379(7)	-487(11)	4048(4)
C12	415(7)	1984(12)	97(3)	4978(6)	-178(10)	3395(4)
C21	-743(7)	-491(11)	848(4)	6863(7)	4297(12)	4622(4)
C22	-1843(7)	1362(13)	770(4)	7196(6)	3615(11)	3934(4)
C31	-956(7)	5181(12)	855(4)	4776(7)	2320(11)	4764(3)
C32	-1151(7)	4048(12)	116(4)	6156(7)	1035(11)	4966(3)
C41	1423(7)	-993(11)	1624(4)	5852(7)	3310(11)	2767(3)
C42	1600(7)	866(13)	2199(4)	4516(6)	4547(10)	2743(3)
C51	1619(8)	4660(13)	2140(4)	2876(7)	2961(15)	3174(5)
C52	1817(8)	5533(13)	1449(4)	3030(7)	892(13)	3657(5)
C61	-842(9)	3988(11)	2051(4)	5142(8)	643(12)	3846(4)
C62	-751(8)	1433(11)	2015(4)	3969(8)	5736(12)	4147(4)

Table 6.1 (continued)

Atom Type	x	y	z
F1	2111(4)	2682(9)	4883(2)
F2	3422(5)	2559(8)	5211(2)
F3	2865(5)	1488(8)	4618(3)
F4	2920(5)	3566(8)	4604(3)
F5	-3648(7)	2726(18)	1918(4)
F6	-2761(7)	2648(14)	1658(4)
F7	-2441(7)	2717(13)	2335(4)
F8	-2980(10)	1260(13)	1990(5)
F9	897(5)	2356(12)	2823(3)
F10	1205(6)	2485(20)	3473(3)
F11	336(12)	3614(11)	3096(5)
F12	472(8)	1919(15)	3129(4)
F13	4273(4)	2206(8)	2036(3)
F14	3059(6)	2998(9)	1849(4)
F15	3228(6)	1149(13)	1650(5)
F16	3395(8)	1548(17)	2254(5)
B1	283(1)	254(2)	484(1)
B2	-292(1)	246(3)	201(1)
B3	68(1)	250(2)	314(1)

Table 6.1 (continued)

Calculated Fractional Atomic Coordinates for the Hydrogen Atoms in stalline $[Ru(DMSO)_6][BF_4]_2$ ($\times 10^4$) [a]

	Cation I [b]			Cation II [b]		
	x	y	z	x	y	z
H111	1960	6358	1562	-1775	1469	1062
H112	1667	5616	1140	-2244	704	663
H113	-1371	4694	917	2042	2292	651
H121	-1216	5850	669	1941	2695	1072
H122	-1235	4815	-28	-125	1645	-29
H123	-1644	3730	136	733	1566	-46
H211	6618	4248	4845	3898	6655	4122
H212	6756	4441	3789	4187	5561	4447
H213	-677	4828	2034	6646	5076	4457
H221	-805	3852	2350	7430	4503	4760
H222	-814	1559	2280	7220	3017	3726
H223	-425	718	2025	7723	3931	4076
H311	1461	3669	646	3082	3737	3085
H312	407	3067	44	2338	3142	3152
H313	2870	2293	2964	2968	376	3429
H321	3450	290	3993	2504	978	3697
H322	6628	-832	3887	6048	-1119	4115
H323	4779	277	3125	6747	-174	4302
H411	4183	2468	4607	4596	-859	3372
H412	6394	580	4889	5469	-549	3412
H413	5978	4106	2760	5006	3158	4848
H421	4142	4341	2826	4788	1918	5035
H422	5569	6143	3776	6034	660	5193
H423	3435	5282	4017	6491	1784	5081
H511	-533	5548	1145	1086	-1429	1752
H512	-962	3275	-89	1957	-1323	1757
H513	1223	-1250	1255	1692	39	2338
H521	1909	1184	2272	1184	1272	2268
H522	-769	-551	1164	-210	-761	858
H523	-2096	2336	588	-1107	-1104	670
H611	-1418	3905	1889	5700	3007	2486
H612	-1298	1275	1797	6328	2878	2932
H613	1205	4675	2279	4362	4602	2447
H621	1919	5408	2223	4739	5358	2861
H622	1896	3942	2208	5296	6927	4094
H623	2195	5128	1510	4837	7045	3616

[a] All hydrogen atoms were assigned an isotropic temperature factor of $U = 0.076 Å^2$.

[b] For details of labelling, see script.

Table 6.2

Thermal Motion Parameters: $Ru(DMSO)_6(BF_4)_2$

($\times 10^3$, $\times 10^4$ for Ru $Å^2$)

Atom type	Cation I						Cation II					
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru	343(6)	395(6)	325(6)	-62(5)	129(4)	-33(5)	300(5)	291(6)	344(6)	-3(5)	92(4)	20(5)
S1	47(2)	62(2)	39(2)	-7(2)	22(2)	-6(2)	52(2)	30(2)	59(2)	7(2)	26(2)	4(2)
S2	49(2)	57(2)	47(2)	-18(2)	15(2)	-10(2)	33(2)	45(2)	56(2)	-4(2)	5(2)	10(2)
S3	47(2)	57(2)	45(2)	-6(2)	7(2)	10(2)	48(2)	49(2)	40(2)	-3(2)	17(2)	7(2)
S4	47(2)	50(2)	52(2)	4(2)	23(2)	5(2)	54(2)	40(2)	41(2)	-3(2)	14(2)	3(2)
S5	49(2)	48(2)	77(2)	-4(2)	18(2)	-17(2)	42(2)	70(3)	70(2)	-8(2)	16(2)	-10(2)
S6	60(2)	54(2)	47(2)	-6(2)	28(2)	-8(2)	54(2)	39(2)	50(2)	8(2)	12(2)	-22(2)
O1	40(5)	66(6)	113(7)	5(5)	-14(5)	42(6)	40(5)	33(5)	42(5)	-2(4)	10(4)	-9(4)
O2	52(5)	34(5)	38(4)	13(4)	15(4)	-3(4)	92(7)	52(6)	67(6)	10(5)	42(5)	-5(5)
O3	83(6)	53(6)	59(5)	-36(5)	26(5)	-3(5)	53(5)	61(6)	78(6)	-25(5)	20(5)	18(5)
O4	52(5)	27(4)	34(4)	-3(4)	14(4)	8(4)	39(5)	43(5)	44(5)	-6(4)	16(4)	3(4)
O5	81(6)	46(5)	88(6)	8(5)	62(5)	7(5)	39(4)	43(5)	41(5)	2(4)	18(4)	-4(4)
O6	32(4)	52(5)	53(5)	-1(4)	12(4)	-5(4)	65(6)	76(7)	35(5)	25(5)	5(4)	-8(5)
C11	67(4)	67(9)	72(9)	-7(8)	3(8)	-18(8)	84(11)	88(12)	72(10)	-14(9)	18(9)	-18(9)
C12	46(7)	64(9)	84(9)	-19(7)	32(7)	-5(8)	101(11)	75(11)	108(12)	-44(9)	45(10)	1(9)
C21	112(12)	52(9)	107(12)	-15(9)	25(10)	7(9)	39(7)	110(11)	45(7)	-11(8)	25(6)	-13(8)
C22	111(11)	73(10)	79(10)	41(9)	41(9)	-8(8)	66(9)	105(11)	40(8)	-6(8)	25(7)	-7(8)
C31	78(9)	65(9)	49(7)	8(8)	32(7)	2(7)	70(10)	62(10)	85(11)	27(8)	24(8)	17(8)
C32	78(9)	79(10)	49(8)	-9(8)	1(7)	38(7)	69(9)	77(11)	52(9)	-10(8)	-13(7)	19(8)
C41	69(9)	65(9)	54(8)	1(7)	27(7)	3(7)	80(10)	36(8)	114(12)	21(7)	46(9)	17(8)
C42	76(9)	45(8)	41(7)	11(7)	7(7)	15(6)	96(11)	97(11)	54(9)	22(9)	31(8)	19(9)
C51	77(9)	50(8)	66(9)	23(7)	-11(8)	24(7)	148(13)	47(9)	112(12)	3(9)	95(11)	-6(8)
C52	49(8)	43(8)	75(9)	-6(7)	10(9)	-4(7)	102(11)	49(9)	89(10)	-5(8)	64(9)	7(8)
C61	41(8)	150(15)	127(12)	16(9)	20(7)	36(11)	87(10)	41(9)	82(11)	-33(8)	9(8)	-5(8)
C62	66(9)	79(11)	141(12)	-25(9)	12(7)	0(10)	47(8)	111(12)	86(10)	-42(8)	32(7)	-31(9)

Table 6.2 (continued)

Atom type	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F1	80(6)	231(11)	109(6)	43(7)	53(5)	18(7)
F2	109(6)	127(7)	68(5)	20(6)	-2(5)	7(6)
F3	115(7)	107(7)	152(8)	16(6)	39(6)	-44(7)
F4	140(8)	116(8)	120(7)	22(6)	62(6)	47(6)
F5	158(11)	539(28)	161(10)	225(14)	49(9)	39(14)
F6	199(12)	294(18)	169(11)	-63(11)	74(10)	22(12)
F7	162(10)	326(19)	158(10)	-100(11)	9(9)	-138(11)
F8	350(22)	137(12)	274(18)	-52(13)	-40(15)	47(12)
F4	132(8)	339(17)	107(7)	-32(9)	80(7)	-85(9)
F10	120(9)	655(35)	94(8)	94(15)	13(7)	5(14)
F11	498(27)	78(9)	295(19)	72(13)	181(19)	15(10)
F12	170(12)	303(19)	277(16)	7(12)	129(12)	59(14)
F13	57(5)	132(8)	150(8)	-9(5)	32(5)	-35(7)
F14	108(8)	68(7)	339(17)	36(6)	2(9)	-15(9)
F15	98(8)	240(14)	298(17)	34(8)	-45(9)	-213(14)
F16	193(13)	356(22)	274(17)	-34(14)	107(13)	151(17)

Isotropic parameters (x 10^2):		U
	B1	66(4)
	B2	89(5)
	B3	89(5)
	B4	75(5)

b The anisotropic temperature factors are of the form:

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

Table 6.3

Structure Factor Listing: $Ru(DMSO)_6(BF_4)_2$ (x10)

Reflections which are considered to be unobserved are denoted by an asterisk

L	FO	FC
H=	0, K=	0
2	644	676
4	4362	-4374
6	39*	-58
8	2231	-2252
10	1648	1629
12	167	87
14	673	584
16	465	-484
18	1200	1216
20	1576	1585
22	979	-980
24	1953	-1965
26	481	-538
28	595	584
30	1175	1142
H=	0, K=	1
30	296	331
29	146*	114
28	330	272
27	484	480
26	457	489
25	366	349
24	175*	117
23	487	-455
22	570	-558
21	924	-940
20	371	-388
19	359	-379
18	801	-804
17	64*	-62
16	224	-237
15	657	-592
14	419	-456
13	106*	17
12	116*	-249
11	1134	1211
10	1515	1606
9	870	957
8	1398	1414
7	1802	-1855
6	960	-952
5	31*	-76
4	998	951
3	423	-428
2	24*	-37
1	271	288
0	8*	0
H=	0, K=	2
0	5253	-4862
1	730	-710
2	355	324
3	1793	-1703
4	428	339
5	133	-149
6	203	167
7	15*	-15
8	633	-589
9	866	-1002
10	3340	-3375
11	17*	343
12	706	703
13	560	649
14	1642	1711
15	423	357
16	426	391
17	183	115
18	396	406
19	423	-493
20	1821	-1768
21	25*	-135
22	336	-347
23	26*	-78
24	1856	1801
25	231*	-277
26	540	554
27	113*	226
28	941	-952
29	157*	95
30	817	-877
H=	0, K=	3
29	396	-298
28	312	384
27	332	301
26	410	385
25	28*	7
24	243	244
23	783	789
22	26*	50
21	643	665
20	1265	-1299
19	378	-403
18	295	-362
17	169*	164
16	306	-239
15	589	-573
14	21*	-232
13	1119	-1119
12	527	730
11	395	-557
10	18*	339
9	417	453
8	241	74
7	1499	1502
6	525	-539
5	427	-432
4	488	-420
3	688	748
2	710	-687
1	1372	-1357
0	14*	0
H=	0, K=	4
0	2328	2349
1	896	-975
2	214	172
3	684	656
4	2512	-2382
5	1815	1744
6	1685	-1612
7	522	-543
8	1548	1512
9	227	35
10	2675	2692
11	21*	180
12	322	321
13	22*	224
14	1919	-1918
15	60*	-235
16	903	-838
17	858	-852
18	457	476
19	25*	-10
20	994	994
21	321	341
22	156*	-101
23	363	331
24	1260	-1212
25	28*	68
26	337	-370
27	173*	-203
28	613	641
H=	0, K=	5
26	459	-432
25	29*	88
24	316	244
23	194*	-227
22	68*	-127
21	198*	-175
20	263	-273
19	314	308
18	761	723
17	510	541
16	770	766
15	734	718
14	114*	-149
13	546	-530
12	455	-471
11	22*	-4
10	959	936
9	1344	1225
8	429	-382
7	655	-569
6	1336	-1306
5	530	-562
4	575	465
3	1062	1018
2	326	-251
1	361	-331
0	110*	0
H=	0, K=	6
0	2331	-2228
1	227	293
2	526	-557
3	301	-467
4	1637	1678
5	634	622
6	750	699
7	908	917
8	1211	-1216
9	586	-584
10	1533	-1609
11	588	-598
12	589	-627
13	25*	-269
14	1093	1105
15	26*	165
16	789	785
17	379	330
18	140*	-150
19	106*	91
20	451	-425
21	120*	-150
22	206*	-243
23	192*	-138
24	956	885
H=	0, K=	7
22	171*	107
21	30*	45
20	192*	-154
19	381	-405
18	124*	41
17	288	235
16	361	402
15	543	578
14	352	-291

L	FO	FC
13	466	-628
12	153*	-34
11	400	-342
10	212	-144
9	628	684
8	453	-504
7	602	575
6	966	989
5	194*	-111
4	24*	134
3	607	-728
2	212	-296
1	24*	49
0	24*	0

H= 0, K= 8

L	FO	FC
0	1265	1222
1	496	486
2	620	588
3	26*	17
4	949	-1043
5	866	-883
6	732	-737
7	385	-350
8	844	805
9	468	554
10	1002	1057
11	262	282
12	28*	18
13	272	396
14	1252	-1303
15	453	387
16	789	-749
17	565	-587
18	704	762

H= 0, K= 9

L	FO	FC
14	100*	13
13	169*	-80
12	30*	24
11	29*	-43
10	83*	-37
9	234*	318
8	177*	234
7	200	192
6	326	229
5	479	-580
4	191*	203
3	28*	200
2	28*	-50
1	49*	-43
0	125*	0

H= 0, K= 10

L	FO	FC
0	579	-570
1	30*	-67
2	206*	-188
3	465	-459
4	609	662

H= 1, K= 10

L	FO	FC
3	392	-376
2	329	291
1	624	556
0	231	214

H= 1, K= 9

L	FO	FC
0	109*	-244
1	197	88
2	836	-822
3	89*	72
4	581	-647
5	130*	-11
6	508	531
7	115*	144
8	654	706
9	180*	205
10	117*	180
11	30*	-37
12	736	-810
13	30*	166

H= 1, K= 8

L	FO	FC
18	283	-219
17	493	-441
16	220*	231
15	260	-313
14	129*	105
13	153*	145
12	243	-272
11	48*	-12
10	267	238
9	189*	203
8	188*	-7
7	71*	35
6	352	331
5	407	376
4	26*	210
3	91*	7
2	26*	-83
1	26*	-156
0	69*	-40

H= 1, K= 7

L	FO	FC
0	607	-624
1	153*	108
2	1509	1537
3	895	922
4	1288	1360
5	721	771
6	1201	-1215
7	882	-928
8	840	-845
9	784	-888
10	155*	188
11	312	-234
12	954	1033
13	27*	-126
14	680	671
15	723	728
16	788	-749
17	179*	160
18	1046	-985
19	227*	-244
20	89*	-50
21	52*	212

H= 1, K= 6

L	FO	FC
24	142*	112
23	129*	165
22	29*	86
21	291	-257
20	187*	-263
19	28*	27
18	739	-736
17	350	426
16	596	-580
15	26*	80
14	518	499
13	56*	30
12	727	785
11	169*	-8
10	68*	-22
9	270	313
8	433	505
7	109*	-32
6	162*	-255
5	646	-688
4	426	-296
3	102*	91
2	305	316
1	22*	56
0	408	-409

H= 1, K= 5

L	FO	FC
0	405	-375
1	442	-455
2	1912	-1839
3	816	839
4	652	-692
5	1385	-1415
6	1374	1401
7	141*	79
8	1740	1663
9	381	479
10	401	-449
11	341	328
12	1855	-1949
13	639	681
14	1150	-1108
15	577	-587
16	1169	1051
17	528	-629
18	427	486
19	26*	75
20	27*	-35
21	27*	267
22	728	-719
23	29*	-46
24	439	-514
25	30*	-231

H= 1, K= 4

L	FO	FC
27	127*	-121
26	372	372
25	29*	55
24	670	670
23	28*	-309
22	440	634
21	860	924
20	26*	234
19	648	640
18	25*	33
17	268	264
16	540	-598
15	573	-575
14	343	-301
13	969	-939
12	186	-127
11	211	208
10	166	170
9	562	-550
8	103*	37
7	219	-315
6	876	-768
5	681	727
4	1105	-1129
3	1066	1012
2	202	-185
1	113*	119

L	FO	FC
H=	1, K=	4
0	456	-482
H=	1, K=	3
0	848	-865
1	82*	-177
2	2580	2486
3	1113	-1098
4	1673	1624
5	550	592
6	1961	-1956
7	675	-654
8	2231	-2099
9	303	288
10	587	589
11	217	208
12	2666	2717
13	21*	-151
14	1323	1245
15	842	821
16	763	-711
17	371	-840
18	1836	-1973
19	24*	-295
20	255	-439
21	26*	199
22	1372	1362
23	27*	5
24	95*	129
25	28*	38
26	1154	-1150
27	65*	-144
28	594	-665
H=	1, K=	2
29	273	230
28	174*	-77
27	342	270
26	549	-553
25	387	438
24	193*	-63
23	240	275
22	339	-360
21	515	-567
20	154*	347
19	588	-587
18	23*	-68
17	413	-494
16	491	-475
15	743	-733
14	254	304
13	690	-635
12	540	566
11	616	596
10	1071	-1093
9	1218	1208
8	2288	-2236
7	540	-554
6	377	342
5	1893	-1909
4	3032	2984
3	653	629
2	600	-592
1	231	230
0	605	612
H=	1, K=	1
0	303	-278
1	379	390
2	5518	-5545
3	1043	1076
4	3570	-3517
5	317	-368
6	552	-509
7	506	519
8	761	743
9	981	-1020
10	169	105
11	142	172
12	468	-406
13	234	248
14	399	-353
15	202	159
16	859	832
17	22*	262
18	1385	1401
19	23*	-397
20	248	-283
21	25*	161
22	2191	-2175
23	299	319
24	326	-418
25	27*	-220
26	1248	1329
27	193*	-194
28	1077	1070
29	289	276
H=	1, K=	0
30	184*	198
28	345	355
26	219	-227
24	691	-675
22	160*	-192
20	818	-815
18	806	827
16	1102	1094
14	266	317
12	2704	2697
10	293	271
8	2137	-2137
4	265	291
6	1104	1097
2	1046	-1087
0	7*	181
H=	2, K=	0
0	5409	6007
2	1692	1624
4	2070	-1958
6	1075	-1067
8	1643	-1726
10	2473	2573
12	886	903
14	632	-690
16	168	140
18	1253	1219
20	2069	2111
22	261	276
24	1501	-1493
26	807	-797
28	328	287
H=	2, K=	1
29	30*	30
28	139*	-180
27	257	226
26	315	324
25	96*	-28
24	27*	-97
23	194*	-252
22	51*	-104
21	103*	-113
20	531	-533
19	381	-361
18	1426	-1411
17	409	-386
16	460	452
15	290	260
14	377	340
13	76*	-13
12	933	-956
11	293	256
10	289	-289
9	1780	1814
8	167	-109
7	644	682
6	1937	1905
5	309	-330
4	1140	-1132
3	1380	-1371
2	653	-723
1	854	-939
0	1449	-1379
H=	2, K=	2
0	925	-883
1	299	279
2	791	-752
3	1236	-1205
4	2932	2791
5	15*	15
6	165	104
7	941	952
8	411	-405
9	377	-392
10	2926	-2849
11	562	-584
12	169	-225
13	294	-319
14	957	981
15	440	481
16	2087	2160
17	195	208
18	414	373
19	337	-287
20	2549	-2520
21	26*	44
22	562	-509
23	27*	-78
24	1519	1559
25	28*	34
26	803	805
27	29*	84
28	833	-790
H=	2, K=	3
27	385	432
26	29*	168
25	29*	140
24	89*	-277
23	361	442
22	519	-584
21	318	319
20	220	-169
19	504	-495
18	544	549
17	294	-308
16	223	138
15	677	-601
14	423	-370

L	FO	FC
13	22*	-145
12	769	734
11	224	-142
10	744	784
9	523	466
8	1250	-1236
7	1311	1284
6	1740	-1818
5	708	-728
4	526	486
3	391	-338
2	1066	1057
1	913	-883
0	97*	-167

H= 2, K= 4

L	FO	FC
0	2137	2067
1	496	517
2	156	-198
3	794	800
4	1789	-1863
5	548	525
6	1539	-1553
7	57*	14
8	20*	124
9	465	-495
10	2413	2231
11	932	-950
12	963	976
13	597	624
14	1658	-1712
15	797	811
16	1204	-1291
17	119*	-107
18	362	408
19	203	182
20	617	596
21	27*	6
22	141*	124
23	28*	109
24	909	-929
25	29*	-259
26	597	-625

H= 2, K= 5

L	FO	FC
25	333	353
24	149*	-234
23	151*	-102
22	167*	-79
21	243	-167
20	28*	-59
19	479	471
18	148*	-116
17	26*	131
16	412	438
15	197*	270
14	940	878
13	935	-911
12	548	-530
11	653	-633
10	418	-425
9	1064	1138
8	215	-169
7	22*	-87
6	21*	128
5	529	-492
4	1145	1173
3	51*	-222
2	437	-399
1	709	829
0	825	-868

H= 2, K= 6

L	FO	FC
0	981	-1031
1	1066	-1185
2	1637	-1587
3	516	-512
4	479	492
5	604	623
6	1543	1575
7	939	825
8	247	-257
9	587	685
10	1407	-1420
11	75*	-140
12	811	-795
13	648	-688
14	1161	1134
15	698	-713
16	750	806
17	102*	-65
18	443	-450
19	106*	-111
20	1105	-1142
21	77*	-69
22	710	-707
23	30*	163

H= 2, K= 7

L	FO	FC
20	368	326
19	335	-299
18	29*	-59
17	29*	-48
16	75*	-73
15	483	500
14	777	-797
13	27*	13
12	117*	34
11	95*	-127
10	770	756
9	296	252
8	328	248
7	475	572
6	66*	71
5	448	-544
4	553	-597
3	538	-454
2	236	-278
1	685	658
0	619	-554

H= 2, K= 8

L	FO	FC
0	1178	1206
1	124*	207
2	581	655
3	207*	-299
4	874	-898
5	27*	-93
6	683	-677
7	219	-143
8	27*	117
9	135*	-97
10	440	373
11	109*	-66
12	340	387
13	399	452
14	727	-801
15	437	410
16	910	-923
17	426	-450

H= 2, K= 9

L	FO	FC
12	494	-459
11	481	-486
10	613	-539
9	214*	254
8	217*	167
7	498	495
6	387	500
5	287	-274
4	641	709
3	226	314
2	28*	45
1	69*	17
0	303	-330

H= 2, K= 10

L	FO	FC
0	627	-645
1	128*	-69

H= 3, K= 9

L	FO	FC
0	151*	88
1	90*	143
2	157*	-313
3	170*	250
4	804	-820
5	183*	104
6	167*	38
7	171*	-248
8	644	665
9	67*	-68
10	318	268
11	30*	59

H= 3, K= 8

L	FO	FC
16	205*	54
15	218*	-234
14	330	-390
13	51*	14
12	414	-370
11	314	283
10	210*	334
9	253	337
8	370	343
7	140*	-48
6	400	475
5	133*	44
4	298	-303
3	365	-364
2	707	-738
1	184*	185
0	27*	-27

H= 3, K= 7

L	FO	FC
0	1538	-1537
1	463	503
2	416	414
3	143*	-316
4	1290	1342
5	590	685
6	165*	-183
7	576	584
8	524	-528
9	662	-655
10	65*	-235
11	266	-310
12	441	413
13	28*	-32
14	517	480
15	28*	-11

L	FO	FC
H=	3, K=	7
16	852	-873
17	87*	-92
18	1138	-1128
19	30*	-87
H=	3, K=	6
22	226*	183
21	30*	47
20	470	-487
19	413	352
18	356	-323
17	206*	270
16	627	-670
15	191*	-173
14	349	273
13	26*	-67
12	1561	1584
11	662	-649
10	421	399
9	25*	-86
8	860	-907
7	571	554
6	1431	-1434
5	291	-236
4	354	358
3	247	170
2	623	566
1	23*	27
0	982	-951
H=	3, K=	5
0	220	110
1	150*	219
2	894	-784
3	83*	-75
4	2469	-2467
5	1268	-1270
6	22*	112
7	546	-499
8	2228	2344
9	241	-235
10	786	793
11	206	207
12	1838	-1816
13	1486	1448
14	810	-825
15	295	-278
16	978	1048
17	593	-598
18	660	604
19	230*	279
20	49*	95
21	160*	-171
22	1125	-1141
23	473	-440
24	789	-793
H=	3, K=	4
25	85*	94
24	179*	-151
23	430*	-420
22	28*	-194
21	333	343
20	560	-508
19	84*	55
18	190*	-217
17	89*	-129
16	478	508
15	232	-230
14	659	-688
13	427	-429
12	875	-879
11	1178	1155
10	689	714
9	201	82
8	782	817
7	776	-705
6	402	-415
5	63*	-201
4	1021	-929
3	604	625
2	346	310
1	143	-95
0	679	731
H=	3, K=	3
0	747	788
1	938	925
2	2352	2310
3	923	-960
4	870	843
5	529	537
6	220	-174
7	523	537
8	1134	-1251
9	19*	-20
10	387	-398
11	199	267
12	2190	2183
13	220	-203
14	2357	2269
15	311	313
16	297	-251
17	433	-416
18	1398	-1374
19	109*	12
20	137*	-7
21	190*	233
22	936	931
23	123*	-48
24	376	378
25	176*	115
26	769	-687
H=	3, K=	2
27	30*	-82
26	367	-404
25	86*	4
24	225	169
H=	3, K=	3
23	28*	-48
H=	3, K=	2
22	603	637
21	222	-221
20	958	964
19	456	427
18	288	-274
17	524	-491
16	753	-767
15	1136	-1163
14	629	605
13	140*	147
12	955	992
11	87*	-210
10	153	-12
9	264	-207
8	1806	-1842
7	224	199
6	270	-225
5	1380	1428
4	2834	2806
3	1268	1290
2	1457	1513
1	1331	-1286
0	3271	-3299
H=	3, K=	1
0	824	830
1	56*	58
2	1186	-1192
3	1186	1218
4	130	147
5	57*	24
6	34*	31
7	456	-466
8	1816	1848
9	340	411
10	1051	1020
11	199	174
12	2566	-2617
13	21*	56
14	1521	-1484
15	286	-330
16	1024	995
17	490	-488
18	1878	1856
19	25*	156
20	198	157
21	298	219
22	1751	-1733
23	27*	53
24	572	-591
25	28*	-25
26	424	429
27	84*	245
28	601	576
H=	3, K=	0
28	717	689
26	395	-412
24	866	-867
22	175*	208
20	278	-318
18	235	200
16	1668	1613
14	1403	-1388
H=	4, K=	0
12	307	-273
H=	3, K=	0
12	404	-433
10	440	469
8	1225	-1269
6	1030	1021
4	172	216
2	1116	-1070
0	1467	1459
H=	4, K=	0
0	854	798
2	3357	3500
4	1610	-1669
6	1854	-1863

L	FO	FC
8	1561	-1552
10	2479	2520
14	3064	-2980
16	575	-564
18	148*	-137
20	1386	1354
22	616	645
24	236	-302
26	246	-208

H= 4, K= 1

L	FO	FC
27	231	215
26	749	755
25	458	416
24	95*	145
23	108*	31
22	454	-411
21	318	302
20	476	-489
19	283	-254
18	439	-420
17	875	-917
16	1290	1301
15	292	300
14	726	792
13	521	502
12	21*	141
11	150*	196
10	615	-630
9	1180	1169
8	235	-256
7	1858	1904
6	2643	2707
5	436	-406
4	1777	1789
3	2269	-2291
2	602	-568
1	1242	-1284
0	2120	-2184

H= 4, K= 2

L	FO	FC
0	3018	-3137
1	909	892
2	1689	-1647
3	175	200
4	1531	1590
5	190	-175
6	1131	1076
7	669	668
8	786	787
9	135*	-114
10	2466	-2428
11	682	-722
12	2090	-2058
13	605	-598
14	1874	1819
15	190*	310
16	2177	2187
17	654	586
18	414	303
19	262	317
20	1150	-1122
21	108*	36
22	482	-517
23	98*	24
24	438	466
25	29*	13
26	557	568

H= 4, K= 3

L	FO	FC
25	73*	-65
24	564	-559
23	172*	235
22	162*	-121
21	117*	-12
20	439	435
19	26*	-46
18	765	-747
17	479	515
16	677	-650
15	274	-390
14	170*	-214
13	46*	94
12	137*	-82
11	1149	-1136
10	811	765
9	568	-577
8	557	-543
7	119*	-114
6	1462	-1410
5	798	784
4	947	820
3	1407	1325
2	1743	1881
1	355	-261
0	304	235

H= 4, K= 4

L	FO	FC
0	1836	1865
1	248	264
2	671	745
3	735	721
4	1057	-1112
5	723	690
6	2230	-2057
7	543	544
8	504	-543
9	366	365
10	1240	1321
11	1108	-1107
12	1414	1386
13	226	171
14	676	-568
15	212	110
16	327	-367
17	350	-299
18	185*	194
19	86*	61
20	328	298
21	28*	84
22	180*	208
23	172*	146
24	713	-727

H= 4, K= 5

L	FO	FC
23	30*	-31
22	636	-638
21	324	-360
20	175*	-78
19	28*	-52
18	28*	144
17	269	-354
16	337	348
15	64*	-75
14	1425	1432
13	196*	-282
12	132*	-112
11	24*	-30
10	1691	-1585
9	662	751
8	900	-885
7	601	570
6	869	853
5	340	-355
4	1199	1183
3	954	-884
2	1028	-1108
1	21*	-44
0	472	-430

H= 4, K= 6

L	FO	FC
0	210	-202
1	23*	30
3	837	-858
4	86*	109
5	371	-327
6	1899	1923
7	688	659
8	459	421
9	258	123
10	785	-790
11	263	179
12	605	-656
13	27*	16
14	938	923
15	321	-393
16	818	817
17	166*	162
18	390	-406
19	158*	-164
20	1152	-1154
21	449	-512

H= 4, K= 7

L	FO	FC
18	347	-324
17	338	379
16	556	-622
15	29*	-57
14	716	-653
13	174*	-165
12	178*	56
11	27*	50
10	341	337
9	186*	-219
8	487	526
7	149*	132
6	416	-359
5	115*	193
4	986	-985
3	144*	-104
2	845	916
1	418	408
0	286	264

H= 4, K= 8

L	FO	FC
0	946	967
1	359	-401
2	875	875
3	106*	-138
4	296	-362
5	517	526
6	369	-387
7	143*	-166
8	49*	-44
9	447	-403
10	316	320
11	140*	225
12	450	410
5	517	526
6	369	-387
7	143*	-166
8	49*	-44

L	FO	FC
H=	4, K=	8
9	447	-403
10	316	320
11	140*	225
12	450	410
13	143*	181
14	767	-746
H=	4, K=	9
9	349	334
8	403	479
7	458	508
6	656	636
5	202*	-67
4	625	606
3	180*	-168
2	601	-587
1	159*	-161
0	1004	-1042
H=	5, K=	9
0	611	633
1	190*	199
2	29*	-117
3	30*	83
4	992	-964
5	30*	16
6	112*	56
7	193*	-274
H=	5, K=	8
13	201*	-226
12	79*	-43
11	203*	219
10	718	763
9	186*	25
8	29*	108
7	379	-364
6	75*	-94
5	28*	-29
4	578	-560
3	164*	95
2	744	-817
1	515	552
0	320	303
H=	5, K=	7
0	830	-816
1	311	320
2	198*	334
3	223	-255
4	762	712
5	444	376
6	200	101
7	100*	196
8	342	-338
9	598	-647
10	183*	-268
11	101*	-33
13	29*	71
14	749	692
15	29*	6
16	524	-550
17	30*	-4
H=	5, K=	6
19	30*	102
18	703	-697
17	65*	18
16	29*	-190
15	189*	-166
14	295	241
13	27*	-73
12	997	1051
11	205	-76
10	549	489
9	68*	-125
8	967	-913
7	185*	150
6	1079	-1069
5	224	249
4	1217	1206
3	124*	-75
2	469	544
1	1048	-1091
0	1610	-1622
H=	5, K=	5
0	1547	1515
1	604	582
2	523	-584
3	602	591
4	1959	-1945
5	23*	98
6	112*	-87
7	24*	36
8	1952	1861
9	81*	-4
10	823	816
11	128*	62
12	575	-555
13	198*	193
14	830	-880
15	685	-680
16	227	250
17	28*	51
18	532	558
19	352	396
20	88*	54
21	30*	112
H=	5, K=	4
23	162*	-66
22	349	-300
21	230	224
20	467	423
19	160*	11
18	705	755
17	506	496
16	493	505
15	143*	-3
14	745	-773
13	25*	8
12	891	-889
11	492	392
10	712	706
9	1042	-913
8	806	800
7	136*	-154
6	22*	-8
5	21*	-120
4	609	-595
3	137*	-120
2	212	214
1	1004	1009
0	1577	1478
H=	5, K=	3
0	954	-935
1	876	922
2	1911	1873
3	336	-378
4	651	736
5	412	-358
6	117	-210
7	693	-738
8	2154	-2150
9	392	-374
10	854	-868
11	631	620
12	945	954
13	304	296
14	1056	1142
15	491	513
16	308	216
17	107*	123
18	189*	125
19	141*	215
20	28*	-69
21	162*	-226
22	355	354
23	560	-473
24	532	537
H=	5, K=	2
25	183*	218
24	441	419
23	229	188
22	423	449
21	78*	16
20	372	407
19	693	689
18	1311	-1321
17	394	-479
16	504	-510
15	1108	-966
14	966	955
13	23*	-98
12	205	-197
11	22*	76
10	678	-596
9	273	238
8	1506	-1571
7	1238	1252
6	600	-612
5	1894	1961
4	1701	1747
3	525	-569
2	1635	1713
1	1648	-1703
0	1040	-1016
H=	5, K=	1
0	2392	2456
1	659	-635
2	1955	-2009
3	179	-205
4	3004	-3038
5	287	249
6	936	-956
7	439	458
8	2152	2245
9	210	210
10	286	284
11	364	346
12	1902	-1962
13	193*	283
14	1155	-1087
15	1282	-1274

L	FO	FC
16	369	303
17	569	-549
18	1441	1417
19	639	619
20	924	863
21	119*	52
22	422	-383
23	29*	-28
24	473	-423
25	238	248
26	136*	-33

H= 5, K= 0

L	FO	FC
26	182*	-203
24	897	-849
22	28*	86
20	669	630
18	1264	1301
16	24*	90
14	616	-677
12	816	-786
10	1021	1031
8	2670	2734
6	780	812
4	2294	-2332
2	266	-264
0	3221	-3345

H= 6, K= 0

L	FO	FC
0	1253	1251
2	2062	2184
4	589	-586
6	548	-553
8	1192	-1173
10	429	438
12	455	520
14	1214	-1252
16	1262	-1291
18	672	-629
20	523	528
22	416	375
24	30*	-12

H= 6, K= 1

L	FO	FC
24	95*	-24
23	29*	92
22	365	-342
21	166*	-188
20	729	-700
19	330	-355
18	274	271
17	323	-355
16	1671	1659
15	271	198
14	283	-226
13	402	462
12	1658	-1712
11	165	-213
10	1693	-1655
9	21*	57
8	123*	13
7	915	921
6	2472	2453
5	114*	-109
4	616	673
3	882	-926
2	2016	-2019
1	17*	-161
0	1064	-1093

H= 6, K= 2

L	FO	FC
0	1272	-1301
1	794	-832
2	2260	-2333
3	1327	1376
4	685	693
5	643	601
6	1393	1384
7	69*	-61
8	973	956
9	509	-536
10	1988	-1921
11	253	-201
12	1307	-1262
13	1018	-1041
14	882	863
15	560	-624
16	583	602
17	901	981
18	550	563
19	320	220
20	156*	-128
21	217	271
22	491	-509
23	287	283
24	212*	183

H= 6, K= 3

L	FO	FC
23	630	604
22	597	600
21	142*	-214
20	625	602
19	218	-304
18	224	166
17	526	512
16	982	-917
15	479	-392
14	25*	60
13	168*	-216
12	1460	1485
11	230	-145
10	204	186
9	499	-543
8	367	-368
7	768	812
6	811	-899
5	980	997
4	190	237
3	748	708
2	1558	1547
1	425	-418
0	1326	1417

H= 6, K= 4

L	FO	FC
0	1174	1200
1	413	-420
2	1570	1485
3	22*	17
4	777	-769
5	247	192
6	1093	-1153
7	766	-780
8	285	-278
9	922	933
10	615	635
11	766	762
12	774	758
13	307	259
14	424	373
15	27*	34
16	81*	74
17	330	-299
18	102*	-176
19	330	-317
20	105*	124
21	295	-323
22	332	313

H= 6, K= 5

L	FO	FC
20	599	-590
19	170*	171
18	487	467
17	190*	41
16	808	786
15	209*	226
14	661	679
13	511	-483
12	623	-623
11	417	-422
10	1201	-1145
9	118*	-102
8	182*	-185
7	112*	-71
6	1040	1082
5	722	762
4	510	429
3	52*	-4
2	1814	-1763
1	664	-634
0	231	-190

H= 6, K= 6

L	FO	FC
0	640	-605
1	167*	132
2	1207	-1218
3	143*	-19
4	25*	-15
5	195	14
6	694	743
7	416	433
8	521	542
9	125*	-73
10	202*	-153
11	152*	-108
12	1008	-991
13	28*	-84
14	461	496
15	41*	-164
16	1297	1254
17	176*	152
18	223*	-159

H= 6, K= 7

L	FO	FC
15	184*	-100
14	182*	-257
13	29*	18
12	752	784
11	301	229
10	178*	219
9	304	-209
8	372	-313
7	181*	145
6	416	-439
5	483	429
4	407	-387
3	27*	35
2	868	809
1	673	-630
0	1001	989

H= 6, K= 8

L	FO	FC
H=	6, K=	8
0	350	411
1	152*	137
2	573	600
3	28*	44
4	370	-348
5	239	121
6	856	-844
7	522	-500
8	202*	97
9	359	-315
10	195*	249
11	161*	271
H=	6, K=	9
5	137*	-106
4	30*	136
3	198*	-180
2	516	-654
1	234*	-335
0	750	-763
H=	7, K=	9
0	577	614
1	110*	184
H=	7, K=	8
9	146*	23
8	297	332
7	585	-589
6	590	-636
5	29*	-86
4	953	-958
3	330	332
2	183*	-157
1	359	411
0	737	730
H=	7, K=	7
0	276	183
1	454	476
2	384	384
3	617	650
4	295	385
5	454	485
6	352	258
7	232	191
8	370	-264
9	345	-253
10	555	-570
11	30*	-74
12	189*	230
13	297	-306
H=	7, K=	6
16	30*	-65
15	261	319
14	1153	1144
13	29*	9
12	543	545
11	489	-513
10	639	-634
9	368	-348
8	622	-659
7	299	-274
6	290	-285
5	141*	28
4	1160	1200
3	45*	-74
2	754	785
1	25*	-7
0	1329	-1371
H=	7, K=	5
0	548	617
1	119*	77
2	921	-903
3	379	405
4	920	-900
5	669	-644
6	401	-354
7	25*	-110
8	300	344
9	664	602
10	1046	1037
11	27*	-57
12	94*	161
13	251	-216
14	786	-827
15	57*	-120
16	127*	13
17	30*	-86
18	636	618
19	101*	165
H=	7, K=	4
20	875	822
19	326	-361
18	919	865
17	264	-230
16	151*	-128
15	165*	-137
14	1089	-1111
13	580	-627
12	476	-486
11	451	527
10	1178	1231
9	552	487
8	1236	1206
7	604	594
6	673	-669
5	247	163
4	1690	-1676
3	616	-616
2	22*	-81
1	349	-352
0	1096	1167
H=	7, K=	3
0	925	-972
1	1075	1048
2	1126	1099
3	342	390
4	847	814
5	22*	94
6	98*	-80
7	736	-731
8	1013	-1053
9	415	-506
10	701	-683
11	254	212
12	174*	96
13	243	-138
14	232	-186
15	424	416
16	201*	185
17	558	595
18	263	-254
19	237	212
20	344	-348
21	155*	-47
22	279	328
H=	7, K=	2
22	366	331
21	29*	-107
20	182*	-173
19	162*	79
18	780	-815
17	184*	-183
16	145*	192
15	26*	4
14	1661	1637
13	117*	13
12	151*	-135
11	24*	-155
10	1170	-1209
9	417	520
8	779	-798
7	403	311
6	555	525
5	414	440
4	1800	1847
3	148*	148
2	1236	1254
1	756	-781
0	999	-1040
H=	7, K=	1
0	864	879
1	647	-633
2	230	112
3	853	-862
4	735	-700
5	782	775
6	766	-749
7	22*	-195
8	345	290
9	304	-284
10	480	500
11	895	916
12	952	-1000
13	192*	117
14	678	-653
15	1250	-1148
16	83*	-77
17	165*	-207
18	753	734
19	382	377
20	662	686
21	199*	-252
22	246	-245
23	30*	18
H=	7, K=	0
22	345	-307
20	388	376
18	1518	1511
16	904	-936
14	2613	-2607
12	679	-667
10	1129	1073
8	1883	1949
6	613	-601
4	2493	-2711
2	1378	-1404
0	1299	1284

L	FO	FC
H=	8, K=	0
0	172	-280
2	590	628
4	695	705
6	1135	1086
8	46*	74
10	485	-481
12	1122	1095
14	597	-535
16	905	-936
18	339	-370
20	474	494
22	689	671
H=	8, K=	1
21	316	-295
20	765	-736
19	478	-449
18	113*	110
17	364	296
16	1558	1557
15	256	280
14	400	-332
13	289	-336
12	1518	-1562
11	311	270
10	910	-902
9	103*	-161
8	1259	1325
7	217	-146
6	2311	2218
5	170	142
4	811	-804
3	240	-227
2	1818	-1810
1	746	-778
H=	8, K=	2
0	252	276
1	406	-361
2	838	-848
3	447	378
4	140*	-114
5	221	-158
6	388	394
7	318	-410
8	24*	44
9	195	203
10	492	-462
11	205	212
12	133*	-105
13	591	-616
14	688	641
15	295	-277
16	367	400
17	221	197
18	186*	109
19	124*	-97
20	479	-492
21	113*	220
H=	8, K=	3
20	678	604
19	440	-433
18	256	-230
17	29*	72
16	942	-950
15	161*	136
14	27*	2
13	381	372
12	1237	1210
11	26*	-100
10	519	500
9	311	-306
8	1212	-1262
7	125*	-227
6	1810	-1814
5	474	501
4	23*	158
3	571	540
2	1416	1417
1	307	-361
0	167*	245
H=	8, K=	4
0	108*	205
1	450	-529
2	24*	24
3	374	430
4	433	-449
5	100*	37
6	390	-376
7	538	-533
8	703	-696
9	367	377
10	652	-633
11	213	187
12	799	801
13	87*	-10
14	370	375
15	28*	-44
16	297	-339
17	138*	-194
18	30*	-36
19	180*	-187
H=	8, K=	5
17	86*	-153
16	1091	1077
15	29*	-176
14	29*	-21
13	890	-897
12	1344	-1273
11	480	-452
10	747	-804
9	268	227
8	422	521
7	860	905
6	1279	1263
5	1134	1138
4	134*	137
3	150*	216
2	1545	-1533
1	309	-299
0	255	193
H=	8, K=	6
0	82*	-81
1	476	-477
2	201*	-97
3	46*	-11
4	304	-387
5	234	-263
6	367	267
7	27*	75
8	603	708
9	323	290
10	28*	-199
11	108*	144
12	1171	-1108
13	239	233
14	137*	145
15	118*	44
H=	8, K=	7
11	30*	-143
10	421	422
9	382	-417
8	929	-977
7	96*	-159
6	863	-863
5	338	350
4	247	123
3	317	376
2	989	1058
1	651	-643
0	708	723
H=	8, K=	8
0	223	231
1	650	644
2	484	500
3	530	443
4	123*	-214
5	30*	-29
6	537	-486
7	315	-318
H=	9, K=	8
4	1419	-1401
3	168*	200
2	170*	-123
1	642	656
0	1255	1319
H=	9, K=	7
0	120*	-16
1	223*	242
2	296	-205
3	237	198
4	305	370
5	77*	37
6	29*	147
7	359	378
8	108*	-212
9	148*	139
H=	9, K=	6
13	222*	-140
12	370	345
11	871	-831
10	1315	-1322
9	148*	-15
8	799	-750
7	269	247
6	476	417
5	247	186
4	626	662
3	187*	152
2	138*	99
1	137*	-145
0	793	-854
H=	9, K=	5
0	204	-245
1	329	309
2	26*	-24

L	FO	FC
H=	9, K=	5
3	826	825
4	189*	-13
5	213	-180
6	377	-347
7	454	-414
8	162*	-83
9	324	246
10	897	932
11	483	-493
12	112*	18
13	481	-467
14	622	-597
15	135*	-45
H=	9, K=	4
17	324	-333
16	529	-465
15	29*	-42
14	1277	-1267
13	106*	-102
12	451	-388
11	630	610
10	1010	1049
9	561	577
8	1341	1317
7	26*	-136
6	799	-775
5	879	-824
4	1885	-1942
3	685	-743
2	628	722
1	540	561
0	2059	2091
H=	9, K=	3
0	915	-824
1	23*	149
2	111*	109
3	613	-643
4	182*	208
5	161*	-191
6	379	418
7	146*	-200
8	120*	-115
9	191*	199
10	288	-326
11	385	461
12	27*	133
13	190*	-232
14	211*	267
15	28*	99
16	243	-183
17	29*	163
18	431	-421
H=	9, K=	2
19	173*	-253
18	792	-758
17	303	-270
16	212*	243
15	333	342
14	604	595
13	38*	-60
12	192*	235
11	150*	-150
10	426	-421
9	987	918
8	1020	-992
7	379	431
6	768	786
5	407	-491
4	1857	1825
3	85*	-114
2	350	-350
1	739	-788
0	1591	-1579
H=	9, K=	1
0	1127	1112
1	22*	-64
2	204	200
3	376	380
4	173*	279
5	366	345
6	530	-605
7	463	-426
8	560	-576
9	24*	47
10	25*	116
11	95*	135
12	758	-829
13	26*	-98
14	500	-517
15	122*	-72
16	180*	196
17	28*	195
18	497	468
19	29*	-70
20	546	533
H=	9, K=	0
20	345	404
18	1571	1559
16	299	-324
14	1553	-1593
12	183	-102
10	1025	1080
8	1390	1404
6	908	-946
4	2248	-2372
2	68*	100
0	2151	2248
H=	10, K=	0
0	289	319
2	107*	-14
4	792	769
6	108*	183
8	728	-659
10	324	284
12	331	396
14	28*	4
16	297	-187
18	495	-515
H=	10, K=	1
18	576	584
17	197*	231
16	1339	1352
15	523	465
14	130*	-94
13	179*	-263
12	615	-606
11	272	278
10	241	-163
9	108*	52
8	700	700
7	1259	-1327
6	1117	1128
5	346	-293
4	734	-723
3	817	827
2	1224	-1317
1	234	-196
0	575	-507
H=	10, K=	2
0	174*	181
1	363	307
2	349	-367
3	24*	27
4	319	-286
5	482	-490
6	376	363
7	25*	69
8	45*	-34
9	225	-124
10	274	-316
11	167*	-23
12	198*	200
13	328	305
14	402	373
15	65*	55
16	291	309
17	211	-119
H=	10, K=	3
16	1000	-971
15	29*	-70
14	29*	85
13	166*	107
12	510	464
11	344	-298
10	550	556
9	60*	-94
8	531	-457
7	425	558
6	1526	-1519
5	486	432
4	582	596
3	618	685
2	2012	2016
1	450	-429
0	24*	86
H=	10, K=	4
0	352	-400
1	883	-829
2	444	-449
3	26*	-145
4	164*	-199
5	230	250
6	27*	30
7	194	199
8	565	-574
9	615	585
10	268	-306
11	139*	182
12	531	515
13	29*	63
14	30*	104
15	213*	-259
H=	10, K=	5
13	323	-270
12	1373	-1347
11	178*	-274

L	FO	FC
10	385	-391
9	499	521
8	984	907
7	556	566
6	726	769
5	72*	177
4	27*	-101
3	326	-403
2	980	-925
1	293	-188
0	26*	29

H= 10, K= 6

L	FO	FC
0	410	515
1	151*	158
2	133*	-194
3	28*	94
4	316	-224
5	427	-465
6	246	296
7	195*	175
8	102*	-114
9	181*	-210
10	255	-291

H= 10, K= 7

L	FO	FC
6	940	-948
5	440	503
4	298	317
3	455	424
2	1313	1336
1	236	-167
0	158*	215

H= 11, K= 7

L	FO	FC
0	243	-201
1	123*	257
2	327	-298
3	269	131

H= 11, K= 6

L	FO	FC
7	242	219
6	619	598
5	191*	191
4	673	678
3	328	-310
2	311	-267
1	234	-195
0	487	-508

H= 11, K= 5

L	FO	FC
0	61*	-157
1	72*	83
2	254	-186
3	28*	-56
4	196*	-136
5	90*	-91
6	332	355
7	379	344
8	109*	-7
9	308	329
10	134*	-13
11	30*	-114

H= 11, K= 4

L	FO	FC
13	139*	-10
12	321	304
11	138*	170
10	1204	1194
9	29*	-198
8	665	658
7	187*	201
6	386	-363
5	376	-433
4	1305	-1320
3	27*	-44
2	212	-24
1	864	841
0	1452	1493

H= 11, K= 3

L	FO	FC
0	107*	78
1	80*	123
2	581	574
3	396	-419
4	79*	206
5	322	-270
6	142*	-73
7	27*	-82
8	245	277
9	153*	157
10	371	-332
11	81*	-3
12	140*	58
13	233	179
14	268	153

H= 11, K= 2

L	FO	FC
15	300	308
14	800	770
13	495	508
12	223	-219
11	174*	131
10	235	-188
9	694	694
8	521	-505
7	260	-228
6	225	177
5	1154	-1133
4	1105	1125
3	963	-999
2	620	-619
1	35*	-64
0	1581	-1615

H= 11, K= 1

L	FO	FC
0	493	470
1	373	393
2	25*	-114
3	349	313
4	245	-182
5	604	-613
6	144*	-31
7	26*	92
8	127*	64
9	393	398
10	312	282
11	511	-497
12	152*	-23
13	29*	-166
14	322	253
15	481	427
16	30*	-149

H= 11, K= 0

L	FO	FC
16	480	-457
14	1137	-1123
12	146*	158
10	963	949
8	643	669
6	696	-786
4	1136	-1078
2	741	714
0	1619	1665

H= 12, K= 0

L	FO	FC
0	80*	107
2	26*	-88
4	235	-221
6	155*	-196
8	28*	-41
10	201*	-225
12	417	-365
14	381	315

H= 12, K= 1

L	FO	FC
14	865	-869
13	155*	141
12	672	-677
11	321	-266
10	178*	41
9	328	-333
8	647	668
7	511	-522
6	656	629
5	182*	-212
4	1015	-975
3	830	861
2	1018	-994
1	799	785
0	208	-115

H= 12, K= 2

L	FO	FC
0	540	-488
1	202	221
2	26*	-107
3	345	-349
4	444	447
5	235	-185
6	27*	72
7	375	389
8	312	-265
9	293	-236
10	376	415
11	83*	2
12	504	504
13	359	389

H= 12, K= 3

L	FO	FC
12	1017	1003
11	187*	112
10	142*	-3
9	29*	151
8	649	-685
7	664	684
6	774	-760
5	28*	-79
4	716	627
3	67*	62
2	1189	1189
1	445	-324
0	270	242

H= 12, K= 4

L	FO	FC
0	154*	150

L	FO	FC
H= 12, K= 4		
1	250	115
2	266	-240
3	424	-391
4	419	-438
5	137*	-69
6	198*	-125
7	272	-201
8	29*	-26
9	182*	-42
10	148*	-201
H= 12, K= 5		
8	932	968
7	30*	-40
6	636	613
5	29*	226
4	314	-285
3	164*	-143
2	484	-445
1	117*	-49
0	57*	14
H= 12, K= 6		
0	248	170
1	451	-432
2	116*	-69
3	239	-111
4	514	546
H= 13, K= 6		
0	557	-571
H= 13, K= 5		
0	303	-316
1	238	-97
2	494	-458
3	496	-530
4	30*	58
H= 13, K= 4		
7	176*	-65
6	1052	-1041
5	30*	46
4	704	-677
3	219	-105
2	256	252
1	29*	126
0	697	690
H= 13, K= 3		
0	623	620
1	275	328
2	586	624
3	380	-356
4	169*	-213
5	180*	95
6	382	-371
7	129*	190
8	528	491
9	186*	-115
H= 13, K= 2		
10	813	-814
9	30*	97
8	66*	95
7	428	-395
6	1224	1175
5	370	-335
4	785	819
3	312	-317
2	586	-619
1	195*	97
0	848	-876
H= 13, K= 1		
0	27*	90
1	703	666
2	298	-344
3	184*	-165
4	502	512
5	517	-480
6	658	606
7	391	365
8	349	-416
9	29*	30
10	589	-508
11	526	-468
H= 13, K= 0		
10	841	798
8	29*	64
6	1515	-1491
4	793	-824
2	132*	285
0	562	482
H= 14, K= 0		
0	28*	128
2	733	-720
4	689	-691
6	596	607
8	599	615
H= 14, K= 1		
8	1167	1132
7	94*	-92
6	418	436
5	354	292
4	1175	-1171
3	29*	53
2	637	-626
1	430	452
0	292	272
H= 14, K= 2		
0	660	-688
1	197*	33
2	763	790
3	126*	-184
4	572	525
5	78*	22
6	982	-923
7	30*	128
H= 14, K= 3		
6	289	-251
5	73*	58
4	1155	1145
3	220*	217
2	836	820
1	187*	-191
0	627	-588
H= 14, K= 4		
0	352	339
1	441	395
2	313	-381
3	138*	72
4	442	-412
H= 14, K= 5		
0	579	563
H= 15, K= 3		
0	917	909
1	195*	205
2	306	349
H= 15, K= 2		
4	280	-263
3	100*	-42
2	1303	-1283
1	273	-332
0	880	-826
H= 15, K= 1		
0	1088	-1036
1	72*	59
2	553	-546
3	284	-309
4	615	666
5	86*	89
H= 15, K= 0		
4	524	-529
2	838	833
0	410	433
H= 16, K= 0		
0	117*	-12
H= 16, K= 1		
0	578	573
H= 1, K= 0		
-28	135*	194
-26	456	-506
-24	1276	-1242
-22	344	-422
-20	682	661
-18	385	-349
-16	389	-409
-14	2049	2029
-12	1372	1385
-10	1374	-1375
-8	2504	-2558
-6	441	-431
-4	692	653
-2	1288	1244
H= 1, K= 1		
-1	354	306
-2	5781	5661
-3	302	322
-4	3065	2854

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-5	61*	28	-5	348	-390	-13	137*	32	-16	496	538
-6	2862	-2628	-4	2053	-1962	-12	947	943	-15	26*	-83
-7	1172	1161	-3	248	-308	-11	88*	-82	-14	25*	6
-8	2106	-2063	-2	1024	955	-10	613	-566	-13	240	316
-9	1168	-1210	-1	65*	97	-9	884	881	-12	491	-496
-10	979	911				-8	804	-807	-11	24*	-9
-11	323	-274	H=	1, K=	3	-7	266	-248	-10	311	-304
-12	1079	1063				-6	1149	1134	-9	348	-440
-13	449	474	-1	1980	-1942	-5	446	-457	-8	737	795
-14	345	-338	-2	311	-319	-4	1317	1298	-7	143*	-2
-15	107*	135	-3	1332	-1225	-3	594	506	-6	447	439
-16	407	-432	-4	812	-723	-2	17*	-193	-5	541	517
-17	162	109	-5	1438	1387	-1	336	-296	-4	182	-256
-18	746	-690	-6	3937	3897				-3	118*	-142
-19	22*	60	-7	571	579	H=	1, K=	5	-2	22*	141
-20	1023	967	-8	3394	3298				-1	149*	-251
-21	154*	21	-9	150	-153	-1	490	-467			
-22	1775	1781	-10	330	-374	-2	2543	2433	H=	1, K=	7
-23	227	161	-11	325	343	-3	1915	1739			
-24	26*	115	-12	3737	-3590	-4	435	471	-1	752	-738
-25	306	-317	-13	447	418	-5	347	-301	-2	1583	-1551
-26	1040	-1052	-14	315	244	-6	2100	-2153	-3	602	644
-27	330	-408	-15	21*	89	-7	547	-503	-4	985	-968
-28	863	-841	-16	2054	2075	-8	1325	-1346	-5	1000	931
-29	92*	215	-17	843	-829	-9	81*	-101	-6	1576	1504
-30	663	642	-18	849	908	-10	96*	192	-7	1646	-1672
-31	285	293	-19	877	-903	-11	141*	23	-8	1502	1522
			-20	69*	59	-12	1359	1269	-9	851	-806
H=	1, K=	2	-21	25*	64	-13	286	-315	-10	560	-522
			-22	1350	-1388	-14	282	317	-11	432	416
-30	30*	42	-23	183*	166	-15	131*	-217	-12	1714	-1735
-29	173*	-59	-24	283	-274	-16	1025	-1000	-13	177*	207
-28	91*	-100	-25	395	434	-17	914	952	-14	432	-458
-27	28*	-35	-26	853	897	-18	655	-675	-15	625	649
-26	325	296	-27	29*	-18	-19	201*	208	-16	1008	1029
-25	568	-547	-28	376	345	-20	515	540	-17	28*	2
-24	639	595	-29	186*	56	-21	27*	-13	-18	452	461
-23	824	-804				-22	901	927	-19	524	-530
-22	907	-882	H=	1, K=	4	-23	28*	74	-20	543	-498
-21	221	242				-24	137*	112	-21	111*	105
-20	252	-215	-28	459	-484	-25	598	-603	-22	683	-741
-19	100*	-8	-27	190*	185	-26	801	-832			
-18	207	-240	-26	103*	-10	-27	184*	-237	H=	1, K=	8
-17	272	-402	-25	250	-209						
-16	313	-287	-24	178*	201	H=	1, K=	6	-19	216*	240
-15	1171	1179	-23	179*	174				-18	965	-981
-14	779	803	-22	812	815	-25	374	457	-17	490	420
-13	294	295	-21	342	-363	-24	66*	79	-16	278	-264
-12	699	-749	-20	747	695	-23	29*	87	-15	342	-282
-11	176	-213	-19	298	-366	-22	523	500	-14	609	636
-10	171	-128	-18	308	-167	-21	63*	93	-13	335	-369
-9	898	-856	-17	214	-194	-20	300	-293	-12	131*	158
-8	1026	981	-16	474	-477	-19	191*	105	-11	154*	139
-7	582	-582	-15	111*	-148	-18	93*	-55	-10	324	343
-6	141	143	-14	288	-327	-17	659	-571	-9	118*	48

L	FO	FC
H= 1, K= 8		
-8	384	-441
-7	595	498
-6	309	-345
-5	26*	132
-4	209*	271
-3	698	-666
-2	757	-773
-1	316	244
H= 1, K= 9		
-1	28*	175
-2	324	330
-3	28*	-15
-4	432	476
-5	311	-345
-6	594	-595
-7	220*	-210
-8	528	-545
-9	370	395
-10	484	486
-11	195*	136
-12	780	810
-13	123*	-84
-14	196*	137
H= 1, K= 10		
-5	169*	-44
-4	30*	-78
-3	163*	-65
-2	218	40
-1	30*	-102
H= 2, K= 10		
-1	382	439
-2	142*	-97
-3	568	554
-4	626	612
H= 2, K= 9		
-14	476	471
-14	476	471
-13	137*	149
-12	287	302
-11	371	319
-10	198*	-54
-9	284	253
-8	178*	-220
-7	175*	239
-6	202*	-205
-5	609	-631
-4	170*	-128
-2	113*	-30
-1	201	-112
H= 2, K= 8		
-1	210	-153
-2	401	371
-3	418	-398
-4	1332	-1278
-5	566	605
-6	1023	-1013
-7	570	532
-8	514	510
-9	380	-275
-10	1015	1058
-11	226	-346
-12	28*	-151
-13	318	-281
-14	1536	-1576
-15	334	-348
-16	29*	-128
-17	258	110
-18	1176	1220
-19	67*	84
H= 2, K= 7		
-23	411	-414
-22	293	255
-21	491	-532
-20	722	735
-19	432	-455
-18	305	343
-17	481	468
-16	806	-845
-15	193*	227
-14	676	-691
-13	188*	-271
-12	188*	-201
-11	321	357
-10	650	591
-9	25*	-119
-8	808	831
-7	165*	44
-6	384	-329
-5	825	857
-4	25*	128
-3	386	-409
-2	331	-381
-1	623	-599
H= 2, K= 6		
-1	877	-865
-2	214	279
-3	323	359
-4	2317	2222
-5	260	336
-6	1326	1343
-7	270	-361
-8	802	-776
-9	376	428
-10	1102	-1100
-11	142*	162
-12	24*	-6
-13	25*	8
-14	955	936
-15	232	-262
-16	597	623
-17	316	-256
-18	273	-242
-19	611	549
-20	306	-295
-21	350	307
-22	235	310
-23	174*	103
-24	843	895
-25	156*	-106
H= 2, K= 5		
-27	498	-505
-26	167*	170
-25	249	-226
-24	28*	-210
-23	150*	183
-22	655	689
-21	120*	-124
-20	26*	-17
-19	688	693
-18	802	-882
-17	459	463
-16	525	630
-15	640	-679
-14	408	470
-13	574	-490
-12	282	-348
-11	333	311
-10	968	-903
-9	190	240
-8	167*	211
-7	865	-824
-6	841	749
-5	833	821
-4	96*	161
-3	293	347
-2	217	215
-1	573	-672
H= 2, K= 4		
-1	158	-151
-2	926	914
-3	987	-954
-4	2431	-2247
-5	472	-449
-6	1159	-1261
-7	683	635
-8	1757	1753
-9	466	415
-10	2246	2214
-11	262	234
-12	1089	-1091
-13	222	-202
-14	2648	-2573
-15	560	569
-16	780	-749
-17	607	647
-18	1501	1461
-19	1084	-1132
-20	1508	1510
-21	437	-371
-22	214*	-370
-23	200*	-230
-24	1309	-1367
-25	176*	-112
-26	224	115
-27	327	303
-28	838*	833
-29	30*	57
H= 2, K= 3		
-30	291	289
-29	150*	-161
-28	289	267
-27	423	413
-26	280	-265
-25	204*	-276
-24	1502	-1463
-23	26*	171
-22	626	-635
-21	126*	-47
-20	930	934
-19	306	-287
-18	599	627
-17	669	718
-16	84*	-144
-15	150*	83
-14	452	-470
-13	394	-422
-12	95*	-97
-11	265	269

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-10	1549	1568	-23	177*	-170	-10	1269	1299	-18	22*	107
-9	409	391	-22	847	837	-8	170	174	-17	550	-568
-8	29*	-80	-21	369	-362	-6	698	-714	-16	888	802
-7	506	-485	-20	476	-524	-4	320	-361	-15	439	428
-6	1955	-1830	-19	172	130	-2	1589	1697	-14	121*	16
-5	436	-447	-18	806	-826				-13	488	476
-4	547	543	-17	698	-687	H=	3, K=	1	-12	1981	-1989
-3	519	542	-16	845	839				-11	350	389
-2	962	895	-15	565	-555	-1	943	-963	-10	896	-909
-1	515	487	-14	424	-413	-2	3678	3458	-9	240	209
			-13	330	300	-3	397	-425	-8	2583	2564
H=	2, K=	2	-12	863	-868	-4	752	-672	-7	242	-248
			-11	494	464	-5	1101	1144	-6	1071	-1092
-1	797	-781	-10	500	-496	-6	329	-303	-5	1466	-1356
-2	2293	2145	-9	1421	1407	-7	1050	1006	-4	969	-976
-3	1571	1496	-8	1119	1106	-8	1363	-1373	-3	1340	-1301
-4	348	328	-7	313	-316	-9	1072	-1057	-2	408	446
-5	949	900	-6	425	427	-10	1799	1778	-1	724	-760
-6	1068	1010	-5	628	-682	-11	1208	-1188			
-7	196	204	-4	3392	3259	-12	2616	2630	H=	3, K=	3
-8	1727	-1726	-3	121	-89	-13	309	-322			
-9	546	543	-2	272	289	-14	552	-603	-1	1692	-1685
-10	3323	-3319	-1	57*	-47	-15	249	225	-2	1529	-1474
-11	17*	13				-16	1027	-1040	-3	974	-987
-12	784	819	H=	2, K=	0	-17	153*	-171	-4	1262	1311
-13	309	-331				-18	1568	-1542	-5	1739	1689
-14	2953	3000	-2	870	-540	-19	178	81	-6	1203	1071
-15	659	-696	-4	5124	-5151	-20	1145	1106	-7	180	208
-16	425	408	-6	4199	-4122	-21	730	748	-8	720	665
-17	262	-251	-8	1524	1554	-22	2242	2320	-9	743	-691
-18	1030	-998	-10	2262	2310	-23	218	232	-10	2622	-2508
-19	278	282	-12	1891	-1909	-24	221	-166	-11	253	148
-20	1027	-1034	-14	784	-760	-25	301	-280	-12	3963	-4017
-21	245	163	-16	306	-341	-26	717	-781	-13	140*	256
-22	110*	42	-18	1065	1085	-27	27*	-87	-14	245	197
-23	335	382	-20	2119	2129	-28	410	-437	-15	382	375
-24	843	864	-22	1265	-1252	-29	133*	39	-16	2234	2246
-25	145*	119	-24	1909	-1935	-30	315	299	-17	591	-534
-26	133*	206	-26	103*	-171	-31	173*	-146	-18	846	831
-27	319	-329	-28	592	547				-19	402	-409
-28	509	-536	-30	680	707	H=	3, K=	2	-20	1436	-1479
-29	116*	127							-21	246	-194
-30	693	-736	H=	3, K=	0	-31	52*	-66	-22	1284	-1309
-31	176*	39				-30	518	-511	-23	26*	32
			-32	1152	1153	-29	168*	-148			
H=	2, K=	1	-30	721	694	-28	74*	103	H=	1, K=	0
			-28	147*	99	-27	285	343			
-31	141*	-98	-26	88*	-159	-26	511	524	-30	339	364
-30	29*	-244	-24	914	-850	-25	118*	121			
-29	29*	-113	-22	1319	1335	-24	557	505	H=	3, K=	3
-28	571	-524	-20	917	890	-23	271	-251			
-27	414	430	-18	1955	-1940	-22	948	-958	-24	473	451
-26	807	-838	-16	137	-99	-21	24*	55	-25	425	389
-25	638	672	-14	173	229	-20	725	-690	-26	606	599
-24	337	337	-12	458	-458	-19	717	-677	-27	348	-334

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	3, K=	3	-16	390	-363	-11	227	-179	-14	485	495
			-17	1016	1065	-12	1408	-1407	-13	465	505
-28	228	241	-18	544	-578	-13	385	241	-12	381	386
-29	135*	-75	-19	191*	107	-14	600	-621	-11	357	428
-30	256	-300	-20	349	348	-15	377	448	-10	51*	-81
			-21	866	-835	-16	1156	1140			
H=	3, K=	4	-22	1186	1145	-17	219*	142	H=	4, K=	6
			-23	161*	84	-18	229	197			
-29	463	417	-24	562	-533	-19	81*	-9	-9	112*	-25
-28	767	-774	-25	29*	-93	-20	785	-797			
-27	400	368	-26	1465	-1478	-21	285	-219	H=	4, K=	9
-26	698	-636	-27	250	-190	-22	94*	-318			
-25	289	-242	-28	177*	-67	-23	128*	272	-8	523	-521
-24	344	-342							-7	71*	-28
-23	378	-364	H=	3, K=	6	H=	3, K=	8	-6	293	270
-22	1192	1211							-5	470	-558
-21	544	-527	-26	30*	94	-19	347	395	-4	452	487
-20	1157	1135	-25	561	589	-18	934	-922	-3	71*	8
-19	250	173	-24	121*	121	-17	179*	177	-2	329	-381
-18	566	-563	-23	462	461	-16	803	-747	-1	238	211
-17	573	508	-22	28*	-117	-15	177*	79			
-16	167*	-103	-21	301	258	-14	395	380	H=	4, K=	8
-15	185	-83	-20	720	-625	-13	257	-188			
-14	426	397	-19	179*	175	-12	259	328	-1	272	165
-13	158*	-90	-18	532	567	-11	146*	-190	-2	201*	-172
-12	1124	1075	-17	349	-375	-10	414	403	-3	166*	-51
-11	458	381	-16	554	524	-9	82*	-58	-4	1422	-1393
-10	292	-197	-15	597	-583	-8	27*	-39	-5	277	257
-9	441	-389	-14	289	-146	-7	856	884	-6	914	-884
-8	1578	-1497	-13	193*	-263	-6	174*	160	-7	688	640
-7	681	-654	-12	760	-758	-5	27*	199	-8	871	867
-6	18*	-116	-11	492	449	-4	297	298	-9	123*	-37
-5	666	-597	-10	957	-975	-3	1200	-1230	-10	770	734
-4	322	325	-9	243	190	-2	164*	-255	-11	410	-437
-3	537	486	-8	544	479	-1	289	360	-12	306	-254
-2	465	465	-7	23*	29				-13	359	-327
-1	299	-290	-6	1449	1508	H=	3, K=	9	-14	919	-989
			-5	609	619				-15	129*	-163
H=	3, K=	5	-4	922	861	-1	86*	237	-16	71*	-125
			-3	146*	89	-2	890	819	-17	29*	-7
-1	1257	1135	-2	546	-490	-3	374	-366	-18	955	958
-2	1677	1740	-1	453	-409	-4	653	611	-19	209*	203
-3	778	792				-5	455	-543			
-4	381	359	H=	3, K=	7	-6	716	-691	H=	4, K=	7
-5	426	-420				-7	135*	-167			
-6	1557	-1538	-1	534	-517	-8	406	-363	-23	348	-438
-7	367	338	-2	1977	-1896	-9	353	429	-22	119*	-151
-8	904	-868	-3	364	-459	-10	437	406	-21	267	-314
-9	527	-469	-4	354	-376	-11	609	583	-20	437	437
-10	1319	1292	-5	848	921	-12	483	486	-19	95*	-29
-11	199	282	-6	1442	1474	-13	30*	-38	-18	792	795
-12	1759	1772	-7	651	-690	-14	145*	-158	-17	408	-463
-13	696	683	-8	1173	1085				-16	413	-405
-14	149*	167	-9	748	-787	H=	4, K=	9	-15	354	-348
-15	353	-387	-10	68*	15				-14	580	-606

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-13	451	462	-18	641	-619	-28	652	668	-25	216	236
-12	102*	-59	-17	184*	140	-27	284	347	-26	120*	-103
-11	613	556	-16	173*	120	-26	262	-297	-27	175*	-111
-10	719	756	-18	443	-619	-25	140*	-130	-28	28*	-20
-9	448	-373	-14	159*	-35	-24	1207	-1200	-29	601	561
-8	1039	990	-13	302	280	-23	152*	-129	-30	504	-506
-7	124*	113	-12	23*	145	-22	775	-760	-31	160*	-89
-6	25*	-25	-11	23*	70	-21	316	-342			
-5	731	742	-10	930	-1051	-20	534	514	H=	4, K=	1
-4	239	-207	-9	327	-356	-19	441	-477			
-3	716	-730	-8	1981	-1822	-18	1806	1820	-32	507	524
-2	832	-816	-7	327	-234	-17	173*	171	-31	29*	-132
-1	717	-715	-6	616	625	-16	157*	78	-30	303	-295
			-5	184	109	-15	454	-418	-29	28*	123
H=	4, K=	6	-4	1959	1832	-14	1836	-1870	-28	457	-384
			-3	205	158	-13	19*	-49	-27	27*	16
-1	384	-280	-2	1075	1053	-12	357	-387	-26	261	-226
-2	1695	1689	-1	293	367	-11	775	760	-25	302	352
-3	192	169				-10	1949	1881	-24	987	914
-4	1563	1519	H=	4, K=	4	-9	18*	-18	-23	314	358
-5	298	188				-8	1297	1233	-22	24*	40
-6	353	407	-1	268	266	-7	961	-906	-21	390	406
-7	314	-238	-2	223	133	-6	1280	-1321	-20	1070	-1070
-8	1354	-1304	-3	1865	-1870	-5	734	-732	-19	320	327
-9	95*	-25	-4	334	-251	-4	123*	130	-18	1213	-1223
-10	1237	-1190	-5	132*	88	-3	671	-662	-17	556	-577
-11	69*	-16	-6	830	797	-2	1710	-1746	-16	155	148
-12	403	-414	-7	1310	1241	-1	447	450	-15	532	-505
-13	925	874	-8	1814	1793				-14	1770	1838
-14	329	353	-9	330	-306	H=	4, K=	2	-13	1193	-1164
-15	158*	-188	-10	1668	1647				-12	59*	-163
-16	448	466	-11	167*	217	-1	1221	-1167	-11	985	971
-17	712	-710	-12	170*	-452	-2	1435	1463	-10	196	-48
-18	38*	135	-12	340	-452	-3	252	234	-9	2564	2619
-19	307	341	-13	245	-264	-4	129*	140	-8	2258	-2184
-20	28*	-14	-14	1683	-1653	-5	332	-358	-7	806	817
-21	28*	79	-15	196	-202	-6	481	-501	-6	2490	-2494
-22	571	507	-16	244	-222	-7	16*	-102	-5	99*	103
-23	29*	83	-17	328	421	-8	1652	-1596	-4	839	854
-24	939	956	-18	1629	1589	-9	1520	1515	-3	409	445
-25	30*	-89	-19	782	-756	-10	2136	-2091	-2	317	-292
-26	465	-488	-20	1171	1164	-11	17*	-12	-1	685	729
			-21	542	458	-12	621	615			
H=	4, K=	5	-22	966	-890	-13	793	-762	H=	4, K=	0
			-23	100*	171	-14	1899	1777			
-28	544	-564	-24	1449	-1483	-15	670	-638	-2	1592	-1689
-27	405	-418	-25	301	-273	-16	150*	-79	-4	1546	1508
-26	241	145	-27	126*	38	-17	560	-558	-6	2661	-2453
-25	538	-529	-28	789	807	-18	1907	-1886	-8	1156	1019
-24	637	640	-29	141*	-139	-19	473	-505	-10	1930	1858
-23	330	-325				-20	1228	-1271	-12	2352	-2329
-22	749	771	H=	4, K=	3	-21	197	-144	-14	2363	-2331
-21	223	-134				-22	848	828	-16	519	463
-20	780	-689	-30	515	570	-23	924	922	-18	1976	2034
-19	1021	971	-29	194*	-254	-24	460	476	-20	2631	2638

L	FO	FC
H=	4, K=	0
-22	24*	-139
-24	1752	-1762
-26	26*	-44
-28	780	827
-30	205	208
-32	821	-855
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-18	1301	-1312
-16	545	-563
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-22	542	537
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-18	513	-615
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-16	647	-696
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-14	863	-747
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-12	119*	36
-11	379	373
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-8	1139	-984
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-17	195	145
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-17	127*	63
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-15	138*	-70
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-12	607	-589
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-19	64*	-43
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-13	27*	105
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-20	127*	-276
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-18	700	-707
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-15	239	-245
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-10	1182	-1209
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-8	2353	-2354
-7	241	-208
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-24	169*	-206
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-20	24*	56
-19	135*	179
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L	FO	FC
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-16	576	-636
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-22	933	897
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-20	998	-998
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-10	149	182
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-14	127*	110
-15	636	-653
-16	78*	-207
-17	586	595
-18	237	-175
-19	806	817
-20	1210	1233
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-22	232	-164
-23	25*	16
-24	457	-485
-25	26*	-73
-26	461	487
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-22	501	-509
-21	777	-761
-20	2739	-2794
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-18	183*	-163
-17	71*	103
-16	2282	2363
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-8	412	445
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-12	185	-144
-13	162	83
-14	1011	980
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-16	92*	-8
-17	383	-383
-18	165*	99
-19	24*	-179
-20	210	-274
-21	431	-435
-22	389	-381
-23	517	-496
-24	639	600
-25	726	678
-26	432	451
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-28	153*	51

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-26	768	-732	-27	470	472				H=	8, K=	7
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-24	672	-618							-22	1073	-1143
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-20	1376	1292	-24	724	744	-15	142*	117	-18	965	960
-19	620	677	-23	29*	-11	-14	557	-607	-17	209*	152
-18	377	406	-22	29*	-145	-13	222*	-226	-15	241	204
-17	210	202	-21	28*	59	-12	132*	238	-14	56*	-38
-16	831	-821	-20	1225	-1183	-11	29*	123	-13	412	-421
-15	387	-432	-19	352	-313	-10	1219	1230	-12	915	-917
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-13	725	-681	-17	167*	-163	-8	325	-243	-10	207	-178
-12	834	933	-16	946	929	-7	149*	17	-9	389	427
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-6	2092	-2053	-10	1371	-1311	-1	190*	-137	-3	869	977
-5	127*	-56	-9	484	-461				-2	482	-477
-4	398	-374	-8	549	573	H=	7, K=	9	-1	410	-510
-3	104*	59	-7	819	-764						
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-1	245	-190	-1	1095	1150	-6	317	-334	-4	685	675
-2	1016	948				-7	260	355	-5	211	208
-3	575	-632	H=	7, K=	7	-8	301	445	-6	125*	32
-4	615	-573				-9	205*	201	-7	163*	-164
-5	980	-975	-1	264	-241	-10	461	471	-8	1273	-1215
-6	533	-547	-2	459	-445				-9	276	-190
-7	952	958	-3	632	-657	H=	8, K=	8	-10	235	-220
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-9	494	443	-5	732	-738	-1	244	130	-12	527	544
-10	745	788	-6	836	827	-2	29*	94	-13	531	528
-11	245	-180	-7	27*	-32	-3	173*	-27	-14	488	471
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-14	445	-400	-10	596	-607	-6	81*	135	-17	109*	-47
-15	132*	68	-11	285	-343	-7	457	-519	-18	537	-534
-16	622	-653	-12	166*	200	-8	132*	-130	-19	28*	46
-17	63*	76	-13	190*	271	-9	87*	-142	-20	415	402
-18	219	241	-14	587	609	-10	699	-753	-21	289	-258

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
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-23	204*	-133	-20	156*	49	-10	971	-922	-2	803	863
-24	123*	-5	-21	708	707	-11	347	-359	-1	104*	-75
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-26	446	-442	-27	198*	212	-17	371	-343	-6	213	162
-25	29*	-23	-28	145*	187	-18	62*	36	-8	442	-420
-24	664	654	-29	408	-399	-19	696	691	-10	2177	2169
-23	167*	85				-20	117*	-200	-12	441	417
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-21	320	384				-22	407	386	-16	203	-190
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-19	210*	-209	-29	265	-187	-24	26*	-17	-20	888	899
-18	1525	-1608	-28	742	793	-25	27*	15	-22	1243	-1144
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-16	352	-255	-26	847	853	-27	111*	31	-26	27*	115
-15	260	-246	-25	273	-249	-28	40*	-144	-28	789	-783
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-13	418	370	-23	492	-545	-30	29*	-5	-32	117*	-123
-12	812	812	-22	1474	-1455	-31	418	-399			
-11	1179	1161	-21	204	-58				H=	9, K=	0
-10	1041	-1028	-20	66*	-50	H=	8, K=	1			
-9	866	856	-19	135*	-102				-30	1296	1288
-8	1789	-1872	-18	1386	1386	-32	1423	1446	-28	825	829
-7	136*	-211	-17	131*	51	-31	30*	-64	-26	131*	107
-6	203	-142	-16	943	942	-30	253	148	-24	1277	-1279
-5	734	-761	-15	564	615	-29	374	293	-22	134*	-82
-4	845	886	-14	896	-876	-28	833	-845	-20	1495	1499
-3	760	-834	-13	1038	925	-27	309	-303	-18	589	-528
-2	1793	1856	-12	955	-948	-26	1126	-1141	-16	1738	-1712
-1	451	-411	-11	300	-230	-25	305	-414	-14	262	-332
			-10	1240	1170	-24	453	463	-12	1119	1150
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			-8	2510	2467	-22	1353	1438	-8	1469	1438
-1	578	-528	-7	359	-431	-21	508	500	-6	1082	-1045
-2	106*	-189	-6	510	-382	-20	737	-822	-4	1482	-1504
-3	409	-467	-5	428	-349	-19	23*	-54	-2	965	1012
-4	93*	184	-4	2180	-2295	-18	1479	-1493			
-5	1075	1057	-3	337	267	-17	1147	-1109	H=	9, K=	1
-6	262	300	-2	998	-1008	-16	988	-974			
-7	227	324	-1	143*	77	-15	22*	44	-1	901	965
-8	179*	230				-14	2049	2050	-2	453	-418
-9	76*	-103	H=	8, K=	2	-13	111*	181	-3	434	459
-10	23*	145				-12	1652	1672	-4	251	194
-11	461	458	-1	726	-670	-11	212	-257	-5	882	-909
-12	749	-736	-2	1610	1595	-10	88*	-53	-6	569	632
-13	556	-538	-3	742	706	-9	694	705	-7	115*	-42
-14	722	-714	-4	446	406	-8	959	-978	-8	1151	-1118
-15	24*	80	-5	335	366	-7	290	342	-9	144*	-69
-16	295	-301	-6	58*	323	-6	757	-765	-10	859	816

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-11	807	-764				-7	284	198	-9	37*	-45
-12	620	686	-1	268	-286	-6	1919	-1915	-8	230	-135
-13	22*	-30	-2	1208	1236	-5	594	611	-7	415	-514
-14	498	-503	-3	113*	-5	-4	1406	-1363	-6	1213	1217
-15	511	472	-4	371	344	-3	395	345	-5	919	-924
-16	195	-315	-5	381	377	-2	180*	180	-4	446	455
-17	1188	1166	-6	529	-472	-1	326	-288	-3	196*	221
-18	134*	-125	-7	22*	18				-2	776	-791
-19	226	209	-8	553	563	H=	9, K=	5	-1	644	648
-20	761	748	-9	1062	1087						
-21	611	-629	-10	1000	-973	-1	25*	-73	H=	9, K=	7
-22	159*	166	-11	826	-827	-2	417	-407			
-23	536	-518	-12	23*	31	-3	701	-764	-1	745	-700
-24	515	-567	-13	1206	-1242	-4	35*	76	-2	257	285
-25	126*	-185	-14	446	462	-5	853	-838	-3	278	-351
-26	423	393	-15	413	514	-6	548	-607	-4	290	-337
-27	68*	76	-16	256	264	-7	181*	100	-5	48*	31
-28	156*	-204	-17	168*	-266	-8	231	92	-6	191*	-227
-29	203*	-223	-18	369	409	-9	285	254	-7	28*	-61
-30	346	-333	-19	276	323	-10	867	892	-8	28*	-156
-31	258	266	-20	96*	-19	-11	829	839	-9	231	258
			-21	26*	56	-12	642	653	-10	74*	-78
H=	9, K=	2	-22	334	-353	-13	445	476	-11	28*	-39
			-23	27*	-58	-14	124*	58	-12	206*	-176
-31	30*	228	-24	159*	-14	-15	365	-358	-13	140*	-28
-30	1298	-1269	-25	311	283	-16	314	-242	-14	177*	162
-29	29*	-36	-26	28*	87	-17	122*	-22	-15	412	376
-28	810	-775	-27	155*	-235	-18	97*	-9	-16	329	250
-27	460	-460	-28	29*	2	-19	699	-735	-17	29*	-106
-26	1044	1026	-29	30*	-10	-20	253	254	-18	561	-578
-25	67*	45	-30	117*	-55	-21	28*	2	-19	250	-243
-24	1114	1139				-22	113*	-164	-20	291	-280
-23	205	88	H=	9, K=	4	-23	368	327	-21	30*	23
-22	666	-651				-24	462	-464			
-21	25*	-20	-28	328	318	-25	30*	43	H=	9, K=	8
-20	1512	-1512	-27	206*	203	-26	397	454			
-19	336	-349	-26	684	-702	-27	718	749	-15	217*	135
-18	116*	-47	-25	29*	-185				-14	886	-939
-15	124*	-54	-24	531	-502	H=	9, K=	6	-13	165*	-90
-14	854	887	-23	152*	77				-12	127*	-184
-13	215	-256	-22	200*	178	-24	975	1024	-11	305	350
-12	831	-796	-21	439	471	-23	329	279	-10	883	903
-11	453	440	-20	1331	1325	-22	238	-213	-9	203*	-195
-10	2517	-2504	-19	87*	171	-21	29*	180	-8	30*	173
-9	104*	17	-18	665	666	-20	1654	-1669	-7	217*	-201
-8	586	-573	-17	245	286	-19	409	-357	-6	662	-663
-7	276	311	-16	1143	-1136	-18	344	-225	-5	29*	3
-6	2348	2295	-15	145*	76	-17	28*	-65	-4	414	-447
-5	234	203	-14	939	-913	-16	995	931	-3	386	-349
-4	821	888	-13	722	-756	-15	448	448	-2	576	647
-3	57*	186	-12	652	608	-14	431	416	-1	66*	79
-2	750	-778	-11	747	-708	-13	27*	71			
-1	358	-353	-10	1855	1936	-12	111*	46	H=	10, K=	8
			-9	428	418	-11	46*	-34			
H=	9, K=	3	-8	522	467	-10	929	-985	-1	101*	31

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H= 10, K= 8			-18	147*	28	-18	340	342	-10	924	-946
			-19	386	-394	-19	180*	216	-11	1116	-1016
-2	30*	-59	-20	161*	214	-20	882	869	-12	99*	125
-3	176*	-167	-21	438	-398	-21	324	314	-13	115*	-27
-4	218*	202	-22	30*	-35	-22	165*	171	-14	177	-165
-5	30*	116	-23	229*	226	-23	94*	67	-15	170*	-228
-6	257	248				-24	167*	156	-16	166*	-129
-7	171*	-155	H= 10, K= 5			-25	323	355	-17	701	723
-8	406	-391				-26	72*	8	-18	482	-504
-9	244	-273	-26	662	-655	-27	79*	-3	-19	709	702
-10	210*	-308	-25	237*	-285	-28	306	-352	-20	310	-248
-11	30*	29	-24	263	315				-21	233	182
-12	431	463	-23	316	258	H= 10, K= 3			-22	419	466
			-22	1320	1266				-23	123*	96
H= 10, K= 7			-21	29*	-97	-29	105*	-213	-24	119*	-3
			-20	28*	115	-28	1122	1115	-25	454	-458
-19	468	-482	-19	212*	-207	-27	101*	-179	-26	174*	250
-18	1017	1033	-18	1460	-1441	-26	381	423	-27	213*	-236
-17	52*	39	-17	159*	-86	-25	98*	-147	-28	105*	-60
-16	695	694	-16	565	-605	-24	646	-697	-29	304	-295
-15	147*	113	-15	197*	-58	-23	27*	61	-30	135*	-194
-14	158*	93	-14	470	589	-22	753	-694			
-13	151*	-226	-13	137*	-125	-21	377	284	H= 10, K= 1		
-12	1027	-997	-12	1199	1173	-20	172*	79			
-11	187*	169	-11	622	652	-19	283	-260	-31	96*	119
-10	259	-313	-10	396	400	-18	1097	1094	-30	363	360
-9	141*	177	-9	413	432	-17	314	-229	-29	457	485
-8	1033	1035	-8	1681	-1584	-16	1170	1213	-28	824	-837
-7	174*	-169	-7	26*	-143	-15	355	244	-27	224*	250
-6	29*	114	-6	832	-934	-14	210	-259	-26	1000	-1001
-5	417	464	-5	175*	134	-13	618	625	-25	412	-339
-4	673	-728	-4	649	653	-12	1953	-1968	-27	28*	250
-3	29*	-21	-3	504	-501	-11	428	441	-23	189*	-194
-2	944	-910	-2	1074	1028	-10	311	-260	-22	1151	1186
-1	816	-776	-1	105*	-153	-9	88*	-10	-21	158*	181
						-8	2405	2344	-20	636	-692
H= 10, K= 6			H= 10, K= 4			-7	124*	-53	-19	350	-365
						-6	1663	1697	-18	1517	-1530
-1	195*	-181	-1	525	-552	-5	118*	46	-17	377	-372
-2	340	-328	-2	50*	108	-4	1125	-1091	-16	647	-645
-3	206	130	-3	153*	56	-3	169*	210	-15	585	613
-4	27*	-145	-4	669	647	-2	1670	-1757	-14	781	759
-5	27*	-79	-5	1130	1113	-1	1044	-1043	-13	23*	12
-6	190*	255	-6	733	795				-12	1336	1331
-7	252	-280	-7	179*	199	H= 10, K= 2			-11	23*	32
-8	519	-480	-8	242	-303				-10	110*	-85
-9	291	-302	-9	574	643	-1	150*	120	-9	334	-317
-10	523	-468	-10	595	-583	-2	756	788	-8	1956	-2004
-11	27*	-50	-11	732	665	-3	1238	1109	-7	1167	-1183
-12	110*	101	-12	418	423	-4	328	-330	-6	2695	-2672
-13	426	389	-13	1183	-1152	-5	400	403	-5	286	-276
-14	401	470	-14	114*	67	-6	23*	-19	-4	1951	1929
-15	161*	142	-15	483	-464	-7	332	-267	-3	1118	1161
-16	28*	-138	-16	799	-783	-8	504	522	-2	2055	2083
-17	169*	-95	-17	87*	93	-9	754	-835	-1	290	236

L	FO	FC
H= 10, K= 0		
-2	635	635
-4	164*	-127
-6	343	-294
-8	873	-799
-10	487	476
-12	23*	102
-14	866	928
-16	121*	42
-18	424	-377
-20	87*	98
-22	989	-1014
-24	27*	91
-26	150*	39
-28	258	-359
-30	406	459
H= 11, K= 0		
-30	840	874
-28	987	1007
-26	49*	174
-24	1191	-1195
-22	221	-169
-20	1179	1142
-18	324	345
-16	1469	-1541
-14	1800	-1803
-12	569	-558
-10	1790	1855
-8	1018	1022
-6	2894	-2933
-4	1904	-1948
-2	905	854
H= 11, K= 1		
-1	178	-78
-2	151*	-165
-3	208	260
-4	691	595
-5	752	-811
-6	84*	164
-7	970	-950
-8	1294	-1390
-9	23*	52
-10	484	-447
-11	267	178
-12	673	-672
-13	161*	-197
-14	293	261
-15	686	641
-16	1364	1377
-17	1196	1190
-18	141*	87
-19	469	-441
-20	135*	-36
-21	559	-529
-22	136*	-38
-23	413	-487
-24	340	-316
-25	334	-425
-26	189*	-46
-27	29*	181
-28	748	-669
-29	149*	192
-30	182*	-11
H= 11, K= 2		
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-28	160*	-278
-27	320	-301
-26	975	961
-25	533	-574
-24	400	488
-23	255	-185
-22	27*	-69
-21	158*	169
-20	718	-747
-19	26*	54
-18	716	-685
-17	193	57
-16	858	858
-15	25*	-76
-14	1807	1736
-13	313	-324
-12	252	267
-11	423	-381
-10	1657	-1706
-9	782	-763
-8	517	-547
-7	293	251
-6	1705	1744
-5	1305	1363
-4	1614	1657
-3	375	336
-2	445	-451
-1	359	376
H= 11, K= 3		
-1	533	591
-2	558	546
-3	430	416
-4	363	373
-5	421	514
-6	742	-711
-7	130*	-41
-8	186*	-254
-9	543	493
-10	859	877
-11	808	-743
-12	773	785
-13	811	-903
-14	661	-701
-15	325	361
-16	276	-254
-17	330	329
-18	1025	1015
-19	231	219
-20	239	-235
-21	304	-250
-22	348	-383
-23	353	304
-24	29*	-20
-25	192*	264
-26	230	-237
-27	298	-226
H= 11, K= 4		
-27	31*	157
-26	686	-721
-25	30*	-90
-24	773	-777
-23	407	362
-22	208*	-128
-21	160*	86
-20	921	934
-19	87*	-111
-18	764	754
-17	171*	64
-16	1011	-955
-15	27*	-93
-14	1292	-1282
-13	123*	-25
-12	469	-499
-11	245	-250
-10	1758	1792
-9	280	223
-8	1425	1423
-7	226	115
-6	1418	-1425
-5	136*	-47
-4	1561	-1530
-3	149*	-262
-2	452	389
-1	471	-492
H= 11, K= 5		
-1	254	-331
-2	517	-468
-3	685	-611
-4	270	229
-5	204*	241
-6	71*	-82
-7	457	507
-8	134*	205
-9	220*	-259
-10	372	415
-11	719	701
-12	208	54
-13	159*	224
-14	27*	99
-15	877	-899
-16	28*	-163
-17	294	-257
-18	758	-746
-19	214	152
-20	483	-465
-21	143*	182
-22	30*	81
-23	30*	-7
-24	295	252
-25	225	65
H= 11, K= 6		
-22	81*	169
-21	343	339
-20	926	-950
-19	202*	154
-18	463	-519
-17	29*	25
-16	896	839
-15	29*	-108
-14	821	885
-13	29*	77
-12	155*	159
-11	69*	129
-10	1289	-1312
-9	452	-403
-8	311	-227
-7	315	-268
-6	990	965
-5	112*	121
-4	247	211
-3	206*	320
-2	75*	56
-1	362	365
H= 11, K= 7		
-1	30*	31
-2	289	280
-3	314	-314

L	FO	FC
H=	11, K=	7
-4	30*	-27
-5	196*	-233
-6	286	-346
-7	172*	-200
-8	156*	35
-9	30*	-45
-10	426	462
-11	338	337
-12	155*	-54
-13	187*	267
-14	369	-335
-15	30*	4
-16	96*	-101
-17	30*	115
H=	12, K=	7
-13	193*	168
-12	1143	-1150
-11	647	-628
-10	293	-271
-9	154*	-106
-8	1113	1105
-7	581	568
-6	588	619
-5	556	519
-4	336	-329
-3	169*	65
-2	960	-962
H=	12, K=	6
-1	343	-345
-2	29*	-11
-3	145*	-197
-4	50*	-105
-5	29*	-69
-6	29*	139
-7	652	693
-8	225	173
-9	29*	237
-10	119*	-176
-11	41*	14
-12	335	-292
-13	249	223
-14	363	325
-15	371	-404
-16	336	344
-17	149*	-145
-18	390	464
-19	230*	-196
H=	12, K=	5
-23	192*	-162
-22	1034	1023
-21	122*	-123
-20	680	679
-19	65*	-53
-18	751	-756
-17	167*	-110
-16	735	-752
-15	28*	-25
-14	292	350
-13	56*	51
-12	1268	1224
-11	353	235
-10	503	503
-9	151*	12
-8	1377	-1404
-7	28*	-53
-6	461	-474
-5	194*	-159
-4	462	496
-3	549	-515
-2	122*	239
-1	40*	174
H=	12, K=	4
-1	196	111
-2	784	762
-3	27*	-92
-4	551	608
-5	816	869
-6	344	321
-7	428	-443
-8	168*	-137
-9	38*	-76
-10	903	-879
-11	569	553
-12	289	181
-13	801	-789
-14	295	324
-15	239	-251
-16	839	-849
-17	407	428
-18	344	-361
-19	267	245
-20	736	732
-21	290	-328
-22	623	617
-23	128*	-200
-24	89*	57
-25	271	298
H=	12, K=	3
-27	363	-317
-26	447	448
-25	164*	-187
-24	279	-302
-23	236	145
-22	1193	-1206
-21	211	116
-20	734	-737
-19	268	-200
-18	578	611
-17	145*	61
-16	1046	1028
-15	167*	115
-14	26*	-49
-13	26*	36
-12	1350	-1354
-11	124*	-119
-10	820	-854
-9	175*	-224
-8	1196	1223
-7	516	486
-6	1504	1538
-5	483	542
-4	1214	-1215
-3	186*	275
-2	1465	-1476
-1	844	-944
H=	12, K=	2
-1	506	484
-2	26*	92
-3	217	292
-4	36*	-24
-5	211	-227
-6	753	755
-7	126*	208
-8	481	522
-9	553	-568
-10	291	-307
-11	595	-587
-12	820	-826
-13	26*	-45
-14	743	-785
-15	333	-306
-16	628	672
-17	579	581
-18	218	248
-19	623	566
-20	161*	-107
-21	153*	-45
-22	249	214
-23	306	297
-24	95*	83
-25	419	-436
-26	234	293
-27	453	-544
-28	151*	-15
H=	12, K=	1
-29	360	338
-28	497	-595
-27	223*	146
-26	730	-742
-25	29*	-30
-24	167*	-264
-23	28*	-15
-22	870	923
-21	275	-285
-20	753	727
-19	243	-199
-18	820	-800
-17	357	406
-16	1489	-1395
-15	72*	90
-14	212	126
-13	276	351
-12	1750	1802
-11	817	850
-10	648	665
-9	672	-717
-8	1347	-1392
-7	1373	-1322
-6	864	-892
-5	342	289
-4	1292	1298
-3	103*	210
-2	1320	1370
-1	316	-306
H=	12, K=	0
-2	433	-383
-4	183	-50
-6	1700	-1733
-8	594	-582
-10	616	648
-12	179	118
-14	1777	1792
-16	117*	-64
-18	1539	-1605
-20	524	-451
-22	659	664
-24	28*	100
-26	836	-834
-28	158*	139
H=	13, K=	0

L	FO	FC
-28	1099	1034
-26	84*	18
-24	709	-688
-22	426	-502
-20	712	689
-18	1800	1771
-16	269	-251
-14	2134	-2139
-12	339	-331
-10	1748	1715
-8	573	589
-6	1153	-1168
-4	564	-588
-2	689	711
H=	13, K=	1
-1	283	276
-2	350	363
-3	518	-543
-4	651	716
-5	26*	5
-6	174*	-194
-7	260	-212
-8	1008	-999
-9	702	-662
-10	287	-249
-11	353	381
-12	313	-346
-13	343	380
-14	445	516
-15	59*	42
-16	1073	1090
-17	522	530
-18	545	-573
-19	167*	-14
-20	575	-584
-21	385	-377
-22	28*	36
-23	199*	-230
-24	687	635
-25	303	-302
-26	175*	168
-27	30*	43
-28	1075	-1076
H=	13, K=	2
-27	30*	-32
-26	202*	229
-25	102*	-12
-24	927	968
-23	111*	-136
-22	419	461
-21	28*	125
-20	794	-804
-19	192*	201
-18	1151	-1119
-17	283	-277
-16	85*	153
-15	241	-239
-14	729	737
-13	507	480
-12	180*	-85
-11	26*	23
-10	391	-328
-9	1032	-1025
-8	536	-605
-7	101*	-90
-6	755	780
-5	479	525
-4	1037	1053
-3	272	94
-2	377	-459
-1	498	550
H=	13, K=	3
-1	27*	71
-2	146*	-163
-3	90*	-5
-4	980	-998
-5	38*	94
-6	401	-446
-7	143*	-164
-8	136*	-36
-9	435	465
-10	27*	242
-11	27*	-92
-12	440	475
-13	314	-280
-14	592	-590
-15	229	-300
-16	525	-483
-17	28*	2
-18	605	578
-19	221	152
-20	28*	147
-21	232	-222
-22	352	-336
-23	280	296
-24	365	-366
-25	439	373
-26	142*	-241
H=	13, K=	4
-24	1246	-1254
-23	73*	-80
-22	382	-374
-21	29*	-106
-20	894	929
-19	479	489
-18	944	909
-17	28*	130
-16	105*	-254
-15	299	-268
-14	855	-876
-13	202*	193
-12	337	-401
-11	319	-366
-10	1064	1084
-9	126*	-131
-8	906	938
-7	198*	189
-6	1170	-1192
-5	129*	-7
-4	944	-941
-3	28*	52
-2	385	394
-1	127*	-101
H=	13, K=	5
-1	710	730
-2	97*	-141
-3	369	378
-4	168*	172
-5	129*	-49
-6	70*	141
-7	154*	59
-8	199*	228
-9	510	-491
-10	190*	10
-11	29*	-19
-12	29*	96
-13	174*	-4
-14	339	376
-15	369	-312
-16	256	167
-17	333	292
-18	511	-504
-19	421	394
-20	807	-778
-21	244*	284
H=	13, K=	6
-16	530	547
-15	219*	-156
-14	1001	991
-13	648	575
-12	124*	-206
-11	85*	70
-10	1133	-1116
-9	473	-485
-8	265	-284
-7	235	-143
-6	447	441
-5	30*	56
-4	580	560
-3	145*	21
-2	610	610
-1	277	356
H=	14, K=	5
-18	651	-610
-17	341	-293
-16	655	-679
-15	144*	-49
-14	30*	96
-13	112*	-80
-12	794	813
-11	212*	-230
-10	490	453
-9	30*	2
-8	753	-749
-7	195*	79
-6	568	-626
-5	425	385
-4	161*	-61
-3	156*	-116
-2	656	638
-1	217*	-209
H=	14, K=	4
-1	334	336
-2	932	904
-3	539	-559
-4	417	373
-5	403	-410
-6	511	-481
-7	223	208
-8	237	-282
-9	379	335
-10	29*	76
-11	91*	49
-12	141*	72
-13	29*	3
-14	29*	113
-15	259	228
-16	268	-339
-17	214*	-204
-18	318	-348
-19	30*	56
-20	515	546
-21	182*	-79

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=	13, K=	3	-10	537	-558	-7	85*	-174			
			-11	680	-708	-6	361	-354	H=	15, K=	1
-24	459	442	-12	165*	-190	-5	133*	175			
-23	30*	128	-13	28*	-35	-4	400	402	-1	439	392
-22	1069	-1033	-14	377	-380	-3	324	-300	-2	463	-432
-21	451	-395	-15	215	145	-2	592	624	-3	562	-535
-20	652	-641	-16	519	489	-1	28*	-77	-4	578	541
-19	416	-446	-17	205*	234				-5	216	-178
-18	754	707	-18	85*	202	H=	14, K=	0	-6	165*	-72
-17	135*	67	-19	325	285				-7	28*	224
-16	322	392	-20	614	-577	-2	190	-102	-8	594	-633
-15	49*	221	-21	159*	134	-4	269	239	-9	379	-404
-14	28*	37	-22	220	-199	-6	325	-311	-10	214	-150
-13	600	610	-23	30*	61	-8	270	218	-11	261	300
-12	196*	-244	-24	90*	263	-10	556	573	-12	152*	215
-11	28*	71	-25	125*	-235	-12	196	95	-13	673	693
-10	537	-488				-14	165*	269	-14	837	822
-9	397	-390	H=	14, K=	1	-16	673	-733	-15	219*	-263
-8	552	551				-18	661	-656	-16	95*	-67
-7	346	287	-26	642	-648	-20	761	704	-17	327	-275
-6	806	820	-25	361	305	-22	802	850	-18	1020	-1066
-5	311	-267	-24	418	-391	-24	354	282	-19	330	364
-4	586	-574	-23	29*	52	-26	1338	-1339	-24	846	860
-3	270	-242	-22	534	554						
-2	1104	-1127	-21	333	-349	H=	15, K=	0	H=	15, K=	2
-1	91*	-103	-20	1055	1043						
			-19	176*	186	-24	460	-419	-23	31*	7
H=	14, K=	2	-18	831	-787	-22	324	-297	-22	351	333
			-17	290	265	-20	588	618	-21	265	264
-1	390	341	-16	1274	-1303	-18	1232	1246	-20	403	-442
-2	933	-906	-15	229	-188	-16	513	-514	-19	30*	8
-3	28*	-42	-14	67*	-194	-14	1529	-1566	-18	418	-430
-4	168*	-57	-13	161*	115	-12	235	-283	-17	362	-370
-5	380	-311	-12	877	839	-10	460	488	-16	298	290
-6	1209	1186	-11	346	305	-8	525	506	-15	302	-347
-7	411	362	-10	339	304	-6	74*	-188	-14	394	347
-8	67*	136	-9	194*	-235	-4	574	-539	-13	128*	99
-9	317	-279	-8	603	-514	-2	203	147	-12	174*	192

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
-11	221	136							-7	160*	202
-10	252	197	-18	350	293	-1	31*	-98	-6	767	-751
-9	29*	49	-17	161*	119	-2	1100	-1073	-5	301	-321
-8	670	-635	-16	61*	-207	-3	218	-96	-4	177*	-200
-7	275	256	-15	396	348	-4	30*	-74	-3	173*	-91
-6	29*	174	-14	606	-551	-5	370	-360	-2	620	618
-5	214	155	-13	391	361	-6	1441	1441	-1	308	277
-4	1026	996	-12	182*	-208	-7	30*	5			
-3	29*	129	-11	166*	-143	-8	572	489	H=	16, K=	0
-2	225	191	-10	533	574	-9	51*	-13			
-1	114*	114	-9	304	-254	-10	716	-717	-2	563	533
			-8	772	764	-11	30*	-35	-4	527	514
H=	15, K=	3	-7	524	-517	-12	497	-496	-6	255	-295
			-6	409	-395	-13	408	350	-8	51*	66
-1	30*	34	-5	285	-249	-14	177*	66	-10	435	289
-2	193*	-162	-4	881	-856	-15	228*	263	-12	630	589
-3	30*	-16	-3	321	361	-16	797	795	-14	441	-346
-4	1430	-1423	-2	269	-267	-17	145*	-114	-16	1517	-1490
-5	29*	47	-1	43*	193	-18	30*	59	-18	30*	8
-6	232	-242				-19	31*	-92	-20	1187	1150
-7	165*	50	H=	16, K=	3						
-8	898	897				H=	16, K=	1	H=	17, K=	0
-9	50*	90	4	174*	784						
-10	396	334	-16	31*	168	-21	31*	67	-14	875	-849
-11	458	-413	-15	81*	73	-20	465	457	-12	713	-684
-12	29*	-18	-14	30*	-41	-19	30*	58	-10	205*	-112
-13	58*	41	-13	396	382	-18	620	-576	-8	904	846
-14	316	-243	-12	151*	-243	-17	167*	-210			
-15	102*	-35	-11	313	329	-16	902	-885	H=	17, K=	1
-16	209	94	-10	346	-356	-15	181*	208			
-17	240	-186	-9	249	232	-14	224	-53	-8	765	-739
-18	484	457	-8	364	364	-13	30*	-9	-9	230*	172
-19	441	440	-7	363	324	-12	426	435	-10	406	-417
-20	30*	79	-6	716	719	-11	442	-451	-11	154*	140
-21	31*	7	-5	385	-379	-10	866	850	-12	492	532
						-9	111*	75	-13	31*	57
H=	15, K=	4	H=	16, K=	2	-8	94*	113	-14	1266	1221

Table 6.4

Bond Lengths and Angles: $Ru(DMSO)_6(BF_4)_2$

a) Distances (Å). Values in square brackets are corrected for thermal motion, the light atom considered to be riding on the heavy atom.

	Cation I	Cation II
Ru-S1	2.260(3)[2.268(3)]	2.250(3)[2.259(3)]
Ru-S2	2.237(3)[2.247(3)]	2.239(3)[2.249(3)]
Ru-S3	2.260(3)[2.270(3)]	2.255(3)[2.264(3)]
Ru-O4	2.118(6)[2.123(6)]	2.117(6)[2.123(5)]
Ru-O5	2.138(6)[2.141(5)]	2.129(6)[2.138(5)]
Ru-O6	2.121(6)[2.125(5)]	2.137(6)[2.150(5)]
S1-O1	1.492(7)[1.516(7)]	1.479(7)[1.501(6)]
S2-O2	1.475(7)[1.489(6)]	1.469(7)[1.510(7)]
S3-O3	1.479(7)[1.500(6)]	1.495(7)[1.521(7)]
S4-O4	1.536(6)	1.555(6)
S5-O5	1.522(6)	1.515(6)
S6-O6	1.547(6)	1.542(7)
S1-C11	1.76 (1)	1.79(1)
S1-C12	1.77(1)	1.78(1)
S2-C21	1.77(1)	1.76(1)
S2-C22	1.77(1)	1.76(1)
S3-C31	1.77(1)	1.77(1)
S3-C32	1.78(1)	1.80(1)
S4-C41	1.75(1)	1.77(1)
S4-C42	1.78(1)	1.79(1)
S5-C51	1.76(1)	1.75(1)
S5-C52	1.75(1)	1.75(1)
S6-C61	1.78(1)	1.76(1)
S6-C62	1.77(1)	1.76(1)

b) Angles (deg)

	Cation I	Cation II
S1-Ru-S2	90.3(1)	90.5(1)

Table 6.4 (continued)

b) Angles (deg)

	Cation I	Cation II
S1-Ru-S3	94.9(1)	93.9(1)
S2-Ru-S3	97.7(1)	96.3(1)
S1-Ru-O4	91.3(2)	92.4(2)
S1-Ru-O5	90.0(2)	8.9(2)
S1-Ru-O6	175.2(3)	175.5(2)
S2-Ru-O4	89.2(2)	88.7(2)
S2-Ru-O5	170.5(2)	172.7(2)
S2-Ru-O6	88.9(2)	90.6(2)
S3-Ru-O4	170.7(2)	171.9(2)
S3-Ru-O5	91.8(2)	91.0(2)
S3-Ru-O6	89.8(2)	90.4(2)
O4-Ru-O5	81.2(2)	84.1(2)
O4-Ru-O6	83.9(2)	83.2(3)
O5-Ru-O6	90.0(2)	89.5(2)
Ru-S1-O1	113.0(3)	112.8(3)
Ru-S2-O2	118.8(3)	117.9(3)
Ru-S3-O3	112.7(3)	114.6(3)
Ru-O4-S4	121.2(4)	122.5(4)
Ru-O5-S5	129.7(4)	131.8(4)
Ru-O6-S6	120.1(4)	119.5(4)
Ru-S1-C11	111.8(4)	110.1(4)
Ru-C1-C12	117.5(4)	117.2(4)
Ru-S2-C21	111.1(4)	112.5(4)
Ru-S2-C22	112.3(4)	112.2(4)
Ru-S3-C31	111.1(4)	110.9(4)
Ru-S3-C32	120.3(4)	120.2(4)
O1-S1-C11	107.9(5)	108.9(5)
O1-S1-C12	106.1(5)	106.8(5)
O2-S2-C21	106.4(5)	106.9(5)
O2-S2-C22	106.5(5)	106.6(5)
O3-S3-C31	106.5(5)	106.0(5)
O3-S3-C32	106.6(5)	105.5(5)
O4-S4-C41	103.2(5)	104.8(5)
O4-S4-C42	103.5(5)	103.0(4)

Table 6.4 (continued)

b) Angles (deg)

	Cation I	Cation II
O5-S5-C51	104.3(5)	103.5(5)
O5-S5-C52	105.7(5)	106.1(5)
O6-S6-C61	101.3(5)	101.6(5)
O6-S6-C62	105.2(5)	104.9(5)
C11-S1-C12	99.4(5)	100.2(5)
C21-S2-C22	100.0(6)	98.8(6)
C31-S3-C32	98.2(6)	97.6(5)
C41-S4-C42	99.5(6)	98.0(5)
C51-S5-C52	97.3(6)	99.7(7)
C61-S6-C62	98.9(5)	100.9(6)

v. Discussion

The $Ru(DMSO)_6^{2+}$ Cation Geometry

The two crystallographically distinct cations found in the asymmetric unit are very nearly identical with respect to interatomic parameters and geometrical configuration, with only small crystallographically (but not chemically) significant differences occuring for several angular parameters (table 6.4); the labelling of the two cations has been chosen to reflect their close similariry. A perspective view of one of the cations is shown in figure 6.1.

Each ruthenium atom is coordinated with irregular octahedral geometry to six DMSO ligands; three ligands bond via their sulphur atoms and three via their oxygen atoms to give the facial isomer. This result continues a trend for ruthenium-DMSO complexes: both $Ru(DMSO)_4Cl_2$[125] and $Ru(DMSO)_3Cl_3^-$[128] also adopt geometries which place S-bonded ligands mutually cis- to one another, and trans- to chloride or O- bonded DMSO ligands. The choice of linkage and geometrical isomers in DMSO complexes has always been considered to be a balance between electronic and steric effects.[125] In the present case, the angles subtended at the central ruthenium atom between the three S-bonded ligands are greater than 90 deg (mean 94.2 deg), while those between the O-bonded ligands are less than 90 deg (mean 85.0 deg). Similar, but smaller deviations from regular octahedral geometry in $Ru(DMSO)_3Cl_3^-$ prompted another group to attribute the observed geometry to predominantly steric factors. These deviations, however, are not large, and may simply reflect the flexibility of the coordination sphere to relieve steric interactions

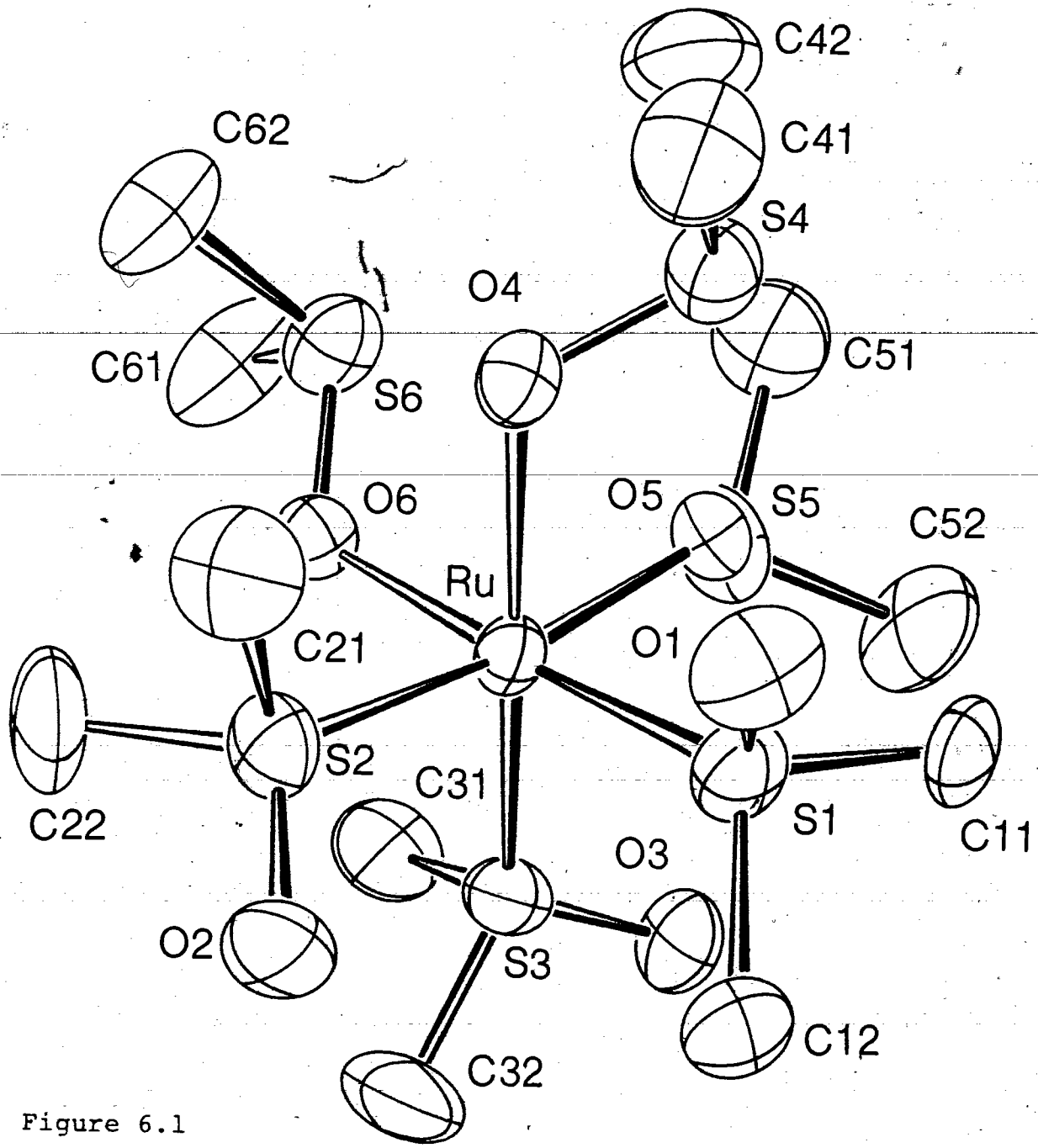

Figure 6.1

Perspective View of the $Ru(DMSO)_6^{2+}$ Cation

resulting from an electronically-determined structure. Furthermore, steric interactions would have been more easily and effectively relieved in these complexes by adoption of a different geometric isomer (e.g. meridional), or a different linkage isomer (e.g. a trans- isomer, containing 2 sulphur-bonded and four oxygen bonded ligands).

Other examples[119,131,132] of complexes where the adopted isomer places S- and O- bonded ligands trans- to one another (when steric factors would favour a different isomer) can be included with these Ru(DMSO) complexes in an interpretation of the observed geometries in terms of stabilization by the "trans influence" of the sulphur atoms. The trans influence is broadly defined[133] as the thermodynamic weakening of a bond (M - X) which is trans- to any ligand (L) under consideration. This may or may not be related to the kinetic "trans effect", which concerns the lability of the ligand X.

The classical polarization theory of the trans influence (the charge on the the metal induces a dipole in L which in turn induces a corresponding dipole in the metal atom, which opposes the natural polarity of X) favours a structure which locates the more polarizable sulphur on one side of the coordination sphere, and the oxygen atoms on the other. An attempt at interpreting this from an orbital point of view for d^6 octahedral systems has been made[134]. A high degree of correlation has been found between the the trans influence series of a number of ligands (L), and that obtained by ordering the ligands according to their $S^2/\Delta E$ ratios (where S is the overlap integral between and E the energy between inter-

acting orbitals on the metal and ligand, and which may be taken as a measure of the bond strength). Furthermore, on the basis of this correlation, it can be deduced that the trans influence of a ligand arises principally from its inductive σ-donor ability, transmitted to its trans- ligand via the appropriate metal p orbital. The magnitude of this effect is modified if the influencing ligand L has π-acceptor properties.

An inspection of the bond lengths in $Ru(DMSO)_6^{2+}$, $Ru(DMSO)_4Cl_2$, and $Ru(DMSO)_3Cl_3^-$ shows that such a model is applicable to these systems. In $Ru(DMSO)_6^{2+}$, the variation in Ru-S and Ru-O distances in both cations, while not crystallographically significant, is chemically sensible; i.e. the longest Ru-S bond lengths occur trans- to the shortest Ru-O bond lengths (table 6.2). The Ru-S bond length, corrected for thermal motion (the light atom assumed to be riding on the heavy atom) is 2.259A (mean value), and is very close to the only other value available for S- bonded DMSO trans- to oxygen (2.252(1)A), and may be compared to values of 2.277(1)A trans- to Cl (where the competition for π-donor orbitals on the metal increases), and 2.188(3)A in $Ru(NH_3)_5(DMSO)^{2+}$[135], where no competition exists. These distances are consistent with sulphur as a weak π-acceptor, and, in absence of large steric influences (as in, for instance, the 2-methyl sulphoxide $Pd(R_2SO)_4^{2+}$,[127] the geometrical and linkage isomer is chosen to reduce competition for the π-donor electrons on metal.

Whether the ruthenium to oxygen bond in

$Ru(DMSO)_6^{2+}$ is weakened is difficult to assess, since there is little in the way of comparison to "normal" Ru-O distances. Using Pauling's value of 0.99A for the covalent radius of chlorine,[136] and an average Ru-Cl distance of 2.376A for Cl *trans*- to Cl (as for example in $RuCl_5NO^{2-}$), leads to an effective octahedral covalent radius for Ru(II) of 1.39A. This is in good agreement with Pauling's estimate of 1.33A, and also with the value found by similar reference to $Ru-NO_2$ bonds (*trans*- to NO_2) in $Ru(NO)(OH)(NO_2)_4^{2+}$ and to the $Ru-NH_3$ bons in $Ru(NH_3)_5DMSO^{2+}$. Using this value, and a covalent radius of 0.66A for oxygen,[136] an Ru-O covalent bond length of approximately 2.04A is predicted. Hence the Ru-O bond in $Ru(DMSO)_6^{2+}$ (mean value 2.133A, corrected as before for thermal motion), appears to be weaker than 'normal', i.e. its σ-donor ability is reduced when *trans*- to sulphur. Two important points should be noted: the weakening, if it exists, is very small; also, a separate, and even more indirect estimate of the Ru-O bond length, based on the Fe-O distance in *trans*-$FeCl_2(DMSO)_2$ (O-bonded)[137], plus the difference in covalent radii for the two metal ions of 0.12A, leads to a value of approximately 2.13A, similar to that found in this work and for the O-bonded ligand in $Ru(DMSO)_4Cl_2$.[125]

The *trans* influence of S- bonded DMSO ligands is illustrated more clearly in the mean Ru-Cl bond distance of 2.426A in $Ru(DMSO)_3Cl_3^-$,[128] which is significantly longer than those for the mutually *trans*- chlorine ligands in the octahedral systems $RuCl_3(N_2C_6H_4Me)PPh_3$,[138] Me_2O and $RuCl_3(NO)(PMePh_2)_2$.[139]

The possible relationship of the trans influence to any kinetic trans effect is discussed with the catalytic properties of the Ru-DMSO complexes (section 6vi).

The average sulphur-oxygen atom bond lengths in $Ru(DMSO)_6^{2+}$ are 1.482A (and 1.506A when corrected for the oxygen atom riding on the sulphur) for S-bonded, and 1.536A for O-bonded ligands, showing loss of sulphur-oxygen double bond character upon coordination via oxygen. This distance is, however, still considerably shorter than the S - O single bond distance of 1.70A.[137] The geometry of the DMSO ligands is very similar to that found in free DMSO.[123] Average O-S-C, C-S-C angles and S - C bond lengths for the S- bonded ligands are 106.7 deg, 98.8 deg, and 1.77A respectively. For the O- bonded ligands, corresponding values are 104.0 deg, 99.1 deg, and 1.76A, while for free DMSO, they are 107 deg, 98 deg, and 1.80-1.82A.[123]

The packing within the unit cell can be considered to approximate the fluorite structure, each $Ru(DMSO)_6^{2+}$ cation being surrounded by eight anions at the corners of an irregular cube, and each BF_4^- anion being surrounded by four $Ru(DMSO)_6^{2+}$ cations in an irregular tetrahedral array. No unusually short interatomic contacts are found.

Spectroscopic Data (Professor Brian James et al., University of British Columbia).

The i.r. spectra of dimethyl sulphoxide complexes are diagnostic of the bonding mode; S-bonding usually causes an increase of ν(S-O) to about 1100 cm^{-1} (from the 1055cm^{-1} value

for free DMSO), whereas a shift to the lower range of 1000-900 cm^{-1} is indicative of donation from oxygen.[123,128] A strong band around 1100 cm^{-1} for the $Ru(DMSO)_6^{2+}$ cation is attributed to S- bonded ν(S-O); a strong, sharp band at 935 cm^{-1} is assigned to O- bonded DMSO. This latter assignment is somewhat complicated by the presence of other bands in this region: there is a BF_4^- stretch at 990 cm^{-1}[140] (and at 525 cm^{-1}), and methyl rocking vibrations in the 950-1000 cm^{-1} region are also present.[123,128] However, the infrared of the fully deuterated complex which gives a band at 930 cm^{-1}, confirms the assignment of[128,129,141] ν(S-O), O- bonded. The assignment at 935 cm^{-1} is further confirmed in that it fits well to an observed correlation found between frequency shift of ν(S-O), on coordination of O-bonded sulphoxide, versus ν(M-O), the ν(Ru-O) stretch[128] being observed at 480 cm^{-1} in the present $Ru(DMSO)_6^{2+}$ cation.

In the nmr spectrum, downfield shifts of up to 1ppm are usually characteristic of S- bonded methyl protons, while the O- bonded ligands, in which the protons are further removed from the metal, show considerably less variation from the free value, (τ= 7.40).[128,129] The measured spectra of the $Ru(DMSO)_6^{2+}$ cation in various solvents at room temperature show singlets in the region τ= 6.70-6.90 due to S- bonded DMSO, together with singlets in the τ= 7.15-7.40 region due to O- bonded or free DMSO.

The nmr spectrum in d_6-DMSO at room temperature changes with time. Two minutes after dissolution of the cation, the spectrum shows free DMSO (τ= 7.40), O- bonded DMSO (τ= 7.15), and S- bonded DMSO (τ= 6.80 and 6.64), in the ratios

of ca. 1:2:3. This shows that one O- bonded DMSO is rapidly displaced; the resulting species should then have two S- bonded ligands (τ= 6.64) trans- to O- bonded DMSO and one S- bonded DMSO (τ= 6.80) trans- to d^6-DMSO. Integration of the peaks in the S- bonded region shows about a 2:5:1 ratio which is reasonably consistent considering that the peaks share a somewhat broad base line and that the spectra are time dependent. On standing, the intensity of the free DMSO peak increases with concomitant decreasing of the other three peaks; the ratio of the peaks in the S- bonded region remains close to 2:1, while the peak of the O- bonded DMSO decreases more rapidly than those of the S-bonded ligands. After 1 hour, the ratio of free DMSO:O- bonded:S- bonded is about 5:1:3. Slower exchange of the S-bonded compared to O- bonded DMSO seems typical of Ru(II) sulphoxide complexes.[129,142]

The nmr spectrum in D_2O at room temperature is of interest in that it shows the presence of four S- bonded, one O- bonded, and one free DMSO, a few minutes after dissolution. On standing, the O- bonded DMSO is displaced while the S-bonded ones are not exchanged, and after 30 minutes, the spectrum shows a multiplet in the S- bonded region and a singlet for free DMSO with an intensity ratio of 2:1, again consistent with four S- bonded DMSO ligands. The multiplet is not well resolved, but it could presumably result from the presence of a mixture of cis- and trans- isomers of $Ru(DMSO)_4(D_2O)_2$, (DMSO = S- bonded DMSO), or a five- coordinate species.

vi. Catalytic Properties

Detailed investigation of the catalytic properties of Ru-DMSO complexes has been made, and the following discussion is based substantially on the reported results.[142]

In N,N-dimethylacetamide solution at 60 deg C and 1 atmosphere H_2, the activated substrate acrylamide (0.8M) is reduced homogeneously with an initially linear rate of 5.0 x 10^{-6}M s^{-1} to propionamide, using a catalyst concentration of 10^{-2}M. The activity is similar using cis-$Ru(DMSO)_4Cl_2$, fac-$Ru(DMSO)_3Cl_3^-$, or fac-$Ru(DMSO)_6^{2+}$.

A mechanistic scheme which fits the observed kinetic data qualitatively and semi-quantitatively has been described[142] which involves activation of hydrogen and olefin via formation of a metal-hydride complex, and decomposition of the metal-alkyl species via protonolysis. This pathway; which is olefin dependent, relates in some aspects the structural results reported here and the accompanying spectral data. Rapid addition of H_2 to $Ru(DMSO)_3(DMSO)_3^{2+}$ leads to formation of the hydride $Ru(DMSO)_2(DMSO)_3H^+$. The loss of an O- bonded ligand is consistent with the ground-state Ru-O bond weakening implied in the crystal structure, and also with the increased lability of the O- bonded over the S- bonded ligands as seen in the nmr. The resulting hydride then undergoes rapid exchange with olefin at the now-labilised S- bonded DMSO trans- to H^-. The trans-$HRu(DMSO)_2(DMSO)_2(olefin)^+$ undergoes slow isomerisation to the cis- complex before the rapid insertion reaction to $Ru(DMSO)_2(DMSO)_2(alkyl)^+$ occurs. This trans- to cis-isomerisation is the rate-determining step in the overall reaction. Isomerisation

of six-coordinate complexes is usually considered to be slow,[122] and only a few hydrido-olefin complexes of unknown stereochemistry are known.[122] The step may proceed via either a five-coordinate intermediate, or, less likely, a seven-coordinate intermediate.

The final insertion step involves promotion of the electrons of the Ru-H bond into the olefin anti-bonding orbital which already contains considerable electron density due to effective π back-bonding from the metal. Since the insertion is fast, however, some electronic redistribution is implied.

vii Afterword

The chemistry of the Ru(II)/sulphoxide complexes discussed in this chapter is currently being extended in a number of areas, for instance in their interactions with nucleosides, purines, and pyrimidines[143]. Furthermore, the ratio of S-bonded to O-bonded sulphoxide ligands has been found to vary in different solvents and with variation in the alkyl substituents. Thus, these complexes serve as very flexible systems with which to study the catalytic abilities of a range of closely related complexes, with a view to being able to design within narrow specifications a complex with any desired catalytic activity.[144]

Appendix

The Nickel(II) Dihydrazone/2,3-Butanedione Reaction: Details of Syntheses and Spectra

The work described in this Appendix was carried out in the laboratory of Professor Neil Curtis, Department of Chemistry, Victoria University of Wellington, New Zealand. The author is grateful to Professor Curtis for supplying these unpublished results.

The ligand designations used (L0 through L4) are consistent with those used in Chapters 1, 2 and 3 of the text.

The infra red spectra included in this Appendix were recorded for samples prepared as KBr discs. The ultra violet/visible data were obtained from diffuse reflectance spectra.

Ai. $Ni(L1)(ClO_4)_2$

Preparation: At room temperature, the orange complex $Ni(L0)(ClO_4)_2$ (L0 = 3,5,5,10,10,12-hexamethyl-1,2,6,9,13,14-hexaaza-tetradeca-2,12-diene) dissolved readily in methanol containing 2,3-butanedione (1.2 mol equivalents). In minutes, a violet solution was formed, which deposited violet crystals over a period of several hours. This compound dissolved easily in water to give a violet solution, from which blue-violet crystals of $Ni(L1)(ClO_4)_2.H_2O$ were obtained.

Analysis: Found.....C,33.5; H,6.3; Ni,9.1%

$NiCl_2O_{11}N_6C_{16}H_{42}$ requires

(this assumes L1 = $C_{18}H_{40}N_6O_2$) C,33.4; H,6.5; Ni,9.1%

Spectra: u.v./visible shows two peaks characteristic of a triplet ground state Ni^{2+} ion.

18,200 cm^{-1}, ε = 1.6 mol^{-1} m^2

11,700 cm^{-1}, ε = 0.9 mol^{-1} m^2

i.r. - see figure A.1 (spectrum for $Ni(L0)(ClO_4)_2$ is given in figure A.2).

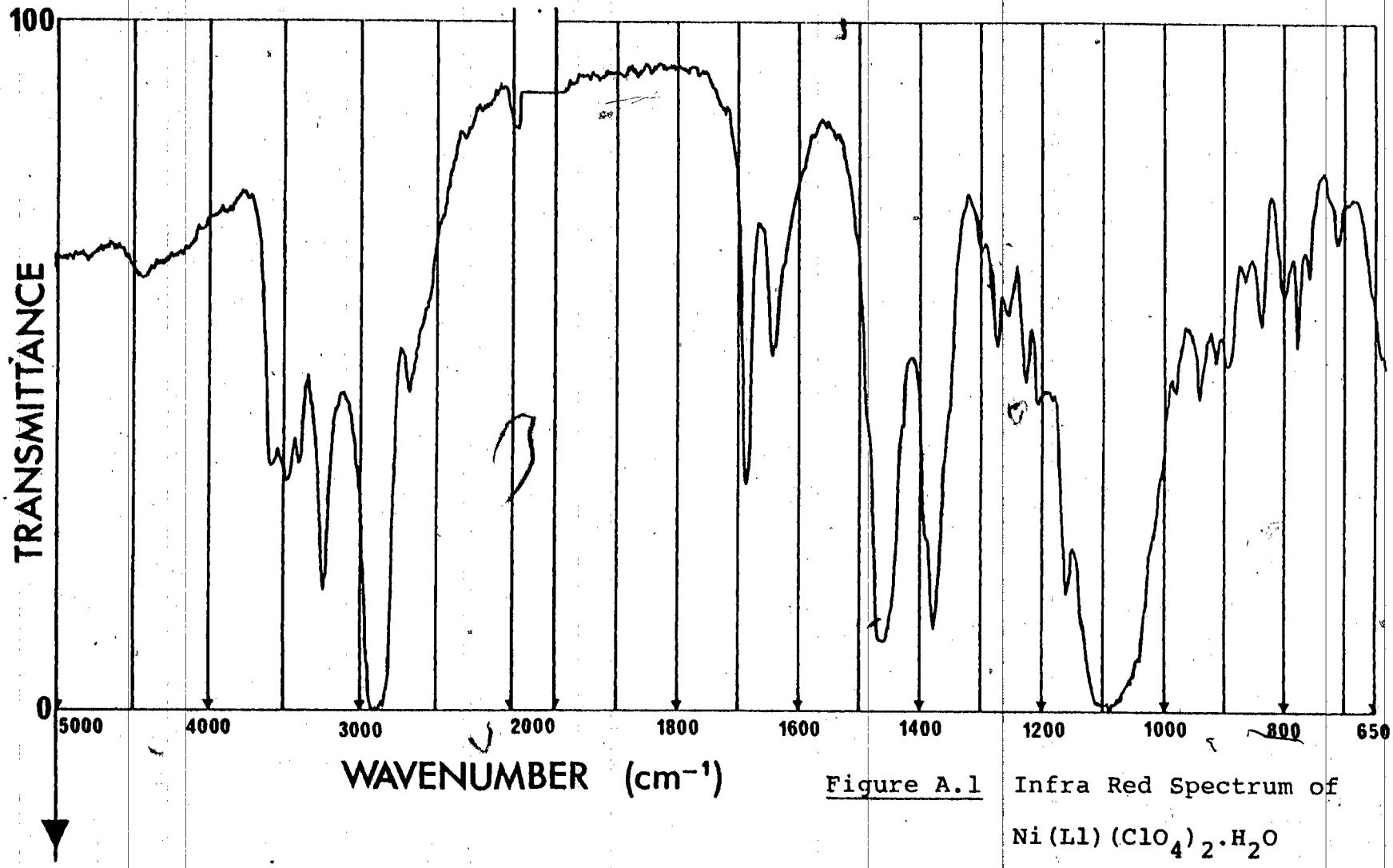

Figure A.1 Infra Red Spectrum of $Ni(Ll)(ClO_4)_2.H_2O$

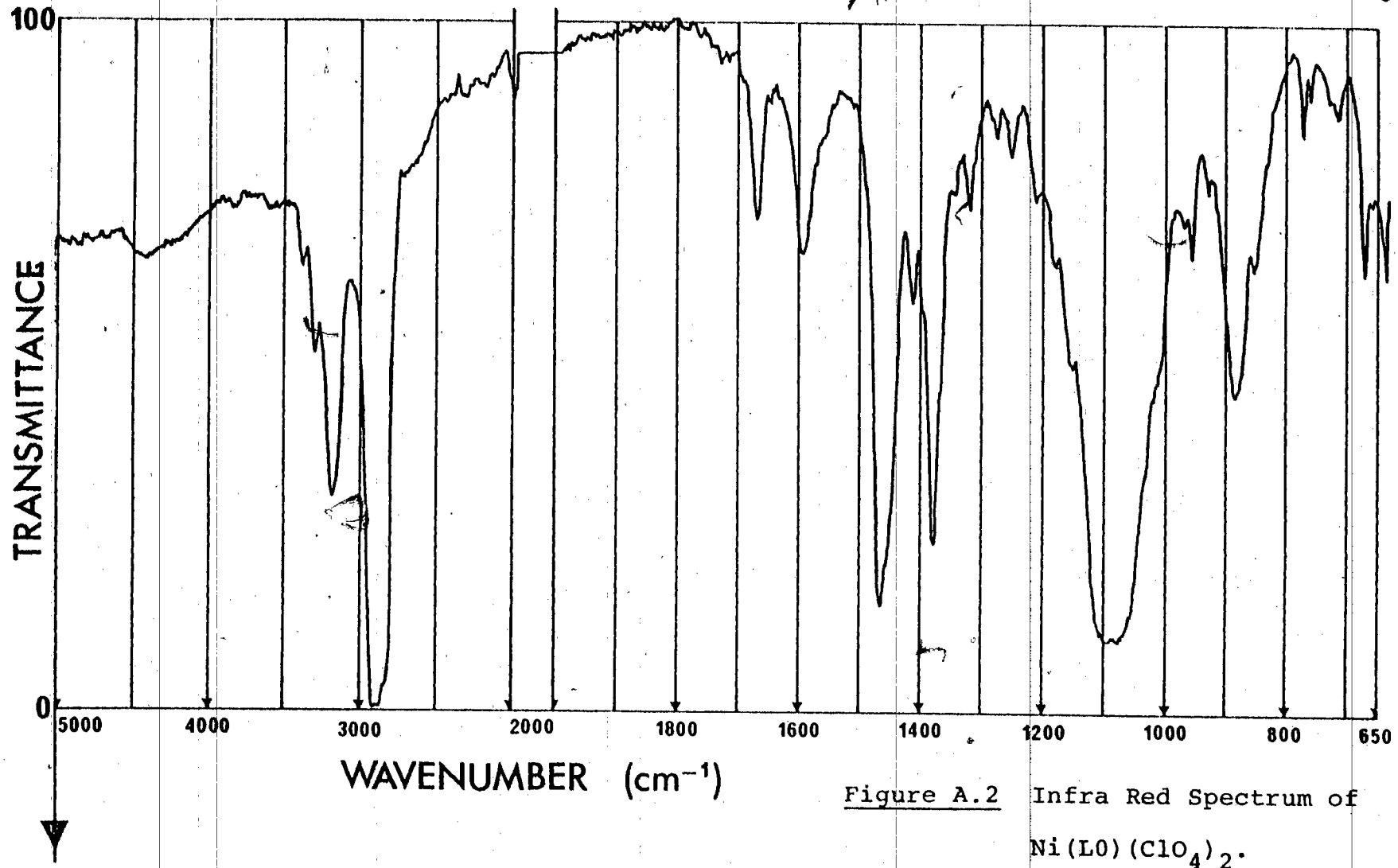

Figure A.2 Infra Red Spectrum of $Ni(L0)(ClO_4)_2$.

Aii. $\underline{Ni(L0)(NCS)_2.H_2O}$

Preparation: Addition of a concentrated blue/violet solution of $Ni(L1)(ClO_4)_2$ in acetonitrile to an ice-cold solution of sodium thiocyanate (2.2 mol equivalents) in water gave a deep blue solution from which blue crystals of $Ni(L0)(NCS)_2.H_2O$ were deposited over a period of several hours, and which were not further recrystallised.

Analysis: Found.....C,41.3; H,7.3; Ni,10.1%

$NiS_2N_8C_{16}H_{34}O$ requires...C,40.3; H,7.2; Ni,12.3%
(assuming L0)

$NiS_2N_8C_{20}H_{40}O$ requires...C,43.9; H,7.4; Ni,10.7%
(assuming L1)

Spectra: i.r. - see figure A.3

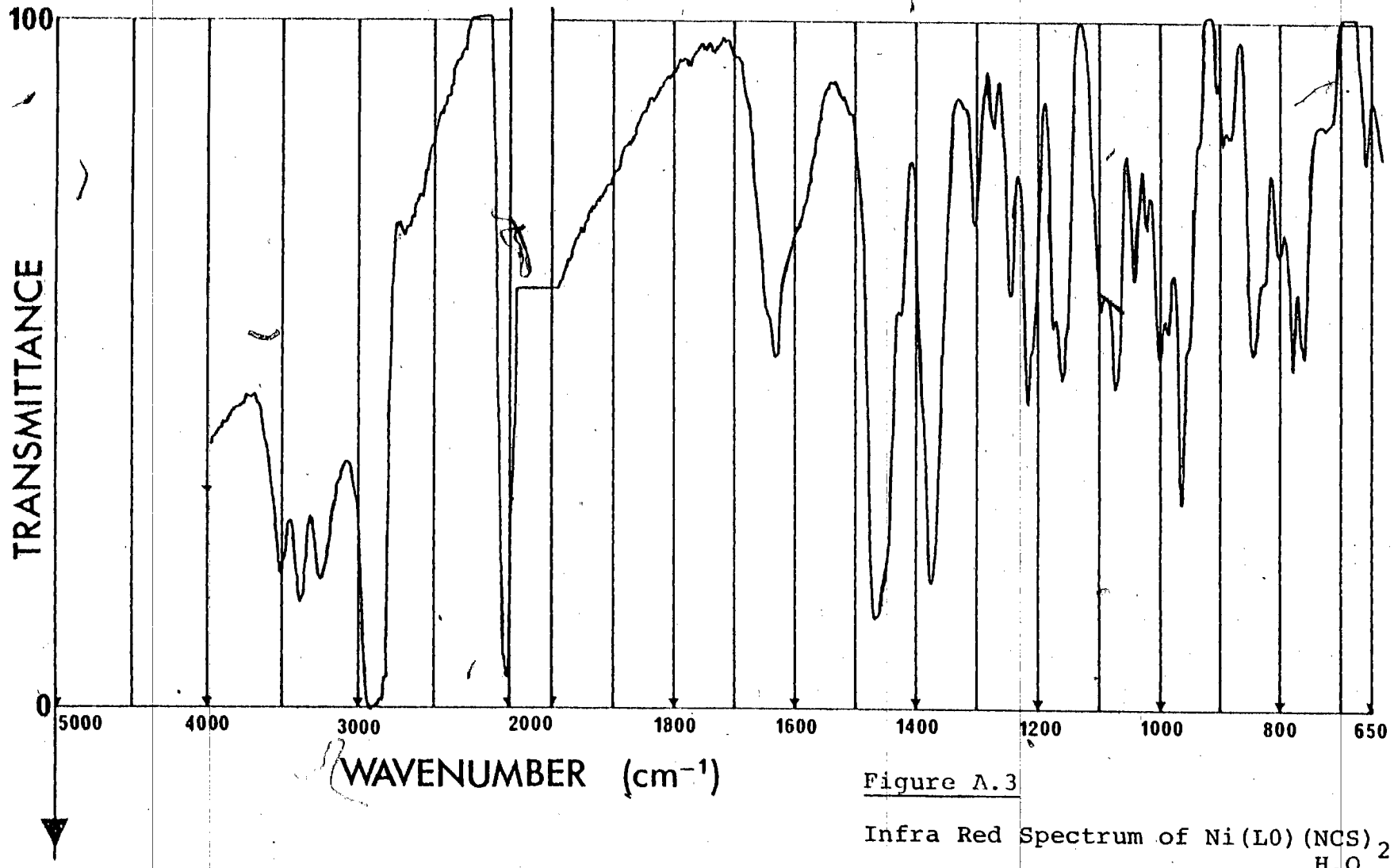

Figure A.3

Infra Red Spectrum of $Ni(L0)(NCS)_2 \cdot H_2O$

Aiii. $\underline{Ni(L0)NO_2(ClO_4)}$

Preparation: A concentrated blue/violet solution of $Ni(L1)(ClO_4)_2$ in acetonitrile was added to an ice-cold solution of sodium nitrite (1.2 mol equivalents) in water. Dark blue crystals of $Ni(L0)NO_2(ClO_4)$ were isolated from this solution after several hours at 0 deg C, and they were not further recrystallised.

Analysis: Found.....C,35.5; H,6.7; Ni,11.5%

$NiClO_6N_7C_{14}H_{32}$ requires C,34.5; H,6.6; Ni,12.0% (assuming L0)

$NiClO_8N_7C_{18}H_{38}$ requires C,37.7; H,6.7; Ni,10.2% (assuming L1)

Spectra: i.r - see figure A.4

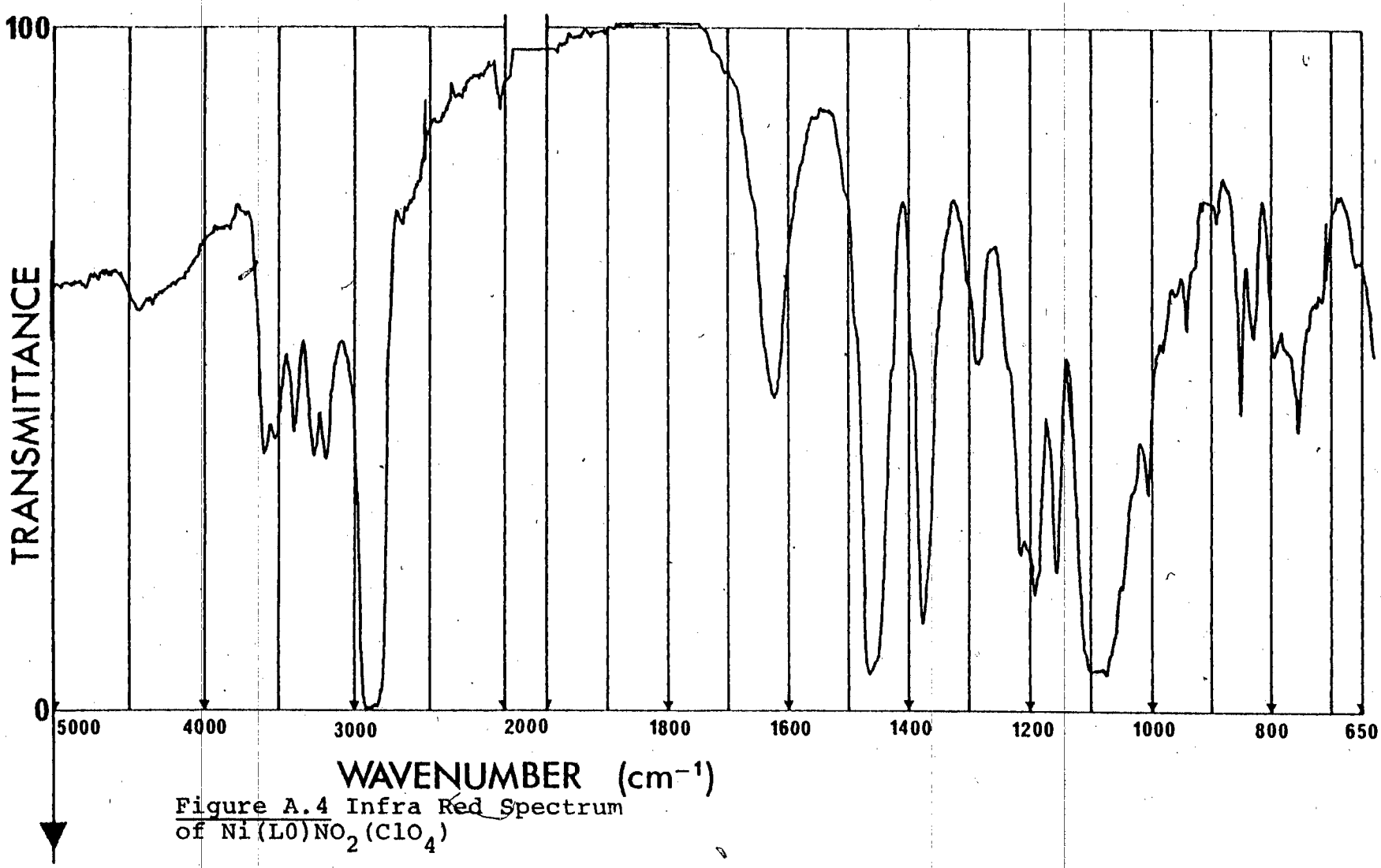

Figure A.4 Infra Red Spectrum of $Ni(L0)NO_2(ClO_4)$

Aiv. $\underline{Ni(L2)H_2O(ClO_4)_2.3H_2O}$

Preparation: When the blue/violet compound $Ni(L1)(ClO_4)_2$ was dissolved in water and allowed to stand for a period of hours, blue crystals of $Ni(L2)H_2O(ClO_4).3H_2O$ were obtained.

Analysis: Found.....C,32.3; H,6.5; Ni,8.6%

$NiCl_2O_{13}N_6C_{18}H_{44}$

requires.....C,31.7; H,6.5; Ni,8.6%

Spectra: u.v./visible - shows the two peaks characteristic of triplet ground state Ni^{2+}

18,300 cm^{-1}; ε = 2.0 $mol^{-1}m^2$

11,300 cm^{-1}; ε = 1.8 $mol^{-1}m^2$

i.r. - see figure A.5

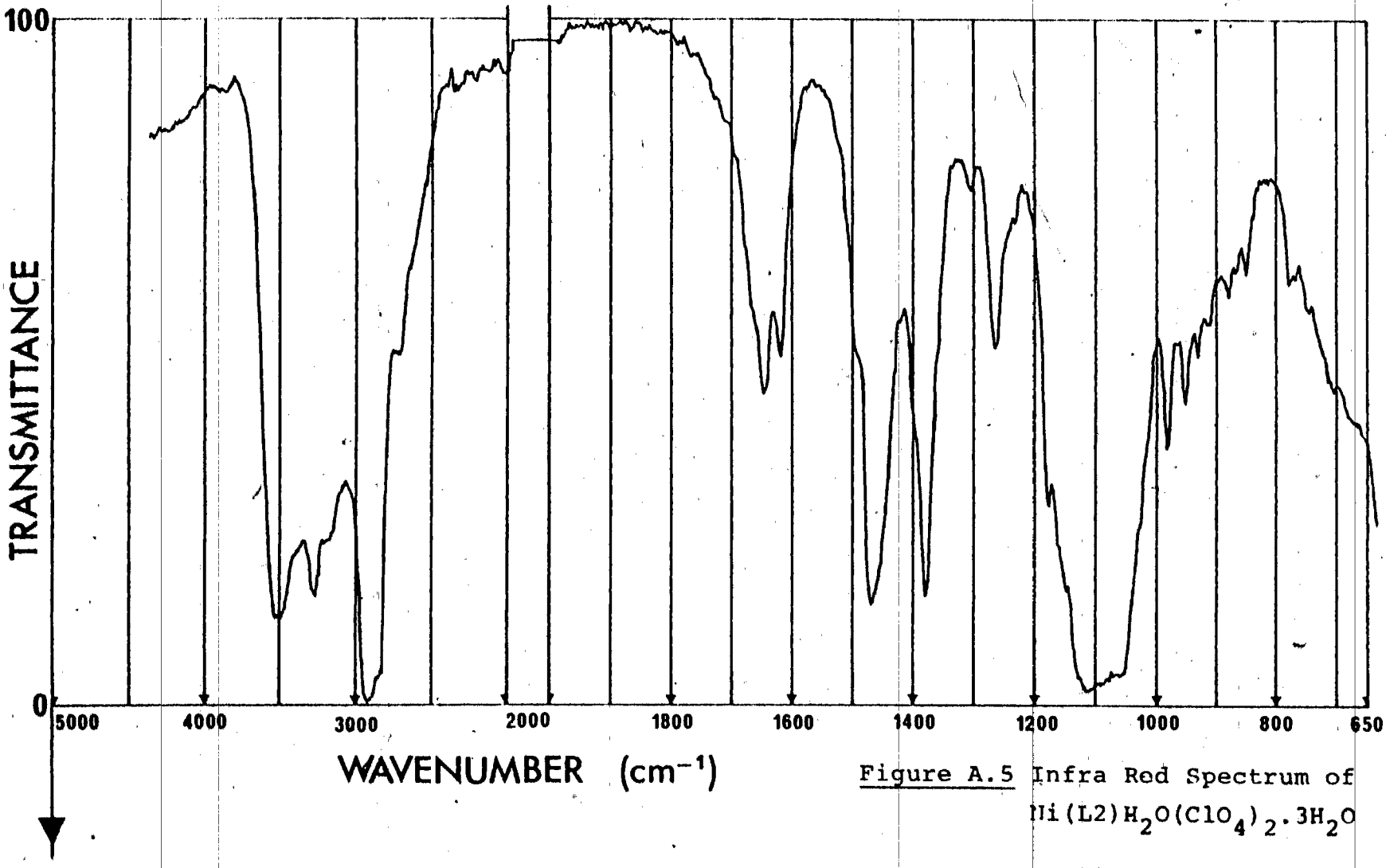

Figure A.5 Infra Red Spectrum of $Ni(L2)H_2O(ClO_4)_2.3H_2O$

Av. $\underline{Ni(L3)(ClO_4)_2}$

Preparation: A solution of $Ni(L1)(ClO_4)_2$ in methanol was allowed to stand at room temperature for ca. 24 hours, during which time, orange crystals of $Ni(L3)(ClO_4)_2$ were deposited. These crystals were filtered off and recrystallised from a solution in hot methanol.

Analysis: Found.....C,35.7; H,6.0; Ni,9.5%

$NiCl_2O_9N_6C_{18}H_{36}$ requires C,35.4; H,6.0; Ni,9.6%

Spectra: u.v./visible - shows a single maximum at 22,400 cm^{-1} (ε = 13.9 $mol^{-1}m^2$) consistent with singlet ground state Ni^{2+}.

i.r. - see figure A.6.

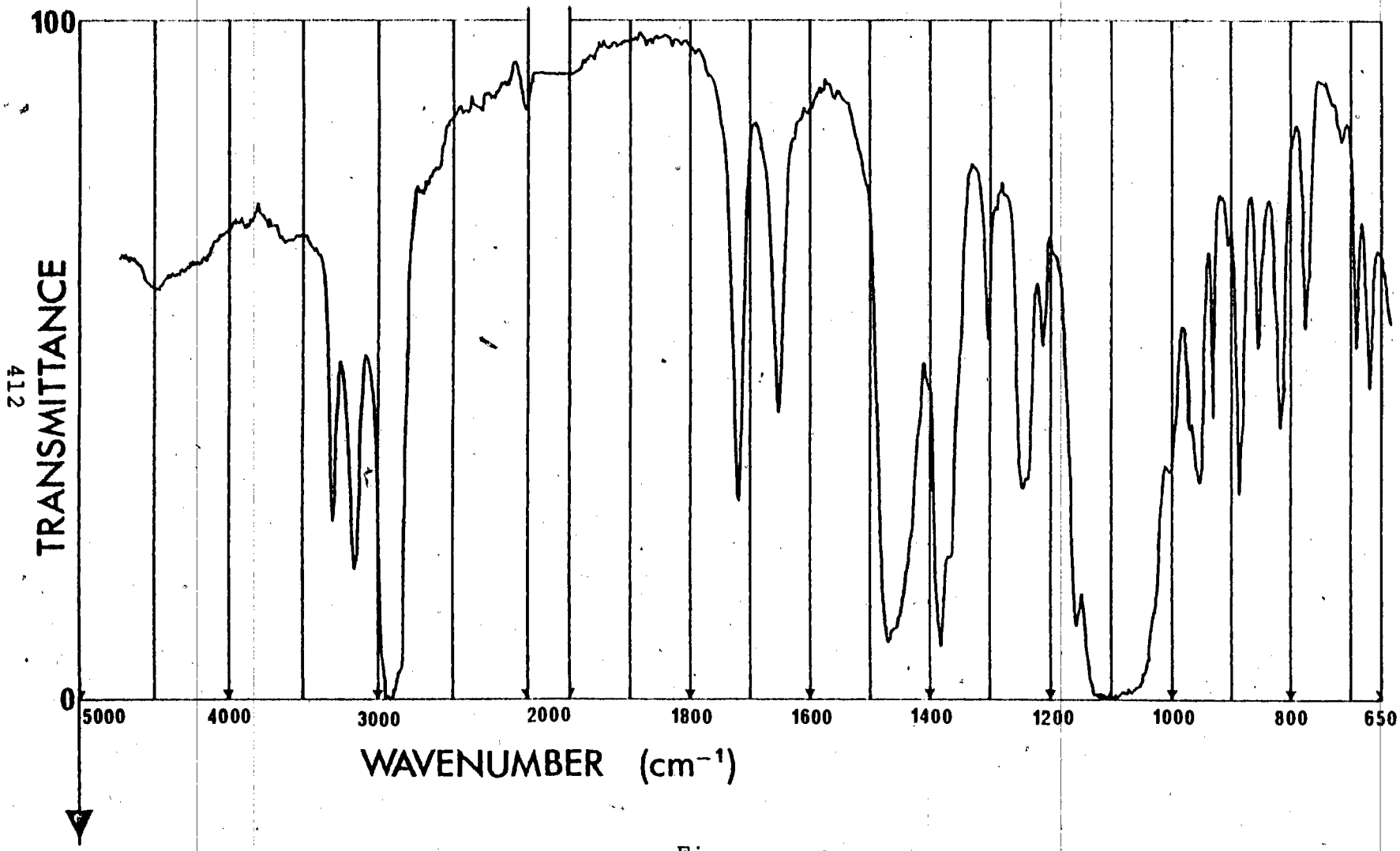

Figure A.6 Infra Red Spectrum of $Ni(L3)(ClO_4)_2$

Avi. α-$Ni(L3)NO_2(ClO_4)$

Preparation: A concentrated solution of the orange complex $Ni(L3)(ClO_4)_2$ and sodium nitrite (1.2 mol equivalents) in water gave an immediate lavender-coloured solution of α-$Ni(L3)NO_2(ClO_4)$. The compound isolated from this solution was recrystallised from an isopropanol/acetonitrile solvent mixture.

Analysis: Found.....C,38.8; H,6.5; Ni,10.6%

$NiClO_7N_7C_{18}H_{38}$ requires....C,38.8, H,6.5; Ni,10.6%

(this assumes L3 as in $Ni(L3)(ClO_4)_2$)

Spectra: u.v./visible - shows two maxima characteristic of triplet ground state Ni^{2+}, at 19,800 cm^{-1} and 10,500 cm^{-1}.

i.r. - see figure A.7

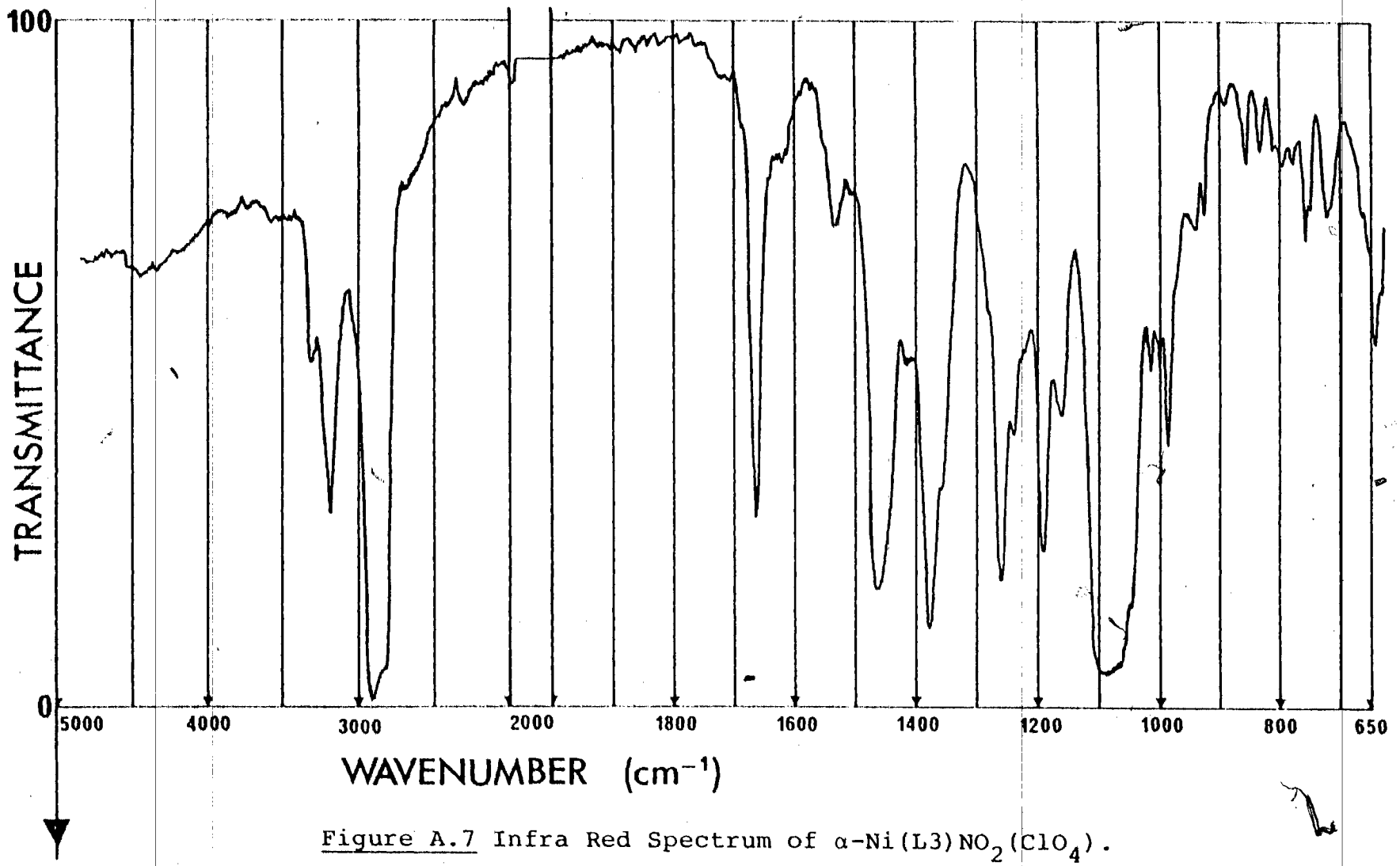

Figure A.7 Infra Red Spectrum of α-Ni(L3)$NO_2(ClO_4)$.

Avii. β-$Ni(L3)NO_2(ClO_4).\frac{1}{2}H_2O$

Preparation: The orange complex $Ni(L3)(ClO_4)_2$ was dissolved in methanol and added to a solution of sodium nitrite (1.2 mol equivalents) in methanol. Initial formation of a lavender solution was observed (presumed to be α-$Ni(L3)NO_2(ClO_4)$ see below), but if the solution was allowed to stand for approximately one week, blue crystals were obtained which were filtered off and recrystallised from a hot methanol/water solvent mixture. The same blue compound could be prepared from dissolution of α-$Ni(L3)NO_2(ClO_4)$ in methanol to give a mixture which was allowed to stand for several days.

Analysis: Found.....C,38.2; H,6.6; Ni 10.6%

$NiClO_{7.5}N_7C_{18}H_{37}$
requires...C,38.2; H,6.6; Ni,10.4%

Spectra: u.v./visible - shows two maxima characteristic of triplet ground state Ni^{2+}, at 17,200cm^{-1} and 11,000cm^{-1}.

i.r. - see figure A.8.

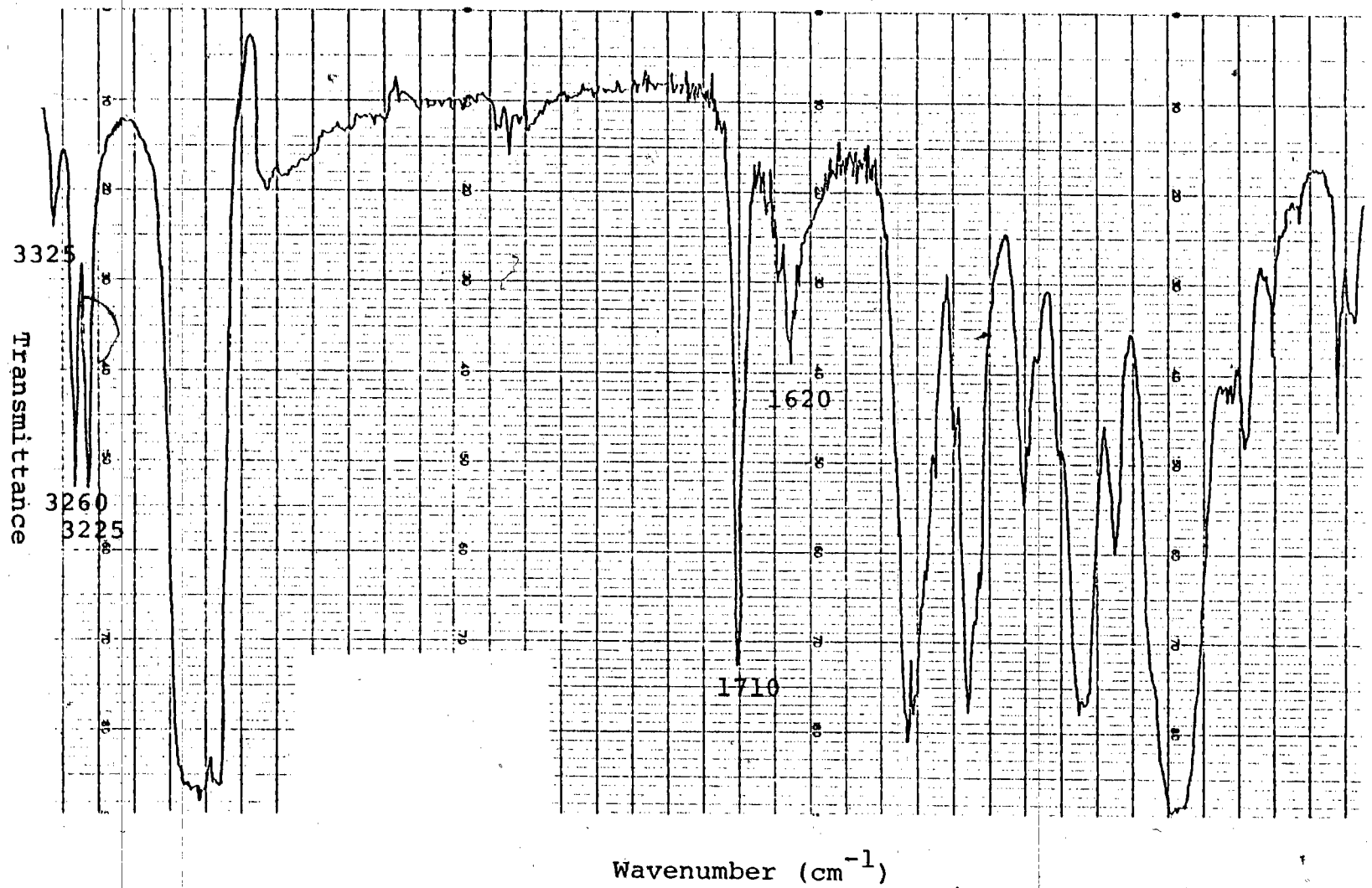

Figure A.8 Infra red spectrum of β-Ni(L3)$NO_2(ClO_4).\frac{1}{2}H_2O$

Aviii. $\underline{Ni(L4)(ClO_4)_2}$.

Preparation: When a solution of $Ni(L1)(ClO_4)_2$ in water was allowed to stand for 2 to 3 days, a red solution was formed from which salmon - red crystals were obtained. These were recrystallised from hot water.

Analysis: Found.....C,36.8; H,5.9; Ni,10.0%

$NiCl_2O_8N_6C_{18}H_{34}$ requires C,36.5; H,5.9; Ni,9.9%

Spectra: u.v./visible - shows a single maximum at 21,500 cm^{-1} (ε = 4.7 $mol^{-1}m^2$), characteristic of singlet ground state Ni^{2+}.

i.r. - see figure A.9.

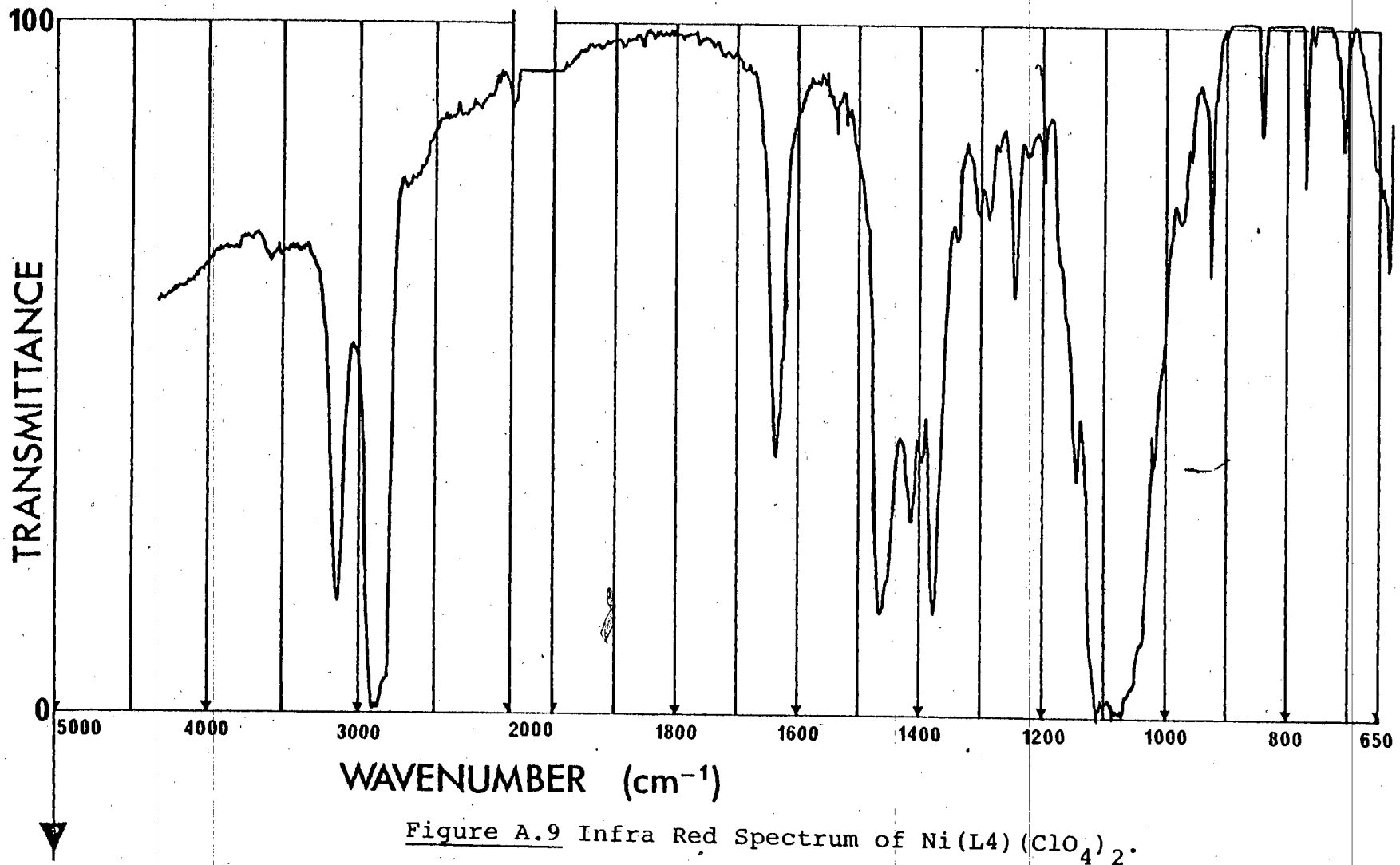

Figure A.9 Infra Red Spectrum of $Ni(L4)(ClO_4)_2$.

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