CRYSTAL STRUCTURE DETERMINATIONS
OF
μ-OXO BIS SULFATO TETRAKIS (2,2'-BIPYRIDINE)-VANADIUM(III)-15-WATER
AND
fac-BROMO (PHENYL BIS(3,5-DIMETHYLPYRAZOLYL)-PHOSPHINO) TRIS CARBONYL RHENIUM (I)

by

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ABSTRACT

The crystal structures of two compounds, $(bipy)_2(SO_4)VOV(SO_4)(bipy)_2 \cdot 15H_2O$, where bipy is 2,2'-bipyridine, and $Re(CO)_3Br(P(Me_2pz)_2(C_6H_5))$, where Me_2pz is 3,5-dimethylpyrazolyl, were determined by single crystal X-ray diffraction. The first compound had a monoclinic unit cell, space group C2/c, with a=12.764(8), b=21.80(2), c=19.08(1)Å, β=96.04(3), Z=4, and D_{calc}=1.516. The structure was refined by full-matrix least-squares procedures to a conventional R factor of 0.086 for 1286 independent observations. The molecule consists of a dimer with a slightly bent (170(1)°) oxo oxygen bridge with V-O=1.776(4)Å. The two halves of the dimer are related by a crystallographic 2-fold axis which passes through the bridging oxygen. Each vanadium atom is coordinated to two bipyridine ligands and a monodentate sulfate group located cis to the sixth coordination site occupied by the bridging oxygen. The structural model is consistent with the composition given but other oxidation states for the vanadium atom cannot be ruled out. The water molecules link the dimeric units throughout the lattice via hydrogen bonds to the sulfate groups and among themselves.

The unit cell for the rhenium compound was also monoclinic, space group $P2_1/c$, with a=8.964(4), b=14.441(10), c=18.156(8)Å, β=111.32(4)°, Z=4, D_{meas}=1.94, and D_{calc}=1.969. The structure was refined by full-matrix least-squares procedures to a conventional R factor of 0.085 for 1362 independent observations. The rhenium atom is coordinated to three carbonyl groups, a bromine atom, and one nitrogen atom from each of the 3,5-dimethylpyrazolyl rings. The three carbonyl groups define one of the triangular faces of the octahedron of coordination. The six-membered ring defined by the rhenium, nitrogen, and phosphorous atoms has a skewed boat configuration.

The relatively poor agreement obtained in the refinement of both structures can be attributed to systematic errors which possibly arose from uncorrected misorientation of the crystals during data collection.

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INTRODUCTION

Original Research Proposal

The original research proposal for this degree was to determine the X-ray diffraction crystal structure of three vanadium compounds which were reported in the literature to be mixed-valent in character. In each case the species in question was thought to consist of two vanadium ions of different oxidation states joined by one or two hydroxo or oxo species and surrounded by various ligands. The ligands which were involved in the three compounds proposed were 2,2'-bipyridine, cyanide ion, and 2,2',2"-terpyridine. It was hoped that the proposed research would definitely determine whether the compounds were indeed specimens of a class of complexes known[1] as Class II mixed-valence compounds. These complexes are described as consisting of coordinated metal ions forming a polymer with each metal site possessing a slightly different ligand field. The differences in the ligand field strengths are large enough to permit the isolation of two different oxidation states but small enough to permit a small amount of electron exchange between the different metal sites.

The earliest reports[2,3] of the existence of the first compound were short comments which proposed that the compound consisted of hydroxo-bridged vanadium centres, each of which was coordinated to two 2,2'-bipyridine ligands. A later, more detailed, study[4] proposed the formulation $V_2L_4(OH)_2(SO_4)\cdot nH_2O$, where L is 2,2'-bipyridine and n=8,11,14, based mainly upon elemental analyses of various samples. In this second study there was some ambiguity concerning the type and number of bridging species. This ambiguity, as well as unusual magnetic and spectral properties, prompted these authors to postulate that the compound was mixed-valent in character. The magnetic moment of $3.3\pm.2$ B.M. appeared to indicate that

V(II) centres were present in the compound along with the expected V(III) ions since V(III) ions alone produce a magnetic moment of only 2.9 B.M. or less. The u.v.-visible spectra consisted mainly of two high intensity peaks. The peak positions (16,000 and 19,000 $cm.^{-1}$) as well as the molar extinction coefficients (1200) were not characteristic of normal V(III) species. Three possible mechanisms were put forward by Murray and Sheahan as possible explanations for the high extinction coefficients. These mechanisms were: 1) relaxation of the Laporte rule by charge transfer between the metal orbitals and the ligand orbitals, 2) the possibility of an intensity enhancement arising from an exchange-induced mechanism which works better with oxo-bridged species than with hydroxo-bridged species, and 3) mixed-valence charge transfer. The mustard yellow species[3] $(VL_2Cl_2)^{2+}$ showed no intense bands and indicated that relaxation of the Laporte rule was not likely to occur with the V(III)-bipy system although a V(II)-bipy system $(VL_3)^{2+}$ was known to utilize this mechanism. The assumption that hydroxy bridges were present in the dimer tended to eliminate an exchange-induced mechanism since hydroxo-bridged species are very poor at promoting intensity enhancement. These arguments left only mixed-valence charge transfer as a likely explanation of the high intensity. The high magnetic moment appeared to support this view. The compound was thus postulated to be a V(II)-V(III) mixed-valent dimer with the configuration of the bridge open to some doubt about the number of bridging hydroxy species.

The second compound which was considered was observed[5] to be the initial product formed when V(III) was added to saturated potassium cyanide solutions. If these dark blue solutions were left at room temperature for several hours, they would decompose to a deep wine coloured solution from which $K_4V(CN)_7$ was isolated. If, however, the initial solution was cooled, then a compound with the formula $K_{3.5}V(CN)_{5.5}(OH)_{0.5}$ was isolated as a dark blue solid. From the elemental analysis reported, this solid has an average oxidation state which indicates that it is mixed-valence in character. This idea is supported by the electronic spectrum which consists of a single, intense band (17,000 $cm.^{-1}$) which is uncharacteristic of V(III) and is suggestive of mixed-valence compounds. The bridge is postulated as a hydroxo species since the infrared spectrum has an O-H stretching frequency at 3450 $cm.^{-1}$ but has no H_2O bending bands. As well, a band at 610 $cm.^{-1}$ is thought to indicate the presence of a V-OH-V bridge. If only one hydroxo entity is present, then the eleven cyanide ions must be arranged in one of several possible and very interesting configurations. One of these possibilities consists of one vanadium atom surrounded by five cyanide groups and the bridging hydroxo group while the other vanadium is coordinated to six cyanide groups and the bridge. The presence of unequal coordination numbers could help stabilize the two different oxidation states in geometries which are sufficiently different to produce different ligand fields with sufficient similarity to permit partial electron exchange as in Class II mixed-valence compounds. Another possibility involves two vanadium atoms in identical coordination spheres consisting of five terminal cyanide groups and one bridging hydroxo group and one bridging cyanide group. This combination would result in a Class II mixed-valence compound if the different oxidation states are partially localized or a Class IIIA mixed-valence compound if the two metal sites are fully sharing the two oxidation states. There are, however, no infrared bands which are characteristic of bridging cyanide groups in the spectrum of this compound. All this speculation of mixed-valence character depends solely upon the number of hydroxo or cyanide groups being correct.

The third compound which was proposed for structural research was postulated[6] as a dimer and was thought to be formed when a solution of 5×10^{-4}M V(III) and 5.7×10^{-4}M 2,2',2"-terpyridine developed a red color with peaks at 685 and 474 mμ. This was the only data available on this compound and any attempt to propose a structure would be pure speculation unsupported by any concrete physical data. The proposal that a dimeric species was present was put forward because the peak at 474 mμ was similar to a peak produced by an aquo dimer of vanadium[7] whose existence is transient and has an equilibrium constant of $10^{-3.9}$ for its formation from two aquated V(III) ions:

$$2V(H_2O)_6^{3+} \rightleftharpoons 2H^+ + 2H_2O + ((H_2O)_4V(OH)_2V(H_2O)_4)^{4+}$$

If the vanadium-terpyridine dimer does exist, then a number of important questions about its structure can be answered. It can be determined whether the terpyridine ligands are tris-chelating or only bis-chelating. The number and type of bridging species, as well as the number of coordinated water molecules, can also be determined.

Pitfalls

Of the three compounds mentioned, it was possible to obtain the structure of only one, $(bipy)_2(SO_4)VOV(SO_4)(bipy)_2 \cdot 15H_2O$. No serious attempt was made to obtain any of the vanadium-terpyridine compound, although it might be possible to obtain some by a procedure analogous to that used to obtain crystals of the vanadium-bipyridine compound (see Experimental section).

A considerable amount of time was spent trying to obtain suitable crystals containing the $(V_2(CN)_{11}(OH))^{7-}$ species. Following the reported procedure for preparing the potassium salt, it was possible to obtain only a powder, or, at best, a micro-crystalline collection of needle-like particles that were much too small to do anything with. The small particle size was thought to be due to the fact that the solid material precipitated rather quickly over a period of only two hours. Attempts at replacing potassium by other larger cations such as tetraethyl ammonium or hexaammine cobalt(III) were unsuccessful. The failure to secure the tetraethyl ammonium salt appears to have been due to the fact that the charge on the cation was quite different from that on the anion even though the sizes of the two ions were much more similar than in the potassium system. The use of the hexaammine cobalt(III) cation appeared to overcome this problem but the low solubility of the chloride salt of the cation in aqueous solutions appeared to be the limiting factor in the hoped for preparation. Because of the large charge of the anion, an attempt was then made to use a unipositive cation smaller than potassium in an effort to increase the solubility sufficiently to permit the precipitation to proceed slow enough to produce good crystals. The first attempt in this direction was the use of sodium in the form of a saturated solution of sodium cyanide to which the vanadium (III) salt was added. At temperatures at or below the freezing point of water, the very deep blue solutions were as stable as the potassium cyanide solutions, but precipitation did not occur as quickly as it did in the potassium cyanide solution. In fact, no precipitate was observed for a full week after which time plate-like crystals were observed to form. When the precipitation was complete, the solution was observed to be wine red in color and therefore indicated that some decomposition had occurred even though the temperature had been kapt rather low. The crystals, when dissolved in water, produced the same intense blue color as the potassium salt had done. The very quick loss of color in a few seconds as the anion decomposed in solution was also similar to the behaviour of the potassium salt.

Attempts were then made to obtain the unit cell parameters. The first photographs obtained were totally blank and showed no evidence of diffraction. When larger crystals were placed in the X-ray beam, a powder pattern was observed. Visual inspection under normal light showed that there was no apparent change in shape or the condition of the surface. Fresh crystals taken from the mother liquor and plaed on a filter paper showed extinction when viewed through a polarizing lens. The same crystals, when placed upon a microscope slide upon the stage of a polarizing binocular microscope, quickly became opaque to all light and no longer showed extinction through the polarizing lens. The only differences that were apparent were the intensity of the light on the crystal and the warmth of the microscope stage due to the light bulb underneath. By exposing fresh crystals to very bright lights while they are still on the filter paper, it was decided that light sensitivity was not the problem. It soon became apparent that the crystals were undergoing a change when their temperature was raised even a small amount above room temperature. From the lack of success at obtaining useful photographs, it was determined that the crystals were only stable for short periods at room temperature. Because of this quasi-stability, it was possible to obtain two photographs from which some information concerning the unit cell parameters was obtained. An oscillation photo, which was relatively easy to obtain with each new crystal before it decomposed, showed that one axial repeat distance was 8.95 Å. A zero level Weissenberg photo, which was the only one ever obtained, showed two reciprocal axes lengths and the angle between them to be 0.1356 and 0.1833 r.l.u. and 84.7°. From the dimensions obtained and the symmetries exhibited by the photos, the unit cell appears to be triclinic. Using the empirical formula $Na_7V_2(CN)_{11}(OH)$, the possible densities are integral multiples of 1.09. A very rough density measurement, made by dropping one crystal in carbon tetrachloride and another in chloroform, indicated that the density of the material is intermediate between the two (1.48 to 1.59). This, however, does not agree with any of the calculated values and indicates either that the molecular formula is wrong in some way i.e. inclusion of water) or that the unit cell volume is wrong. Either or both could be the cause of this anomaly. However, the answer to this and other questions concerning this compound will have to wait until a procedure is found to maintain the crystals at a low temperature at all times or another cation is found which will produce crystals with greater thermal stability.

After having so little success with the proposed compounds, a search was made to find other compounds whose structures had not been done and were interesting in a chemical sense. An attempt was also made to keep within the guidelines given in the original research proposal; to determine the structure of materials reported to be mixed-valence.

An attempt was made to synthesize a vanadium compound which possessed mixed-valence character but which had not been found in any search of the literature. The synthesis is based upon the reaction between vanadium II and

IV solutions uder acidic conditions in which a brown intermediate is observed[7] before forming vanadium III. It was hoped that this intermediate could be stabilized by putting chelating ligands on the metal ions before the reaction took place and, in order to keep the main reaction free from acidic hydrolysis, carry it out in an organic solvent like benzene or pyridine. In the reaction attempted, the ligand used was acetylacetone. The vanadium IV species was bis acetylacetonato oxo vanadium(IV) while the vanadium II species was bis acetylacetonato bis pyridine vanadium(II)[8]. The preparation of the second compound was complicated by rapid aerial oxidation while it was in solution. The only solid product ever obtained upon the combination of these two compounds was tris acetylacetonato vanadium(III). It was hoped that the product would be a species consisting of two vanadium atoms bridged by the oxo oxygen of the vanadium IV entity. The vanadium atom which started with the higher oxidation state would also be coordinated to a square planar arrangement of chelating ligands and possibly a pyridine molecule in the position trans to the oxo bridge. The coordination sphere of the other metal atom would depend very much upon the nature of the vanadium II starting material. Since the reporte d synthesis of this material did not state whether the two pyridine ligands were cis or trans to each other, some ambiguity arises when trying to predict the configuration of any reaction products. If the pyridines were trans to each other, then the coordination sphere of the second vanadium ion in the final complex would be essentially identical to that of the other vanadium atom. If, instead, the cis conformation of the precursor was the true form, then the final complex could be formed with the two ends of the molecule with different coordination spheres; one end as described and the other with a pyridine cis to the bridge. No matter whether the configurations of the two ends are the same or not, it will still be possible to determine if the material is mixed-valence in character by comparing the bond lengths around the two metal atoms. This is apparent when both configurations are different since the end with the cis configuration has one vanadium-oxygen bond which has essentially the same environment as all the vanadium-oxygen bonds on the other end of the molecule. In order to obtain any of this material in the future, it will be necessary to work in an absolutely oxygen free environment. It would also be helpful to determine the best solvent to use in the coupling reaction in order to prevent proton addition to the bridge or oxidation of the vanadium II entity. As well, displacement of the ligands by the solvent must be avoided. Although it is not necessary, it would also be interesting to determine the configuration of the vanadium II starting material.

A second compound which was looked at was an aqueous chromium dimer with the bridge postulated[9] as either a single oxo oxygen or two hydroxo species. This material was formed either by shaking an acidic solution of chromous perchlorate with oxygen or by boiling a chromic perchlorate solution. This dimeric species was isolated in the solid state by producing an acid sulfate salt. In attempting to produce this material, the solid obtained consisted of microcrystalline particles which were much too small to use in any attempt at single crystal X-ray diffractometry. Because of this difficulty and the lack of success at increasing the particle size by recrystallization, the investigation of this compound was curtailed. It was hoped that if the investigation was successful, then the character of the bridge and the environment of the metal atoms could be clarified.

A material reported[10] as $1.2(K_4Mn(CN)_6)0.7(K_3Mn(CN)_6)\cdot 0.25H_2O$, and characterized as a mixed-valence material, was sufficiently intriquing to warrant an attempt to clarify the structure. The fact that the physical characteristics of this compound were different from, and intermediate between, both $K_4Mn(CN)_6 \cdot 3H_2O$ and $K_3Mn(CN)_6$ suggested that an investigation of this compound would be worthwhile. However, when the crystals were examined, they were found to consist of very thin needles which were too thin for single crystal work. The initial report of this material stated that shorter, thicker crystals, as well as needle-like crystals, were obtained. No such luck was encountered in this laboratory. This lack of success would appear to be the result of the difference in growth times. The literature method reports that it took up to two weeks for the crystals to form while they were obtained within two days by this lab.

In the course of the reduction of chlorotungstates[11] in concentrated hydrochloric acid solutions, a deeply violet compound of tungsten is formed. This material was initially reported[12] to be $K_2W(OH)Cl_5$ but an infrared study[13] showed that the compound should be formulated as an oxygen-bridged dimer, $K_4(Cl_5WOWCl_5)$, with a bent bridge. As well, a comparison of the electronic spectrum of other oxygen-bridged species suggests that the tungsten atoms are not tungsten IV, but are, instead, in two different oxidation states, tungsten III and tungsten V. This mixed-valence character is also supported by a polarographic study[14] which showed that the coulometric reduction of chlorotungstates proceeds directly from tungsten V to tungsten III. If this is indeed a mixed-valence material, then it must be either Class II or Class IIIA. In preparing this material, crystals were obtained which were much too small to use in single crystal diffractometry. Because of the very high acidity used in the preparation and the tendency of the material to decompose by oxidative hydrolysis, attempts at recrystallization in order to increase the crystal size were unsuccessful. There is, however, hope that larger crystals can be produced by controlling the reaction conditions since previous workers report obtaining dark red square platelets.

Dr. Sams of U.B.C. produced a material formulated as Fe(OEP)ClO_4·2EtOH, where OEP is octaethylporphyrin, which exhibited a spin crossover when the ethanol molecules of solvation were removed under vacuum. It became apparent that the crystals supplied were also losing ethanol by evaporation and the remaining portion of the molecule compensated for this loss by shifting enough to disturb the long range order of the crystal. The unit cell is either monoclinic, with $\beta=90^\circ$, or orthorhombic with a=10.13, b=18.14, c=11.73, and Z=2. The ambiguity in the symmetry of the unit cell arose from the apparent lack of symmetry of the oscillation photograph obtained about the <u>a</u> axis which could be the result of a misalignment of the crystal. Because of the lack of stability of the crystals, the ambiguity could not be conclusively resolved although the orthorhombic cell is preferred.

The Second Compound

After obtaining the structure of $(SO_4)L_2VOVL_2(SO_4 \cdot 15H_2O$ and experiencing numerous difficulties searching for other compounds whose structures had not been done and were worth investigating, a sample was kindly provided by Dr. L.K. Peterson. The compound was formulated[15] as $Re(CO)_3Br(P(Me_2pz)_2C_6H_5)$ where Me_2pz is 3,5-dimethylpyrazolyl. Elemental analysis, ^{31}P and ^{1}H n.m.r. spectra, and mass spectra confirmed this formulation and indicated that, besides coordination by the three carbonyl groups and the bromide ion, the rhenium atom was coordinated by the 2-N sites of the two pyrazolyl rings of the phosphine ligand. This particular ligand is one of a series of ligands which can be described as $(P(pz)_n(C_6H_5)_{3-n})$ where n can be 1,2, or 3 and pz is either pyrazolyl or 3,5-dimethylpyrazolyl. An analogous series of ligands which has been investigated more extensively than the above mentioned series are the polypyrazolylborate anions[16] $(B(pz)_nR_{4-n})^-$ where n is 1,2,3, or 4 and R is an organic group or hydrogen. The boron series has been observed to always coordinate to metal species through the 2-N sites on the pyrazolyl rings. Since the boron atom is tetrahedrally surrounded by organic groups of one sort or another, the ligands can, at best, utilize a maximum of three pyrazolyl groups to coordinate to a metal species. In this respect the actions of the phosphine ligands are similar since the phosphorous atom also experiences tetrahedral coordination with the fourth site being occupied by a lone pair of electrons. This lone pair of electrons permits the phosphine ligands to exhibit coordination radically different from that of the borate ligands when the number of pyrazolyl entities on the ligands is low. Thus, when there are no pyrazolyl groups, the well known triphenylphosphine results. This popular ligand always coordinates to metal sites through the lone pair. When one pyrazolyl group is attached to the phosphorous atom a strange state of affairs arises. It has been observed[15,17] that this ligand coordinates to a metal species through both the phosphorous and the 2-N nitrogen atoms. Apparently the lone pair on the phosphorous atom is sufficiently active to compete with the lone pair on the nitrogen atom. An intermediate was isolated[15] in which only the phosphorous atom was coordinated. This appeared to indicate that the phosphorous lone pair was slightly stronger than the nitrogen lone pair in the ability to coordinate to a metal site. The question which is to be answered by a crystal structure study of the aforementioned rhenium compound is whether the phosphorous atom is still capable of coordination when there are two pyrazolyl units attached or, as indicated by the ^{31}P and ^{1}H n.m.r. and the mass spectra, the two pyrazolyl groups are sufficiently electron withdrawing to neutralize the coordinating ability of the phosphorous atom and instead coordinate to the metal themselves as in the borate ligand series.

EXPERIMENTAL

$(bipy)_2(SO_4)VOV(SO_4)(bipy)_2 \cdot 15H_2O$

In making this compound, a departure was made from the reported[4] procedure which consisted of adding 2,2'-bipyridine to V(III) alum and obtaining a powder. The procedure, which was successful in producing good crystals, consists of adding 0.5 gm.(3.03 mmole) of 2,2'-bipyridine to a solution of 0.24 gm.(1.52 mmole) VCl_3 in 1 ml. H_2O. 0.75 gm. K_2SO_4 in 5 ml. hot water was then added to this purple solution. After warming the solution to dissolve any crystals formed at this stage and subsequently cooling the solution to -4° in the refrigerator overnight, the resulting small cluster of fairly large crystals (0.3-2.0 mm.) was filtered. After this disturbance, another crop of very much smaller crystals precipitated.

The compound prepared in this way was not chemically analysed, nor was the average oxidation state of the vanadium determined by titration for reasons given by other workers[4]. The U.V.-visible spectrum and the magnetic moment were not measured and in retrospect these measurements would have been desirable in order to confirm that the compound studied was the same as that reported by Murray and Sheahan[4].

$Re(CO)_3Br(P(Me_2pz)_2(C_6H_5))$

The following procedure was supplied by Dr. Peterson[15] and was the method used in his lab to produce the crystals used in this study.

A mixture of $(Re(CO)_4Br)_2$ (0.19 mmole) and $(C_6H_5)P(Me_2pz)_2$ (0.38 mmole) in benzene (10 ml.) was heated at 95-100° for 8 hours. The evolved carbon monoxide (0.36 mmole) was determined, the solution was evaporated to dryness under vacuum to give a residue which was recrystallized twice from chloroform-hexane and identified as $Re(CO)_3Br(P(Me_2pz)_2(C_6H_5))$.

STRUCTURE DETERMINATION AND REFINEMENT

$(bipy)_2(SO_4)VOV(SO_4)(bipy)_2 \cdot 15H_2O$

The purple-black plate-like crystals had a monoclinic unit cell with a=12.764(8), b=21.80(2), c=19.084(10)Å, β=96.04(3)°, and Z=4. Various photographs of reciprocal lattice layers indicated that the spacegroup was either Cc or C2/c. Structure solution and refinement was carried out successfully utilizing the latter space group. With a θ-2θ scan of base width 1.5 degrees in 2θ at a rate of 2° per minute and a 20 second background count on each side of a peak, intensity data for 2480 independent reflections with 2θ less than 40° was collected using a Picker FACS-I automatic diffractometer controlled by a PDP 8/E minicomputer. Nb filtered Mo Kα radiation was used. The 1286 reflections with $I>3\sigma(I)$, $(\sigma(I)=(N_{pk}+(t_{pk}/t_{bg})^2N_{bg})^{\frac{1}{2}}$, where N_{pk} is the peak count, N_{bg} is the total background count, t_{pk} is the time required for the peak count, and t_{bg} is the total time for the background count) were used in the subsequent analysis* and were given unit weights. The scattering factor tables were taken from Cromer and Waber[18] as were the tables for neutral atomic species. No attempt was made to correct for anomalous dispersion. A Patterson map enabled the positions of one vanadium atom and one oxygen atom to be determined. These two atoms were used to determine the signs of the structure factors. A Fourier map computed at this stage yielded the coordinates of the non-hydrogen atoms of the various ligands. An electron density difference map produced the coordinates of the water molecules of crystallization while the positions of the hydrogen atoms of the 2,2'-bipyridine ligands were calculated at 0.95Å from the ring carbon atoms. After all non-hydrogen atoms were refined with anisotropic temperature factors, the final R factor was 0.086 $(R=\Sigma||F_o|-|F_c||/\Sigma|F_o|)$ and would not go any lower. At this point, a difference map was calculated and did not reveal the presence of any more atoms, but did indicate that the anisotropic temperature parameters of the vanadium atom were not representing a perfectly accurate model of the electron density of the metal atom. There were three regions of excess electron density of approximately 1.0 electron per cubic Ångstrom ($eÅ^{-3}$) and one region of deficient electron density of approximately 1.6 $eÅ^{-3}$ in an electron density difference map with a standard error of 0.16 $eÅ^{-3}$. The final positional and temperature parameters are listed in Table I and the structure factors are in Table II.

* All calculations were performed on an IBM 370/155 computer. Programs used were FORDAP, crystallographic Fourier summation and peak searching (A. Zalkin); BUCILS, crystallographic structure factors and full-matrix least-squares (University of Canterbury); ORFFE, Fortran crystallographic function and error program (W.R. Busing, K.O. Martin, and H.A. Levy); ORTEP, Fortran thermal ellipsoid plot program for crystal structure illustrations (C.K. Johnson); and MEANPLANE, calculation of weighted mean planes through atom groups with esd's (M.E. Pippy and F.R. Ahmed).

TABLE I

Positional and Thermal Parameters of the Vanadium Compound

Positions in fractional coordinates x 10^4.

Atom	x	y	z
V	1011(2)	1312(2)	3210(2)
O	0	1381(10)	2500
O1	2112(9)	1813(6)	2790(7)
O2	3453(10)	2417(9)	3402(7)
O3	2954(12)	2573(11)	2150(9)
O4	1826(12)	2916(8)	2981(9)
O5	0	3588(11)	2500
O6	4606(12)	3079(8)	1546(9)
O7	1840(14)	1574(10)	-348(9)
O8	2816(14)	1722(12)	1032(10)
O9	3288(14)	657(10)	-423(10)
O10	4975(17)	1489(12)	3239(13)
O11	252(13)	4452(11)	1391(9)
O12	4349(15)	554(12)	971(10)
S	2586(5)	2434(4)	2832(3)
N1	436(12)	1992(8)	3814(9)
N2	1633(12)	500(10)	2877(9)
N3	176(12)	618(9)	3682(8)
N4	2025(11)	1291(9)	4204(8)
C11	-338(18)	2359(12)	3600(11)
C12	-806(16)	2792(12)	4025(13)
C13	-348(19)	2861(12)	4688(12)
C14	472(16)	2472(11)	4942(11)
C15	885(14)	2065(9)	4480(11)
C21	2393(22)	474(14)	2437(14)
C22	2821(18)	-92(18)	2233(14)
C23	2384(24)	-633(14)	2454(13)
C24	1613(18)	-608(13)	2924(13)
C25	1279(15)	-38(14)	3085(10)

TABLE I (continued)

C31	-614(17)	726(12)	4106(11)
C32	-1141(17)	245(13)	4378(12)
C33	-855(21)	-340(15)	4249(16)
C34	-80(17)	-447(13)	3826(13)
C35	429(15)	51(13)	3560(10)
C41	2812(17)	893(11)	4368(11)
C42	3456(15)	902(13)	4994(13)
C43	3164(18)	1302(14)	5518(11)
C44	2357(16)	1712(11)	5372(10)
C45	1755(13)	1670(9)	4706(11)

Thermal[a] parameters x 10^3.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
V	19(2)	68(2)	37(2)	-2(2)	3(1)	4(2)
O	41(10)	105(17)	14(9)	0	21(7)	0
O1	24(8)	68(11)	74(10)	-19(8)	13(6)	-8(8)
O2	45(9)	185(19)	57(10)	-13(10)	-10(7)	-21(10)
O3	75(13)	258(27)	81(13)	-94(15)	11(10)	41(15)
O4	53(10)	98(14)	121(14)	20(10)	-18(10)	-20(12)
O5	70(15)	112(21)	93(17)	0	9(12)	0
O6	80(12)	126(17)	121(15)	7(11)	50(10)	29(12)
O7	109(15)	190(23)	95(14)	3(14)	12(11)	11(14)
O8	102(15)	267(29)	115(16)	20(16)	19(12)	-51(17)
O9	93(15)	162(20)	132(17)	-11(13)	34(12)	15(15)
O10	136(18)	184(26)	204(23)	34(17)	23(16)	-19(20)
O11	70(12)	207(22)	92(14)	-6(13)	-9(10)	-15(14)
O12	93(15)	239(28)	126(18)	-33(16)	10(12)	36(17)
S	45(4)	112(7)	56(4)	-31(4)	-2(3)	7(4)
N1	14(9)	84(15)	54(13)	0(10)	-22(9)	14(11)
N2	9(10)	102(18)	38(12)	-4(11)	0(8)	26(12)
N3	39(12)	54(14)	45(12)	10(10)	-3(9)	-20(10)
N4	20(10)	82(14)	53(12)	10(10)	9(8)	8(12)

TABLE I (continued)

C11	54(15)	79(19)	59(16)	-15(15)	-16(13)	-7(15)
C12	39(14)	97(21)	73(18)	20(13)	7(13)	-30(16)
C13	75(18)	100(21)	56(17)	-2(16)	14(14)	-20(16)
C14	44(14)	78(18)	72(16)	18(14)	-11(12)	19(16)
C15	23(12)	45(14)	62(16)	12(11)	12(11)	-4(13)
C21	63(21)	98(24)	68(19)	2(18)	-20(15)	7(17)
C22	46(17)	130(29)	88(21)	14(20)	15(14)	-5(22)
C23	97(24)	97(26)	52(18)	12(19)	12(15)	-13(17)
C24	50(17)	86(24)	76(20)	11(16)	-3(13)	22(17)
C25	31(14)	68(19)	47(15)	22(14)	-11(11)	18(15)
C31	40(15)	112(23)	41(15)	4(15)	-5(12)	4(15)
C32	40(15)	74(20)	78(18)	-21(15)	26(12)	30(16)
C33	57(21)	104(28)	120(27)	-4(17)	-6(18)	25(21)
C34	24(14)	111(24)	84(19)	-3(15)	16(13)	-4(17)
C35	27(12)	71(20)	34(13)	-12(13)	-2(10)	-13(13)
C41	44(14)	77(18)	68(17)	24(13)	2(12)	-10(13)
C42	28(14)	127(24)	58(18)	6(14)	-28(12)	30(17)
C43	52(16)	128(24)	40(15)	-5(17)	-24(12)	2(18)
C44	36(13)	85(18)	45(14)	-17(13)	-14(11)	12(13)
C45	27(12)	28(13)	58(15)	2(10)	14(11)	6(12)

Calculated positions of hydrogen atoms (all with isotropic temperature parameters equal to 6.0) x10^4.

Atom	x	y	z
H11	-638	2357	3119
H12	-1406	3079	3862
H13	-656	3156	4971
H14	758	2540	5374
H21	2592	763	2275
H22	3302	-148	1895
H23	2603	-1056	2273
H24	1312	-988	3163
H31	-831	1196	4201
H32	-1723	324	4660

TABLE I (continued)

H33	-1237	-657	4484
H34	97	-885	3749
H41	3000	635	3993
H42	4094	630	5125
H43	3586	1326	5991
H44	2159	1986	5731
H6	1016	2113	-1766
H9	2868	2023	1443
H1'	4428	1827	3299

a The form of the anisotropic ellipsoid is $\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$.

$Re(CO)_3Br(P(Me_2pz)_2(C_6H_5))$

The colorless crystals had a monoclinic unit cell with a=8.964(4), b=14.441(10), c=18.156(8)Å, β=111.32(4)°, Z=4, D_{meas}=1.94 gm/ml., and D_{calc}= 1.969 gm/ml. The density was measured by floatation in a mixture of diiodomethane and iodobenzene. Photographs of layers of the reciprocal lattice indicated that the space group was $P2_1/c$. A crystal in the form of a rectangular prism of dimensions 0.09 mm.x0.25 mm.x0.33 mm. was used for data collection. With a θ-2θ scan of base width 1.5 degrees in 2θ at a rate of 2° per minute and a 20 second background count on each side of a peak, intensity data for 2057 independent reflections with 2θ less than 40° was collected using a Picker FACS-I automatic diffractometer controlled by a PDP 8/E minicomputer. The 1362 reflections with $I>3\sigma(I)$, $(\sigma(I)=(N_{pk}+(t_{pk}/t_{bg})^2N_{bg})^{\frac{1}{2}}$, where N_{pk} is the peak count, N_{bg} is the total background count, t_{pk} is the time required for the peak count, and t_{bg} is the total time for the background count), were used in the subsequent analysis* The scattering factor table for rhenium was taken from the International Tables for X-Ray Crystallography[19] while the tables for the rest of the atoms were obtained from Cromer and Waber[18]. Anomalous dispersion corrections were applied to the rhenium, bromine, and phosphorous atoms. After calculating structure factors with only the rhenium atom, which was located from a Patterson map, a Fourier synthesis was used to locate the bromine and phosphorous atoms. A difference Fourier map then revealed the positions of all other non-hydrogen atoms. Upon examination of the structure factors it was noted that the data could be split into four groups. This differentiation was based upon a comparison of the observed and calculated structure factors. A group of data was given its own scale factor if the majority of the data had the magnitudes of the observed structure factors larger than the magnitudes of the calculated structure factors or vice versa. No definite explanation for the fluctuation of the data was arrived at but it is possible that movement of the crystal away from the centered position could cause this behaviour. With the three heaviest atoms being treated as anisotropic and the lighter atoms remaining isotropic, the R factor was 0.085. With all non-hydrogen atoms being treated as anisotropic, the R factor was 0.078, but this decrease appeared to be due only to the increased number of parameters and was not a true indication of improved refinement since the lighter atoms showed no indication of anisotropy. Because of this, the lighter atoms were refined as isotropic and a difference map calculated on this basis revealed that there was still some electron density remaining around the site of the rhenium atom. There were four regions of excess electron density of approximately 1.4-2.2 $e\text{Å}^{-3}$ and two regions of deficient electron density of approximately 3.3 $e\text{Å}^{-3}$ in an electron density difference map with a standard error of 0.35 $e\text{Å}^{-3}$. Attempts to account for this by varying the weighting scheme from the unit weights used up to this point were unsuccessful. It was apparent that the reflection data was causing this problem but no systematic means of solving it was apparent. The refinement was halted at this point. The final positional and temperature parameters are listed in Table III and the structure factors are in Table IV.

* All calculations were performed on an IBM 370/155 computer. Programs used were FORDAP, crystallographic Fourier summation and peak searching (A. Zalkin); BUCILS, crystallographic structure factors and full-matrix least-squares (University of Canterbury); ORFFE, Fortran crystallographic function and error program (W.R. Busing, K.O. Martin, and H.A. Levy); ORTEP, Fortran thermal ellipsoid plot program for crystal structure illustrations (C.K. Johnson); and MEANPLANE, calculations of weighted mean planes through atom groups with esd's (M.E. Pippy and F.R. Ahmed).

TABLE III

Positional[a] and Thermal[b,c] Parameters for the Rhenium Compound

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re	-3(3)	2069(2)	817(1)	63(2)	38(1)	18(1)	10(2)	21(2)	-1(1)
Br	-1766(9)	3334(5)	-145(4)	93(6)	62(5)	34(4)	25(4)	10(4)	9(3)
P	535(20)	2960(12)	2843(8)	91(12)	42(10)	22(7)	5(10)	23(8)	2(8)

Atom	x	y	z	B
N11	127(5)	323(3)	150(2)	2.8(9)
N12	149(5)	347(3)	227(2)	3.2(9)
C11	237(7)	419(4)	254(3)	4.2(12)
C12	301(8)	452(5)	195(4)	5.6(16)
C13	230(7)	390(4)	134(3)	4.2(13)
C14	280(8)	464(5)	335(4)	5.8(16)
C15	241(7)	394(4)	50(4)	5.3(14)
N21	-169(4)	221(3)	145(2)	2.2(8)
N22	-125(6)	271(4)	216(3)	5.2(12)
C21	-270(7)	287(5)	229(3)	5.3(14)
C22	-399(7)	245(5)	169(4)	5.3(14)
C23	-320(8)	210(5)	128(4)	5.2(14)
C24	-280(9)	331(5)	307(4)	6.9(18)
C25	-422(7)	179(4)	34(4)	5.3(15)
C31	145(6)	184(4)	309(3)	3.1(11)
C32	314(7)	177(5)	339(4)	4.8(15)
C33	392(7)	99(4)	370(3)	4.4(14)
C34	303(7)	25(4)	379(3)	4.6(13)
C35	141(7)	25(4)	352(3)	4.5(13)
C36	61(7)	109(4)	317(3)	4.3(13)
C1	-98(8)	109(5)	28(4)	5.5(16)
O1	-175(6)	44(4)	-16(3)	7.1(12)
C2	110(6)	199(4)	12(3)	3.6(12)
O2	195(5)	186(3)	-24(2)	4.7(9)
C3	124(6)	118(4)	147(3)	3.0(11)
O3	225(6)	63(3)	179(3)	6.4(11)

TABLE III (continued)

a Parameters for Re, Br, and P are $\times 10^4$; those for other atoms are $\times 10^3$.

b Parameters for Re, Br, and P are $\times 10^3$.

c The form of the anisotropic ellipsoid is $\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$ and the isotropic thermal parameter is $8\pi^2\bar{u}^2$, where $\bar{u}^2$ is the mean-square amplitude of vibration.

DISCUSSION

$(bipy)_2(SO_4)VOV(SO_4)(bipy)_2 \cdot 15H_2O$

The structure consists of dimeric neutral molecules with the molecules in the unit cell being linked by a network of hydrogen-bonded water molecules linked to the sulfate oxygens. The geometry of the dimer is shown in Figure 1. A crystallographic 2-fold axis passes through the bridging oxygen atom and is perpendicular to the V-V vector. The complex consists of two approximately octahedrally coordinated V(III) centres which are bridged by the oxide anion. Each vanadium atom is coordinated to two cis 2,2'-bipyridine ligands, an oxygen atom of the sulfate group, and the bridging oxide. As is apparent from the figure, the pseudo-octahedron of one vanadium atom is rotated approximately 90° around the V-O vector relative to the coordination polyhedron around the other vanadium so that the V-O1 vector is approximately perpendicular to the V'-O1' vector. The molecule as a whole, as seen in Figure 1, has a Δ configuration. Necessarily there are an equal number of Δ and Λ dimers in the centrosymmetric space group C2/c. The bond lengths and angles associated with the molecule are listed in Table V.

The V-O distance of 1.776 Å is indicative of considerable multiple bonding between the metal atoms and the bridging oxygen atom. While there are no V^{III}-O-V^{III} systems known to me with which I may make a comparison, the Fe^{III}-O-Fe^{III} distances in a variety of oxo-bridged iron(III) dimers[20-27] are in the range 1.76-1.8 Å which is comparable to the present value. The V-O separation is comparable with those in linear Cr^{III}-O-Cr^{III} systems[28,29] (1.82 Å) and are much shorter than the values reported for Cr^{III}-O bonds involving hydroxide bridges[30] (1.94 Å) in which there is no multiple bonding. Evidently there is no structural evidence for a direct through space metal-metal interaction since the V-V separation is 3.53 Å.

TABLE V

Interatomic Distances and Angles for the Vanadium Compound

Distances in Å (e.s.d.'s)

V-0	1.776(4)	V-N2	2.066(19)
V-01	2.012(13)	V-N3	2.106(18)
V-N1	2.060(18)	V-N4	2.182(15)

S-01	1.481(14)	S-03	1.461(16)
S-02	1.470(13)	S-04	1.479(16)

N1-C11	1.304(25)	N4-C41	1.338(24)
N1-C15	1.346(22)	N4-C45	1.337(22)
C11-C12	1.416(28)	C41-C42	1.377(27)
C12-C13	1.345(28)	C42-C43	1.407(30)
C13-C14	1.394(29)	C43-C44	1.371(30)
C14-C15	1.392(26)	C44-C45	1.417(24)
C15-C45	1.436(24)		

N2-C21	1.351(29)	N3-C31	1.378(24)
N2-C25	1.333(26)	N3-C35	1.306(24)
C21-C22	1.420(35)	C31-C32	1.376(28)
C22-C23	1.390(35)	C32-C33	1.356(31)
C23-C24	1.400(32)	C33-C34	1.361(33)
C24-C25	1.359(29)	C34-C35	1.388(30)
C25-C35	1.499(28)		

Angles in Degrees (e.s.d.'s)

0-V-01	97.6(6)	01-V-N4	89.0(6)
0-V-N1	95.3(7)	N1-V-N2	163.7(7)
0-V-N2	96.3(7)	N1-V-N3	93.0(7)
0-V-N3	91.6(6)	N1-V-N4	75.0(7)
0-V-N4	169.1(5)	N2-V-N3	75.2(7)
01-V-N1	97.8(6)	N2-V-N4	92.2(7)
01-V-N2	92.0(7)	N3-V-N4	83.9(6)
01-V-N3	165.1(6)	V-0-V	170.2(14)

01-S-02	107(1)	02-S-03	112(1)
01-S-03	108(1)	02-S-04	109(1)
01-S-04	113(1)	03-S-04	108(1)

TABLE V (continued)

V-N1-C11	125(1)	V-N4-C41	125(2)
V-N1-C15	118(1)	V-N4-C45	116(1)
N1-C11-C12	126(2)	N4-C41-C42	124(2)
C11-C12-C13	116(2)	C41-C42-C43	116(2)
C12-C13-C14	120(2)	C42-C43-C44	121(2)
C13-C14-C15	119(2)	C43-C44-C45	118(2)
C14-C15-N1	121(2)	C44-C45-N4	122(2)
C15-N1-C11	117(2)	C45-N4-C41	118(2)
C14-C15-C45	122(2)	C44-C45-C15	124(2)
N1-C15-C45	117(2)	N4-C45-C15	114(2)

V-N2-C21	124(2)	V-N3-C32	124(2)
V-N2-C25	121(1)	V-N3-C35	117(1)
N2-C21-C22	122(3)	N3-C31-C32	121(2)
C21-C22-C23	118(2)	C31-C32-C33	120(2)
C22-C23-C24	120(3)	C32-C33-C34	120(3)
C23-C24-C25	116(2)	C33-C34-C35	119(3)
C24-C25-N2	128(2)	C34-C35-N3	123(2)
C25-N2-C21	116(2)	C35-N3-C31	118(2)
C24-C25-C35	121(3)	C34-C35-C25	121(3)
N2-C25-C35	111(2)	N3-C35-C25	116(2)

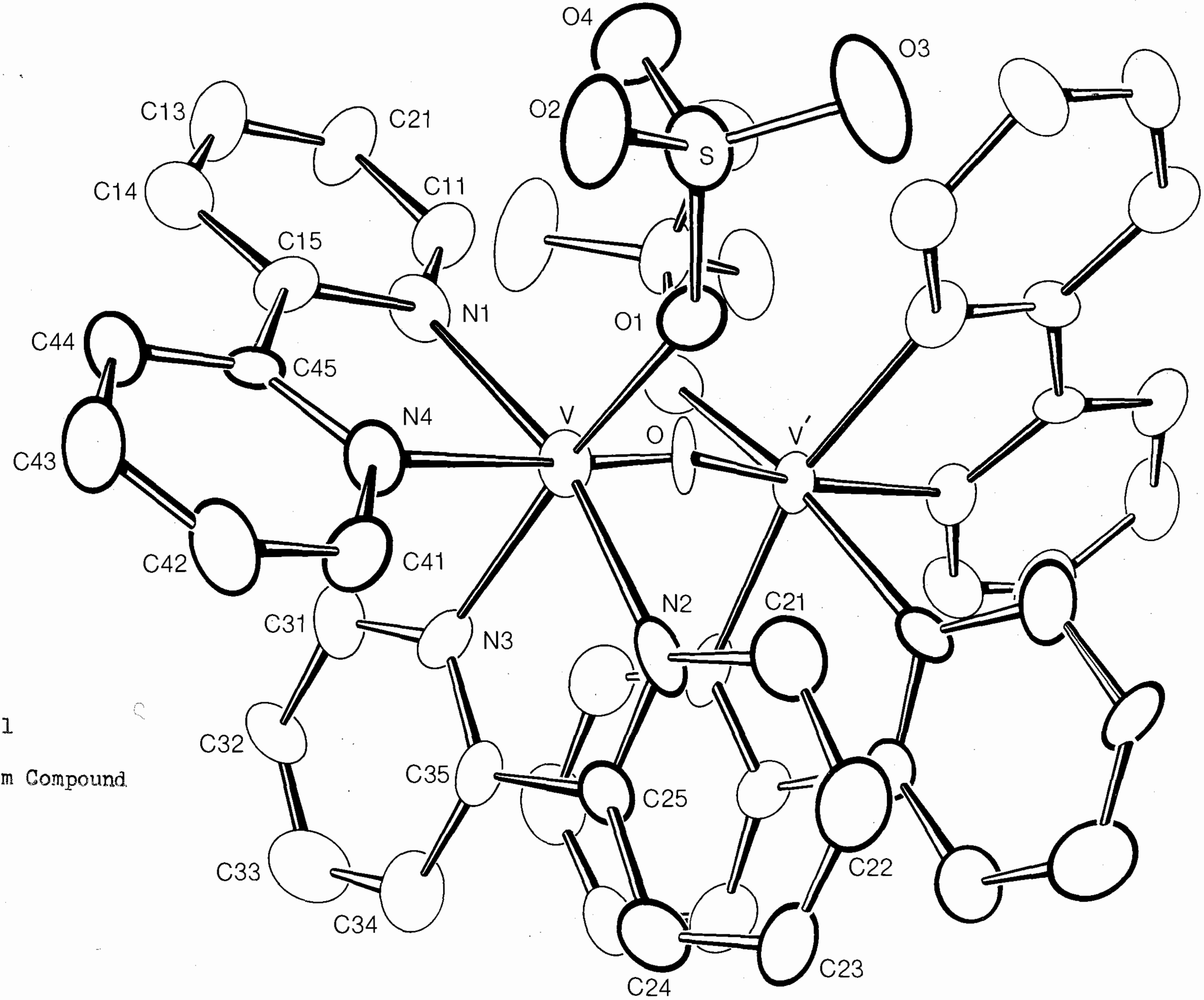

Figure 1

Vanadium Compound

The four V-N distances are in the range 2.06-2.18 Å with an average of 2.10 Å; this distance is probably not significantly different from the V-O1 distance of 2.01 Å. The absence of any significant shortening of the V-N bonds relative to other distances suggests that there is very little multiple bonding between the metal atom and the aromatic ligand. A similar observation has been made for chromium(III) complexes[31,32] of the related 1,10-phenanthroline (phen) ligand.

The non-linear nature of the bridge appears to result mainly from steric interactions of the ligands on the two halves of the molecule. The sulfate groups interact with the bipyridine groups whose planes are parallel to the metal-metal direction while the remaining bipyridine ligand is opposite its symmetry related counterpart. The dihedral angle by which these last bipyridine ligands are displaced about the metal-metal axis is 14.2°. The major steric interaction appears to be between the sulfate groups and the opposing bipyridine ligands. Thus C11 and its hydrogen atom protrude across the gap surrounding the bridge and interact with the sulfate group to such a degree (2.74 Å) that the bridge is bent 10° from linearity and the angle between the planes defined by O1, N1, N2, N3, and their symmetry related counterparts is 12.4°. As well, the planes of the bipyridine ligands opposite to these steric interactions are 7.7° apart. The result of this interaction is to bend the molecule as a whole and to place two bipyridine ligands essentially parallel to each other with almost maximum overlap when viewed perpendicular to the planes of the ligands (Figure 2). The closest intramolecular interatomic approaches between these two ligands (3.57, 3.58 Å) occur between N2 and N3', and C21 and C31'. These distances are very similar to non-interacting intermolecular distances (3.45-3.65 Å) of a number of planar organic compounds[33-35]. Besides these intramolecular separations, there were also some relatively

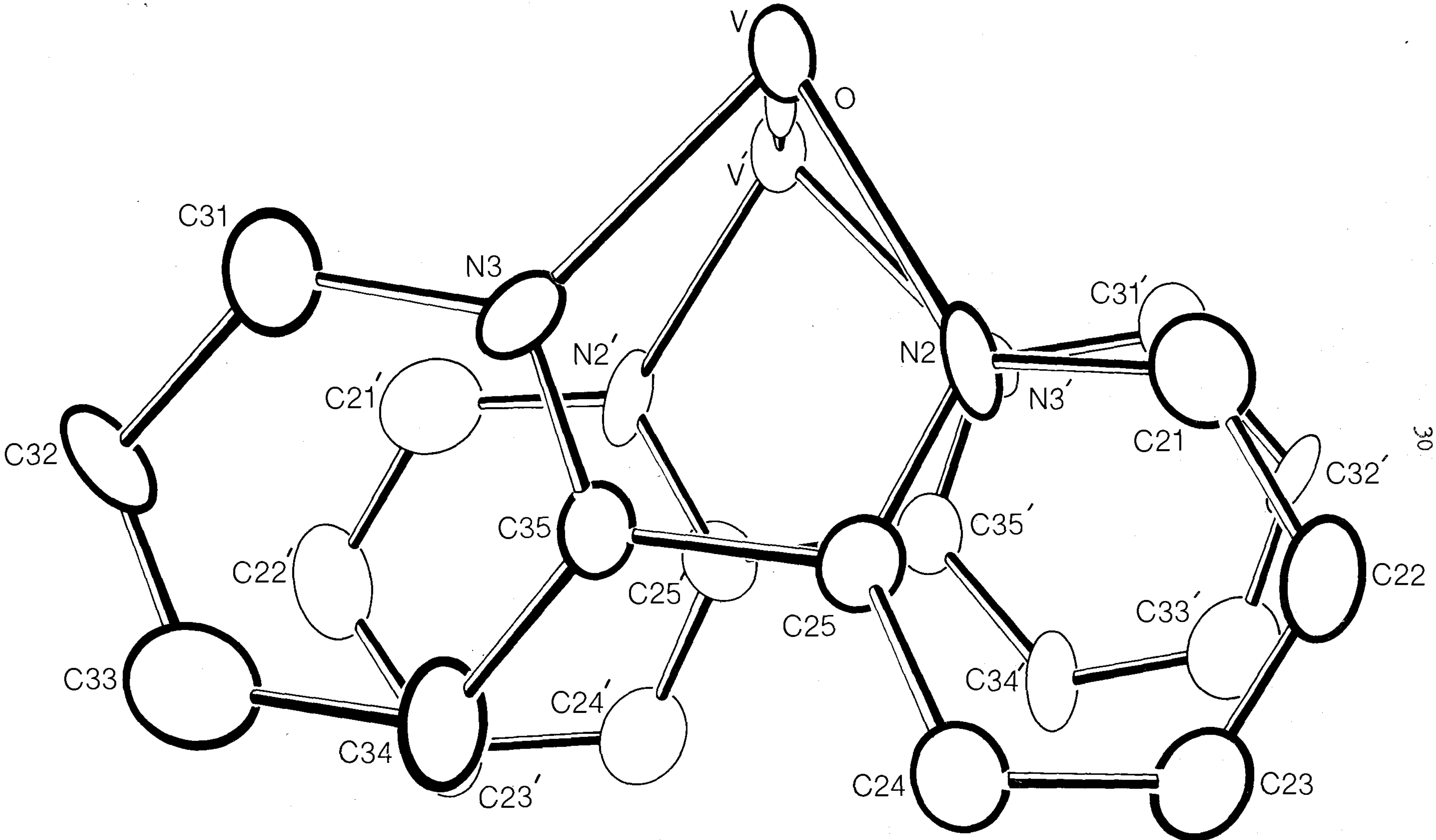

Figure 2: Ligand Overlap

short intermolecular approaches (C33-C32", 3.46 Å; C31-C33", 3.58 Å).

The groups coordinated to the vanadium do not appear to have undergone any major distortions. The sulfate group is very close to being an ideal tetrahedron with the angle subtended at the coordinating oxygen of 140.7°. The bipyridine entities are both composed of pairs of essentially planar pyridine rings (Table VI). One ligand has the rings coplanar within 3.1° while the other is within 1.9°. As well, the vanadium atom is also very close to being coplanar with the bipyridine ligands (0.094, 0.005 Å).

Of the fifteen water molecules surrounding each dimer, only one is situated on a special position, a 2-fold axis, and is hydrogen-bonded to O4 of each half of the molecule thus forming another bridge. Three of the remaining seven unique water species are coordinated by hydrogen bonds to the two other free oxygen atoms of the sulfate group. The remaining solvent molecules form a hydrogen-bonded network throughout the crystal lattice (Table VII).

The crystallographic two-fold symmetry of the molecule simplifies the quest for an answer to the question of why this compound has such intense bands in its u.v.-visible spectrum. This symmetry element eliminates the mechanism of mixed-valence charge transfer. This leaves two other possible answers: relaxation of the Laporte rule and/or oxo-induced exchange. It was shown earlier (see Introduction) that a relaxation of the Laporte rule by electron exchange between the metal orbitals and the ligand orbitals of the 2,2'-bipyridine ligands was unlikely since the $(V(bipy)_2Cl_2)^+$ species did not exhibit this phenomenon. If, however, an electron exchange is postulated between the metal orbitals and the orbitals of the bridging oxygen ligand, then the relaxation of the Laporte rule becomes identical with the oxo-induced mechanism. This particular situation has been observed with another dimeric species[36] $(Cr(bipy)_2OH)_2^{+4}$. The behaviour of this chromium compound was observed over a

TABLE VI

Ring Planes and X^2 for Vanadium Compound Ligands[a]

Ring nitrogen	A	B	C	D	X^2
N1	0.6671	0.6876	-0.2867	0.7868	6.72
N2	-0.6125	-0.0143	-0.7903	-5.2519	2.81
N3	-0.5871	-0.0068	-0.8095	-5.3674	0.76
N4	0.6520	0.6788	-0.3377	0.3264	10.38
N1+N4	0.6561	0.6858	-0.3150	0.5595	34.25
N2+N3	-0.6006	-0.0091	-0.7995	-5.2791	9.4

[a] Equation of plane is $Ax+By+Cz-D=0$.

TABLE VII

Hydrogen-Bonded Inter-Oxygen Distances and Angles

Distances in Å (e.s.d.'s)

02-06'	2.86(2)	07-08	2.81(3)
02-010	2.84(3)	07-09	2.74(3)
03-06	2.74(2)	09-011	2.77(3)
03-08	2.82(3)	09-012	2.86(3)
04-05	2.82(2)	010-010'	2.83(5)
05-011	2.88(3)	010-012'	2.63(3)
06-07	2.88(3)	011-012	2.75(3)

Angles in Degrees (e.s.d.'s)

04-05-04'	117.5(11)	07-09-012	105.3(9)
04-05-011	104.7(5)	011-09-012	109.4(9)
04-05-011'	115.2(5)	02-010-010'	101.3(9)
011-05-011'	98.1(11)	02-010-012	132.5(10)
02-06-03	119.0(8)	010'-010-012	122.1(8)
02-06-07	130.2(7)	05-011-09	125.4(8)
03-06-07	89.1(8)	05-011-012	135.1(8)
06-07-08	153.8(7)	09-011-012	100.2(8)
06-07-09	122.4(8)	09-012-010'	124.6(12)
08-07-09	84.1(8)	09-012-011	119.1(9)
03-08-07	140.4(11)	010'-012-011	114.2(10)

wide range of pH values. In acidic solutions the cation consisted of the diol as represented but upon raising the pH, first one and then the other hydrogens were reversibly lost to produce first the mixed hydroxo-oxo and then the dioxo bridged species. As this change proceeded, the u.v.-visible spectrum changed. The initial acidic species produced a yellow solution while the basic species yielded a brown solution of greater intensity. It was also observed that when the dihydroxo species was allowed to decompose in an acidic medium the maxima shifted and increased in intensity. This change in the spectrum was postulated to be due to the presence of an intermediate product which possessed only one OH bridge. This study indicates that intensity enhancement can occur when hydroxo species are converted to oxo species and when the number of bridging species is reduced from two to one. In the present vanadium compound the molecule is the end result of both of these mechanisms. If a $(V(bipy)_2OH)_2^{+4}$ species exists, it would be expected to be paler than a similar compound with one bridging hydroxo group which would, in turn, be paler than the present compound. Thus the presence of a single oxo anion as the bridging species appears to account for the high intensity of the absorption maxima.

The linearity of the bridge and the short V-O bond length indicate that there is a great deal of double bond character in the bridge. The orbitals involved in the bridge bonding can be deduced by examining the ligand placement about the two metal sites. When viewed down the V-V vector, the ligands are in an eclipsed conformation with the sulfate entities rotated 90° from each other. The orbitals of the oxo oxygen can be described in the following manner: two sp_z hybrid orbitals forming σ bonds to the two metal atoms and the full p_x and p_y orbitals extending perpendicular to them. The metal d orbitals are arranged as follows: the d_{z^2} orbital forms σ bonds with the bridging oxygen and N4, $d_{x^2-y^2}$ forms σ bonds with the other four coordinating atoms, and d_{xy}, d_{xz}, and d_{yz} occupy their usual positions. The shortness of the V-O bond length indicates that the energy of the d_{z^2} orbital will be slightly higher than that of the $d_{x^2-y^2}$ orbital and that the energies of the d_{xz} and d_{yz} orbitals will be a small amount higher than the d_{xy} orbital energy. The two d level electrons of each approximately octahedrally coordinated vanadium atom will be in the d_{xy} and one of d_{xz} or d_{yz} orbitals. When the p_x and p_y orbitals of the oxygen atom are combined with the d_{xz} and d_{yz} orbitals of the two vanadium atoms, six molecular π orbitals are formed in degenerate pairs. The six electrons available fill the two bonding M.O.'s and half-fill the two non-bonding M.O.'s. This bonding scheme has also been suggested by other workers for another oxo-bridged dimer[37]. The end result of this bonding scheme is a linear three atom system held together by four filled bonding molecular orbitals consisting of two σ and two π bonds.

The above bonding scheme helps to explain why this compound has a bridge system which is very close to being linear while similar iron systems[20-23] are usually bent (139-152°) as a result of the extra electrons being placed in antibonding molecular orbitals.

The structural information obtained in this study very strongly suggests that both vanadium atoms are in the +3 oxidation state with identical coordination spheres. This conclusion cannot, however, be accepted as an absolute fact. Because there was a choice of space groups, there is a possibility that the dimeric molecule is not situated on a symmetry element. Moreover, since no attempt was made to determine the oxidation state of the vanadium by, for example, titration, there is some question as to the precise oxidation state of vanadium in this compound. The presence of undetected hydrogen ions in the crystal lattice would of course change the formal vanadium oxidation state.

Since the u.v.-visible spectrum and magnetic moment of the compound were not measured, there is the slight possibility that the compound studied here was not that previously investigated by other workers[4].

It may be noted however, that if this compound was the same as that studied by Murray and Sheahan, a magnetic moment of 3.3 B.M. would not be inconsistent with vanadium in the 3+ oxidation state, since an orbital contribution could increase the magnetic moment above the spin-only value of 2.9 B.M.

Many possibilities for future work arise from modifications of the present system. The simplest modification consists of replacing the sulfate anions by other species. Thus it would be very simple to obtain the perchlorate salt in which it is quite possible that water molecules occupy the sixth coordination site of the vanadium atoms. By varying the identity of the anion it should be possible to vary the species which occupies this position and determine the resulting distortions arising from the differing steric requirements of the coordinating species. Compact entities such as water and the nitrite ion would be expected to produce very little steric interaction between the two halves of the molecule with the result that the V-O-V system should be more linear than in the present compound. If bulkier species such as R_3PO or R_2SO, where R is an alkyl species such as CH_3, can be induced to coordinate to the vanadium atom, then the bridge will be bent. If a large deviation from linearity does occur, then, if the intensity of the peaks in the electronic spectrum is a result of the pi system of the bridge, the resulting compounds should be paler in color. The main difficulty with bulky ligands is the initial formation of the complex since the bipyridine ligands trans to the coordination sites will be forced closer together. Another anion to be investigated, for a different reason, is PF_6^-. It was reported[4] that the species isolated did not include solely PF_6^- but also included the chloride ion so that the anionic content was $((PF_6)_{1.3}Cl_{0.7})$ for each vanadium atom. It would be interesting to find out how the two types of anions are distributed in the unit cell. Another interesting arrangement of coordinated species would result in the destruction of the two-fold symmetry of the dimer by placing different molecules on the two metal sites.

If the unusual electronic spectrum is due to the presence of the linear oxo bridge, then the spectrum can be drastically changed by altering the nature of the bridge. Changing the presently well protected oxo spcies to a hydroxo species by proton addition in an acidic medium would probably result in a dihydroxy bridged material. The second hydroxo group would form a bridge after the sulfate anions were forced to break away as the molecule bent to accomodate the presence of the first hydroxo group. Another way to produce a bent molecule would be to change the bipyridine ligand by placing sterically bulky groups on the rings, i.e. 6,6'-dimethyl-2,2'-bipyridine. With such ligands it would be very difficult to form a dimer analogous to the one studied. However, if a dimer were formed, it would most likely involve a double bridge of either oxo or hydroxo groups.

Future work to determine the exact cause of the unusual electronic spectrum of this compound involves many different approaches to the problem and will greatly improve the understanding of polymeric transition metal complexes which have oxo or hydroxo bridging species.

$Re(CO)_3Br(P(Me_2pz)_2(C_6H_5))$

A single crystal diffraction study of $Re(CO)_3Br(P(Me_2pz)_2(C_6H_5))$, where Me_2pz is 3,5-dimethylpyrazolyl, revealed that the rhenium atom was coordinated to three carbonyl entities, one bromine atom, and one nitrogen atom from each 3,5-dimethylpyrazolyl portion of the phosphine ligand. The six coordinated atoms are arranged in an octahedral configuration (Figure 3) with the three carbonyl groups defining one of the triangular faces. There were no solvent molecules incorporated into the unit cell and there were no indications of intermolecular interactions. Table VIII lists the interatomic distances and angles.

The Re-Br distance of 2.623(7) Å is very close to the expected distance of 2.68 Å which is the sum of the crystal ionic radii of Re^{4+} (Re^{1+} was not available) and Br^-.[38] When the experimental value is corrected for the riding motion of the bromine atom with respect to the metal atom, a value of 2.639(7) Å is obtained and is somewhat closer to the expected value. The three carbonyl groups appear to deviate very little from linearity with the angles subtended at the carbon atoms being very close to 180°. A comparison of the bond lengths connected with these groups is very hard to make since the electron density immediately surrounding the rhenium atom severely limits the ability of the least-squares process to resolve the light atoms (C,N,O,H) in the neighborhood of the heavy metal atom. This difficulty is especially apparent with carbonyl groups which have a relatively large amount of electron density between the carbon and oxygen atoms. In order to sidestep the problem, a comparison of the overall Re-O distances can be made with the result that all three groups appear to be identical (3.01-3.06 if linearity is assumed; 2.97-3.05 if allowance is made for non-linearity).

The rhenium atom, the four nitrogen atoms, and the phosphorous atom form

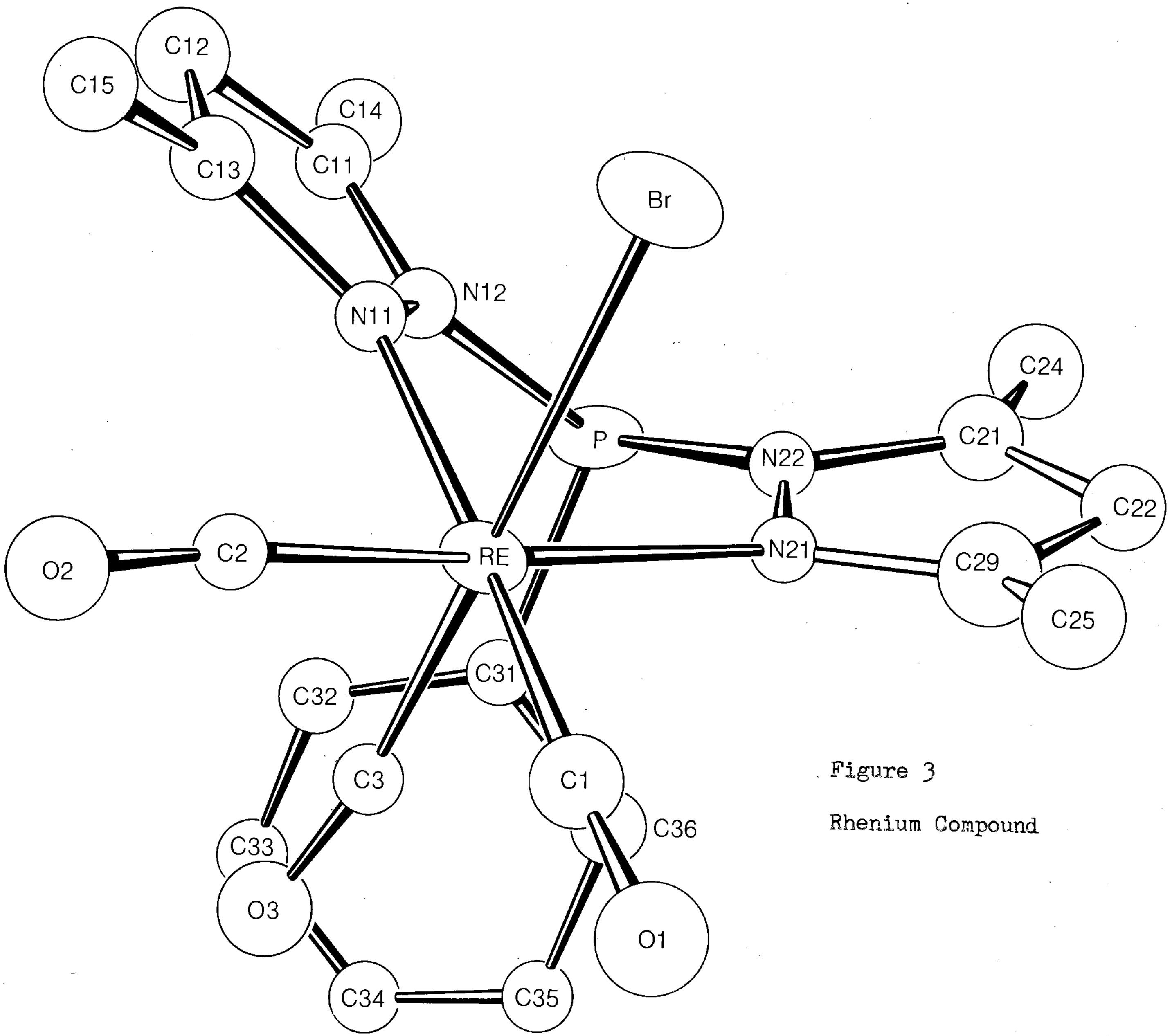

Figure 3

Rhenium Compound

TABLE VIII

Interatomic Distances and Angles for the Rhenium Compound

Distances in Å (e.s.d.'s)

Re-N11	2.15(4)	Re-C1	1.76(7)
Re-N21	2.21(4)	Re-C2	1.87(6)
Re-Br	2.623(7)	Re-C3	1.83(6)

P-N12	1.73(4)	P-N22	1.67(5)
N11-N12	1.38(5)	N21-N22	1.41(6)
N12-C11	1.30(6)	N22-C21	1.42(7)
C11-C12	1.47(8)	C21-C22	1.41(8)
C12-C13	1.40(8)	C22-C23	1.32(8)
C13-N11	1.44(7)	C23-N21	1.28(7)
C11-C14	1.52(8)	C21-C24	1.59(9)
C13-C15	1.55(8)	C23-C25	1.67(9)

P-C31	1.79(6)	C1-O1	1.27(7)
C31-C32	1.42(8)	C2-O2	1.19(6)
C32-C33	1.34(8)	C3-O3	1.18(6)
C33-C34	1.38(8)		
C34-C35	1.35(7)		
C35-C36	1.43(8)		
C36-C31	1.37(7)		

Angles in Degrees(e.s.d.'s)

Br-Re-N11	85(1)	N11-Re-C3	96(2)
Br-Re-N21	85(1)	N21-Re-C1	94(2)
Br-Re-C1	98(2)	N21-Re-C2	170(2)
Br-Re-C2	86(2)	N21-Re-C3	96(2)
Br-Re-C3	178(2)	C1-Re-C2	82(3)
N11-Re-N21	87(1)	C1-Re-C3	81(3)
N11-Re-C1	177(2)	C2-Re-C3	93(2)
N11-Re-C2	98(2)		

Re-N11-N12	129(3)	Re-N21-N22	121(3)
Re-N11-C13	130(3)	Re-N21-C23	136(4)
P-N12-N11	126(3)	P-N22-N21	131(4)
P-N12-C11	118(4)	P-N22-C21	122(4)
N11-N12-C11	116(4)	N21-N22-C21	106(4)
N12-C11-C12	109(5)	N22-C21-C22	111(5)
C11-C12-C13	101(5)	C21-C22-C23	98(6)
C12-C13-N11	114(5)	C22-C23-N21	124(6)
C13-N11-N12	100(4)	C23-N21-N22	102(5)
N12-C11-C14	128(5)	N22-C21-C24	124(5)

TABLE VIII (continued)

C12-C11-C14	123(5)	C22-C21-C24	124(6)
N11-C13-C15	120(5)	N21-C23-C25	115(5)
C12-C13-C15	126(6)	C22-C23-C25	118(6)
P-C31-C32	119(4)	N12-P-N22	101(2)
P-C31-C36	122(4)	N12-P-C31	104(2)
C31-C32-C33	123(6)	N22-P-C31	103(3)
C32-C33-C34	118(6)	Re-C1-O1	174(6)
C33-C34-C35	123(6)	Re-C2-O2	171(5)
C34-C35-C36	118(6)	Re-C3-O3	165(5)
C35-C36-C31	121(5)		
C36-C31-C32	117(5)		

a six-membered ring with a boat configuration. Although the molecule as a whole has approximate mirror symmetry, a comparison of similar sections of the boat ring indicates that the symmetry is not very exact in this region. Table IX shows that the dihedral angles of the different portions of the ring, as viewed in Newman projections down the various bonds, are sufficiently different to indicate a slightly skewed configuration for the boat ring. The skewing of the boat ring appears to be an example of a puckered chelate ring. With the present ligand there is the possibility of eight different conformations with four being associated with the boat configuration and four associated with the chair configuration. By analogy with five-membered ring systems which have only two configurations, the molecule as represented in Figure 3 has the ligand in the δ boat configuration with the phenyl ring in the axial position. It was mentioned by Trofimenko[16] that models indicate that the chair conformation should be preferred since it entails much less non-bonding interactions between the substituents in position 3 than in the boat conformation. It is not known what models were used but the present compound would indicate that the boat conformation is preferred since only in the boat form can the pyrazolyl rings maintain linear or almost linear bonds to both the phosphorous and metal atoms.

In the present compound the dimensions of the two pyrazolyl rings are very irregular. This is probably due to the inability of the refinement process to accurately account for all of the electron density. Despite this problem, the average bond lengths of these rings (N-N, 1.39 Å; N-C, 1.38 Å; C-C, 1.40 Å) are not very different from those obtained from a compound utilizing the analogous borate ligand[39] (N-N, 1.364 Å; N-C, 1.335 Å; C-C, 1.386 Å).

When the two N-Re-Br angles (85°) and the two N-Re-C3 angles (96°) are compared, it appears that the boat ring is being displaced toward the bromine

TABLE IX

Dihedral Angles From Newman Projections For Boat Ring

Atoms involved	View down	Dihedral angle
Re,N11,N12,P	N11-N12	9(6)
N11,N12,P,N22	N12-P	164(4)
N12,P,N22,N21	P-N22	127(6)
P,N22,N21,Re	N22-N21	25(7)
N22,N21,Re,N11	N21-Re	160(4)
N21,Re,N11,N12	Re-N11	153(4)

atom. This small effect could be due to an interaction between the phenyl ring and the neighboring carbonyl group. This possibility arises when it is noted that the phenyl group is situated close to C3 (C3-C31, 3.04(7) Å). The proximity of these two groups could be due to a pi-pi interaction between molecular orbitals of the two groups. Another possibility which could explain this near approach involves the overall shape of the whole molecule and the packing of the molecules in the unit cell. If the phenyl group was positioned at the site occupied by the phosphorous lone pair, then it would point away from the rest of the molecule and would give the molecule the appearance of a ball with a long flat extension. By occupying a position near the carbonyl group, however, the general shape of the complex is much more spherical and this shape would permit easier packing of the complex molecules into the unit cell than would the other more irregular shape. The proximity of the phenyl group to the carbonyl group appears to indicate that, if the conditions were appropriate, further intramolecular reactions are possible. Acylation of the phenyl group would occur if a hydrogen atom could be removed from one of the ortho carbons of the ring and a tris-chelating phosphine ligand would result. A loss of both a carbonyl group and an ortho hydrogen would result in an ortho-metallated complex which would again produce a tris-chelating phosphine ligand.

The behaviour of the phosphine ligand in this and other compounds is mainly due to the two pyrazolyl rings. The electron withdrawing ability of a pyrazolyl ring is so great that the coordinating power of the phosphorous lone pair of electrons is decreased well below the coordinating power of the ring nitrogens. Because of this arrangement of electron density the rhenium compound is incapable of serving as a phosphine ligand to other metal complexes. This inability to coordinate through the phosphorous atom makes the ligand very similar to other ligands utilizing pyrazolyl rings. The best known series is $(R_nB(pz)_{4-n})^-$ but other less familiar series are known[16] in which the boron atom is replaced by carbon to yield neutral ligands or by beryllium to yield dinegative ligands. It should also be possible to make a ligand series in which nitrogen replaces phosphorous in order to observe the competition between two identical atoms. The behaviour of all of these various ligands is mainly governed by the pyrazolyl rings and the total charge of the ligand. Variations in stability of complexes with respect to degradation by air or water are observed when R is varied or alkyl groups are put on the rings but it is the presence of the rings which permits coordination in the first place. A complete structural study of polypyrazolyl ligands would be very time consuming but it would help to explain the manner in which the various components of the ligand-metal system interact. Thus changing the central ligand atom (i.e. from boron to carbon) may indicate that chair conformations are preferred to boat conformations for some dipyrazolyl systems. The same effect can be examined by varying the coordinated metal atom. Varying the number of pyrazolyl rings may reveal unexpected products such as the monopyrazolyl phosphine mentioned earlier. Steric interactions of alkyl groups on the pyrazolyl rings and/or on the central atom would possibly reveal how various complexes utilizing these ligands are more stable than similar compounds lacking such groups. All in all a study of these ligands would be very interesting and would help to open up a new field of study in coordination chemistry. The present study is a small step in this direction.

TABLE II Structure Factors For the Vanadium Compound

L	FO	FC
H=	0, K=	0
2	221	-216
4	66	66
6	21	-12
8	65	-77
10	15*	0
12	50	-41
14	12*	-13
16	13*	-5
18	24*	6
H=	0, K=	2
0	116	-155
1	225	-252
2	30	39
3	21	-24
4	97	-92
5	122	124
6	146	-145
7	20	16
8	18*	22
9	157	162
10	39	-32
11	26	32
12	47	38
13	65	-74
14	4*	2
15	27*	30
16	63	67
17	17*	-30
18	33	-39
H=	0, K=	4
0	106	144
1	56	72
2	115	-143
3	50	-54
4	14*	1
5	47	-46
6	29	-36
7	6*	-13
8	100	102
9	20*	26
10	40	35
11	7*	6
12	112	-115
13	23*	-7
14	140	144
15	24*	-24
16	67	-76
17	15*	4

L	FO	FC
H=	0, K=	6
0	61	-71
1	128	143
2	13*	22
3	18*	-24
4	11*	-26
5	103	-110
6	37	33
7	137	141
8	64	-63
9	86	-93
10	56	-52
11	31	-27
12	3*	3
13	92	95
14	90	-87
15	27*	-43
16	24*	17
17	39	34
H=	0, K=	8
0	21*	-12
1	64	-69
2	123	-136
3	76	82
4	50	43
5	20	18
6	117	121
7	31	-26
8	133	-136
9	38	34
10	10*	26
11	21*	-8
12	73	78
13	46	-48
14	4*	-5
15	4*	8
16	22*	24
H=	0, K=	10
0	179	-182
1	62	-69
2	79	78
3	32	35
4	52	-57
5	40	47
6	14*	8
7	104	-106
8	25	-17
9	3*	6
10	3*	-2
11	65	58

L	FO	FC
12	19*	-3
13	31	-33
14	16*	11
15	36	35
16	17*	12
H=	0, K=	12
0	34	-43
1	54	57
2	24	35
3	24*	-18
4	72	76
5	88	-84
6	34	22
7	20*	27
8	61	54
9	21*	-17
10	4*	4
11	20*	-3
12	36	-29
13	20*	14
14	71	62
15	15*	-1
H=	0, K=	14
0	49	52
1	27	31
2	3*	-20
3	3*	-14
4	39	-42
5	3*	-20
6	12*	17
7	16*	9
8	18*	-25
9	46	-39
10	12*	-14
11	6*	7
12	22*	20
13	39	38
H=	0, K=	16
0	111	107
1	14*	8
2	88	-86
3	48	-51
4	18*	-11
5	25*	27
6	33	33
7	15*	-20
8	16*	-10
9	4*	21
10	13*	15

L	FO	FC
11	17*	28
H=	0, K=	18
0	23*	-21
1	55	-49
2	27*	12
3	13*	2
4	4*	0
5	32	34
6	10*	-4
7	21*	-14
8	30	23
9	28*	15
H=	0, K=	20
0	4*	-5
1	60	38
2	13*	-10
3	35	-31
4	4*	2
5	7*	4
H=	1, K=	19
0	32	-25
1	18*	-11
2	4*	3
3	4*	-12
4	52	37
5	12*	12
6	35	-27
7	21*	10
H=	1, K=	17
0	15*	25
1	27*	-28
2	11*	-2
3	40	-41
4	38	-41
5	37	38
6	61	51
7	29	-24
8	13*	-12
9	13*	10
10	4*	17
H=	1, K=	15
0	85	69
1	31	-18
2	3*	-10
3	6*	0

```
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC    2

   4    47    -49       6   16*     -4
   5    42    -40       7    70    -68       0   15*     -8       0   106    108
   6    31     28       8    32    -39       1    72    -76       1    62     51
   7    37     33       9   17*    -13       2    75    -74       2    82    -92
   8   13*      1      10    73    -65       3   111    131       3   158   -142
   9   21*    -23      11    82     84       4   13*     16       4   299   -271
  10    32    -28      12    41     38       5    2*      5       5    25     23
  11    4*     20      13   24*    -34       6   137   -149       6    98   -100
  12    53     40      14   13*      7       7    36    -41       7   123   -117
                       15    4*      0       8   19*     13       8    45    -41
H=    1, K=   13      16   15*      7       9    43    -53       9    61    -61
                                          10    33     35      10    47     49
   0    53    -44    H=    1, K=    7      11   129    142      11    49     54
   1   111    100                         12   22*    -24      12    55    -62
   2   15*     21       0    78     84      13   11*    -22      13    61    -68
   3    55     51       1    42    -47      14   15*     12      14    69     72
   4   18*     24       2    22     17      15   22*     26      15    4*     17
   5    3*      8       3    60     66      16    4*      4      16    42    -39
   6    34     35       4    29    -36      17    7*     23      17   19*     25
   7    34     36       5   13*    -36
   8   10*     26       6    52     57    H=    1, K=    1    H=    2, K=    4
   9    36     34       7   15*     27
  10   11*      2       8    46    -45       0   252    276       0   15*     -1
  11    54    -50       9   18*    -19       1    9*     -3       1    59    -75
  12   16*    -14      10    57    -68       2   16*      6       2   236    239
  13    47     41      11    57    -58       3   173   -175       3    48    -53
  14   18*     14      12   112    112       4   195   -204       4   159   -162
                       13   24*     34       5   143    145       5    27    -14
H=    1, K=   11      14    39    -36       6   119    115       6    3*    -23
                       15    27    -20       7   106   -109       7    62     63
   0   21*    -26      16   15*      8       8   19*    -15       8    50    -51
   1   10*    -22      17    4*     -5       9    51    -43       9   16*     -9
   2    9*    -16                           10   16*    -20      10    58     58
   3    9*    -21    H=    1, K=    5      11    39    -41      11    30    -32
   4    42     37                           12    32     33      12    41    -46
   5    40    -45       0    77     80      13   19*     -8      13    4*    -13
   6    43    -45       1    28    -26      14    37    -37      14   11*    -14
   7    55    -53       2    19     21      15    42     46      15   26*    -27
   8    44     44       3   101   -120      16    35     41      16    67     62
   9    3*     12       4    49    -52      17   19*     -9      17   14*     -7
  10   14*      2       5    65     64      18    4*     -7
  11   12*     14       6    24    -27                         H=    2, K=    6
  12    40    -42       7    26     24    H=    2, K=    0
  13   27*    -23       8    53     56                            0   17*     33
  14    4*     12       9   11*      9       0    48    -74       1   127    132
  15   30*     30      10    3*     15       2   368    359       2    42    -52
                       11    66    -73       4   825   -781       3   113    125
H=    1, K=    9      12    55    -60       6   406    403       4    60     55
                       13    99    111       8   102     99       5   157   -162
   0    23     16      14    47     56      10    52    -56       6    22     21
   1   11*    -31      15   25*    -39      12   155    163       7    36     44
   2    8*      8      16    4*      8      14    85    -94       8    8*     20
   3    7*    -29      17   14*    -14      16    34     44       9   102     98
   4    32    -37                                                 10   23*    -25
   5    56     64    H=    1, K=    3    H=    2, K=    2      11    96   -104
```

H= 2, K= 6

L	FO	FC
12	28	25
13	37	33
14	43	46
15	18*	0
16	4*	-3

H= 2, K= 8

L	FO	FC
0	18*	-9
1	45	44
2	23	26
3	87	-90
4	91	102
5	41	49
6	71	70
7	64	-63
8	44	48
9	9*	11
10	114	-116
11	44	42
12	101	107
13	13*	17
14	48	-53
15	4*	1
16	4*	0

H= 2, K= 10

L	FO	FC
0	18*	21
1	3*	-12
2	3*	12
3	3*	-18
4	34	34
5	56	58
6	49	-46
7	34	-39
8	8*	-1
9	14*	-23
10	4*	-4
11	95	96
12	64	-63
13	4*	-2
14	4*	-1
15	6*	-1

H= 2, K= 12

L	FO	FC
0	105	-111
1	17*	11
2	61	-59
3	16*	23
4	41	37
5	17*	-30
6	21*	-22
7	3*	13
8	9*	1
9	32	36
10	46	49
11	45	-44
12	31	22
13	10*	17
14	23*	29

H= 2, K= 14

L	FO	FC
0	83	75
1	40	-37
2	3*	12
3	57	56
4	30	-27
5	21*	-21
6	12*	12
7	12*	20
8	25*	24
9	4*	4
10	41	-44
11	4*	-14
12	19*	-15

H= 2, K= 16

L	FO	FC
0	12*	0
1	50	-45
2	78	80
3	9*	-6
4	68	-75
5	5*	-3
6	62	65
7	23*	26
8	4*	6
9	25*	-20
10	37	-36
11	4*	5

H= 2, K= 18

L	FO	FC
0	18*	-13
1	4*	-4
2	22*	-4
3	29	-37
4	4*	-3
5	34	36
6	4*	2
7	16*	6
8	16*	-3

H= 2, K= 20

L	FO	FC
0	4*	7
1	18*	-15
2	32	20
3	36	34
4	4*	12

H= 3, K= 19

L	FO	FC
0	4*	0
1	10*	-22
2	4*	-4
3	25*	-8
4	18*	16
5	6*	19

H= 3, K= 17

L	FO	FC
0	15*	-9
1	4*	14
2	4*	13
3	18*	-15
4	9*	-15
5	19*	18
6	12*	-3
7	44	44
8	18*	29
9	44	-45

H= 3, K= 15

L	FO	FC
0	4*	4
1	16*	-25
2	106	107
3	25*	-6
4	60	-65
5	9*	-11
6	28	21
7	16*	-5
8	37	39
9	6*	6
10	33	-37
11	34	-29

H= 3, K= 13

L	FO	FC
0	20*	24
1	47	-54
2	23*	-32
3	59	65
4	29	23
5	67	-62
6	4*	-16
7	12*	-1
8	4*	5
9	72	73
10	4*	-9
11	16*	16
12	6*	9
13	32	21

H= 3, K= 11

L	FO	FC
0	41	42
1	109	101
2	19*	-21
3	55	-60
4	44	37
5	7*	2
6	3*	-17
7	31	-33
8	39	-42
9	4*	-5
10	66	61
11	30	-21
12	20*	-9
13	4*	-16
14	12*	3

H= 3, K= 9

L	FO	FC
0	106	108
1	24	30
2	5*	12
3	34	36
4	43	47
5	57	59
6	44	41
7	33	41
8	7*	14
9	106	-106
10	48	-48
11	83	80
12	16*	13
13	13*	-9
14	23*	31
15	47	-48

H= 3, K= 7

L	FO	FC
0	176	-186
1	87	88
2	25	22
3	59	-67
4	76	-78
5	63	-64
6	9*	-12
7	38	-37
8	31	27
9	55	57
10	85	-83

L	FO	FC
11	40	-46
12	20*	21
13	13*	10
14	11*	18
15	46	46
16	34	-37
H=	3, K=	5
0	8*	23
1	198	-201
2	56	-50
3	167	166
4	13*	-3
5	110	106
6	21*	-23
7	35	-30
8	16*	7
9	14*	11
10	41	44
11	47	-31
12	4*	2
13	33	33
14	8*	3
15	4*	-6
16	12*	9
H=	3, K=	3
0	70	56
1	20	44
2	115	-118
3	66	-79
4	2*	-8
5	192	178
6	38	37
7	68	58
8	74	-76
9	11*	-7
10	66	67
11	6*	12
12	64	-67
13	10*	-2
14	14*	-9
15	13*	-14
16	32	28
17	22*	-18
H=	3, K=	1
0	51	-42
1	50	-51
2	222	197
3	46	-36
4	365	-342

L	FO	FC
5	35	27
6	16*	-4
7	195	192
8	195	190
9	183	-181
10	23*	-17
11	94	98
12	35	29
13	47	-43
14	9*	-5
15	10*	-17
16	6*	-15
17	71	62
H=	4, K=	0
0	244	223
2	229	-194
4	6*	-21
6	341	-330
8	390	385
10	146	-148
12	49	-55
14	57	52
16	78	-80
H=	4, K=	2
0	131	-131
1	132	119
2	39	38
3	90	-85
4	87	-87
5	11*	5
6	34	32
7	162	146
8	69	70
9	56	-53
10	51	-51
11	18*	9
12	65	68
13	19*	9
14	43	-41
15	19*	-27
16	43	37
H=	4, K=	4
0	82	91
1	46	49
2	98	-99
3	92	-78
4	163	160
5	86	-82
6	57	50

L	FO	FC
7	45	-43
8	26	34
9	7*	-11
10	91	85
11	4*	19
12	54	-58
13	14*	26
14	23*	19
15	19*	23
16	6*	8
H=	4, K=	6
0	24	-31
1	15*	-23
2	48	46
3	70	67
4	85	-86
5	36	-38
6	57	-53
7	51	-48
8	21*	14
9	125	118
10	34	-38
11	17*	-28
12	36	29
13	32	-31
14	30	-30
15	44	42
H=	4, K=	8
0	93	-97
1	17*	-14
2	31	25
3	7*	3
4	17*	-31
5	38	-37
6	53	-39
7	43	47
8	37	30
9	54	-48
10	11*	2
11	31	30
12	4*	-11
13	14*	-2
14	90	100
15	4*	-4
H=	4, K=	10
0	68	-68
1	140	134
2	86	84
3	41	-42

L	FO	FC
4	13*	-1
5	20*	28
6	15*	15
7	21*	13
8	39	-38
9	56	-53
10	25*	14
11	13*	4
12	11*	-13
13	10*	-7
14	39	-35
H=	4, K=	12
0	80	85
1	27	-16
2	50	-50
3	55	62
4	40	40
5	18*	-14
6	31	21
7	11*	-8
8	79	-78
9	14*	14
10	18*	17
11	4*	3
12	39	-39
13	15*	-20
H=	4, K=	14
0	52	-45
1	61	-66
2	49	50
3	41	45
4	24*	-26
5	30	24
6	31	-23
7	52	-53
8	50	50
9	42	49
10	29*	-27
11	16*	-3
H=	4, K=	16
0	4*	10
1	48	52
2	37	34
3	38	-30
4	4*	-3
5	28*	27
6	48	-45
7	4*	11
8	79	72

L	FO	FC
H=	4, K=	16
9	29*	-19
H=	4, K=	18
0	4*	6
1	26*	-18
2	4*	-10
3	36	-23
4	13*	-4
5	10*	5
6	17*	-1
H=	5, K=	19
0	36	21
1	4*	-16
H=	5, K=	17
0	38	40
1	38	37
2	14*	0
3	24*	-13
4	15*	-5
5	7*	-2
6	30	-21
H=	5, K=	15
0	49	-55
1	13*	-12
2	46	43
3	4*	14
4	5*	10
5	7*	-2
6	93	-85
7	4*	-7
8	84	77
9	28*	-25
H=	5, K=	13
0	19*	-3
1	4*	-11
2	12*	9
3	7*	20
4	25*	-22
5	85	73
6	25*	27
7	106	-94
8	35	-31
9	54	45
10	4*	-10

L	FO	FC
11	10*	-19
H=	5, K=	11
0	57	57
1	22*	-13
2	30	-32
3	16*	23
4	3*	-5
5	96	-88
6	50	40
7	52	48
8	46	-50
9	4*	-10
10	20*	-10
11	11*	4
12	4*	-20
H=	5, K=	9
0	141	-135
1	96	101
2	105	107
3	42	-41
4	3*	-16
5	34	-26
6	35	34
7	62	55
8	15*	17
9	4*	3
10	31	34
11	51	52
12	41	42
13	49	50
H=	5, K=	7
0	96	-96
1	76	-87
2	103	97
3	95	99
4	65	62
5	40	-40
6	94	-85
7	19*	24
8	16*	15
9	17*	-20
10	62	-52
11	7*	-8
12	44	-45
13	24*	-18
14	56	59
H=	5, K=	5

L	FO	FC
0	50	39
1	62	-56
2	63	63
3	17*	9
4	31	-38
5	197	188
6	51	49
7	171	-158
8	35	-34
9	54	47
10	21*	17
11	23*	-21
12	21*	20
13	37	-40
14	28*	-24
15	59	51
H=	5, K=	3
0	28	35
1	29	-30
2	154	-150
3	77	-70
4	19*	-6
5	112	-111
6	55	42
7	138	130
8	26	36
9	156	-155
10	16*	14
11	4*	-8
12	16*	10
13	33	29
14	38	-36
15	47	-44
H=	5, K=	1
0	120	-120
1	45	50
2	18*	7
3	99	88
4	14*	4
5	25	-21
6	167	-165
7	11*	8
8	214	213
9	7*	2
10	3*	-4
11	42	-45
12	74	-73
13	33	25
14	22*	8
15	4*	-18

L	FO	FC
H=	6, K=	0
0	3*	-7
2	89	94
4	73	65
6	20*	36
8	28	28
10	24*	34
12	87	-94
14	53	50
H=	6, K=	2
0	68	71
1	127	129
2	48	-60
3	82	74
4	65	68
5	103	-97
6	16*	-3
7	89	90
8	33	41
9	28	28
10	50	53
11	50	-52
12	98	-102
13	35	38
14	41	37
H=	6, K=	4
0	47	-35
1	25	-10
2	3*	-3
3	13*	10
4	194	-187
5	41	35
6	142	132
7	31	24
8	38	-36
9	4*	-5
10	31	-27
11	4*	-5
12	57	48
13	37	31
14	39	-39
H=	6, K=	6
0	15*	9
1	35	34
2	42	42
3	34	-36
4	100	87
5	68	58

```
   L    FO      FC       L    FO      FC       L    FO      FC       L    FO      FC    6

   6    77     -77      10    12*     -8       6     4*     -6       4    11*      6
   7    33     -26      11     4*     -6       7    20*      8       5    47      48
   8    10*    -17                             8    23*     23       6     4*      3
   9     4*     -3    H=     6, K=    14                               7    32      29
  10    51      46                          H=     7, K=    11       8    55      52
  11    22*     20       0    22*      9                               9     4*    -13
  12    61     -55       1    40     -36       0    10*     -7      10    41      40
  13    66     -67       2    31     -33       1    33      39      11    70      70
  14     4*     10       3    19*    -22       2    64      61      12    48      48
                         4    49      49       3    15*    -22      13    16*     13
H=     6, K=     8       5    58      54       4    76     -64
                         6    51     -49       5    23*     13    H=     7, K=     3
   0    92     -96       7    23*    -34       6    32      24
   1    16*     22       8    15*     15       7    54     -54       0   124     122
   2    20*     20       9    22*    -27       8    13*     -6       1    25     -26
   3    16*    -16                             9    43      41       2    25      13
   4   101      99    H=     6, K=    16      10    42     -33       3     6*    -13
   5    69     -70                                                   4    91     -85
   6    87     -81       0    31     -25    H=     7, K=     9       5    11*      4
   7    68     -66       1     4*     12                             6    61      56
   8    47      42       2    24*     28       0     4*      0       7    38     -34
   9    16*      8       3    26*     24       1     4*    -14       8    44     -38
  10    55     -56       4     4*      6       2    87     -95       9    19*     17
  11    44     -42       5    23*     -9       3   145     139      10    44     -40
  12     4*     -6       6    42     -39       4    88      89      11    56     -62
  13    40      31                             5   113    -108      12    30*    -37
                      H=     6, K=    18       6    95     -94      13    23*     29
H=     6, K=    10                             7    52      48
                         0    23*     36       8    23*    -17    H=     7, K=     1
   0    21*    -15       1     4*     13       9    29     -27
   1    35      29       2    14*     -5      10     4*    -12       0     8*      6
   2     3*      3                            11    47     -42       1    13*    -14
   3    42      41    H=     7, K=    17                             2     3*      4
   4    31     -23                          H=     7, K=     7       3   111     102
   5    91     -83       0    12*     11                             4    58      51
   6    31     -28       1     4*      8       0    25*    -39       5   145    -133
   7    79      75                             1    16*     16       6    47     -40
   8    22*    -16    H=     7, K=    15       2    52     -43       7    73      67
   9    19*     -7                             3   172    -168       8     4*     -1
  10    66      56       0    13*    -20       4   116     114       9    10*     12
  11    15*     21       1    15*     -5       5    93      86      10   102     104
  12     4*      7       2     7*    -21       6    18*    -13      11    14*     -6
                         3    19*    -24       7    75     -69      12   100    -106
H=     6, K=    12       4    23*     20       8    18*    -10      13    31      30
                         5     4*     16       9    37      37
   0    11*     11       6    23*    -37      10    17*     15    H=     8, K=     0
   1    10*      0                            11     4*      4
   2    31      29    H=     7, K=    13      12    34     -30       0    15*     -8
   3    23*    -13                                                   2   161    -187
   4    68     -66       0    25*     29    H=     7, K=     5       4   106     113
   5     4*     12       1    21*     29                             6     4*     12
   6    67      62       2    24*    -22       0     3*     11       8    43     -47
   7    53     -48       3    41     -41       1    35     -45      10    63      54
   8    15*      4       4    27      15       2    58      54      12    35     -21
   9    32      27       5    22*     20       3    44     -41
```

H= 8, K= 2

L	FO	FC
0	46	49
1	87	-77
2	62	62
3	94	103
4	26*	-36
5	43	-52
6	36	43
7	35	-39
8	34	37
9	49	47
10	24*	-23
11	55	-57
12	19*	-29

H= 8, K= 4

L	FO	FC
0	9*	-8
1	83	85
2	91	98
3	66	-65
4	51	-54
5	25*	-27
6	17*	-17
7	4*	-23
8	55	-48
9	69	-69
10	40	-49
11	27*	-28
12	4*	6

H= 8, K= 6

L	FO	FC
0	4*	-10
1	76	79
2	28	28
3	70	-78
4	4*	13
5	44	37
6	41	-36
7	20*	22
8	42	45
9	8*	-1
10	4*	19
11	36	37

H= 8, K= 8

L	FO	FC
0	71	70
1	5*	5
2	137	-140
3	9*	4
4	102	98
5	12*	-11
6	4*	-4
7	31	35
8	66	-57
9	10*	14
10	92	86

H= 8, K= 10

L	FO	FC
0	64	-62
1	76	-73
2	99	99
3	49	43
4	11*	-14
5	23*	-4
6	27*	-26
7	50	-42
8	14*	12
9	71	70

H= 8, K= 12

L	FO	FC
0	4*	8
1	33	31
2	22*	22
3	34	-36
4	4*	0
5	17*	-16
6	12*	7
7	26*	18

H= 8, K= 14

L	FO	FC
0	24*	-6
1	16*	27
2	29*	-12
3	41	-33
4	12*	-5
5	38	34

H= 9, K= 13

L	FO	FC
0	34	-36
1	62	56
2	18*	17
3	30	-17

H= 9, K= 11

L	FO	FC
0	53	-54
1	53	-51
2	35	31
3	27*	7
4	26*	17
5	56	-53
6	39	-30

H= 9, K= 9

L	FO	FC
0	22*	23
1	61	-62
2	7*	-20
3	24*	-25
4	17*	-1
5	33*	45
6	60	64
7	54	-52
8	34*	-37

H= 9, K= 7

L	FO	FC
0	50	46
1	4*	9
2	76	-83
3	22*	25
4	16*	14
5	79	-83
6	10*	6
7	52	63
8	64	-69
9	47	-44

H= 9, K= 5

L	FO	FC
0	37	-40
1	127	130
2	55	51
3	121	-117
4	21*	-25
5	42	49
6	37	-38
7	22*	-21
8	25*	-26
9	27*	-28
10	22*	-23

H= 9, K= 3

L	FO	FC
0	50	-51
1	75	-76
2	112	129
3	89	94
4	36	-40
5	18*	-13
6	4*	-4
7	25*	36
8	64	66
9	8*	8
10	22*	-23

H= 9, K= 1

L	FO	FC
0	52	57
1	29	-33
2	21*	27
3	40	49
4	4*	-9
5	46	42
6	4*	3
7	32	-33
8	19*	-27
9	94	87
10	29*	21
11	41	37

H= 10, K= 0

L	FO	FC
0	19*	38
2	27*	-28
4	33	-43
6	69	-64
8	102	-109

H= 10, K= 2

L	FO	FC
0	13*	13
1	56	-60
2	31	21
3	4*	0
4	35	-31
5	6*	21
6	47	51
7	61	-57
8	27*	31

H= 10, K= 4

L	FO	FC
0	139	-142
1	23*	25
2	73	79
3	13*	-17
4	29*	33
5	22*	5
6	49	-52
7	47	48
8	63	61

H= 10, K= 6

L	FO	FC
0	87	84
1	66	73
2	18*	-15
3	17*	-9
4	4*	-2
5	39	-52
6	31	18

```
   L    FO      FC       L    FO      FC       L    FO      FC       L    FO      FC    8

   7    63      60                             -10    10*      8      -4    71     -69
                           0    30*     36     -11     6*      4      -5     9*      3
H=  10, K=       8         1    55     -67     -12    35     -47      -6    97     103
                           2    30*     40     -13    20*     12      -7    31      37
   0    45      54         3     4*      2     -14    91     102      -8    31     -24
   1    21*    -13         4     6*    -16     -15    16*      4      -9    16*    -25
   2    26*    -10         5    38     -47     -16    36     -43     -10    20*     29
   3    19*    -13         6     5*      2     -17    14*     39     -11    20*    -19
   4     4*    -24                             -18    17*     26     -12     4*     19
   5    19*      9     H=  12, K=       0                             -13    22*     53
   6    34      29                         H=   1, K=       5         -14    15*    -21
                           0    23*     35                            -15    29*    -53
H=  10, K=      10         2    36      44      -1   117    -128     -16    49      47
                                                -2   109     127
   0     4*      2     H=  12, K=       2      -3    78      77     H=   1, K=      11
   1    21*    -28                              -4    14*    -18
   2     4*      5         0     5*     -3      -5    45     -41      -1    57      55
   3    23*     17         1    15*     40      -6    47      41      -2    59      67
   4     4*     18                              -7    35      33      -3    20*    -16
                       H=  12, K=       4      -8    28      45      -4    53     -58
H=  10, K=      12                              -9   159     166      -5     3*      6
                           0     5*    -14     -10   130    -141      -6    17*     -5
   0    85     -85                             -11     3*    -10      -7    16*     18
                       H=   1, K=       1     -12    21*    -15      -8    15*     16
H=  11, K=       9                             -13    29*    -34      -9    46     -50
                          -1   329     322     -14    30*     33     -10    40     -42
   0    13*      5        -2   217    -202     -15    61      68     -11    29*     33
                          -3    29     -17     -16    20*      6     -12     9*      2
H=  11, K=       7        -4    22      23     -17     4*    -21     -13     9*     -3
                          -5   325     309                           -14    43      41
   0    38      31        -6    87     -82     H=   1, K=       7    -15     4*    -22
   1    34      34        -7   135    -118
   2     4*      2        -8   125    -126      -1   120    -141     H=   1, K=      13
   3    32*    -25        -9     4*     -1      -2    24      19
                         -10    35      27      -3     9*      6      -1    79     -89
H=  11, K=       5       -11    21*      6      -4   107     118      -2     3*     -6
                         -12    29     -30      -5    43      45      -3    26*     38
   0    46     -50       -13    56      58      -6    91      97      -4    12*    -23
   1     4*      9       -14    14*     -1      -7    30     -27      -5    20*     35
   2    23*      0       -15    56     -53      -8    94    -102      -6    18*    -25
   3    73      76       -16     4*     17      -9    83      85      -7    39     -37
   4    23*     25       -17    38      51     -10    91      98      -8     5*      6
   5    74     -78       -18    23*    -25     -11    31     -25      -9    55      61
                                               -12    17*    -15     -10    24*    -22
H=  11, K=       3     H=   1, K=       3     -13    61     -72     -11    28*    -43
                                               -14    53     -61     -12     4*      3
   0    31     -25        -1   108     123     -15    12*      7     -13     4*     -6
   1    31*     33        -2    96     104     -16     4*     15     -14     5*     14
   2    12*    -18        -3    62     -55     -17    38     -36
   3    59     -67        -4    16*      2                           H=   1, K=      15
   4    31      22        -5   136    -134     H=   1, K=       9
   5    28*     33        -6    24      25                            -1     4*    -12
   6    64     -85        -7   105     101      -1    83      99      -2    68     -81
                          -8    19*     25      -2    66     -73      -3    22*     39
H=  11, K=       1        -9    33     -35      -3   137    -169      -4    20*    -24
```

```
   L     FO     FC       L     FO     FC       L     FO     FC       L     FO     FC

H=    1, K=   15                                -7    14*     38      -4    148   -145
                          -1     51     51      -8     34    -31      -5     23     19
  -5    20*     -8        -2    27*    -30      -9     39    -50      -6     47     43
  -6     38     40        -3     42    -49     -10    17*    -20      -7     38    -39
  -7     4*     18        -4     4*      2     -11     74     78      -8    136    135
  -8     36    -46        -5    20*     15     -12    23*    -13      -9     31    -26
  -9    12*    -19        -6    19*     22     -13     7*     -4     -10    150   -145
 -10     44     49        -7    18*      9     -14    19*     16     -11    17*    -37
 -11     4*     -1        -8    21*     19     -15    22*    -31     -12     43     38
 -12     4*     -3        -9    11*    -35     -16    32*    -42     -13     31     34
                         -10    15*     15                           -14    10*     24
H=    1, K=   17         -11    24*     13    H=    2, K=    8       -15     40     44
                                                                     -16    31*    -36
  -1     48     52    H=    2, K=   14          -1     4*      4     -17    22*    -30
  -2     39    -42                              -2     63    -68     -18     9*     13
  -3    31*    -34        -1     61    -68      -3     71    -70
  -4    22*     33        -2     88    -93      -4    151    166    H=    2, K=    2
  -5     6*     -1        -3     56     53      -5     82     78
  -6    16*     -2        -4     49     52      -6    19*    -29      -1    143    135
  -7     4*      0        -5     43    -45      -7     74     81      -2     43    -68
  -8    23*     30        -6     31    -29      -8     36    -45      -3    173   -169
  -9    30*    -19        -7    17*     14      -9     3*     13      -4     66     68
 -10     5*      1        -8    11*    -12     -10     47     53      -5     22     22
                          -9    31*     37     -11     4*     14      -6     36     33
H=    1, K=   19         -10    20*     33     -12     4*     -5      -7     85     79
                         -11     44    -36     -13     8*     34      -8    14*     -1
  -1     4*      6       -12    23*    -17     -14     36    -45      -9     26    -32
  -2    26*     26       -13    10*      7     -15     4*     -2     -10     60     58
  -3     37     27                             -16     54     61     -11     70     68
  -4     44    -30    H=    2, K=   12                               -12     83    -89
  -5    18*    -10                            H=    2, K=    6       -13    22*    -18
  -6     4*     -6        -1     76    -73                           -14     36     44
  -7    21*     16        -2     73     76      -1     2*     -8     -15     88    -93
                          -3     9*      7      -2    334   -359     -16     53    -65
H=    2, K=   20          -4     65    -80      -3    221    235     -17    30*     47
                          -5     3*      4      -4     79     84     -18    32*     30
  -1    31*     27        -6     38     37      -5    108   -118
  -2    16*     19        -7    20*    -10      -6     46    -41    H=    2, K=    0
  -3     4*     23        -8    12*     14      -7     78    -71
  -4    32*    -22        -9    25*     22      -8    116   -122      -2    111    -67
  -5     5*     -4       -10     59    -67      -9     59     56      -4    193   -182
                         -11    22*    -15     -10     3*    -16      -6     31     33
H=    2, K=   18         -12     53     51     -11     80    -89      -8    176    178
                         -13    14*      0     -12    15*      1     -10     53    -51
  -1     7*     13       -14     4*     18     -13    28*    -23     -12     3*      5
  -2     6*      6       -15    21*     11     -14    24*      5     -14    27*    -26
  -3     4*     -5                             -15    14*     16     -16     98    102
  -4    20*    -36    H=    2, K=   10         -16    20*     22     -18     69    -77
  -5    21*     15                             -17     5*    -19
  -6     4*    -20        -1     44     50                          H=    3, K=    1
  -7     4*     11        -2     42    -38    H=    2, K=    4
  -8     9*      2        -3     92   -105                             -1    10*      0
  -9     5*      5        -4     47     52      -1     7*    -39      -2     83     60
                          -5     26    -19      -2    570    602      -3     35     23
H=    2, K=   16          -6    12*     11      -3     80    -84      -4    220    190
```

L	FO	FC
-5	36	20
-6	43	-38
-7	6*	19
-8	19*	16
-9	3*	14
-10	46	-53
-11	99	98
-12	43	-39
-13	63	-57
-14	17*	23
-15	4*	9
-16	48	52
-17	62	68
-18	17*	-19
H=	3, K=	3
-1	110	-109
-2	263	266
-3	233	-224
-4	155	140
-5	148	142
-6	43	40
-7	83	-78
-8	56	58
-9	26	30
-10	123	-131
-11	3*	-19
-12	81	84
-13	20*	-28
-14	47	-49
-15	24*	-26
-16	65	-72
-17	30*	37
-18	4*	13
H=	3, K=	5
-1	56	80
-2	267	-280
-3	209	218
-4	266	-277
-5	178	-179
-6	86	90
-7	131	139
-8	3*	2
-9	17*	-16
-10	12*	-8
-11	65	-72
-12	22*	19
-13	21*	15
-14	4*	12
-15	47	60
-16	10*	-20
-17	14*	-20

L	FO	FC
H=	3, K=	7
-1	113	-119
-2	79	-87
-3	79	81
-4	182	195
-5	133	-130
-6	113	-121
-7	60	-67
-8	39	46
-9	38	40
-10	34	37
-11	36	-41
-12	47	-50
-13	37	38
-14	23*	8
-15	4*	-18
-16	17*	9
-17	4*	-4
H=	3, K=	9
-1	56	56
-2	114	-125
-3	148	-164
-4	85	89
-5	56	63
-6	3*	-4
-7	25*	27
-8	24	-4
-10	22*	29
-11	68	78
-12	64	-72
-13	13*	-19
-14	34	35
-15	4*	-7
-16	4*	-17
H=	3, K=	11
-1	54	-62
-2	12*	13
-3	22*	-31
-4	50	-58
-5	10*	30
-6	51	49
-7	29	-28
-8	15*	2
-9	4*	6
-10	44	-43
-11	4*	9
-12	65	66
-13	4*	6
-14	9*	11

L	FO	FC
-15	4*	-18
H=	3, K=	13
-1	4*	-19
-2	4*	10
-3	71	83
-4	23*	-17
-5	82	-96
-6	4*	4
-7	77	84
-8	4*	4
-9	19*	-16
-10	9*	-6
-11	4*	-4
-12	4*	4
-13	8*	16
-14	23*	19
H=	3, K=	15
-1	4*	3
-2	43	-46
-3	15*	-13
-4	64	71
-5	30	36
-6	37	-47
-7	8*	-15
-8	16*	8
-9	18*	17
-10	4*	-8
-11	30*	-31
-12	25*	-19
H=	3, K=	17
-1	24*	18
-2	4*	10
-3	32*	-25
-4	30*	-29
-5	24*	27
-6	18*	5
-7	6*	17
-8	17*	-3
-9	28*	-10
-10	9*	-3
H=	3, K=	19
-1	27*	-9
-2	12*	-14
-3	5*	-17
-4	48	-40
-5	5*	-12
-6	23*	-11

L	FO	FC
H=	4, K=	18
-1	31*	-23
-2	27*	25
-3	27*	-13
-4	21*	-25
-5	38	31
-6	32*	30
-7	15*	-4
H=	4, K=	16
-1	16*	0
-2	22*	-17
-3	17*	6
-4	29*	23
-5	33	25
-6	32*	-27
-7	12*	-6
-8	19*	3
-9	5*	3
-10	22*	-12
H=	4, K=	14
-1	42	34
-2	4*	13
-3	4*	0
-4	12*	2
-5	36	-36
-6	21*	-25
-7	4*	21
-8	28*	23
-9	12*	-11
-10	42	-45
-11	4*	-15
-12	5*	23
H=	4, K=	12
-1	4*	-15
-2	31	-35
-3	27*	20
-4	4*	-7
-5	44	-47
-6	33	35
-7	19*	21
-8	55	-54
-9	4*	-20
-10	4*	7
-11	4*	-2
-12	4*	14
-13	34*	25
-14	11*	3

```
   L    FO      FC       L    FO      FC       L    FO      FC       L    FO      FC   11

H=   4, K=      10     -17     5*    -17      -1    96    -108     -16    15*     -1
                                              -2    46      44
  -1    22*     16    H=   4, K=       4      -3    27      26    H=   5, K=       7
  -2    13*      7                            -4    20*     15
  -3    35     -37      -1    32     -31      -5   145     134      -1   136     133
  -4    76     -77      -2    74     -80      -6    48      38      -2   146     152
  -5   101      97      -3    45     -35      -7   202    -197      -3    76     -79
  -6    49      54      -4   136    -120      -8    75      72      -4    58      57
  -7   100     -97      -5     3*     -2      -9   153     150      -5    57     -56
  -8    60     -72      -6   174     161     -10    22*     15      -6    58     -55
  -9    15*     22      -7   155     162     -11    50     -56      -7    73      73
 -10    29*    -29      -8    38     -41     -12     4*     13      -8    42      40
 -11     4*     17      -9    54      42     -13    40     -47      -9    91     -91
 -12    50      42     -10    44      34     -14    51      50     -10     7*    -10
 -13    33*    -25     -11    38     -27     -15    30*     54     -11    19*     24
 -14    20*      9     -12    21*      8     -16    29*    -41     -12    16*    -16
 -15     8*     -9     -13    29*     41     -17    39      38     -13    20*    -22
                       -14     4*    -13                           -14    28*     29
H=   4, K=       8     -15     4*      3    H=   5, K=       3     -15    17*     13
                       -16     5*    -32                           -16    39     -43
  -1    63     -66     -17     8*     -2      -1    13*      6
  -2    35      22                            -2    55     -43    H=   5, K=       9
  -3    39     -42    H=   4, K=       2      -3    12*      4
  -4   248     258                            -4   162    -146      -1    49     -59
  -5    27*    -31      -1    58      43      -5    67      54      -2    16*     -5
  -6   111    -119      -2    33       4      -6   186     166      -3    79      76
  -7    22*     21      -3     5*    -10      -7    37     -28      -4   119    -109
  -8    46      43      -4   213    -188      -8   153    -144      -5   145     140
  -9    27*    -31      -5   129     115      -9    70     -76      -6   113    -109
 -10    29*     33      -6    23*    -22     -10    37      40      -7   108    -112
 -11     4*     11      -7   106     -97     -11     4*    -15      -8    69      66
 -12    76     -83      -8    75      84     -12    18*     14      -9    84      85
 -13    25*     12      -9    38     -32     -13    75     -67     -10    52     -49
 -14    44      55     -10   114    -122     -14    48     -51     -11    39     -28
 -15     5*      6     -11    45      34     -15    34      36     -12    25*     18
 -16    55     -44     -12    26*     29     -16    23*     28     -13    12*      6
                       -13    97     -95     -17     7*    -18     -14    16*      2
H=   4, K=       6     -14    44     -48                           -15    29*     22
                       -15    37      46    H=   5, K=       5
  -1   116     113     -16    26*     24                          H=   5, K=      11
  -2    47      49     -17    42      50      -1    54      59
  -3    38     -43                            -2    78     -80      -1    13*     -2
  -4    80      73    H=   4, K=       0      -3    90      87      -2    70     -71
  -5   171    -173                            -4    16*     17      -3    56     -48
  -6    87      93      -2   134    -127      -5   116    -105      -4    38      42
  -7    22*     16      -4   104      91      -6    82      76      -5    49     -49
  -8    39      32      -6    36     -32      -7   101      90      -6   118     122
  -9    11*     14      -8    86      85      -8    10*      2      -7     4*      0
 -10     4*     21     -10    23*     18      -9     4*     10      -8    76     -68
 -11     4*     -1     -12    74     -77     -10    32     -31      -9    46     -43
 -12    20*     28     -14    75      85     -11    28     -19     -10    18*      1
 -13    39      49     -16    14*      5     -12    25*     27     -11    36      41
 -14    27*    -17                           -13    35      39     -12    24*     34
 -15    17*    -15    H=   5, K=       1     -14    39     -45     -13     6*     -7
 -16    27*    -29                           -15    12*    -25     -14    27*    -33
```

```
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC   12

                    H=   6, K=    16     -13    5*     -1     -13   14*    -14
H=   5, K=    13                         -13    5*     -1     -14   59     -52
                      -1   21*    -22    -14    5*     -9     -15   22*     18
  -1   34      46     -2   28*     21                         -16   38*     44
  -2   52      46     -3   19*    -25   H=   6, K=     8
  -3   18*    -43     -4   51     -40                        H=   6, K=     2
  -4   17*     -4     -5   26*    -25     -1   27      27
  -5   13*    -12     -6   24*    -14     -2  129     124      -1   64     -69
  -6    7*     11     -7   42     -41     -3   25*    -25      -2   34      37
  -7    4*     13     -8    8*     18     -4  119    -109      -3   23*     16
  -8   25*     16                         -5   24*     32      -4   50     -49
  -9    4*     -3   H=   6, K=    14      -6   88     -84      -5   67     -71
 -10   29*    -18                         -7   15*    -18      -6   23*      9
 -11   18*     -6     -1   38      31     -8   80      67      -7   88     -72
 -12   20*     20     -2   27*     -5     -9   14*     18      -8   39     -31
 -13   47      45     -3   17*      4    -10   71     -71      -9  169     152
                      -4   23*     17    -11    9*    -17     -10   52      55
H=   5, K=    15      -5    4*     24    -12   94      84     -11   35     -40
                      -6   23*     20    -13   17*     -3     -12   53     -57
  -1   19*    -11     -7   76      68    -14   33*    -21     -13   23*     -9
  -2    4*     -8     -8   26*      8    -15   43      32     -14   29*     36
  -3   35     -31     -9   60     -47                         -15   53      57
  -4   12*    -27    -10   27*    -16   H=   6, K=     6      -16   28*    -18
  -5   41     -42    -11   38      32
  -6   25*    -23                         -1  116     118    H=   6, K=     0
  -7    4*     23   H=   6, K=    12      -2  110    -110
  -8    4*      2                         -3   65     -63      -1   12*      0
  -9   40     -31     -1   35      37     -4    3*     26      -4   55     -46
 -10   18*    -20     -2   17*     16     -5   42     -39      -6  137     116
 -11    5*      9     -3   34     -30     -6   81     -76      -8  166     157
                      -4   34      31     -7   83      77     -10  130    -133
H=   5, K=    17      -5   42      39     -8   45      38     -12    4*     15
                      -6   33*     42     -9   83     -73     -14   19*      3
  -1   17*     -1     -7   16*     -7    -10   28*    -21     -16   14*    -31
  -2   15*     34     -8   67     -59    -11   10*     15
  -3   26*      7     -9   17*     -8    -12   39      48    H=   7, K=     1
  -4    4*     16    -10   26*    -17    -13    4*    -13
  -5   48      45    -11   23*      4    -14    4*    -18      -1   39     -55
  -6    5*      5    -12   25*     19    -15   27*    -25      -2   55     -71
  -7   60     -54    -13   22*      6    -16   28*    -26      -3   51      53
  -8    5*      2                                               -4  104     -96
                    H=   6, K=    10    H=   6, K=     4        -5   53     -51
H=   5, K=    19                                                -6   23*    -24
                      -1   49     -48     -1    9*      3      -7   14*     -8
  -1    5*     -8     -2   74     -71     -2  116    -109      -8   24*      9
  -2   24*    -11     -3  109      96     -3  140    -130      -9   98      96
  -3    5*      3     -4   96      93     -4   25     -22     -10   81     -69
                      -5   63     -61     -5   29*     23     -11   25*     27
H=   6, K=    18      -6   40      42     -6  128     117     -12   31      25
                      -7   65     -68     -7   77      68     -13    4*     -5
  -1   20*    -13     -8   12*     -9     -8  102     -85     -14    4*     -1
  -2   29*     -6     -9   31     -23     -9   62     -55     -15   30*     26
  -3   34*     26    -10   19*     23    -10   72      68     -16   37     -29
  -4   12*      9    -11    4*      6    -11    7*    -15
                     -12   42      43    -12   26*     22    H=   7, K=     3
```

L	FO	FC
H=	7, K=	3
-1	3*	-16
-2	97	-113
-3	73	74
-4	128	127
-5	4*	0
-6	33	-27
-7	60	-54
-8	30	-25
-9	119	103
-10	83	81
-11	142	-119
-12	4*	-8
-13	29*	29
-14	19*	33
-15	5*	8
H=	7, K=	5
-1	47	61
-2	68	-67
-3	73	-71
-4	4*	2
-5	59	52
-6	9*	15
-7	93	93
-8	76	-69
-9	113	-115
-10	73	77
-11	100	91
-12	18*	15
-13	79	-69
-14	18*	-25
-15	17*	10
H=	7, K=	7
-1	4*	-12
-2	65	62
-3	7*	-12
-4	47	-44
-5	17*	32
-6	15*	3
-7	31*	-34
-8	67	68
-9	23*	29
-10	61	-56
-11	45	-36
-12	40	48
-13	11*	15
-14	5*	-15
H=	7, K=	9
-1	22*	9
-2	58	48
-3	61	65
-4	15*	-5
-5	17*	-23
-6	64	62
-7	13*	-16
-8	4*	5
-9	28*	-16
-10	4*	10
-11	4*	-14
-12	4*	24
-13	5*	3
H=	7, K=	11
-1	21*	-20
-2	68	-64
-3	23*	-21
-4	36	39
-5	26*	-14
-6	4*	3
-7	31*	-48
-8	71	-79
-9	32*	26
-10	29*	22
-11	80	-47
-12	5*	5
H=	7, K=	13
-1	32	34
-2	4*	-3
-3	43	40
-4	4*	6
-5	38	37
-6	4*	-18
-7	55	54
-8	48	-46
-9	100	-90
-10	8*	6
-11	52	41
H=	7, K=	15
-1	4*	6
-2	19*	2
-3	44	-50
-4	14*	1
-5	22*	26
-6	60	60
-7	19*	-17
-8	51	43
H=	7, K=	17
-1	18*	-22
-2	5*	-5
-3	40	34
H=	8, K=	14
-1	15*	18
-2	26*	3
-3	21*	-18
-4	4*	21
-5	65	58
-6	70	49
-7	65	-62
H=	8, K=	12
-1	28*	-22
-2	50	-52
-3	4*	-9
-4	16*	10
-5	4*	-14
-6	60	-59
-7	4*	-5
-8	70	-67
-9	5*	-41
-10	59	57
H=	8, K=	10
-1	8*	5
-2	16*	15
-3	31	39
-4	21*	23
-5	32*	28
-6	60	64
-7	16*	-4
-8	66	-62
-9	62	67
-10	57	57
-11	59	-59
-12	5*	-1
H=	8, K=	8
-1	23*	-6
-2	11*	9
-3	25*	21
-4	69	-64
-5	4*	-18
-6	29	23
-7	38	34
-8	16*	-11
-9	4*	-5
-10	8*	-19
-11	55	-41
-12	32*	34
-13	16*	8
H=	8, K=	6
-1	23*	27
-2	27	20
-3	75	-79
-4	44	-45
-5	93	92
-6	33	38
-7	23*	-15
-8	113	-106
-9	4*	-7
-10	26*	19
-11	34	23
-12	43	35
-13	49	-51
-14	5*	-25
H=	8, K=	4
-1	13*	32
-2	34	-39
-3	58	-61
-4	94	82
-5	23*	27
-6	82	-72
-7	19*	13
-8	4*	-1
-9	4*	3
-10	79	76
-11	26*	-32
-12	85	-86
-13	18*	-16
-14	28*	35
H=	8, K=	2
-1	19*	-31
-2	15*	-27
-3	36	43
-4	4*	9
-5	105	-91
-6	14*	-14
-7	91	84
-8	15*	13
-9	62	56
-10	22*	9
-11	106	-108
-12	37	27
-13	12*	13
-14	5*	-8
-15	25*	-8

```
   L    FO    FC      L    FO    FC      L    FO    FC      L    FO    FC   14

 H=    8, K=    0
  -2   64   -83
  -4   53   -53
  -6   52    50
  -8   56    51
 -10   94   -89
 -12   57    59
 -14   12*  -16

 H=    9, K=    1

  -1    4*   13
  -2    4*  -12
  -3   28*  -33
  -4   12*    1
  -5   57   -57
  -6   69    61
  -7   30    25
  -8   33   -27
  -9   66    66
 -10   29*  -32
 -11   82   -79
 -12   45    51
 -13   50    48

 H=    9, K=    3

  -1   31    39
  -2    4*   17
  -3    5*   11
  -4   23*  -31
  -5   59   -51
  -6   71   -76
  -7   78    65
  -8   46    39
  -9   20*  -31
 -10   22*   10
 -11   18*  -11
 -12   24*  -33
 -13   23*    9

 H=    9, K=    5

  -1   37   -49
  -2   11*  -21
  -3   11*  -12
  -4   74    73
  -5   39    42
  -6   50   -54
  -7   53   -61
  -8   37   -30
  -9   66    58
 -10   25*   30

 -11    4*   16
 -12   26*  -32
 -13   20*  -13

 H=    9, K=    7

  -1   17*  -18
  -2   12*    5
  -3   10*  -10
  -4   52   -53
  -5   13*  -11
  -6   23*   21
  -7    4*   10
  -8   48   -51
  -9   32*  -33
 -10   13*   12
 -11   18*   17
 -12   56    58

 H=    9, K=    9

  -1   26*   32
  -2    9*   14
  -3   16*   23
  -4   14*   16
  -5   36    43
  -6    4*    1
  -7   20*    0
  -8   53   -61
  -9    5*   15
 -10    7*   -6
 -11   86   -85

 H=    9, K=   11

  -1   16*  -26
  -2   30*  -38
  -3    4*   24
  -4   68    68
  -5   19*  -15
  -6    5*   -8
  -7   60    73
  -8    5*   18
  -9    7*   -8

 H=    9, K=   13

  -1   22*   -4
  -2   17*   -3
  -3    5*  -21
  -4   18*   14
  -5   72    61
  -6   28*  -12

 H=   10, K=   12

  -1   26*  -13
  -2    8*    8
  -3   22*   -6

 H=   10, K=   10

  -1   26*   12
  -2   31*  -27
  -3   26*   38
  -4   72    78
  -5   29*  -20
  -6   44   -36
  -7   73    78

 H=   10, K=    8

  -1   16*   28
  -2   27*  -25
  -3   19*  -26
  -4    8*   -8
  -5   23*  -29
  -6   16*   -9
  -7    9*    3
  -8   59   -64
  -9    5*   -1

 H=   10, K=    6

  -1   87  -106
  -2   54   -58
  -3    4*   -4
  -4   97   103
  -5   30*   36
  -6    4*   -9
  -7    6*   21
  -8   30*   34
  -9   59    61
 -10    7*   13

 H=   10, K=    4

  -1   14*  -37
  -2   62    79
  -3    4*  -19
  -4    4*  -10
  -5   18*  -25
  -6   49   -56
  -7   25*   35
  -8    4*   23
  -9   18*   12
 -10    5*    5
 -11    5*    0

 H=   10, K=    2

  -1   54    88
  -2    4*   17
  -3   12*  -34
  -4    4*  -21
  -5   27*  -28
  -6    4*  -23
  -7   88    91
  -8   16*   -5
  -9   24*  -21
 -10   19*  -24
 -11   15*  -30
 -12   11*  -11

 H=   10, K=    0

  -2   15*  -26
  -4    4*    7
  -6   63    56
  -8   78   -68
 -10   33    25
 -12   19*   27

 H=   11, K=    1

  -1   39    68
  -2   29*  -47
  -3   18*  -30
  -4    4*   15
  -5   19*   -8
  -6   30    26
  -7   46    41
  -8   33*  -34
  -9   44   -38

 H=   11, K=    3

  -1   36    50
  -2   30*   40
  -3   33   -60
  -4   36   -40
  -5   19*    8
  -6    4*    8
  -7   20*    9
  -8   26*   26
  -9    5*   -6

 H=   11, K=    5

  -1   62   -55
  -3   28*   49
  -4   45    43
  -5   52   -52
  -6   37   -43
  -7   11*   16
```

```
   L     FO     FC      L     FO     FC      L     FO     FC      L     FO     FC   15

 H=   11,  K=    5                            -6      7*    -6     -1     38     30
                       -1     44    -52       -7     17*     3     -2      5*   -20
   -8    21*     9     -3      5*    -2                            -3     18*   -24
                       -4      5*    30    H=   11,  K=    9       -4     47     44
 H=   11,  K=    7     -5     13*    25
```

```
 L     FO     FC      L     FO     FC      L     FO     FC      L     FO     FC   16

H=  12, K=    4      -4      5*  -24      -2     11*    39    H=  12, K=    0
                                          -3     35*   -81
 -1    29*    34    H=  12, K=    2      -4     18*   -23     -2     41    -80
 -2    26*    51                          -5      8*    21     -4     60     87
 -3    26*   -30      -1     29*    37                         -6     53    -57
```

TABLE IV Structure Factors For the Rhenium Compound

L	FO	FC
H=	0, K=	0
2	141	129
4	3*	12
6	19*	-25
8	42	-34
10	111	105
12	161	163
14	102	133
16	50*	-61
H=	0, K=	1
16	86	-78
15	25*	-11
14	71	-79
13	24*	33
12	90	94
11	52	37
10	198	206
9	35	-33
8	181	177
7	79	-83
6	65	74
5	46	-47
4	232	-208
3	37	32
2	261	-277
1	30	20
H=	0, K=	2
0	31*	-416
1	30	-48
2	118	-121
3	219	-244
4	4*	-10
5	25*	-21
6	168	161
7	37	-28
8	70	72
9	59	54
10	91	-93
11	16*	15
12	117	-128
13	80	-90
14	102	-111
15	85	-90
16	63	62
H=	0, K=	3
15	17*	-14
14	78	82
13	56	-71
12	14*	-18
11	45	-50
10	98	-114
9	18*	33
8	102	-98
7	209	204
6	50	-44
5	231	231
4	123	136
3	43	59
2	160	182
1	84	-95
H=	0, K=	4
0	56	71
1	57	61
2	33	-24
3	295	289
4	96	-96
5	129	134
6	120	-131
7	21*	-25
8	81	-78
9	100	-102
10	6*	28
11	60	-61
12	44	55
13	102	113
14	49	45
15	101	121
H=	0, K=	5
15	28*	27
14	35*	-44
13	100	113
12	54	-51
11	82	95
10	16*	23
9	19*	-8
8	20*	2
7	196	-202
6	58	-61
5	169	-186
4	4*	-19
3	21*	-13
2	50	-66
1	179	206
H=	0, K=	6
0	113	108
1	58	-72
2	99	102
3	233	-264
4	78	79
5	67	-65
6	51	64
7	72	89
8	38	42
9	131	145
10	39	45
11	94	106
12	20*	24
13	51	-59
14	7*	19
H=	0, K=	7
14	7*	3
13	107	-129
12	31*	32
11	89	-103
10	89	90
9	23*	-27
8	77	94
7	95	109
6	35	46
5	79	86
4	45	-43
3	5*	-17
2	5*	13
1	224	-239
H=	0, K=	8
0	229	-191
1	60	65
2	71	-70
3	153	152
4	22*	-23
5	17*	20
6	46	50
7	53	-59
8	48	37
9	130	-131
10	42*	-59
11	96	-97
12	56	-67
13	20*	23
H=	0, K=	9
12	20*	-6
11	65	66
10	96	-96
9	30*	23
8	58	-57
7	36*	-38
6	31*	-33
5	29*	-35
4	126	128
3	36	32
2	100	100
1	168	140
H=	0, K=	10
0	151	148
1	40	-31
2	50	43
3	60	-64
4	76	-74
5	11*	9
6	141	-136
7	52	51
8	66	-67
9	49	49
10	7*	29
11	39*	60
H=	0, K=	11
10	71	75
9	7*	12
8	54	51
7	22*	-17
6	12*	-3
5	19*	10
4	155	-145
3	7*	9
2	112	-98
1	64	-47
H=	0, K=	12
0	129	-102
1	23*	-15
2	7*	-19
3	20*	-7
4	78	73
5	7*	-10
6	130	122
7	7*	6
8	72	69
H=	0, K=	13
5	7*	4
4	92	81
3	30*	-29
2	107	92
1	62	-51

H= 1, K= 13

L	FO	FC
0	33*	8
1	42*	-43
2	113	91
3	7*	-14
4	137	113

H= 1, K= 12

L	FO	FC
7	8*	1
6	109	87
5	15*	-12
4	66	49
3	23*	-20
2	57	-44
1	28*	3
0	165	-117

H= 1, K= 11

L	FO	FC
0	49	-41
1	28*	-27
2	171	-133
3	20*	10
4	147	-142
5	32*	40
6	18*	-27
7	33*	17
8	33*	35
9	18*	26

H= 1, K= 10

L	FO	FC
10	56	58
9	66	57
8	79	-79
7	68	59
6	85	-86
5	18*	10
4	67	-62
3	6*	-21
2	46	53
1	17*	13
0	153	142

H= 1, K= 9

L	FO	FC
0	24*	17
1	118	119
2	83	96
3	27*	17
4	127	132
5	82	-83
6	10*	-7
7	72	-70
8	42	-53
9	25*	-13
10	88	-83
11	28*	23

H= 1, K= 8

L	FO	FC
12	32*	-34
11	95	-95
10	25*	-35
9	108	-109
8	57	58
7	99	-106
6	84	85
5	47	48
4	24*	18
3	86	94
2	49	-45
1	11*	10
0	135	-125

H= 1, K= 7

L	FO	FC
0	13*	19
1	171	-196
2	51	49
3	20*	-21
4	9*	19
5	116	117
6	38	37
7	150	149
8	89	84
9	6*	-16
10	90	91
11	72	-74
12	22*	22
13	83	-89

H= 1, K= 6

L	FO	FC
13	51	-54
12	6*	-7
11	99	103
10	15*	-25
9	142	135
8	20*	3
7	104	114
6	21*	-9
5	107	-109
4	11*	13
3	193	-229
2	23*	27
1	64	-67
0	64	61

H= 1, K= 5

L	FO	FC
0	44	-49
1	133	162
2	88	-82
3	4*	25
4	112	-110
5	132	-155
6	61	-63
7	170	-164
8	17*	2
9	22*	30
10	20*	-22
11	120	128
12	36*	-40
13	116	129
14	27*	-25

H= 1, K= 4

L	FO	FC
14	51	60
13	76	81
12	36	38
11	53	-56
10	55	61
9	60	-58
8	41	-32
7	27*	-31
6	124	-121
5	169	174
4	86	-85
3	395	398
2	121	116
1	132	140
0	60	77

H= 1, K= 3

L	FO	FC
0	149	-151
1	110	-133
2	204	215
3	48	-46
4	223	203
5	110	112
6	4*	-4
7	125	122
8	97	-101
9	63	-69
10	91	-91
11	116	-117
12	15*	2
13	111	-122
14	58	70
15	45	-55

H= 1, K= 2

L	FO	FC
15	61	-63
14	72	-74
13	70	-82
12	77	-89
11	6*	-3
10	58	-74
9	43	40
8	107	102
7	37	-36
6	161	153
5	122	-132
4	96	95
3	250	-277
2	119	-123
1	57	-69
0	303	-311

H= 1, K= 1

L	FO	FC
0	34	24
1	81	69
2	146	-120
3	10*	-1
4	146	-138
5	4*	7
6	90	93
7	50	-44
8	197	194
9	29*	35
10	210	208
11	40	37
12	63	63
13	47	46
14	69	-80
15	19*	24

H= 1, K= 0

L	FO	FC
14	78	83
12	95	96
10	80	77
8	138	-127
6	233	-219
4	66	-60
2	181	181
0	470	497

H= 2, K= 0

L	FO	FC
0	28*	32
2	21*	31
4	221	-179

```
   L     FO     FC       L     FO     FC       L     FO     FC       L     FO     FC    3

H=   2, K=       0       5    25*     24      11     84     83       5     5*     -3
                         4    156    151      12    35*    -23       6     55    -56
   6    280   -239       3     55    -55                             7    17*     27
   8    237   -216       2    204    187    H=   2, K=       7       8     44    -56
  10    30*     22       1    301   -277                             9     40     38
  12     71     78       0     45     46      12     7*      6
  14     47     36                            11     51    -54    H=   2, K=      11
                       H=   2, K=       4     10    14*     28
H=   2, K=       1                             9    22*     12       7     40     35
                         0    137    123       8    25*      6       6    15*    -14
  14     98   -104       1    155    152       7    172    165       5    21*     26
  13     48     41       2    110     98       6    13*      8       4    103   -124
  12    24*    -11       3    292    284       5    136    132       3     32     23
  11    35*     39       4    24*    -26       4     44    -49       2     85   -101
  10    154    140       5    155    156       3    18*     12       1    16*     20
   9     49     49       6     71    -75       2     36    -40       0     37    -34
   8    115    114       7     48    -43       1    112   -112
   7     57    -48       8    21*    -24       0    15*     13    H=   2, K=      12
   6     5*     -6       9    111   -109
   5     29    -14      10     70     68    H=   2, K=       8       0    119   -124
   4    233   -201      11     85    -73                             1     5*     -1
   3     56     47      12     48     46       0     52    -47       2     59    -67
   2    102    -80      13    29*     39       1     30     31       3    20*    -21
   1    103     92                             2    30*    -31       4    19*     19
   0     35    -37    H=   2, K=       5       3     78     87       5     6*      2
                                               4     65     73
H=   2, K=       2      13    101    106       5     42     54    H=   2, K=      13
                        12     6*      0       6     97    107
   0    256   -228      11     99    104       7     69    -75       3     6*      8
   1    190   -170      10     6*     18       8     60     72       2     69     68
   2     54    -45       9    33*     27       9     66    -75       1    24*    -26
   3    203   -172       8     5*     22      10     5*     -6       0    22*     17
   4    139    121       7    142   -137      11     60    -66
   5    116   -118       6     5*      3                          H=   3, K=      12
   6    161    169       5     96    -94    H=   2, K=       9
   7    21*      4       4     71    -70                             3    21*     -9
   8    153    147       4     73    -70      10     44    -52       2     61    -56
   9     54     44       3    14*    -10       9     5*    -30       1    22*     13
  10     49    -50       2     84    -85       8     42    -47       0    131   -122
  11     62     48       1    221    211       7     87   -107
  12     82    -78       0     4*     -7       6    10*     22    H=   3, K=      11
  13    23*    -20                             5     76    -88
  14     46    -39    H=   2, K=       6       4    111    132       0    16*    -18
                                               3     31    -31       1    10*      6
H=   2, K=       3       0     28    -33       2     67     82       2     54    -51
                         1     65    -59       1     40     50       3     5*     11
  14     49     50       2     58    -49       0    22*     28       4     78    -81
  13    124   -117       3    175   -177                             5    20*     18
  12     6*      1       4     47    -48    H=   2, K=      10       6     6*      2
  11    106   -106       5    134   -127
  10     96    -88       6     88    -80       0    141    141    H=   3, K=      10
   9     64    -67       7    103     99       1     5*      3
   8     65    -61       8     57    -54       2     60     58       7    12*      2
   7     63     59       9    110    109       3    23*    -19       6     61    -68
   6    27*     25      10     62    -58       4    22*    -35       5     39    -46
```

L	FO	FC
4	14*	-18
3	50	-54
2	63	71
1	43	-45
0	129	131

H= 3, K= 9

L	FO	FC
0	26*	21
1	5*	13
2	70	66
3	43	-40
4	86	91
5	73	-67
6	5*	21
7	94	-89
8	52	-53

H= 3, K= 8

L	FO	FC
9	59	-60
8	49	55
7	26*	-23
6	57	69
5	60	69
4	56	56
3	115	118
2	21*	-7
1	59	65
0	51	-54

H= 3, K= 7

L	FO	FC
0	22*	-21
1	85	-95
2	60	-54
3	36	38
4	82	-87
5	123	133
6	31	-39
7	128	124
8	5*	-13
9	34	26
10	6*	-3

H= 3, K= 6

L	FO	FC
11	58	59
10	16*	-20
9	72	76
8	44	-46
7	82	81
6	31*	-40
5	90	-89
4	42	-43
3	158	-169
2	70	-75
1	48	-40
0	57	-61

H= 3, K= 5

L	FO	FC
0	32	39
1	202	232
2	68	-70
3	10*	-22
4	14*	-6
5	90	-90
6	35	40
7	130	-131
8	38	40
9	5*	2
10	36	46
11	70	72

H= 3, K= 4

L	FO	FC
12	36	41
11	87	-95
10	25*	36
9	115	-120
8	17*	-20
7	92	-90
6	43	-49
5	46	51
4	30	-28
3	94	99
2	47	48
1	60	65
0	136	142

H= 3, K= 3

L	FO	FC
0	56	57
1	209	-232
2	114	116
3	15*	-20
4	141	139
5	16*	21
6	19*	-15
7	81	83
8	69	-64
9	39	-32
10	73	-74
11	65	-70
12	20*	-6

H= 3, K= 2

L	FO	FC
12	77	-81
11	77	76
10	46	-40
9	74	72
8	102	102
7	92	84
6	144	144
5	13*	-15
4	112	109
3	79	-80
2	56	-52
1	14*	-24
0	121	-124

H= 3, K= 1

L	FO	FC
0	18*	-31
1	30	40
2	108	-102
3	4*	12
4	244	-229
5	18*	-5
6	39	-44
7	25*	-26
8	72	63
9	5*	-1
10	75	68
11	30*	34
12	34	-32
13	33*	34

H= 3, K= 0

L	FO	FC
12	83	90
10	45	47
8	142	-143
6	200	-186
4	205	-204
2	49	45
0	71	66

H= 4, K= 0

L	FO	FC
0	124	116
2	105	93
4	78	-69
6	145	-133
8	80	-80
10	72	74

H= 4, K= 1

L	FO	FC
11	17*	14
10	75	68
9	17*	-20
8	78	70
7	32	-31
6	44	-50
5	30	-25
4	194	-184
3	37	-35
2	149	-144
1	47	44
0	73	-72

H= 4, K= 2

L	FO	FC
0	103	-96
1	35	43
2	80	-73
3	8*	-15
4	64	63
5	12*	4
6	98	104
7	69	72
8	58	66
9	86	80
10	49	-52
11	72	65

H= 4, K= 3

L	FO	FC
11	35	-36
10	66	-69
9	35	33
8	63	-66
7	124	130
6	6*	-1
5	70	73
4	92	89
3	16*	15
2	43	48
1	103	-89
0	10*	22

H= 4, K= 4

L	FO	FC
0	86	83
1	7*	17
2	40	29
3	57	56
4	18*	-22
5	38	37
6	54	-56
7	105	-108
8	38	-35
9	83	-83
10	26*	23

H= 4, K= 5

L	FO	FC
H=	4, K=	5
10	35	30
9	45	-48
8	39	41
7	119	-115
6	34	31
5	95	-97
4	19*	17
3	39	-44
2	20*	8
1	143	149
0	7*	4
H=	4, K=	6
0	28	-25
1	61	-67
2	15*	20
3	132	-134
4	22*	-8
5	77	-79
6	15*	-6
7	41	48
8	5*	-2
9	72	71
H=	4, K=	7
8	27*	-7
7	77	86
6	32*	-40
5	82	84
4	58	-60
3	15*	27
2	66	-63
1	103	-107
0	33	-41
H=	4, K=	8
0	72	-78
1	70	68
2	35	-36
3	100	101
4	26*	19
5	70	65
6	50	43
7	5*	-7
8	31*	26
H=	4, K=	9
6	12*	3
5	39	-39
4	61	66
3	5*	6
2	45	56
1	36	31
0	5*	-10
H=	4, K=	10
0	112	101
1	50	-50
2	59	58
3	66	-46
4	41	-29
5	58	-52
H=	4, K=	11
3	22*	-10
2	44	-35
1	5*	-11
0	5*	9
H=	4, K=	12
0	95	-86
H=	5, K=	10
2	34	32
1	30*	-32
0	58	66
H=	5, K=	9
0	5*	-7
1	67	58
2	26*	21
3	5*	12
4	48	46
H=	5, K=	8
5	43	37
4	16*	-13
3	85	84
2	50	-61
1	61	57
0	66	-68
H=	5, K=	7
0	16*	21
1	111	-102
2	44	-42
3	5*	16
4	34	-33
5	44	31
6	5*	2
H=	5, K=	6
7	17*	18
6	28*	16
5	62	-62
4	47	52
3	82	-66
2	68	62
1	92	-99
0	25*	13
H=	5, K=	5
0	8*	-23
1	118	109
2	15*	2
3	33	-39
4	5*	-6
5	88	-86
6	26*	18
7	71	-65
8	17*	10
H=	5, K=	4
8	57	-43
7	47	-47
6	50	-41
5	65	55
4	30*	-30
3	62	55
2	14*	4
1	34	36
0	46	43
H=	5, K=	3
0	6*	-7
1	49	-42
2	64	60
3	40	31
4	48	51
5	79	79
6	20*	-8
7	99	84
8	48	-41
9	57	52
H=	5, K=	2
9	39	39
8	41	38
7	44	32
6	58	52
5	35	-27
4	31	38
3	22*	-13
2	82	-81
1	18*	-9
0	139	-131
H=	5, K=	1
0	36	-35
1	32	31
2	123	-114
3	23*	-10
4	114	-95
5	34	-29
6	5*	-3
7	47	-41
8	71	67
9	20*	-8
H=	5, K=	0
8	30*	-32
6	46	-48
4	19*	-14
2	118	117
0	157	153
H=	6, K=	0
0	140	128
2	100	81
4	48	-37
6	53	-45
H=	6, K=	1
7	23*	-25
6	37	31
5	38	-31
4	66	-61
3	20*	2
2	69	-59
1	22*	13
0	7*	1
H=	6, K=	2
0	112	-107
1	44	-43
2	61	-60
3	61	-52

```
    L    FO   FC        L    FO   FC        L    FO   FC        L    FO   FC     6

    4   49    39
    5   55   -45      H=  6, K=    9      H=  8, K=    1       -1   82   -95
    6   55    53                                               -2   23   -21
    7   11*   12        0   17*    3        0    6*   11       -3  137   126
                                                               -4  104   -92
  H=  6, K=    3      H=  7, K=    6      H=  1, K=    0       -5  273   238
                                                               -6   18*  -13
    6   14*  -11        1   30*  -23      -16   39*  -35       -7  215   210
    5   71    66        0   28*   21      -14  184   179       -8  113   108
    4   64    55                          -12  248   235       -9  136   123
    3   36    32      H=  7, K=    5      -10  156   142      -10  201   178
    2   56    50                           -8   45   -45      -11   27   -20
    1   55   -48        0   31*  -20       -6  109  -112      -12    4*   12
    0   19*    5        1   70    61       -4   75    66      -13   89   -82
                        2   30*  -21       -2   68   102      -14   83   -79
  H=  6, K=    4                                              -15   39    38
                      H=  7, K=    4      H=  1, K=    1      -16   92   -95
    0   32    47
    1   70    73        3   79    66       -1   46    61      H=  1, K=    4
    2    5*   -2        2    5*    8       -2  334   324
    3   82    73        1   44    45       -3    2*    6      -16   45   -45
    4   38   -34        0   34    39       -4   33*  312      -15   93  -104
    5   62    50                           -5  183  -156      -14   45    39
    6   41   -31      H=  7, K=    3       -6   42   -27      -13   89   -83
                                           -7   93   -77      -12   71    69
  H=  6, K=    5        0   18*   17       -8  131  -116      -11   87    94
                        1   53   -54       -9   44   -36      -10    4*   -8
    5   68   -57        2   42    41      -10  166  -165       -9  256   235
    4   28*  -28        3    5*   -9      -11   25*    9       -8   79   -84
    3   14*   -4                          -12   38   -37       -7  119   120
    2   24*  -19      H=  7, K=    2      -13   19*   19       -6  157  -138
    1   93    77                          -14  127   116       -5   41   -35
    0   23*  -18        4   37    29      -15    5*  -15       -4   27   -25
                        3   54   -61      -16  112   119       -3   72   -77
  H=  6, K=    6        2   32*  -30                           -2   64   -58
                        1   40   -34      H=  1, K=    2       -1   55    63
    0   36    48        0   71   -70
    1   75   -75                          -16   34*   42      H=  1, K=    5
    2    9*   20      H=  7, K=    1      -15   84    79
    3   67   -53                          -14  143  -136       -1  138   168
    4   33    23        0    5*   19      -13   55    48       -2   15*  -25
    5   45   -36        1   19*   16      -12  151  -150       -3   34   -39
                        2   42   -38      -11   95   -90       -4   27    26
  H=  6, K=    7        3   11*    5      -10  128  -110       -5  135  -139
                        4   47   -47       -9  174  -151       -6   18*  -23
    3    5*    5                           -8   65    64       -7  272  -254
    2    5*   -4      H=  7, K=    0       -7   58   -46       -8   32   -35
    1   89   -89                           -6  285   246       -9   18*  -25
    0   37    41        4   49   -45       -5   16*  -18      -10   65   -62
                        2   53    42       -4   19*  -12      -11  109   101
  H=  6, K=    8        0   96   100       -3   13*   21      -12    5*   -2
                                           -2   59   -53      -13  121   127
    0   59   -54      H=  8, K=    0       -1   23    26      -14   36    31
    1   25*   29                                              -15    5*  -12
    2   41   -35        0   44    46      H=  1, K=    3
```

L	FO	FC
H=	1, K=	6
-15	112	119
-14	56	53
-12	41	42
-13	67	68
-11	104	-105
-10	80	69
-9	186	-179
-8	37	44
-7	49	-51
-6	50	51
-5	58	55
-4	20*	24
-3	184	202
-2	21*	25
-1	55	64
H=	1, K=	7
-1	154	-188
-2	105	122
-3	15*	-4
-4	75	84
-5	74	69
-6	18*	-22
-7	133	129
-8	10*	-16
-9	18*	-19
-10	71	-67
-11	129	-120
-12	7*	-5
-13	160	-155
-14	33*	30
H=	1, K=	8
-13	39	-44
-12	94	-94
-11	65	72
-10	56	-57
-9	114	117
-8	24*	19
-7	15*	-7
-6	64	68
-5	73	-71
-4	23*	28
-3	186	-206
-2	54	-52
-1	81	-97
H=	1, K=	9
-1	119	129
-2	91	-96
-3	4*	18
-4	104	-89
-5	32	-23
-6	26*	35
-7	58	-54
-8	61	59
-9	44	37
-10	116	113
-11	74	76
-12	5*	8
-13	114	108
H=	1, K=	10
-11	38	-44
-10	26*	27
-9	11*	-23
-8	78	-78
-7	27*	21
-6	154	-147
-5	32	33
-4	50	-47
-3	100	112
-2	19*	21
-1	77	76
H=	1, K=	11
-1	17*	-26
-2	60	66
-3	12*	-15
-4	126	115
-5	20*	-23
-6	32*	-41
-7	5*	3
-8	79	-77
-9	14*	-13
-10	113	-110
H=	1, K=	12
-8	77	73
-7	5*	-4
-6	131	124
-5	17*	1
-4	60	54
-3	5*	-10
-2	27*	-24
-1	16*	17
H=	1, K=	13
-1	53	-47
-2	54	-53
-3	18*	-5
-4	60	-57
-5	13*	15
-6	28*	5
H=	2, K=	13
-5	43	37
-4	72	-67
-3	5*	16
-2	40	-42
-1	34	-31
H=	2, K=	12
-1	22*	11
-2	50	-45
-3	11*	17
-4	15*	13
-5	5*	0
-6	114	115
-7	14*	-7
-8	61	56
H=	2, K=	11
-10	129	-134
-9	21*	-6
-8	102	-104
-7	19*	28
-6	32	-39
-5	15*	20
-4	83	80
-3	12*	-6
-2	63	65
-1	12*	-11
H=	2, K=	10
-1	53	55
-2	34	40
-3	98	103
-4	16*	-29
-5	66	63
-6	135	-140
-7	39	37
-8	67	-64
-9	28*	-40
-10	54	56
-11	18*	-15
-12	85	87
H=	2, K=	9
-13	89	91
-12	20*	-16
-11	41	53
-10	113	113
-9	5*	2
-8	82	77
-7	102	-99
-6	4*	7
-5	74	-79
-4	78	-88
-3	14*	-13
-2	78	-75
-1	75	78
H=	2, K=	8
-1	81	-85
-2	26	-27
-3	201	-211
-4	52	49
-5	102	-108
-6	128	126
-7	19*	13
-8	19*	13
-9	88	94
-10	41	-42
-11	37	36
-12	61	-66
-13	49	-55
-14	69	-70
H=	2, K=	7
-15	22*	-18
-14	48	48
-13	143	-146
-12	53	59
-11	119	-118
-10	5*	2
-9	15*	-2
-8	29	24
-7	181	176
-6	40	40
-5	108	110
-4	86	88
-3	4*	4
-2	132	138
-1	111	-123
H=	2, K=	6
-1	46	47
-2	29	-35
-3	174	181
-4	24	-21
-5	86	88
-6	38	-29

L	FO	FC
-7	30	-28
-8	6*	11
-9	203	-200
-10	15*	26
-11	106	-99
-12	17*	14
-13	95	94
-14	38	34
-15	130	127

H= 2, K= 5

L	FO	FC
-16	8*	3
-15	23*	-18
-14	21*	4
-13	151	148
-12	75	-68
-11	143	135
-10	81	-76
-9	16*	12
-8	67	-73
-7	218	-210
-6	71	-70
-5	102	-105
-4	12*	22
-3	3*	5
-2	42	-52
-1	140	166

H= 2, K= 4

L	FO	FC
-1	41	51
-2	29	37
-3	79	-81
-4	15*	19
-5	18*	11
-6	106	-106
-7	143	138
-8	55	-56
-9	255	251
-10	6*	-5
-11	133	134
-12	105	100
-13	37	-42
-14	47	40
-15	88	-95
-16	52	-46

H= 2, K= 3

L	FO	FC
-16	75	-88
-15	49	51
-14	70	-74
-13	107	-114
-12	4*	-15
-11	88	-82
-10	193	180
-9	47	40
-8	102	100
-7	185	176
-6	3*	-3
-5	79	84
-4	112	-114
-3	49	-48
-2	106	-109
-1	128	-155

H= 2, K= 2

L	FO	FC
-1	10*	6
-2	65	-61
-3	61	59
-4	87	87
-5	37	34
-6	233	229
-7	127	-118
-8	94	82
-9	168	-156
-10	70	-67
-11	99	-99
-12	160	-158
-13	21*	14
-14	115	-116
-15	38	32
-16	44	44
-17	41	41

H= 2, K= 1

L	FO	FC
-17	35*	-41
-16	150	163
-15	8*	-4
-14	158	159
-13	40	40
-12	66	67
-11	12*	-8
-10	167	-153
-9	13*	-6
-8	53	-51
-7	39	-33
-6	77	64
-5	117	-102
-4	305	316
-3	35	21
-2	276	294
-1	93	96

H= 2, K= 0

L	FO	FC
-2	171	159
-4	100	-90
-6	414	-378
-8	91	-85
-10	137	138
-12	185	184
-14	164	165
-16	63	-56

H= 3, K= 0

L	FO	FC
-16	53	-61
-14	91	99
-12	122	117
-10	63	58
-8	190	-196
-6	419	-417
-4	190	-189
-2	78	-80

H= 3, K= 1

L	FO	FC
-1	78	82
-2	174	187
-3	32	29
-4	264	260
-5	44	-44
-6	40	41
-7	44	-49
-8	140	-139
-9	43	37
-10	183	-176
-11	27	30
-12	79	70
-13	66	65
-14	100	111
-15	5*	3
-16	139	168
-17	11*	-18

H= 3, K= 2

L	FO	FC
-17	11*	23
-16	44	52
-15	23*	28
-14	70	-83
-13	22*	2
-12	142	-145
-11	75	-79
-10	43	-38
-9	114	-124
-8	101	98
-7	71	-82
-6	263	251
-5	48	63
-4	83	95
-3	99	124
-2	37	-54
-1	64	80

H= 3, K= 3

L	FO	FC
-1	144	-175
-2	107	-142
-3	71	-84
-4	90	-97
-5	46	46
-6	3*	-3
-7	133	119
-8	113	103
-9	98	-88
-10	126	131
-11	147	-141
-12	4*	-3
-13	133	-139
-14	67	-69
-15	23*	-17
-16	64	-86
-17	38	45

H= 3, K= 4

L	FO	FC
-16	29*	-18
-15	83	-92
-14	33	44
-13	41	-29
-12	91	97
-11	138	146
-10	53	51
-9	195	196
-8	4*	-7
-7	77	74
-6	76	-84
-5	28	-24
-4	17*	29
-3	192	-224
-2	80	93
-1	87	-108

H= 3, K= 5

L	FO	FC
-1	111	126
-2	4*	-14
-3	10*	-4
-4	13*	6
-5	90	-105
-6	4*	17
-7	135	-138
-8	69	-65
-9	14*	10
-10	56	-60

L	FO	FC
H=	3, K=	5
-11	141	142
-12	37	-39
-13	179	178
-14	5*	-5
-15	31*	24
-16	18*	9
H=	3, K=	6
-15	107	115
-14	14*	-15
-13	67	71
-12	19*	-16
-11	98	-84
-10	22*	-23
-9	195	-180
-8	26*	-23
-7	58	-49
-6	88	-74
-5	89	83
-4	91	-99
-3	186	209
-2	32	-37
-1	52	63
H=	3, K=	7
-1	87	-80
-2	62	62
-3	5*	12
-4	36	37
-5	154	154
-6	16*	22
-7	179	181
-8	21*	-18
-9	21*	10
-10	5*	-7
-11	100	-89
-12	53	47
-13	113	-116
-14	45	42
-15	6*	-6
H=	3, K=	8
-14	54	-46
-13	43	-48
-12	56	-54
-11	42	34
-10	12*	-20
-9	128	112
-8	31*	33
-7	5*	18

L	FO	FC
-6	146	133
-5	75	-67
-4	72	69
-3	135	-139
-2	5*	7
-1	45	-35
H=	3, K=	9
-1	42	51
-2	98	-98
-3	5*	-3
-4	88	-90
-5	125	-119
-6	26*	16
-7	135	-117
-8	102	91
-9	33*	-28
-10	111	99
-11	35*	33
-12	12*	-13
-13	44	49
H=	3, K=	10
-12	108	105
-11	6*	7
-10	47	47
-9	66	-58
-8	35	-26
-7	6*	-7
-6	118	-117
-5	57	51
-4	33	-27
-3	53	50
-2	50	47
-1	5*	-16
H=	3, K=	11
-1	6*	-4
-2	123	104
-3	11*	-7
-4	86	78
-5	37	30
-6	8*	-12
-7	28*	33
-8	99	-96
-9	27*	24
-10	126	-118
H=	3, K=	12
-8	30*	25
-7	6*	-7

L	FO	FC
-6	87	92
-5	12*	-8
-4	6*	6
-3	13*	32
-2	66	-62
-1	19*	22
H=	3, K=	13
-1	26*	-8
-2	87	-69
-3	6*	20
H=	4, K=	12
-1	11*	10
-2	35*	-38
-3	6*	13
-4	29*	22
-5	14*	-6
-6	79	83
H=	4, K=	11
-9	16*	24
-8	82	-70
-7	49	47
-6	31*	17
-5	18*	13
-4	89	86
-3	14*	-21
-2	134	119
-1	24*	-15
H=	4, K=	10
-1	24*	-32
-2	48	40
-3	21*	18
-4	23*	-12
-5	33*	26
-6	106	-109
-7	36*	-35
-8	22*	-19
-9	77	-65
-10	34*	49
-11	24*	-29
H=	4, K=	9
-12	9*	-5
-11	10*	24
-10	85	90
-9	37*	-36
-8	87	85

L	FO	FC
-7	106	-107
-6	5*	-3
-5	96	-103
-4	50	-49
-3	8*	16
-2	106	-94
-1	49	39
H=	4, K=	8
-1	15*	9
-2	7*	-5
-3	82	-95
-4	29*	31
-5	36	-33
-6	80	80
-7	34	39
-8	45	33
-9	156	150
-10	21*	-25
-11	45	59
-12	76	-75
-13	6*	-31
H=	4, K=	7
-14	30*	31
-13	96	-105
-12	26*	19
-11	64	-64
-10	54	-58
-9	7*	20
-8	81	-80
-7	146	148
-6	19*	-27
-5	134	135
-4	23*	-16
-3	7*	4
-2	10*	-6
-1	74	-70
H=	4, K=	6
-1	58	61
-2	26*	-21
-3	162	178
-4	30	-39
-5	47	46
-6	14*	-20
-7	52	-48
-8	19*	-21
-9	175	-146
-10	5*	-11
-11	81	-75
-12	8*	-11

```
  L    FO     FC

-13    27*    32
-14    47    -37
-15   115    121

H=     4,  K=   5

-16    23*    29
-15    33*    28
-14     6*    16
-13   176    167
-12    11*    -6
-11   125    119
-10    34    -26
 -9    18*    24
 -8    22*    -1
 -7   125   -115
 -6    31     34
 -5   102   -114
 -4    56     58
 -3     4*    17
 -2    67     75
 -1   110    131

H=     4,  K=   4

 -1   124   -136
 -2    62     70
 -3   203   -235
 -4    16*   -19
 -5    78    -83
 -6    68    -61
 -7    23*    18
 -8    16*     5
 -9   134    123
-10    32     31
-11    82     76
-12    80     87
-13    47    -48
-14    71     70
-15   117   -118
-16     6*    -8

H=     4,  K=   3

-16    96    -99
-15    40*   -45
-14    56    -66
-13   170   -166
-12    12*    10
-11   143   -131
-10   108    101
 -9    85    -82
 -8   133    114
 -7    60     51
 -6     4*   -12
```

```
  L    FO     FC

 -5    47     59
 -4   116   -127
 -3    20*   -24
 -2    71    -81
 -1   119   -136

H=     4,  K=   2

 -1    65     73
 -2    75   -107
 -3   110    117
 -4    60     62
 -5    82     89
 -6   229    213
 -7    14*   -14
 -8    57     49
 -9   130   -123
-10    32    -30
-11    11*   -16
-12   148   -137
-13    34*    28
-14    73    -71
-15    72     71
-16    63     62
-17    33*    31

H=     4,  K=   1

-17     6*   -10
-16   134    147
-15    22*     7
-14    58     72
-13    80     69
-12    17*   -11
-11    67     61
-10   228   -196
 -9    44     30
 -8   202   -173
 -7    46    -43
 -6    67    -60
 -5    16*    -5
 -4   132    142
 -3    11*   -23
 -2    80     93
 -1    40     44

H=     4,  K=   0

 -2    14*    27
 -4    89    -80
 -6   338   -294
 -8   183   -148
-10     5*    15
-12   149    140
-14    22*    29
```

```
  L    FO     FC

-16    42    -61

H=     5,  K=   0

-16    43    -55
-14    24*    33
-12   166    155
-10    24*    25
 -8    54    -52
 -6   202   -187
 -4    30    -34
 -2   132    150

H=     5,  K=   1

 -1    25*    13
 -2    87    102
 -3    18*   -30
 -4    66     76
 -5    42    -33
 -6    30    -28
 -7    43    -45
 -8   183   -163
 -9    22*   -22
-10   238   -213
-11    44     48
-12    33*   -30
-13    60     44
-14    52     58
-15    22*    -2
-16    94     97

H=     5,  K=   2

-16    40     45
-15    92     89
-14    44    -53
-13    34*    30
-12   157   -135
-11     5*    -5
-10    30*   -29
 -9   100    -87
 -8    67     63
 -7     5*     6
 -6   139    131
 -5    53     47
 -4    45     56
 -3    99    125
 -2    78    -90
 -1    65     77

H=     5,  K=   3

 -1    48    -54
 -2    85    -98
```

```
  L    FO     FC   10

 -3    17*    21
 -4    89   -107
 -5   121    121
 -6    22*   -16
 -7   119    113
 -8    86     81
 -9    11*     3
-10   116     99
-11    71    -71
-12    24*    -3
-13   125   -122
-14    30*   -42
-15     6*    -5
-16   107   -106

H=     5,  K=   4

-16    16*   -11
-15   111   -128
-14    53     55
-13    47    -51
-12    79     75
-11    22*    20
-10     5*    16
 -9   110    101
 -8    54    -48
 -7    16*    22
 -6    65    -62
 -5    90    -99
 -4    38    -42
 -3   157   -183
 -2    38     46
 -1    82    -87

H=     5,  K=   5

 -1    96    104
 -2    60     79
 -3    18*    -3
 -4    54     50
 -5   133   -138
 -6    27*    17
 -7   133   -128
 -8    40     32
 -9    20*    18
-10     5*    -6
-11    53     60
-12     5*     4
-13   119    119
-14    31*    36
-15    28*     5

H=     5,  K=   6

-14    17*   -24
```

```
   L   FO      FC      L   FO      FC      L   FO      FC      L   FO      FC   11

H=     5, K=    6     -5   40     -46     -8    6*      5     -1   36     -39
                      -6   30*    -17     -9   70      78     -2   29*     41
 -13   23*     32     -7   73     -71    -10   31*    -26     -3   76    -101
 -12   17*      8     -8   76      83    -11   68      66     -4   48     -59
 -11   67     -69     -9   20*    -15                         -5   30*    -20
 -10    5*      7    -10   73      72    H=     6, K=    7     -6   71     -68
  -9  155    -137    -11   36*     42                         -7   38      39
  -8   19*      8                        -12    6*     -6     -8   51     -40
  -7   48     -53    H=     5, K=   10    -11   66     -60     -9  108     110
  -6   16*    -13                        -10   39     -35    -10   18*     -1
  -5   38      40     -9   71     -62     -9    6*      2    -11   21*     26
  -4   32      27     -8   32*    -28     -8   31*    -44    -12   22*     29
  -3  119     145     -7   23*    -23     -7   67      63    -13   52     -45
  -2   19*     25     -6   93     -98     -6    6*     -2    -14   30*     35
  -1   38      44     -5   33*     24     -5   76      91    -15  110    -115
                      -4   36     -38     -4   23*     14
H=     5, K=    7     -3   13*      8     -3   34     -31    H=     6, K=    3
                      -2   26*     32     -2   17*     27
  -1   83     -87     -1   25*     -7     -1   80     -81    -15    6*     10
  -2   17*     16                                            -14   31*    -39
  -3   32     -25    H=     5, K=   11    H=     6, K=    6    -13   67     -59
  -4    5*     -8                                            -12    6*      6
  -5  104     109     -1   50     -35     -1   37      43    -11   29*    -33
  -6   16*    -34     -2   98      89     -2   18*      9    -10   84      72
  -7  108     107     -3   24*    -20     -3   81     110     -9   42      24
  -8   72     -76     -4   88      81     -4    5*     14     -8   70      57
  -9   25*     15     -5   28*    -11     -5   36      33     -7  121     114
 -10   65     -62     -6    9*     17     -6   16*      9     -6    9*    -17
 -11   65     -67                         -7   56     -63     -5  121     141
 -12   24*    -17    H=     6, K=   10     -8   31*     35     -4   56     -74
 -13  109    -103                         -9  110    -110     -3   23*     31
 -14   22*      9     -4   50     -53    -10    8*     19     -2   77     -88
                      -5   36*     36    -11   65     -57     -1    5*    -18
H=     5, K=    8                        -12   36*     30
                     H=     6, K=    9    -13   42      32    H=     6, K=    2
 -13   24*     -4
 -12   69     -72     -9    6*    -11    H=     6, K=    5     -1   19*     27
 -11   78      73     -8   59      62                         -2   39     -42
 -10   32*    -21     -7   29*    -32    -14    6*     13     -3   43      64
  -9  130     123     -6   14*      6    -13   84      95     -4   34      42
  -8   20*     10     -5   29*    -17    -12    6*     -2     -5   12*      5
  -7   55      59     -4   56     -52    -11   48      52     -6   89      88
  -6   61      62     -3   31*     18    -10   23*     -9     -7   35     -22
  -5   36     -28     -2   73     -73     -9   16*     -7     -8   67      62
  -4   18*     20     -1   54      58     -8    5*      2     -9   67     -59
  -3   56     -64                         -7  109    -115    -10   44     -33
  -2   41     -45    H=     6, K=    8     -6   32*     21    -11   26*    -31
  -1   15*    -21                         -5  116    -127    -12  124    -121
                      -1   45     -48     -4   35      29    -13   39      33
H=     5, K=    9     -2   25*    -28     -3   18*      9    -14   50     -57
                      -3   48     -50     -2   32      28    -15   67      80
  -1   56      49     -4   27*     35     -1   46      43
  -2   74     -79     -5   43     -51                        H=     6, K=    1
  -3   24*     30     -6   31*     39    H=     6, K=    4
  -4   59     -58     -7   27*     32                        -16   88     100
```

L	FO	FC
-15	6*	-3
-14	52	67
-13	23*	29
-12	6*	-22
-11	20*	14
-10	149	-134
-9	16*	-25
-8	150	-131
-7	37	-24
-6	5*	5
-5	43	-60
-4	42	66
-3	26*	-10
-2	90	110
-6	19*	5
H=	6, K=	0
-2	81	91
-4	5*	-30
-6	116	-100
-8	24*	-23
-10	80	66
-12	154	155
-14	89	90
-16	52	-46
H=	7, K=	0
-14	90	85
-12	126	132
-10	46	45
-8	46	-52
-6	57	-61
-4	5*	-38
-2	33*	15
H=	7, K=	1
-1	24*	11
-2	74	110
-3	6*	6
-4	47	67
-5	8*	-30
-6	36	41
-7	37	-22
-8	65	-52
-9	10*	-10
-10	72	-73
-11	6*	14
-12	6*	-17
-13	26*	21
-14	96	98
H=	7, K=	2

L	FO	FC
-14	41*	-49
-13	35*	21
-12	92	-100
-11	23*	-19
-10	31*	-24
-9	62	-51
-8	47	58
-7	37	-38
-6	64	76
-5	22*	13
-4	6*	27
-3	6*	29
-2	8*	-21
-1	10*	2
H=	7, K=	3
-1	38	-37
-2	46	-68
-3	22*	7
-4	39	-47
-5	56	91
-6	27*	-16
-7	54	53
-8	53	46
-9	34*	37
-10	41	46
-11	41	-34
-12	21*	16
-13	24*	-43
-14	51	-52
H=	7, K=	4
-13	46	-39
-12	29*	35
-11	45	44
-10	6*	-14
-9	109	108
-8	36*	-34
-7	35	24
-6	41	-38
-5	14*	-13
-4	38	-33
-3	36	-54
-2	31	20
-1	34*	-24
H=	7, K=	5
-1	35*	44
-2	6*	-7
-3	25*	24

L	FO	FC
-4	6*	10
-5	78	-100
-6	20*	6
-7	72	-79
-8	25*	-25
-9	21*	-23
-10	39	-34
-11	72	65
-12	21*	-8
H=	7, K=	6
-11	52	-45
-10	6*	18
-9	82	-87
-8	6*	14
-7	13*	-25
-6	21*	10
-5	34*	44
-4	6*	-2
-3	72	70
-2	6*	-16
-1	36*	49
H=	7, K=	7
-1	57	-49
-2	33*	36
-3	6*	-16
-4	30*	48
-5	45	55
-6	14*	13
-7	30*	51
-8	12*	-22
-9	6*	8
-10	6*	11
H=	7, K=	8
-6	18*	41
-5	51	-45
-4	6*	27
H=	8, K=	5
-7	47	-48
-6	6*	4
-5	46	-59
H=	8, K=	4
-2	6*	16
-3	46	-43
-4	26*	8

L	FO	FC	12
-5	27*	-38	
-6	26*	-35	
-7	29*	38	
-8	33*	-35	
-9	78	85	
H=	8, K=	3	
-10	53	48	
-9	19*	16	
-8	46	48	
-7	31*	26	
-6	6*	-21	
-5	18*	43	
-4	6*	-33	
-3	6*	-13	
-2	21*	-29	
-1	46	-37	
H=	8, K=	2	
-1	24*	10	
-2	6*	-21	
-3	30*	17	
-4	9*	26	
-5	6*	15	
-6	47	73	
-7	18*	-29	
-8	39*	41	
-9	47	-52	
-10	24*	-29	
-11	12*	-17	
H=	8, K=	1	
-11	28*	31	
-10	70	-56	
-9	26*	8	
-8	41	-44	
-7	10*	-20	
-6	29*	36	
-5	12*	-13	
-4	16*	57	
-3	9*	4	
-2	51	74	
-1	6*	15	
H=	8, K=	0	
-2	12*	-5	
-4	6*	-33	
-6	22*	-74	
-8	45	-51	
-10	23*	20	

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