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THE SHAPE OF EIGHT-COORDINATE SPECIES :
A STRUCTURAL INVESTIGATION OF TWO
TETRAKIS(TROPOLONATO)METAL COMPLEXES

by

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B.Sc.(Honours), University of London, 1972.

A THESIS SUBMITTED IN PARTIAL FULFILLMENT
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ABSTRACT

The crystal and molecular structures of two tetrakis-(tropolonato)metal complexes have been determined from three-dimensional X-ray diffraction intensity data collected by counter methods on a computer controlled Picker four circle diffractometer.

The acid dimer of tetrakis(tropolonato)scandium(III), $(\text{HScT}_4)_2$, (where $\text{T} = \text{C}_7\text{H}_5\text{O}_2^-$), crystallizes in the triclinic space group $\text{P}\bar{1}$ with cell constants $a = 11.624(3)\text{\AA}$, $b = 11.986(3)\text{\AA}$, $c = 10.004(3)\text{\AA}$, $\alpha = 95.33(1)^\circ$, $\beta = 116.27(1)^\circ$, $\gamma = 102.32(1)^\circ$, and $z = 2$. Full matrix least squares refinement of the 2732 reflections considered to be above background gave a final R factor of 5.9%. The molecules exist as centrosymmetrically related hydrogen bonded dimers (O...O separation of $2.484(4)\text{\AA}$). Each scandium atom is eight-coordinate; the oxygen atoms are at the vertices of a polyhedron which is best described as an irregular bicapped trigonal prism, distorted towards a dodecahedron. The two tropolonato ligands involved in the hydrogen bonding are bonded asymmetrically to the metal, and the different bond length alternation in these two rings reflects the asymmetric position of the hydrogen atom in this bond.

The compound $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$ crystallizes in the monoclinic space group $\text{C}2/c$ with cell constants $a = 15.16(1)\text{\AA}$, $b = 13.94(1)\text{\AA}$, $c = 25.88(1)\text{\AA}$, $\beta = 95.46(4)^\circ$, and $z = 4$. A final R factor of 7.5% was obtained after full matrix least squares

refinement of the 1651 reflections considered to be above background. The $(\text{H}_3\text{OCl}_3)^{2-}$ anion contains the H_3O^+ species hydrogen bonded to the chloride ions placed at the corners of the base of a flattened pyramid. A two-fold axis passes through one chloride ion and relates the other two chloride ions. The oxygen atom is disordered either side of the two-fold axis at the apex of the pyramid.

The arrangement of the donor atoms about the central metal atom in complexes of the type $\text{M}(\text{bidentate})_4$ has been shown to be dependent on the parameter b : the ratio of the donor atom separation to the metal-donor atom distance. From the differences in the central metal and in the charge on the $(\text{NbT}_4)^+$ and $(\text{ScT}_4)^-$ species, one would expect a difference in the geometry of the oxygen atoms, assuming the tropolonato ligands to be rigid. However, the average oxygen atom separation within the ligands in the $(\text{NbT}_4)^+$ cation is significantly and unexpectedly small (2.432\AA) compared to that for the $(\text{ScT}_4)^-$ anion (2.501\AA), and the geometries of the two species are similar, corresponding quite closely to the arrangement predicted by theories of high-coordination. The most notable features of the 'NbO₈' polyhedron are two interligand O...O contacts which are very short ($2.410(14)\text{\AA}$ and $2.467(17)\text{\AA}$) compared to other interligand contacts, and occur between oxygen atoms whose lone pairs of electrons overlap. Close contacts in the 'ScO₈' polyhedron and in other high-coordinate complexes are found where the geometry would permit similar overlap of lone pairs. This pattern of non-imposed short

contacts suggests that there is an interaction involving the lone pairs which should be recognised when predictions of high-coordinate geometry are made.

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CHAPTER ONE

INTRODUCTION

High-coordinate compounds in which the central metal atom is bonded to seven or more non-metallic ligand donor atoms have been thoroughly reviewed^{1,2}, with particular emphasis on their structure, and more specifically on the geometry exhibited by the ligand donor atoms. Important to the stabilization of many high-coordinate compounds is the chelate effect, and it is the metal chelates that form by far the largest group within this class of compounds. The most common donor atoms found in the multidentate ligands are oxygen and nitrogen, which satisfy one of the requirements needed to achieve high-coordination : that the donor atoms must be small so that ligand-ligand repulsion can be minimised. For the same reason, the central metal atom must be of sufficiently large effective radius. The filling of the d-electron level across a periodic system causes a decrease in the size of the metal ion, e.g. Ti(IV) has an ionic radius of 0.68Å compared to 0.54Å for Ge(IV), with seven and eight coordinate compounds well known for Ti(IV) but not for Ge(IV). On the other hand, Sn(IV) (d^{10} , ionic radius = 0.71Å) is comparable with Ti(IV) in size and in its ability to form

high-coordinate species. Equally important to the stabilization of a high-coordinate complex is the high positive formal charge necessary to accommodate the electrons contributed by eight bonding ligand atoms.

Comparisons between bidentate ligands can be made in terms of their rigidity, the coplanarity (or lack of) of the ligand atoms, and also by the separation of the donor atoms. The more compact the ligand, and the smaller the 'bite', the more effective is the ligand in generating high-coordinate complexes. Compact ligands with small 'bites' include the coplanar nitrate group (O...O separation of $\sim 2.1\text{\AA}$), the oxalato ligand (O...O $\sim 2.56\text{\AA}$), and the tropolonato anion $\text{C}_7\text{H}_5\text{O}_2^-$ (hereon abbreviated to T^-) which is derived from tropolone, and has an O...O separation which in previously determined structures has ranged from $2.49 - 2.57\text{\AA}$. Considerable stability should be conferred to chelates based on this ligand because of the delocalised π - system. In fact, the lightest covalently bonded eight-coordinate atom known is scandium in the form of the tetrakis-(tropolonato)scandium(III) anion prepared originally by Muetterties and co-workers³, along with a series of similar eight-coordinate complexes of Zr(IV), Nb(V), In(III), Sn(IV), Hf(IV), Ta(V), and all the lanthanide metals.

Geometry

In discrete high-coordination, ~~these~~ polyhedra which are made up mainly or completely of triangular faces are the most common. This is explained simply by the demands of interligand interactions : repulsion forces push the ligands as far apart as

possible whilst keeping a constant distance from the central atom. In polyhedra inscribed in a sphere, moreover, the average edge length increases as the number of sides of the defining polygons decreases. In eight-coordination, the most common polyhedra observed are the dodecahedron, the square antiprism and the bicapped trigonal prism. The latter two can be obtained by simple deformations of the dodecahedron and are themselves interchangeable by a small deformation (Figure 1a, page 5). The criteria which define the extent of distortion of a real geometry from these ideal polyhedra of the dodecahedral class have been established by Porai-Koshits and Aslanov⁴. They extended the concept introduced by Hoard and Silverton⁵ of the ideal dodecahedron and square antiprism inscribed in a sphere to include the bicapped trigonal prism. Parameters which visually characterize the ideal polyhedra can be calculated using these models and used in comparison with the parameters determined from structural investigations of eight-coordinate compounds. This comparison is given in detail in section 4.1.

For a compound of stoichiometry $M(\text{bidentate})_4$, where all four ligands span equivalent polyhedral edges, there are two different isomers of dodecahedral geometry and two of square antiprismatic geometry; these are shown in Figure 1b (page 5), where the square antiprism is most conveniently displayed along the $\bar{4}$ axis, and the dodecahedron is considered in terms of two interpenetrating, mutually perpendicular trapezoids. Blight and Kepert⁶ have produced a description of the effects of

-4-

ligand-ligand repulsion among bidentate ligands on eight-coordinate geometry. Neglecting all other sources of repulsion or attraction, they found that the potential energy surfaces produced by ligand-ligand repulsion are critically dependant on the parameter b : the ratio of the donor atom separation to the metal-donor atom distance. For different values of b , potential energy surfaces incorporating the isomers shown in Figure 1b are given together with structural parameters of the most energetically favourable intermediate geometries. In order to test the results of these calculations, the crystal and molecular structures of two tetrakis(tropolonato)metal complexes (where $M = Sc$ and Nb) have been determined. It was expected that, for a fixed value of the ligand 'bite', there would be a significant difference in the value of b (predicted to be ~ 1.15 for the Sc complex, and ~ 1.25 for the Nb complex), and therefore in the geometry of the two species.

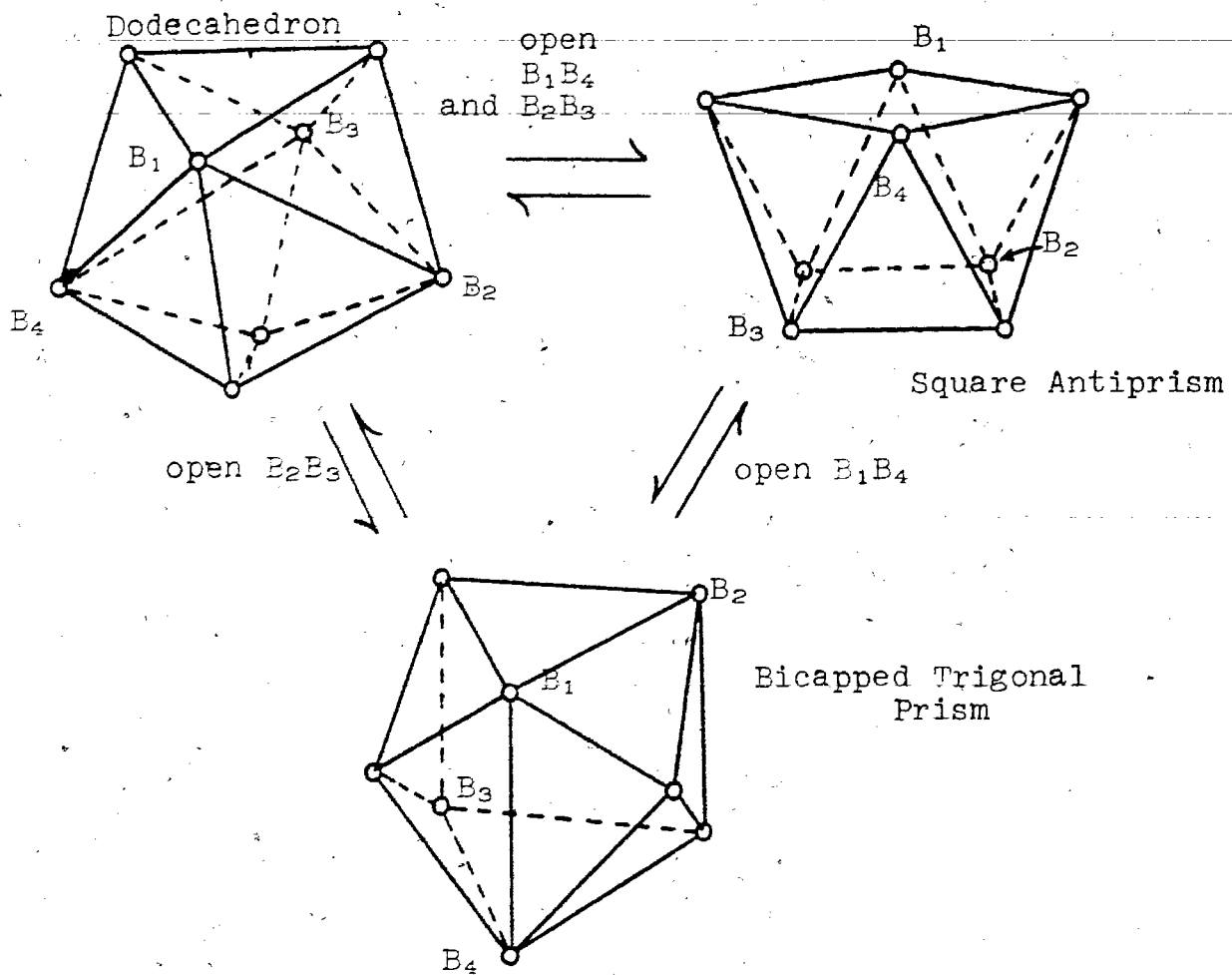


Figure 1a : Regular eight coordinate polyhedra.

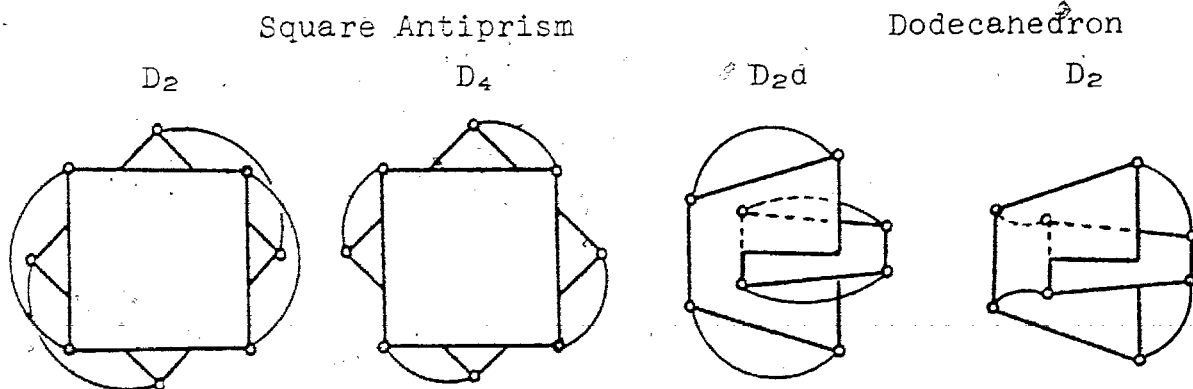


Figure 1b : Stereo isomers of the $M(\text{bidentate})_4$ system where all the bidentates span equivalent edges.

CHAPTER TWO

EXPERIMENTAL

2.1 Preparation of the complexes

The species $(\text{HScT}_4)_2$ and $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$ were prepared according to the methods reported by Muetterties and Wright³. For $(\text{HScT}_4)_2$, scandium chloride (0.01 mole) was dissolved in water and added to a solution of tropolone (0.04 mole) in ethanol; crystallization was carried out by adding acetonitrile to the reaction mixture and allowing the solvent to evaporate slowly over a number of days. Small yellow crystals were obtained, and one of approximate dimensions 0.13 x 0.22 x 0.40 mm was mounted for the purposes of data collection.

$(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$ was prepared by mixing a solution of niobium pentachloride (0.01 mole) dissolved in dichloromethane (200ml) and ether (30ml) with a solution of tropolone (0.04 mole) in dichloromethane (200ml). The product separated slowly from the resulting orange solution; the solvent was evaporated under reduced pressure, and then acetonitrile (400ml) was added to the residue. This was then heated until solution was complete. When cooled, bright orange crystals separated out, and the product was recrystallised from hot acetonitrile.

Crystals obtained from this preparation were very small, and great difficulty was encountered in finding a single crystal of suitable size and quality for investigation. Many attempts were made to obtain larger crystals by repeating the preparation under different conditions and by recrystallizing the products

using a variety of solvents and mixtures of solvents, and under different conditions. Finally, a crystal from the original preparation, of approximate dimensions 0.12 x 0.12 x 0.06 mm, was mounted for the purpose of data collection.

2.2 Preliminary Investigation

The details and results of the preliminary investigation and photography are given in Table 1 (page 8). From the Weissenberg and precession photographs taken (λ Cu radiation : $\lambda = 1.5418\text{\AA}$), the crystal of the Sc complex was assigned triclinic Laue symmetry, and the Nb complex was assigned monoclinic symmetry, with systematic absences for hkl, $h+k = 2n+1$ and h0l, $l = 2n+1$, suggesting the monoclinic space groups C_2 or $C2/c$. For the crystal of the niobium complex, intensities of even the strongest reflections measured by counter methods were weak, and after considerable effort, a new crystal (again from the first preparation) of approximate dimensions 0.12 x 0.08 x 0.08 mm was found. This crystal was mounted, as in the case of the $(\text{HScT}_4)_2$ crystal, with the c axis approximately parallel to the ϕ axis of the diffractometer. In view of the weak intensity data expected, the interface circuitry on the diffractometer control system was modified to read the units digit of the number of counts for each reflection.

Accurate cell dimensions for both crystals were determined from counter measurement of the strongest reflections having $2\theta > 25^\circ$ for $(\text{HScT}_4)_2$, and $2\theta > 20^\circ$ for the Nb complex, using a Picker FACS-1 computer controlled four circle diffractometer, Mo K_{α_1} radiation, and a take-off angle of 1.0° .

Table 1 Crystal Data

Compound :	HScT_4	$(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3)(\text{CH}_3\text{CN})$
Formula weight :	530.4	654.5
Colour :	yellow	red
Zones photographed :		
Weissenberg (Cu K_α) :	hk0,hk1	h0l
Precession (Cu K_α) :	h0l,0k1	0k1,hk0,hkh,hk2h
Systematic absences :	none	hk1,h+k=2n+1 h0l,l=2n+1
Laue symmetry :	$\bar{1}$	2/m
Crystal system :	triclinic	monoclinic
Space group :	$P\bar{1}$	C2/c
Crystal dimensions :	0.13x0.22x0.40mm	0.12x0.12x0.06mm
Accurate Cell Dimensions :		
no. reflections used :	29 ($2\theta > 25^\circ$)	12 ($2\theta > 20^\circ$)
Temperature :	21°C	22°C
Take-off angle :	1.0°	1.0°
Radiation used :	Mo K_{α_1} (0.70926Å)	Mo K_{α_1} (0.70926Å)
Lattice constants :	$\underline{a} = 11.624(3)\text{Å}$ $\underline{b} = 11.986(3)\text{Å}$ $\underline{c} = 10.004(3)\text{Å}$ $\underline{\alpha} = 95.33(1)^\circ$ $\underline{\beta} = 116.27(1)^\circ$ $\underline{\gamma} = 102.32(1)^\circ$	$\underline{a} = 15.16(1)\text{Å}$ $\underline{b} = 13.94(1)\text{Å}$ $\underline{c} = 25.88(2)\text{Å}$ $\underline{\beta} = 95.46(4)^\circ$
Unit cell volume :	1207.2Å ³	5444 Å ³
Calculated density :	1.46g cm ⁻³	1.60g cm ⁻³
Measured density : (flotation)	1.46(2)g cm ⁻³	1.57(2)g cm ⁻³
Z :	2	8
$\mu(\text{Mo K}_\alpha)$	3.69 cm ⁻¹	5.22 cm ⁻¹

2.3 Diffractometry

(HScT₄)₂ :

Reflections for the unique set of data for $\sin\theta < 0.4226$ were collected using a scintillation detector with pulse height analysis. Measurement was made using niobium-filtered molybdenum radiation ($\lambda\text{Mo-K}_{\alpha_1} = 0.70926\text{\AA}$) and a take-off angle of 3.0° with a symmetrical θ - 2θ scan of 1.6° base width increased to allow for d_1 - d_2 dispersion. Background counts of 10s were measured at both scan limits. After each 70 reflections, 2 standard reflections were measured; their variation was $\pm 3.0\%$ over the entire data collection. The intensities were corrected for Lorentz and polarization effects; absorption was neglected since it was estimated to introduce a maximum error of $\pm 3.0\%$ in the net count, I . 4212 reflections were measured, of which 2732 were considered observed (i.e. $> 2.3\sigma^*$).

(NbT₄)₂(H₃OCl₃). (CH₃CN) :

Diffraction data for this complex were collected using monochromatised radiation (graphite monochromator, $\lambda(\text{MoK}_{\alpha}) = 0.70926\text{\AA}$, see Appendix A), with a take-off angle of 3.0° . Reflections for the unique set of data were collected; for data where $\sin\theta < 0.2164$, a scan base width of 1.2° was used, and for the outer data, ($0.2164 < \sin\theta < 0.3827$), a base width of

* $\sigma I_{\text{net}} = [(\text{TC}) + (t_s/t_b)^2(B_1 + B_2) + (kI)^2]^{\frac{1}{2}}$, where TC = total count, B_1 and B_2 are the background counts at each end of the scan range t_s = scan range, t_b = total background time, k is a constant set to 0.03, and I is the net count.

1.0° was used, in a symmetrical θ - 2θ scan at a speed of 1°/min. Separate scales were assigned to the inner and outer shells of data for the purpose of refinement. Background counts of 20 sec. were measured at both scan limits. The intensities were corrected for Lorentz and polarization effects; absorption was neglected since it was estimated to introduce an extreme error in F of 1.0%. 3601 reflections were measured, of which 1666 were considered to be above background (i.e. greater than 2.3σ , see footnote on page 9). The maximum value of I recorded during data collection was 17,409 for the 113 plane.

CHAPTER THREE

STRUCTURE DETERMINATION AND REFINEMENT

3.1 (HScT₄).

Examination of the three-dimensional Patterson function based on all data gave the position of the scandium atom and seven oxygens. Refinement of the scale and these atomic coordinates gave $R = 0.474$ where $R = \frac{\Sigma(|F_o| - |F_c|)}{\Sigma|F_o|}$. A Fourier synthesis revealed the other oxygen and five carbon atoms. Three cycles of refinement and subsequent electron density difference maps gave the remaining carbon atom positions. Hydrogen atom positions (except for the proton) were found after a further cycle of refinement. With the non-hydrogen atoms refined anisotropically and $R = 0.062$, the remaining proton position was found between oxygen atoms O_1 and O_3' on a centrosymmetrically related molecule. Because the O_1-O_3' separation was so short (2.48\AA), a symmetrical arrangement was assumed and the proton was placed at the mid-point of the line joining the oxygen atoms. Upon refinement however, the shifts indicated that this was not a valid assumption, and the final position is that resulting from refinement of the original parameters obtained from the difference map.

Using an inner set of data, hydrogen atom positions and temperature factors, together with the positions of the carbon atoms, and oxygen atoms O_1 and O_3 were refined. Two of the hydrogen temperature factors were not well behaved and the other values were averaged to give a final hydrogen atom temperature factor of 3.4\AA^2 . The hydrogen atomic positions and

isotropic temperature factor of the proton only were included along with all other coordinates and temperature factor parameters in the final two cycles of full matrix least squares refinement which gave an R factor of 0.059 for all the observed data. In the early refinement, constant unit weights were used; in the final stages, weights ($= 1/\sigma^2 F$) were given in terms of $\sigma F = \sigma I / (Lp.2Fo)$. Atomic scattering factors used were taken from references 7a and 7b, and included corrections for anomalous dispersion for the scandium atom ($\Delta f' = 0.2$, $\Delta f'' = 0.5$).

Crystallographic computer programs used in this determination (and that of the niobium complex) have been listed elsewhere⁸. A table of the measured and calculated structure factors ($\times 10$) is given in Appendix B (page 51). Final atomic and thermal motion parameters are listed in Table 2 (page 14), with a perspective view of the acid dimer shown in Figure 2 (page 17).

Thermal Motion

Analysis of the thermal motion parameters shows that the ScT_4^- anion is not well described in terms of rigid body motion (reference 9 gives details of this analysis). However, each of the four ligands gives good agreement (rings 1 and 2 give the best fit, this being consistent with their reduced thermal motion which is attributed to their hydrogen bond participation and 'internal' position in the dimer. An alternative model where each oxygen atom is assumed to ride on the Sc atom, lengthens the Sc-O bond lengths by 0.002Å to 0.006Å for O_1-O_4 and 0.006Å for O_5-O_8 . If the Sc and coordinated oxygen atoms

'kernel' were assumed to form a rigid body, then the corrections would be 0.001Å to 0.004Å. The view adopted of the thermal motion is that the 'ScO₈' riding model gives too large a correction (the oxygen atom motion not being independent) while the 'ScO₈' rigid body model is probably an underestimate. In any event, the uncorrected distances (Sc-O) are too short by at least one standard error.

TABLE 2a

Fractional Atomic Coordinates ($\times 10^4$, $\times 10^3$ for H)
in Crystalline $(\text{HScT}_4)_2$.

(The least squares estimated errors are in parentheses)

Atom Type	Coordinates		
Sc	1231 (1)	-1682 (1)	-484 (1)
O ₁	866 (3)	74 (2)	-1063 (3)
O ₂	3089 (3)	-362 (2)	0 (3)
O ₃	1157 (3)	-695 (2)	1500 (3)
O ₄	2736 (3)	-1879 (2)	1744 (3)
O ₅	157 (3)	-3255 (2)	-146 (4)
O ₆	-901 (3)	-1850 (2)	-1604 (3)
O ₇	2096 (3)	-2951 (2)	-1062 (3)
O ₈	735 (3)	-1863 (3)	-2872 (3)
1C ₁	1832 (4)	901 (3)	-1006 (4)
1C ₂	1604 (5)	1915 (4)	-1497 (5)
1C ₃	2455 (5)	2896 (4)	-1530 (6)
1C ₄	3806 (5)	3155 (4)	-1057 (6)
1C ₅	4626 (5)	2465 (4)	-441 (6)
1C ₆	4338 (4)	1390 (4)	-131 (5)
1C ₇	3115 (4)	627 (4)	-357 (5)
2C ₁	2043 (4)	-630 (4)	2939 (5)
2C ₂	2070 (5)	83 (4)	4100 (5)
2C ₃	2904 (5)	270 (5)	5677 (5)
2C ₄	3866 (6)	-232 (5)	6450 (6)
2C ₅	4274 (5)	-1084 (5)	5861 (6)
2C ₆	3871 (1)	-1560 (5)	4385 (5)
2C ₇	2906 (4)	-1373 (4)	2998 (5)
3C ₁	-1121 (4)	-3641 (4)	-927 (5)
3C ₂	-1796 (5)	-4737 (4)	-891 (6)
3C ₃	-3145 (5)	-5337 (4)	-1677 (6)
3C ₄	-4211 (5)	-5003 (5)	-2690 (6)
3C ₅	-4175 (5)	-3951 (5)	-3139 (6)
3C ₆	-3106 (5)	-2994 (4)	-2748 (6)
3C ₇	-1725 (4)	-2811 (4)	-1785 (5)
4C ₁	1851 (4)	-3263 (4)	-2442 (5)
4C ₂	2296 (5)	-4180 (4)	-2841 (6)
4C ₃	2146 (6)	-4677 (5)	-4226 (7)
4C ₄	1543 (6)	-4395 (5)	-5615 (7)
4C ₅	947 (6)	-3516 (5)	-5962 (6)
4C ₆	731 (5)	-2746 (5)	-5042 (6)
4C ₇	1031 (4)	-2616 (4)	-3486 (6)

TABLE 2a (Cont'd)

1H ₂	72(4)	193(4)	-187(5)
1H ₃	204(4)	352(4)	-195(5)
1H ₄	414(4)	394(4)	-122(5)
1H ₅	559(4)	275(4)	-19(5)
1H _e	503(4)	104(4)	25(5)
2H ₂	148(4)	55(4)	384(5)
2H ₃	270(4)	81(4)	624(5)
2H ₄	428(4)	-7(4)	748(5)
2H ₅	498(4)	-128(4)	662(5)
2H _e	434(4)	-212(4)	421(5)
3H ₂	-123(4)	-516(4)	-26(5)
3H ₃	-330(4)	-612(4)	-145(5)
3H ₄	-503(4)	-556(4)	-311(5)
3H ₅	-505(4)	-386(4)	-387(5)
3H _e	-326(5)	-233(4)	-321(5)
4H ₂	279(4)	-438(4)	-200(5)
4H ₃	253(4)	-532(4)	-419(5)
4H ₄	165(4)	-481(4)	-632(5)
4H ₅	80(4)	-338(4)	-704(5)
4H _e	31(4)	-217(4)	-546(5)
H	-27(5)	31(5)	-127(6)

TABLE 2b

Thermal Motion Parameters in Crystalline $(\text{HSCT}_4)_2$

($\times 10^3 \text{ \AA}^2$, $\times 10^4 \text{ \AA}^2$ for Sc)

Atom Type	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Sc	261(5)	275(5)	293(5)	126(4)	109(4)	73(4)
O ₁	25(2)	28(2)	44(2)	10(1)	17(1)	12(1)
O ₂	35(2)	34(2)	49(2)	16(1)	18(2)	18(2)
O ₃	30(2)	37(2)	27(2)	14(1)	9(1)	8(1)
O ₄	40(2)	47(2)	27(2)	24(1)	13(1)	5(1)
O ₅	29(2)	37(2)	69(2)	15(1)	18(1)	23(2)
O ₆	29(2)	28(2)	51(2)	56(1)	13(2)	16(1)
O ₇	48(2)	44(2)	32(2)	23(2)	19(2)	10(1)
O ₈	59(2)	55(2)	35(2)	36(2)	20(2)	12(2)
1C ₁	33(2)	25(2)	25(2)	9(2)	18(2)	1(2)
1C ₂	39(3)	37(3)	40(3)	18(2)	23(2)	15(2)
1C ₃	49(3)	33(3)	60(3)	18(2)	34(3)	16(2)
1C ₄	56(3)	36(3)	67(4)	14(3)	37(3)	21(3)
1C ₅	36(3)	40(3)	55(3)	5(2)	23(3)	11(4)
1C ₆	27(3)	40(3)	38(3)	11(2)	10(2)	2(2)
1C ₇	29(2)	31(2)	26(2)	8(2)	12(2)	2(2)
2C ₁	29(2)	53(2)	33(3)	12(2)	14(2)	8(2)
2C ₂	43(3)	45(3)	36(3)	23(2)	20(2)	12(2)
2C ₃	65(4)	69(4)	31(3)	35(3)	20(3)	3(3)
2C ₄	70(4)	99(5)	20(3)	44(4)	6(3)	6(3)
2C ₅	54(3)	86(4)	31(3)	41(3)	5(3)	13(3)
2C ₆	44(3)	60(3)	33(3)	30(3)	10(2)	9(2)
2C ₇	26(2)	35(2)	31(3)	10(2)	10(2)	10(2)
3C ₁	37(3)	29(3)	40(3)	14(2)	25(2)	9(2)
3C ₂	39(3)	36(3)	64(4)	15(2)	30(3)	17(3)
3C ₃	57(4)	38(3)	61(4)	11(3)	36(3)	13(3)
3C ₄	45(3)	48(3)	64(4)	-8(3)	24(3)	11(3)
3C ₅	33(3)	68(4)	62(4)	8(3)	11(3)	25(3)
3C ₆	39(3)	43(3)	54(3)	13(3)	12(3)	23(3)
3C ₇	35(3)	35(3)	31(2)	18(2)	16(2)	7(2)
4C ₁	27(2)	34(3)	34(3)	6(2)	16(2)	3(2)
4C ₂	47(3)	46(3)	55(4)	18(3)	24(3)	8(3)
4C ₃	61(4)	49(4)	66(4)	18(3)	37(3)	-4(3)
4C ₄	70(4)	71(4)	54(4)	15(3)	34(3)	-15(3)
4C ₅	66(4)	77(4)	39(3)	13(3)	30(3)	-1(3)
4C ₆	50(3)	62(4)	38(3)	20(3)	12(3)	9(3)
4C ₇	32(3)	37(3)	39(3)	6(2)	14(2)	4(2)

Isotropic temperature factor for tropolonato hydrogen atoms,
 $U = 0.043 \text{ \AA}^2$. Refined isotropic temperature factor for H,
 $U = 0.094 \text{ \AA}^2$.

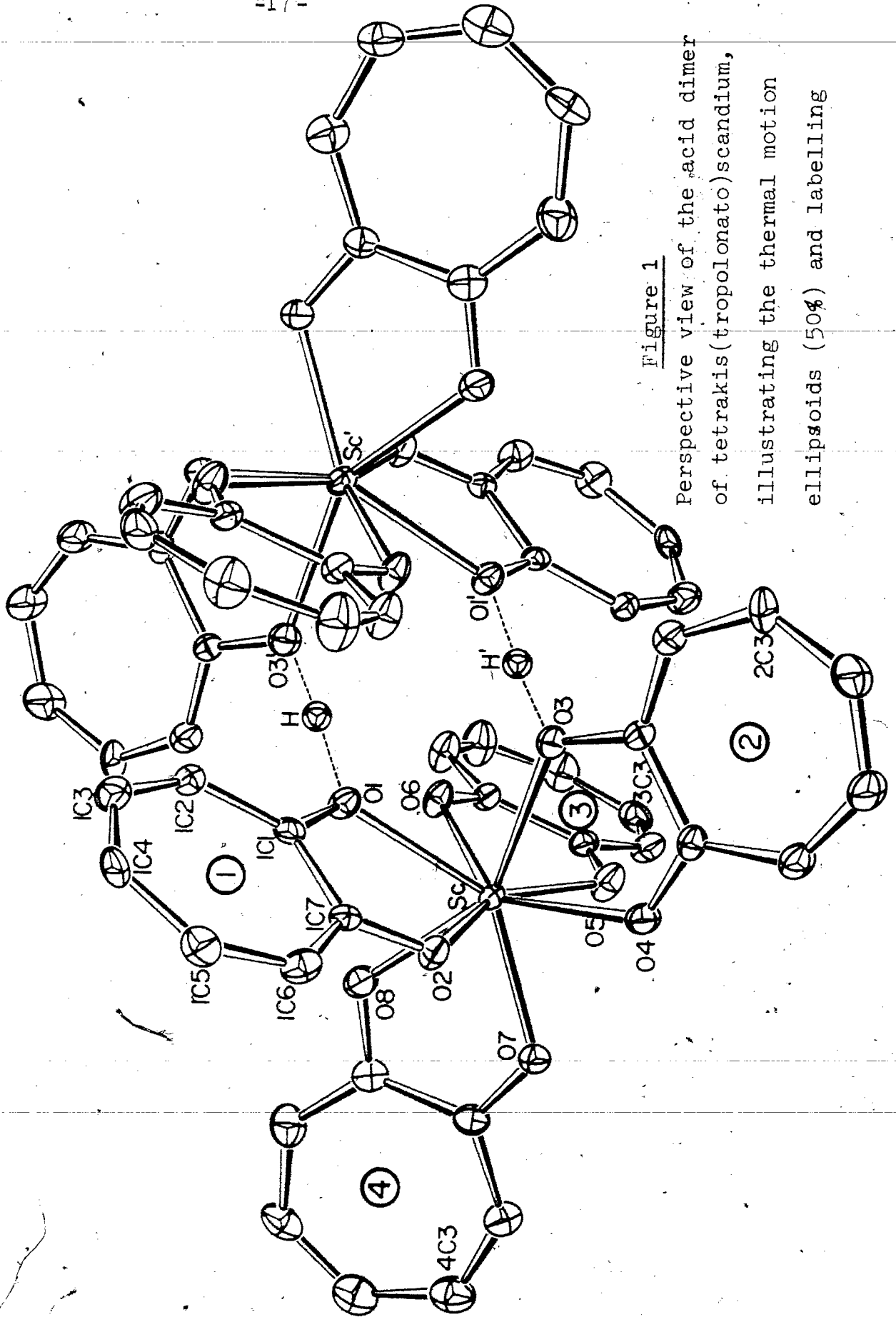


Figure 1

Perspective view of the acid dimer of tetrakis(tropolonato)scandium, illustrating the thermal motion ellipsoids (50%) and labelling

3.2 $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$

A three-dimensional Patterson synthesis based on the inner data ($\sin \theta < 0.2164$) gave the positions of the niobium atom and one chlorine atom. These parameters were refined together with a scale factor to give $R = 0.445$. A fourier synthesis gave the eight oxygen atoms bonded to the niobium. Three cycles of refinement using the full set of data and subsequent electron density difference maps gave all the trolonato carbon atom positions, as well as two prominent peaks on the two-fold axis near to the chlorine atom, and two other peaks (approximately 2.7\AA apart), one of which was on the two-fold axis. In the first case, refinement was continued using a model of $(\text{H}_3\text{OCl}_3)^{2-}$ with one chlorine atom on the two-fold axis which related the other two chlorine atoms in the species to give the base of a flattened pyramid. The oxygen atom formed the apex of this pyramid and was disordered either side of the two-fold axis. The other two peaks were refined as an acetonitrile molecule of crystallization, disordered about the two-fold axis. The extended peak in the general position was split to give the $-\text{C}\equiv\text{N}$ group of this molecule, and refinement of this model gave reasonable final atomic parameters and temperature factors. The remaining hydrogen atom positions (excluding those in the H_3O^+ and CH_3 groups) were calculated with a C-H bond length of 0.96 \AA , and all hydrogen atoms were assigned temperature factors of 0.038 \AA^2 , a value based on the refined isotropic temperature factors of the carbon atoms to which they were bonded. An R factor of 7.7% was obtained after refinement of all

non-hydrogen atom positional and thermal motion parameters, and with niobium, chlorine and oxygen atoms (except for O_9 in H_3O^+) allowed anisotropic thermal motion parameters. The estimated standard deviation (s) of an observation of unit weight was 1.233. (Where $s = (\sum w(|E_o| - |F_c|)^2 / (m-n))^{1/2}$, w are the counter weights given by $1/\sigma_F^2$, and $(m-n)$ is the difference between the number of independent observations and the number of parameters varied).

A listing of the correlation coefficients indicated very strong interactions between the scale factors and niobium thermal motion parameters, and between positional parameters of bonded atoms; in all there were 792 correlation coefficients with values greater than 0.1. Geller has pointed out that these coefficients are directly related to the structure model (e.g. vector overlap in the Patterson map), and it was assumed that the refinement had stopped at some kind of 'false minimum'. Further evidence for this came from a comparison of the least squares estimated errors in the tropolonato bond lengths, and the errors calculated on the basis of the internal consistency within the model. The four tropolonato ligands were assumed to be all chemically equivalent and symmetrically bonded to the metal since all the niobium-oxygen distances were equal. Thus, for a group of n bond lengths with a mean value \bar{l} , the standard deviation (σ_s) for this group is given by $\sigma_s = (\sum(l_n - \bar{l})^2 / (n-1))^{1/2}$, and the estimated standard deviation in \bar{l} is $\sigma_{\bar{l}}$, which is given by $\sigma_{\bar{l}} = (\sum(l_n - \bar{l})^2 / n(n-1))^{1/2}$. Values of σ_s calculated in this way were a factor of two to three times larger than the least squares

estimated errors. The tropolonato ligands were therefore chemically equivalent within the errors expressed by values of σ_s , but significantly different on the basis of the least squares estimated errors.

An analysis of $\frac{\sum w \Delta^2}{n}$ values indicated systematic trends which showed that the strong and/or low angle data were heavily over-weighted. To achieve an acceptable weighting scheme, it was considered necessary to increase the constant k (in the expression used to calculate $\sigma_{I_{net}}$) to down-weight reflections of this type. After some analysis, a value of $k = 0.075$ was determined as appropriate. Refinement was continued using the reprocessed data (1651 'observed' reflections). Large shifts in the parameters of the tropolonato ligands were observed; the least squares estimated errors in the bond lengths were higher than those for the previous model, and generally agreed well with those errors (σ_s) calculated on the basis of the internal consistency (which were slightly lower for the new model). The one exception was the $O_1 \dots O_2$ donor atom separation ($2.476(15)\text{\AA}$) which was significantly longer than those for the other 3 ligands (mean value of $2.418(8)\text{\AA}$). A final R factor of 0.075 based on the 1651 'observed' reflections was obtained. A value of $s = 1.263$ was obtained for the new model; this, however, is a measure of the absolute rather than the relative error in the model, and the even distribution of the $\sum w \Delta^2/n$ values is recognized as the most important improvement. The correlation

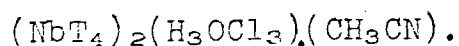
* $\sum w \Delta^2$, where $\Delta = |F_o| - |F_c|$, is the function that is minimised in the least squares refinement.

matrix still showed some large interactions, which would indicate some indeterminacy in the structure. One cycle of refinement using the final parameters and the 2344 reflections $> 1.0\sigma$, however, gave negligible shifts, indicating that the final model was unchanged when 50% more data was included in the refinement. The value of s for this refinement was 1.290.

Atomic scattering factors used were taken from reference 7, and included corrections for anomalous dispersion for the niobium ($\Delta f' = -2.1$, $\Delta f'' = 0.9$) and chlorine ($\Delta f' = 0.1$, $\Delta f'' = 0.2$) atoms. A table of the measured and calculated structure factors is given in Appendix B. Final atomic and thermal motion parameters are given in Tables 3a and 3b (page 22). A projection of the unit cell along the a axis is shown in Figure 3 (page 25).

Table 3a

Fractional atomic coordinates ($\times 10^4$) in crystalline



(The least squares estimated errors are in parentheses)

Atom Type	Coordinates		
	x	y	z
Nb	4544(1)	2816(1)	1013(1)
Cl ₁	0	418(6)	2500
Cl ₂	220(4)	3546(5)	1621(2)
O ₁	5147(6)	2958(8)	1768(4)
O ₂	5790(7)	3390(8)	955(4)
O ₃	5201(7)	1505(8)	1109(4)
O ₄	4836(6)	2307(9)	297(4)
O ₅	3296(7)	2482(8)	628(4)
O ₆	3800(7)	2083(9)	1525(4)
O ₇	4338(7)	3949(9)	474(4)
O ₈	360(14)	2415(19)	2555(11)
N	3403(20)	898(22)	2952(11)
C ₁	5000	729(26)	2500
C ₂	4042(28)	809(31)	2794(16)
1C ₁	5951(11)	3249(12)	1835(7)
1C ₂	6341(11)	3340(13)	2357(7)
1C ₃	7220(11)	3601(14)	2525(7)
1C ₄	7903(12)	3836(14)	2254(7)
1C ₅	7894(11)	3943(14)	1725(7)
1C ₆	7184(12)	3846(13)	1325(7)
1C ₇	6344(10)	3501(12)	1392(6)
2C ₁	5564(12)	1100(14)	721(7)
2C ₂	6091(12)	287(14)	835(7)
2C ₃	6501(13)	-268(16)	487(8)
2C ₄	6512(13)	-159(16)	-37(8)
2C ₅	6094(13)	498(15)	-342(8)
2C ₆	5557(11)	1252(13)	-248(7)
2C ₇	5311(11)	1563(14)	251(7)
3C ₁	2691(10)	2115(14)	877(6)
3C ₂	1843(11)	1954(13)	623(7)
3C ₃	1114(12)	1537(14)	813(7)
3C ₄	1009(12)	1194(15)	1286(8)
3C ₅	1627(12)	1148(14)	1725(7)
3C ₆	2498(12)	1415(14)	1766(7)
3C ₇	2971(12)	1849(12)	1401(7)
4C ₁	3982(10)	4656(13)	590(6)
4C ₂	3863(11)	5473(13)	225(6)
4C ₃	3524(12)	6412(15)	285(7)
4C ₄	3207(13)	6774(16)	710(9)
4C ₅	3177(13)	6416(16)	1198(8)
4C ₆	3385(11)	5512(14)	1368(7)
4C ₇	3755(10)	4760(12)	1108(6)

Table 3a (continued)

The atomic parameters of tropolonato hydrogen atoms, which were calculated using the final carbon atom positions and a C-H distance of 0.96 Å.

1H ₂	7301	4030	985
1H ₃	8453	4106	1607
1H ₄	8464	3928	2455
1H ₅	7354	3623	2897
1H ₆	5964	3190	2623
2H ₂	6190	97	1197
2H ₃	6828	-814	647
2H ₄	6873	-608	-210
2H ₅	6183	417	-703
2H ₆	5327	1612	-548
3H ₂	1739	2166	275
3H ₃	601	1487	575
3H ₄	433	948	1331
3H ₅	1420	880	2036
3H ₆	2820	1322	2095
4H ₂	4030	5320	-112
4H ₃	3547	6819	-16
4H ₄	2958	7414	647
4H ₅	2956	6842	1450
4H ₆	3302	5387	1718

Table 3b
 Thermal Motion Parameters in Crystalline $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$.
 ($\times 10^3 \text{ \AA}^2$)

Anisotropic Atoms		U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Nb	Atom Type	30(1)	35(1)	19(1)	-1(1)	-6(1)	1(1)
Cl ₁		64(5)	59(6)	66(6)	0	23(4)	0
Cl ₂		99(5)	81(5)	63(4)	10(4)	6(4)	13(4)
O ₁		18(6)	53(9)	28(6)	-12(6)	-4(5)	-8(6)
O ₂		30(7)	57(9)	27(7)	-4(6)	-12(6)	11(6)
O ₃		53(8)	37(8)	31(8)	19(7)	-4(6)	12(6)
O ₄		38(6)	48(8)	16(6)	9(6)	11(5)	-5(6)
O ₅		30(7)	51(10)	31(7)	-5(6)	-7(5)	4(6)
O ₆		31(6)	49(9)	27(6)	-6(7)	-2(6)	9(7)
O ₇		35(7)	54(9)	20(6)	2(6)	3(5)	2(6)
O ₈		58(8)	49(9)	35(8)	6(7)	-3(7)	9(7)

Isotropic Atoms		U	Atom Type	U
O ₉		69(9)	2C ₆	41(5)
C ₁		88(11)	2C ₇	35(5)
C ₂		59(12)	3C ₁	32(4)
N		45(9)	3C ₂	41(5)
1C ₁		32(5)	3C ₃	45(5)
1C ₂		34(5)	3C ₄	56(6)
1C ₃		42(5)	3C ₅	48(5)
1C ₄		45(5)	3C ₆	51(6)
1C ₅		45(5)	3C ₇	39(5)
1C ₆		46(5)	4C ₁	26(4)
1C ₇		48(4)	4C ₂	35(5)
2C ₁		44(5)	4C ₃	51(6)
2C ₂		44(5)	4C ₄	61(6)
2C ₃		61(6)	4C ₅	58(6)
2C ₄		61(6)	4C ₆	43(5)
2C ₅		59(6)	4C ₇	28(4)

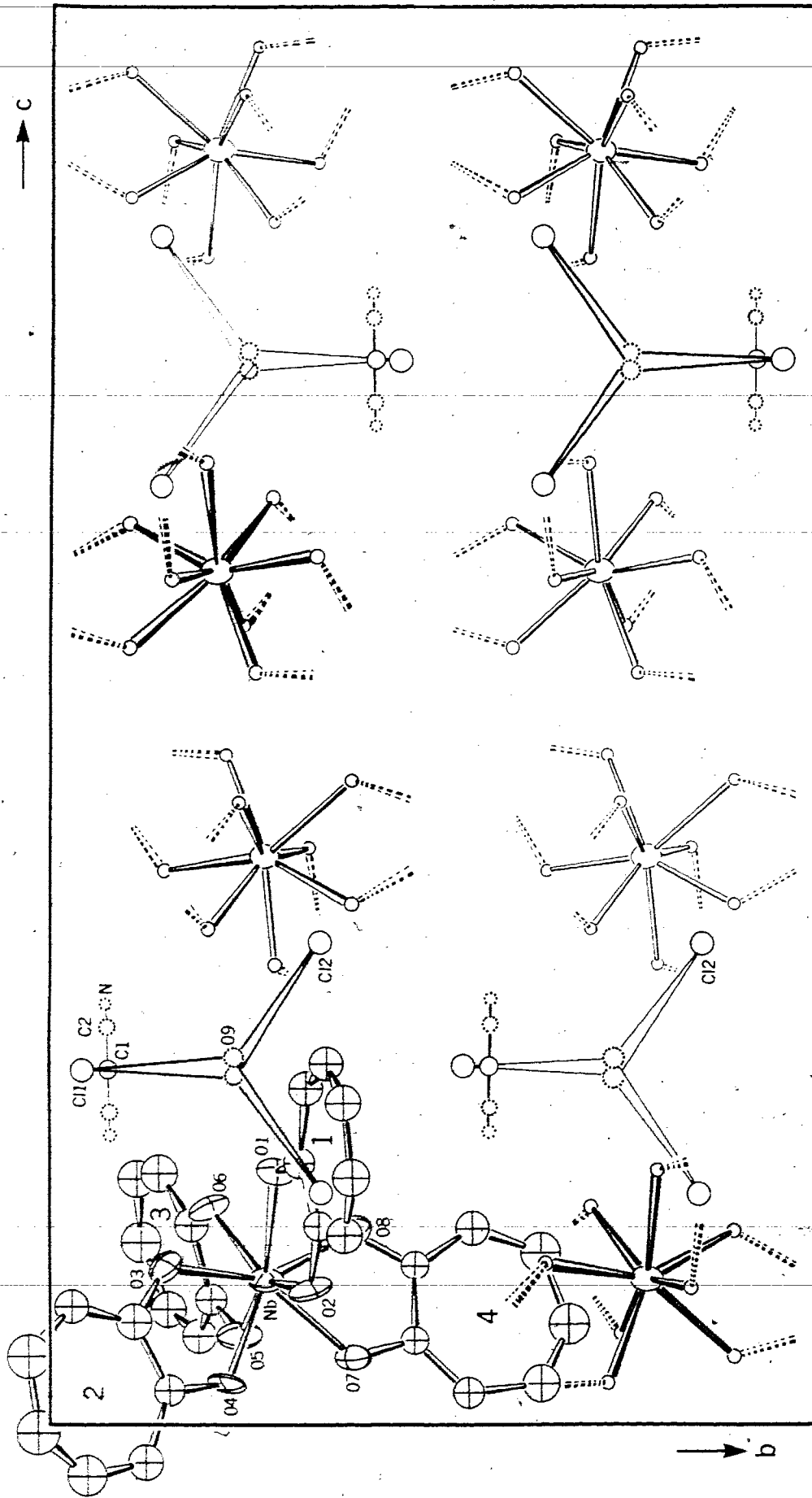


Figure 3 : A view along the a axis of the unit cell of crystalline $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$, illustrating the thermal motion (50%) and labelling in one molecule. The tropolonato ligands of the other cations have been omitted for clarity.

CHAPTER FOUR

DISCUSSION

4.1 The 'MO₈' Polyhedra

"There is a wonderful sentence in Augustine : 'Do not despair, one of the thieves was saved; do not presume, one of the thieves was damned.'

That sentence has a wonderful shape. It is the shape that matters."

Samuel Beckett

In order to establish a useful description of the polyhedra defined by the eight oxygen donor atoms in the two structures, an approach based on criteria established by Porai-Koshits and Aslanov⁴ is used. In treating polyhedra of the dodecahedral class, (the dodecahedron, the square antiprism, and the bicapped trigonal prism), they defined the set of dihedral angles, δ , between pairs of faces which intersect along the 'type B' edges of a dodecahedron. These edges can be seen from Figure 1 (page 5) as those which connect vertices B₁, B₂, B₃ and B₄ at which five edges are joined. These correspond to oxygen atoms O₂, O₃, O₅, and O₈ in the perspective views of the 'MO₈' polyhedra shown in Figure 4 (page 31). An additional criterion given by Porai-Koshits and Aslanov is the degree of non-planarity of the diagonal trapezoids which characterize the dodecahedron shape. Distortions from the regular dodecahedron lead to a twisting in these trapezoids, and the corresponding parameter ϕ has been calculated for the trapezoids (defined by O₁, O₆, O₅, O₂ and O₃, O₄,

O_7, O_8) according to Porai-Koshits and Aslanov's method, and is listed together with values for the ' ScO_8 ' and ' NbO_8 ' polyhedra and the three regular polyhedra of this class in Table 5a (page 33). It is clear from a comparison of these results that the ' MO_8 ' polyhedra are both best described as irregular bicapped trigonal prisms, distorted towards a dodecahedron.

Blight and Kepert⁶ have produced a description of the effect of bidentate ligands on eight-coordination. Neglecting any type of interaction save that of interligand repulsion, they show the dependence of geometry on a parameter b , defined as the ratio of the ligand bite to the metal to donor atom distance. For various values of b , they give the dimensions of a generalised eight-coordinate stereochemistry which is predicted to have the most stable configuration. The generalised sphere is shown in Figure 5 (page 32), and the parameters of the most stable configurations for $b = 1.10$ and $b = 1.15$ are given in Table 5b (page 33), alongside those parameters determined for the ' ScO_8 ' and ' NbO_8 ' polyhedra. Values of b for these structures were obtained from the mean ligand bite and mean metal to oxygen atom distance for each structure, giving $b = 1.13$ for ' ScO_8 ' and $b = 1.16$ for ' NbO_8 '. The agreement between these sets of parameters is seen to be quite close. Bond distances and angles within the two MO_8 polyhedra are given in Tables 4a and b (page 30).

The most striking feature of the ' NbO_8 ' polyhedron is the wide range of interligand O...O distances. In the regular dodecahedron, the ratio of the length of the 'type B' edges to

the other edges (all of which are equivalent) is 1.25; in the 'NbO₈' polyhedron, this ratio (based on the interligand distances) averages 1.20, but varies from 1.10 to 1.40. In particular, the O₁...O₆ (2.410(14)Å) and O₄...O₇ (2.467(17)Å) edges are very short compared to other interligand O...O distances of the same type (which vary from 2.508(15)Å to 2.654(17)Å and average 2.60Å). This pair of short contacts are related by an approximate (non-crystallographic) ionic 4 axis. Such results cannot be rationalized on the basis of interligand repulsion alone. The shortest edges connect tropolonato ligands which are arranged in such a way that the lone pairs of electrons on each of the oxygen atoms involved in the contact overlap in the space between the nuclei of the oxygen atoms. The niobium complex appears to be the most extreme example of a correlation between short interligand O...O distances, and the overlap of lone pairs of electrons on adjacent oxygen atoms. Table 6 (page 34) gives a list of the shortest interligand contacts¹¹⁻¹⁶ in some high-coordinate complexes containing bidentate ligands with oxygen donor atoms. In each case, the geometry involved in these contacts would allow overlap of the lone pairs on the oxygen atoms involved. Also, it is well established that high-coordinate complexes bonded to oxygen atoms contain empty valence shell orbitals.

Epiotis¹⁷ has shown that, for small organic systems, if lone pairs of electrons interact to give a bonding and anti-bonding combination, then this interaction will be attractive if there is an antisymmetric molecular orbital which can interact

with the antisymmetric lone pair combination.

It is tentatively suggested that, for the short contacts listed in Table 6, conditions exist in the arrangement of the lone pairs and empty metal d-orbitals for interactions to occur which would oppose the coulombic repulsive force, thus stabilizing the contact. Such an interaction would need to be included in any theory of those high-coordinate geometries where arrangements of lone pairs could arise. In all the cases listed in Table 6, the lone pairs, oxygen atoms and metal atom involved in the contact are approximately planar. In T_3SnCl^{12} , two short interligand distances (2.52Å : related by an approximate, non-crystallographic, molecular mirror plane) have been observed in addition to that listed in Table 6. One of the tropolonato ligands is approximately perpendicular to the two other, nearly coplanar ligands. The lone pairs on the three oxygen atoms involved in the two contacts can still be envisaged as overlapping, and a similar decrease in the coulombic repulsive forces is suggested.

Table 4

Interatomic distances and angles in the 'MO₈' polyhedra of the ScT₄⁻ and NbT₄⁺ ions.

<u>Distances (Å)</u>			
Sc-O ₁	2.310(3)	Nb-O ₁	2.088(9)
Sc-O ₂	2.209(3)	Nb-O ₂	2.070(11)
Sc-O ₃	2.259(3)	Nb-O ₃	2.084(11)
Sc-O ₄	2.215(3)	Nb-O ₄	2.070(10)
Sc-O ₅	2.172(3)	Nb-O ₅	2.104(9)
Sc-O ₆	2.173(3)	Nb-O ₆	2.070(10)
Sc-O ₇	2.161(3)	Nb-O ₇	2.111(11)
Sc-O ₈	2.173(3)	Nb-O ₈	2.092(13)
O ₁ -O ₂	2.517(4)	O ₁ -O ₂	2.476(16)
O ₃ -O ₄	2.495(4)	O ₃ -O ₄	2.398(14)
O ₄ -O ₆	2.495(4)	O ₅ -O ₆	2.438(14)
O ₇ -O ₈	2.504(4)	O ₇ -O ₈	2.417(17)
O ₁ -O ₃	2.710(4)	O ₁ -O ₃	2.654(17)
O ₁ -O ₆	2.568(4)	O ₁ -O ₆	2.410(14)
O ₁ -O ₈	2.741(4)	O ₁ -O ₈	2.508(15)
O ₂ -O ₃	3.189(4)	O ₂ -O ₃	2.815(17)
O ₂ -O ₄	2.725(4)	O ₂ -O ₄	2.608(14)
O ₂ -O ₇	2.978(4)	O ₂ -O ₇	2.547(14)
O ₂ -O ₈	2.993(4)	O ₂ -O ₈	3.226(18)
O ₃ -O ₅	3.054(4)	O ₃ -O ₅	3.325(14)
O ₃ -O ₆	2.914(4)	O ₃ -O ₆	2.600(16)
O ₄ -O ₅	2.753(4)	O ₄ -O ₅	2.574(15)
O ₄ -O ₇	2.696(4)	O ₄ -O ₇	2.467(17)
O ₅ -O ₇	2.756(4)	O ₅ -O ₇	2.637(16)
O ₅ -O ₈	3.558(4)	O ₅ -O ₈	2.860(16)
O ₆ -O ₈	2.715(4)	O ₆ -O ₈	2.652(18)
<u>Angles (°)</u>			
O ₁ ScO ₂	67.6(1)	O ₁ NbO ₂	73.1(0.4)
O ₃ ScO ₄	67.7(1)	O ₃ NbO ₄	70.5(0.5)
O ₅ ScO ₆	70.1(1)	O ₅ NbO ₆	71.1(0.4)
O ₇ ScO ₈	70.5(1)	O ₇ NbO ₈	70.2(0.5)
O ₁ ScO ₃	72.7(1)	O ₁ NbO ₃	79.0(0.4)
O ₁ ScO ₂	69.8(1)	O ₁ NbO ₆	70.5(0.4)
O ₁ ScO ₈	75.3(1)	O ₁ NbO ₈	73.7(0.4)
O ₂ ScO ₃	91.0(1)	O ₂ NbO ₃	85.3(0.5)
O ₂ ScO ₄	76.0(1)	O ₂ NbO ₄	78.1(0.4)
O ₂ ScO ₇	85.9(1)	O ₂ NbO ₇	75.1(0.4)
O ₂ ScO ₈	86.1(1)	O ₂ NbO ₈	101.6(0.5)
O ₃ ScO ₅	87.1(1)	O ₃ NbO ₅	105.1(0.4)
O ₃ ScO ₆	82.2(1)	O ₃ NbO ₆	77.1(0.5)
O ₄ ScO ₅	77.7(1)	O ₄ NbO ₅	76.1(0.4)
O ₄ ScO ₇	75.3(1)	O ₄ NbO ₇	72.3(0.5)
O ₅ ScO ₇	78.9(1)	O ₅ NbO ₇	77.5(0.4)
O ₅ ScO ₈	109.9(1)	O ₅ NbO ₈	86.0(0.4)
O ₆ ScO ₈	77.3(1)	O ₆ NbO ₈	78.8(0.5)

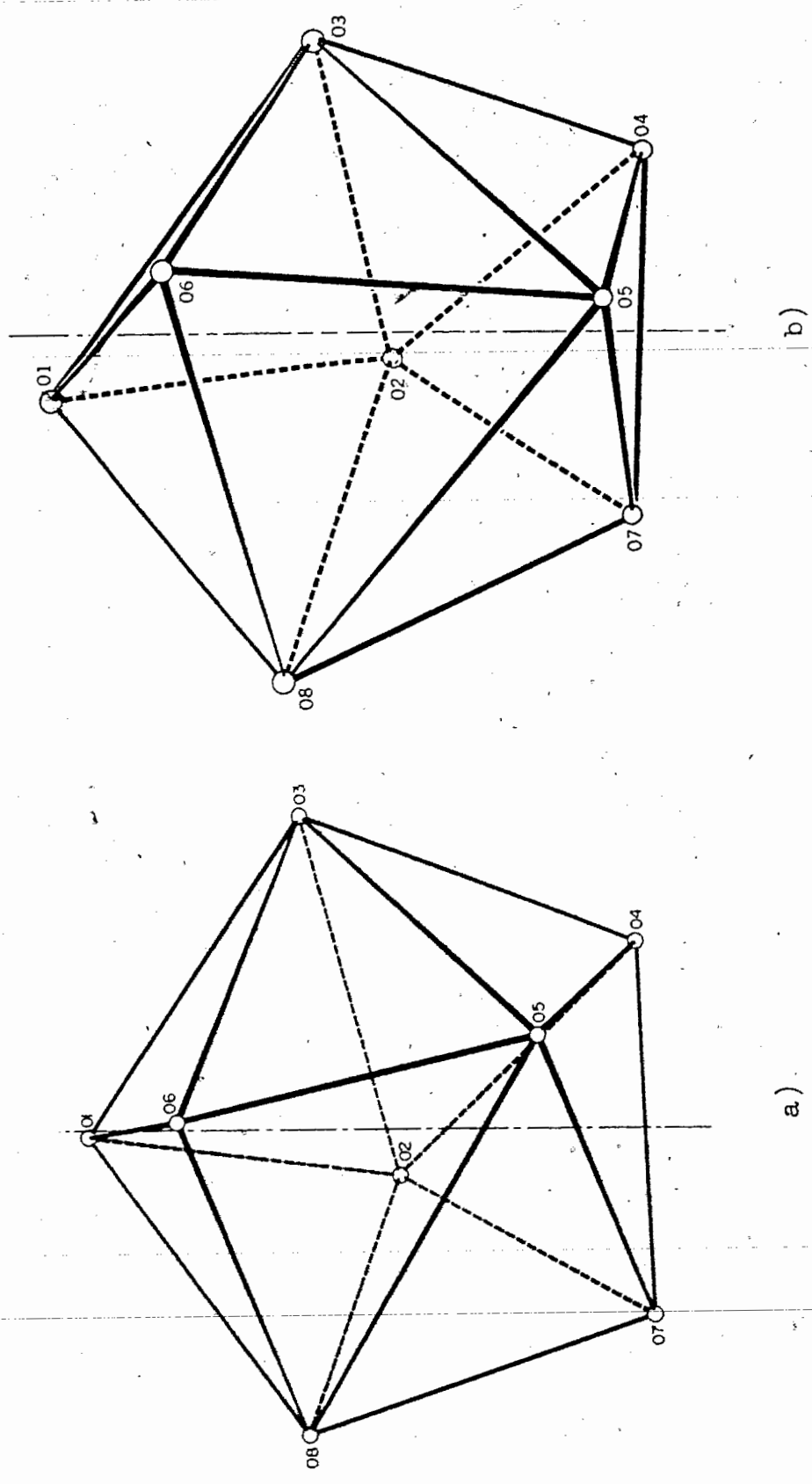


Figure 4 :
Perspective views of the a) 'ScO₈' and b) 'NbO₈' polyhedra.
The vertical broken line shows in each case the direction of
an approximate 4 axis. O₁ and O₄ are the capping oxygens in the
description of the polyhedra as bicapped trigonal prisms.

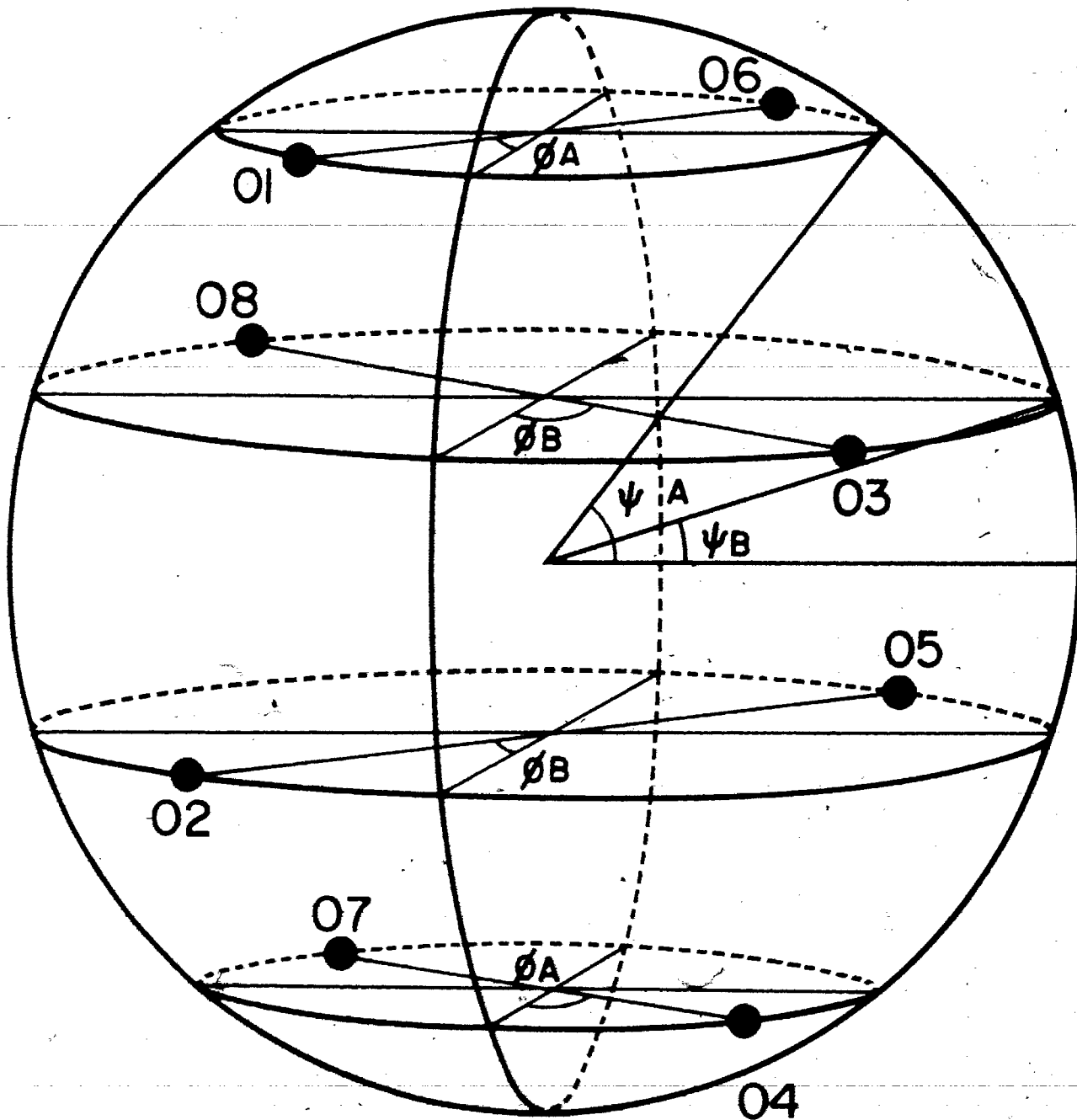


Figure 5 : Generalised eight-coordination

(adapted from reference 6).

Table 5

a) Values of δ and φ (as defined in reference 4) for regular polyhedra of the dodecahedral class, for HScT_4 , and for NbT_4^+ .

	δ (deg.)				φ (deg.)	
Dodecahedron	29.5	29.5	29.5	29.5	0	0
Bicapped Trigonal Prism	0	21.7	48.2	48.2	14.1	14.1
Square Antiprism	0	0	52.5	52.5	24.5	24.5
HScT_4	13.4	29.0	43.0	42.5	10.8	10.8
NbT_4^+	19.4	21.0	42.9	45.1	11.5	13.9

b) Angular parameters for $\text{M}(\text{biden})_4$ of intermediate geometry (from reference 6).

	Predicted values (deg.)		HScT_4	NbT_4^+
	b=1.10	b=1.15	b=1.13	b=1.16
ϕ_A	37.4	34.4	37.8	37.8
ψ_A	50.9	51.2	55.0	54.3
ϕ_B	50.6	53.7	48.3	49.7
ψ_B	14.8	16.9	15.5	16.3

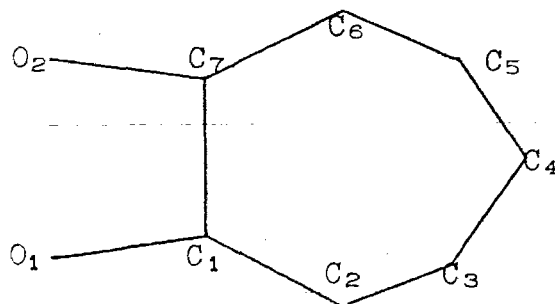
Table 6

Shortest interligand O...O contacts in some high-coordinate complexes. Also given are the bidentate ligand 'bites' in each complex, and the mean M-O distance for these ligands.

Complex	Shortest Interligand Contacts (Å)	Ligand 'Bite' (Å)	Mean M-O Distance	Reference	
NbT ₄ ⁺	2.41	2.48	2.08	} Table 4a	
	2.47	2.44			
		2.42			
		2.40			
ScT ₄ ⁻	2.57	2.52	2.21		
	2.70	2.50			
		2.50			
		2.50			
ThT ₄ .DMF	2.80	2.56	2.45	11	
		2.53			
		2.55			
		2.52			
T ₃ SnOH	2.52	2.54	2.16	12	
		2.54			
		2.60			
T ₃ SnCl	2.53	2.59	2.45	12	
		2.55			
		2.52			
Zr(Oxalato) ₄	2.63	2.55	2.20	13	
	2.51	2.58			related to 2 more by 2-fold axis
Ti(NO ₃) ₄	2.51	2.14	2.07	14	
		2.13			
		2.13			
		2.12			
Sn(NO ₃) ₄	2.72	2.13	2.16	15	
		2.75			2.15
					2.14
					2.13
Fe(NO ₃) ₄ ⁻	2.63 (mean of two values)	2.13 (mean of four values)	2.14	16	

4.2 The Tropolonato Ligands

Earlier crystal structures involving this ligand have been reviewed¹⁸, and certain systematics in the ligand parameters can be recognised. The labelling scheme used in this discussion is shown diagrammatically below :



The key features of the tropolonato ligand based on previous results are the following.

- 1) There is no discernable bond length alternation around the C₇ ring.
- 2) The C₁-C₇ distances are significantly longer than other C-C distances.
- 3) There is a sequential decrease in the C-C bond distances from those nearest to the oxygen atoms to the central C₄ ring atom, and indicate symmetrical bonding.
- 4) There is a remarkable similarity in the ligand parameters for a wide range of compounds (e.g. NaT, FeT₃, T₄Th.DMF).
- 5) The range of intraligand O...O separations is quite narrow, 2.490-2.593Å.

For the ScT₄⁻ anion, the parameters for ligands 3 and 4 (i.e. those not involved in the hydrogen bond) can be compared to these general results. The C₇ rings in both ligands are

non-planar, the oxygen atoms showing larger deviations from the C_7 plane than do the carbon atoms (least squares mean planes are given in Table 9a). In discussing similar non-planar ligands, Day and Hoard¹¹ have noted that because the bite of the tropolonato ligand is small and therefore contributes to the loose packing of the ligand, the molecular arrangement is susceptible to distortion in the solid state as a result of packing forces. The dihedral angles between the least squares mean planes of the C_7 rings and the corresponding ScO_2 atoms are 12.8° for ligand 3, and 6.0° for ligand 4. Bond lengths in the C_7 rings of these ligands follow those reported for other structures, with a steady decrease in the C-C length with increasing distance from the oxygen atoms, and indicate symmetrical bonding. The C_1-C_7 distance is longest, this being attributed to the small aromatic character in this bond, and the oxygen atom separations (2.495(4), 2.504(4)) are among the shortest found for tropolonato ligands. Carbon-hydrogen distances in all four ligands are all identical within the accuracy of the determination, and average $0.96(3)\text{\AA}$. Bond lengths in the tropolonato ligands in the ScT_4^- anion are given in Table 7a, along with the average values for previously determined structures. Bond angles in the tropolonato ligands of both complexes are given in Table 8.

As a consequence of the hydrogen bond, the ligand parameters in ligands 1 and 2 are different from those in 3 and 4. The asymmetry of the bond is reflected in the bond lengths around the tropolonato ligands. The C_7 ring in ligand 2 has bond lengths which alternate, (the differences being significant, see Table 7a),

and this can be explained by assuming a bond between the C_3 and H atoms which leads to double bond character in C_1-C_2 (1.332(5)), C_3-C_4 (1.349(7)) and C_5-C_6 (1.357(2)), and single bond character in C_1-C_7 (1.463(5)), C_2-C_3 (1.403(6)), C_4-C_5 (1.398(7)) and C_6-C_7 (1.421(6)). The bond lengths in the C_7 ring of ligand 1 indicate bonding which is intermediate between that of 2 and the symmetrical ligands 3 and 4. The C_7 ring in ligand 1 is the only planar ring in the structure (within our limits of error) with the oxygen atoms placed either side of this plane (as was found for the other rings). The C_7 ring of ligand 2 has the largest deviations from the least-squares plane for all four ligands.

Because of the large errors in the parameters of the four tropolonato ligands in the NbT_4^+ cation, a rather different approach is taken in their discussion. Shown in Table 7b (page 40) are the mean values \bar{l} of the bonds within the ligands (which are considered to be chemically equivalent on the basis of equal Nb-O distances), $\sigma_{\bar{l}}$ (the standard deviation in this mean), and σ_s (error based on the internal consistency of the structure; as defined in Chapter 3.2). The corresponding values of \bar{l} for all previously determined structures involving this ligand are also listed. It can be seen that the mean values in the NbT_4^+ cation are, within the error expressed by $\sigma_{\bar{l}}$, equal to the general mean values, except in the case of the C_1-C_7 bond lengths. A comparison of bond lengths in those structures reported¹⁸ shows that increasing strength of the complexing bonds is accompanied by some lengthening in the C-O bond length, and also a shortening of the C_1-C_7

bonds. The values of the C₁-C₇ bond lengths (which average 1.408(10)Å) do not differ significantly from values for strongly complexing tropolonato ligands as in T₃SnCl¹² (1.439(15)Å). The short intraligand O...O contacts in these ligands have been discussed in the previous section. It is clear that the characterization of the tropolonato ligand as having a rigid ligand bite must be reconsidered.

Three of the C₇ rings in the NbT₄⁺ cation are statistically planar (relevant mean planes are given in Table 9b, page 43), and the fourth has distortions from planarity which are not chemically significant. Deviations of the corresponding oxygen atoms are small (0.001 to 0.057 Å), though larger deviations of the niobium atom (0.099 to 0.218 Å) are observed.

Table 7a.

Bond lengths in the tropolonato ligands of $(\text{HScT}_4)_2$. Also given are the mean values of the same bonds calculated for previously determined structures ^{18,19}.

Bond	1(O ₁ ,O ₂)	2(O ₃ ,O ₄)	3(O ₅ ,O ₆)	4(O ₇ ,O ₈)	Previous Mean
O ₁ -C ₁	1.306(5)	1.332(5)	1.283(5)	1.280(5)	1.287(2)
C ₂ -C ₇	1.261(5)	1.253(5)	1.270(5)	1.274(5)	
C ₁ -C ₇	1.468(5)	1.463(5)	1.464(5)	1.454(6)	1.462(6)
C ₁ -C ₂	1.386(6)	1.361(6)	1.391(6)	1.406(6)	1.405(4)
C ₂ -C ₃	1.379(6)	1.403(6)	1.384(7)	1.376(7)	1.384(2)
C ₃ -C ₄	1.376(7)	1.349(7)	1.377(7)	1.364(8)	1.380(2)
C ₄ -C ₅	1.375(6)	1.393(7)	1.376(7)	1.370(8)	1.380(2)
C ₅ -C ₆	1.357(6)	1.357(7)	1.376(7)	1.381(7)	1.384(2)
C ₆ -C ₇	1.429(6)	1.421(6)	1.412(6)	1.407(6)	1.405(4)

Table 7b

Bond lengths in the tropolonato ligands of the NbT_4^+ cation, with mean values (\bar{l}) of chemically equivalent bonds, together with $\sigma_{\bar{l}}$ and σ_s (as defined in the text). Also given are the mean values of the same bonds calculated from previously determined structures 18, 19.

Bond Type	Ligand Type				$\bar{l}(\sigma_{\bar{l}})$	σ_s^*	Previous Mean Value
	1	2	3	4			
C ₁ -O ₁	1.281(17)	1.317(21)	1.277(18)	1.296(18)			
C ₂ -O ₂	1.351(16)	1.275(19)	1.309(18)	1.294(18)	1.300(9)	0.025	1.287(2)
C ₁ -C ₇	1.387(22)	1.397(23)	1.431(22)	1.415(41)	1.408(10)	0.020	1.462(6)
C ₁ -C ₂	1.427(21)	1.401(23)	1.406(20)	1.374(21)			
C ₆ -C ₇	1.390(22)	1.445(23)	1.379(25)	1.392(22)	1.402(9)	0.024	1.405(4)
C ₂ -C ₃	1.411(21)	1.377(26)	1.406(20)	1.419(25)			
C ₅ -C ₆	1.427(22)	1.366(25)	1.367(23)	1.362(25)	1.392(9)	0.027	1.384(2)
C ₃ -C ₄	1.344(24)	1.369(26)	1.337(24)	1.342(26)			
C ₄ -C ₅	1.377(29)	1.329(25)	1.404(23)	1.364(27)	1.358(9)	0.025	1.380(2)

* These values can be compared to the least squares errors given in parentheses after each bond length (see page 19).

Table 8

a)

Bond angles in the tropolonato ligands of $(\text{HScT}_4)_2$.

(degrees)

Angle	Ligand : 1	2	3	4
$\text{C}_7\text{C}_1\text{C}_2$	126.7(0.4)	129.4(0.4)	126.6(0.4)	125.6(0.4)
$\text{C}_1\text{C}_2\text{C}_3$	131.3(0.4)	129.2(0.4)	130.2(0.5)	130.9(0.5)
$\text{C}_2\text{C}_3\text{C}_4$	129.6(0.5)	129.4(0.3)	129.9(0.5)	129.6(0.5)
$\text{C}_3\text{C}_4\text{C}_5$	126.9(0.5)	128.1(0.5)	127.2(0.5)	127.8(0.5)
$\text{C}_4\text{C}_5\text{C}_6$	130.0(0.5)	129.3(0.5)	130.1(0.5)	129.4(0.6)
$\text{C}_5\text{C}_6\text{C}_7$	131.9(0.4)	131.2(0.5)	130.2(0.5)	130.6(0.5)
$\text{C}_6\text{C}_7\text{C}_1$	123.6(0.4)	123.1(0.4)	125.6(0.4)	125.8(0.4)
$\text{O}_1\text{C}_1\text{C}_7$	112.3(0.4)	110.5(0.3)	112.8(0.4)	114.3(0.4)
$\text{O}_2\text{C}_7\text{C}_1$	116.0(0.4)	116.7(0.3)	114.9(0.4)	114.2(0.4)
$\text{O}_1\text{C}_1\text{C}_2$	121.0(0.4)	120.2(0.4)	120.7(0.4)	120.0(0.4)
$\text{O}_2\text{C}_7\text{C}_6$	120.4(0.4)	120.2(0.4)	119.5(0.4)	120.0(0.4)

b)

Bond angles (degrees) in the tropolonato ligands of

 $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$

Angle	Ligand: 1	2	3	4
$\text{C}_7\text{C}_1\text{C}_2$	126.1(1.6)	131.2(1.9)	125.2(1.7)	128.3(1.7)
$\text{C}_1\text{C}_2\text{C}_3$	127.5(1.7)	126.9(1.8)	129.0(1.6)	128.5(1.8)
$\text{C}_2\text{C}_3\text{C}_4$	130.9(1.6)	129.3(2.0)	130.2(1.7)	126.8(2.0)
$\text{C}_3\text{C}_4\text{C}_5$	127.6(1.6)	127.9(2.2)	128.9(1.9)	131.8(2.1)
$\text{C}_4\text{C}_5\text{C}_6$	130.1(1.8)	133.1(2.1)	128.1(2.0)	127.8(2.1)
$\text{C}_5\text{C}_6\text{C}_7$	125.5(1.8)	126.7(1.7)	128.8(1.8)	129.3(1.8)
$\text{C}_6\text{C}_7\text{C}_1$	131.4(1.5)	124.6(1.8)	129.6(1.6)	127.2(1.6)
$\text{O}_1\text{C}_1\text{C}_7$	116.5(1.4)	111.4(1.3)	114.8(1.3)	111.5(1.5)
$\text{C}_2\text{C}_7\text{C}_2$	112.4(1.4)	113.9(1.7)	111.0(1.5)	113.9(1.5)
$\text{O}_1\text{C}_1\text{C}_2$	117.3(1.6)	117.3(1.7)	119.9(1.4)	120.1(1.6)
$\text{O}_2\text{C}_7\text{C}_6$	116.1(1.5)	121.5(1.5)	119.4(1.6)	118.8(1.6)

Table 9a

Atomic displacements from the least-squares planes* relevant to discussion of structure in the acid dimer of tetrakispropolonato scandium.

Equations of the L-S planes

		** χ^2
P	$0.3288X - 0.2320Y - 0.9155Z - 1.2880 = 0$	3.2
Q	$0.6391X + 0.7686Y - 0.0286Z + 0.2568 = 0$	133.7
R	$0.5973X - 0.2335Y - 0.7673Z - 1.5874 = 0$	32.9
S	$-0.7502X - 0.6265Y - 0.2115Z + 0.4834 = 0$	60.3

Displacements (Å)

Ligand 1	2	3	4
L-S plane P	Q	R	S
O ₁ -0.023	O ₃ -0.078	O ₅ 0.040	O ₇ -0.030
O ₂ 0.022	O ₄ 0.111	O ₆ 0.006	O ₈ 0.085
1C ₁ 0	2C ₁ -0.028	3C ₁ 0.012	4C ₁ -0.014
1C ₂ -0.004	2C ₂ -0.011	3C ₂ -0.022	4C ₂ -0.012
1C ₃ 0.003	2C ₃ 0.028	3C ₃ 0	4C ₃ 0.018
1C ₄ 0	2C ₄ 0.020	3C ₄ 0.020	4C ₄ 0.021
1C ₅ 0.003	2C ₅ -0.035	3C ₅ -0.003	4C ₅ -0.028
1C ₆ -0.006	2C ₆ -0.014	3C ₆ -0.016	4C ₆ -0.012
1C ₇ 0.004	2C ₇ 0.039	3C ₇ 0.006	4C ₇ 0.028
Sc 0.217	Sc 0.152	Sc 0.415	Sc 0.193

* for footnotes, see next page
**

Table 9b

Atomic displacements from the least-squares planes* relevant to the discussion of structure in $(\text{NbT}_4)(\text{H}_3\text{OCl}_3)(\text{CH}_3\text{CN})$.

Equations of the L-S planes

P	0.296X - 0.952Y - 0.072Z + 2.163	χ^2 **	30.1
Q	-0.799X - 0.586Y - 0.131Z + 7.740		2.4
R	0.313X - 0.901Y - 0.299Z + 2.108		4.1
S	-0.894X - 0.336Y - 0.298Z + 7.93		6.5

Displacements (Å)

Ligand	1	2	3	4
L-S plane	P	Q	R	S
O_1	0.016	O_3 0.049	O_5 0.021	O_7 -0.056
O_2	0.016	O_4 -0.049	O_6 0.001	O_8 0.057
$1C_1$	0.048	$2C_1$ -0.005	$3C_1$ -0.015	$4C_1$ 0.008
$1C_2$	-0.033	$2C_2$ 0.005	$3C_2$ -0.001	$4C_2$ 0.014
$1C_3$	-0.027	$2C_3$ 0.012	$3C_3$ 0.012	$4C_3$ 0.017
$1C_4$	0.037	$2C_4$ -0.017	$3C_4$ -0.003	$4C_4$ 0.0214
$1C_5$	0.027	$2C_5$ -0.004	$3C_5$ -0.023	$4C_5$ -0.005
$1C_6$	-0.060	$2C_6$ 0.017	$3C_6$ 0.020	$4C_6$ 0.008
$1C_7$	0.005	$2C_7$ -0.010	$3C_7$ 0.008	$4C_7$ -0.015
Nb	0.218	Nb -0.212	Nb -0.131	Nb -0.099

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

The weights used in the calculation of L-S planes are given

$$\text{by } W_i = \frac{W_{i1}}{\sigma^2} = \frac{3}{\sigma^2(X_i) + \sigma^2(Y_i) + \sigma^2(Z_i)}$$

** χ^2 for a plane $lX + mY + nZ - p = 0$ for N atoms is given by

$$\sum_{i=1}^{i=N} (P_i^2 / \sigma^2(P_i)), \text{ where } \sigma^2(P_i) = l^2\sigma^2(X_i) + m^2\sigma^2(Y_i) + n^2\sigma^2(Z_i),$$

and P_i is the distance of atoms i from the plane.

4.3 The hydrogen bond in $(\text{HScT}_4)_2$

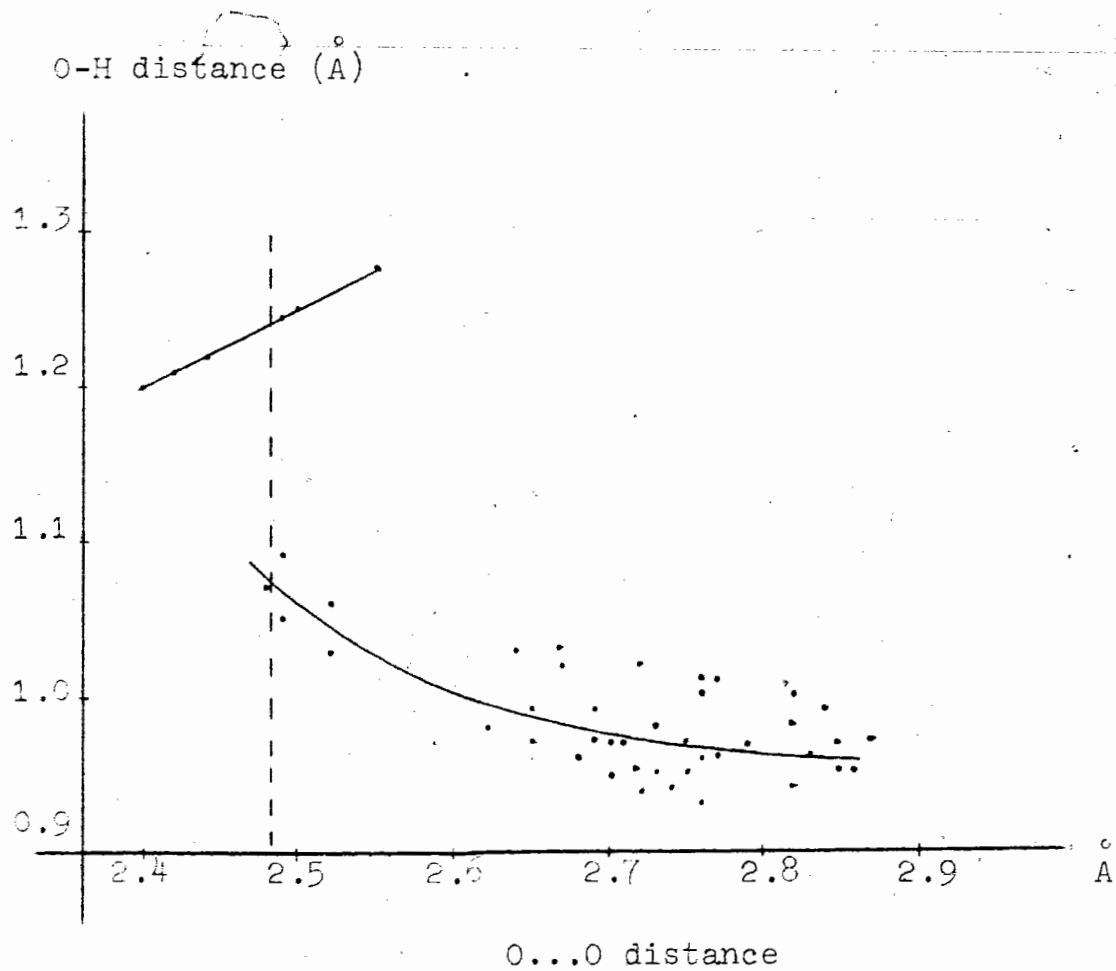
The effect of this bond on the associated tropolonato ligands and the Sc-O bond lengths has already been noted, and these results indicate clearly that this bond is not symmetrical.

Ibers and Hamilton²⁰ have published a graph relating O-H distance to O...O separation for hydrogen bonds based on neutron diffraction data. Their graph has two discontinuous curves - one for short O...O separations (2.38 - 2.55Å) where the proton is symmetrically placed - the other for O...O separations of 2.48 - 2.87Å where the proton is asymmetrically placed. The O...O separation in this bond is 2.484(4)Å and so falls in the region where there is overlap between both curves. While the O-H distance of 1.17(6)Å is within the limits of error of either the symmetric or asymmetric curves, the data from the tropolonato ligands indicate very strongly an asymmetric proton position. Ibers and Hamilton's curve is shown in Figure 6 (page 45). The O-H...O angle is 167(2)°.

Infra-red stretching frequencies as a function of distances in hydrogen bonded systems have been reviewed²¹, and for an O...O separation of 2.48Å, an O-H stretching frequency of 1975 cm^{-1} is predicted on the basis of other results. The infra-red spectrum of the $(\text{HScT}_4)_2$ acid dimer shows a small, broad band at 1976 cm^{-1} in agreement with this prediction.

Figure 6

O-H distance as a function of O...O distance as determined by neutron diffraction for a number of compounds containing O-H...O bonds. The curved line represents the best least squares fit to the points, but the deviations of some of the points are significant. Adapted from reference 20.



4.4 The $(\text{H}_3\text{OCl}_3)^{2-}$ anion

The arrangement of a flattened pyramidal hydroxonium ion (H_3O^+), triply bonded to three chlorine atoms at the vertices of the base of the pyramid ($\text{O}\dots\text{Cl} = 2.87(3)\text{\AA}$) has been found previously in the structures of hydrogen chloride monohydrate²² ($\text{O}\dots\text{Cl} = 2.95(1)\text{\AA}$) and caesium chloride.1/3 hydroxonium bichloride ($\text{O}\dots\text{Cl} = 2.92(2)\text{\AA}$)²³. It is interesting that the same type of disorder is proposed in all three structures, with equal probability that the oxygen will be above or below the plane formed by the three chlorine atoms. No evidence for the hydrogen atom positions in this anion was found from the data, which is not surprising in view of the occupancy numbers of 0.25 and 0.5 which would be assigned to them. Bond lengths and angles for this anion and for the acetonitrile molecule of crystallization are included in Table 10.

Table 10

Bond lengths and angles in the $(\text{H}_3\text{OCl}_3)^{2-}$ anion and in the CH_3CN molecule of crystallization in the crystal structure of the niobium complex.

Distances (\AA)	Angles ($^\circ$)
$\text{O}_9\text{-Cl}_1$ 2.84(3)	$\text{Cl}_1\text{O}_9\text{Cl}_2$ 119.8(0.9)
$\text{O}_9\text{-Cl}_2$ 2.88(2)	$\text{Cl}_2\text{O}_9\text{Cl}_2'$ 108.7(0.9)
$\text{Cl}_1\text{-Cl}_2$ 4.94(1)	C-NC_2 174(4)
$\text{Cl}_2\text{-Cl}_2'$ 4.67(1)	
$\text{O}_9\text{-O}_9'$ 1.11(2)	
$\text{C}_1\text{-C}_2$ 1.71(5)	
$\text{C}_1\text{-N}$ 2.80(3)	
$\text{C}_2\text{-N}$ 1.09(5)	

CONCLUSION

The structure of the acid dimer of tetrakis(tropolonato)-scandium chloride was published in Inorganic Chemistry, 13, 1880, (1974). This structure was determined simultaneously and independently by Anderson, Neuman and Melson, and was published as the following paper. The unit cell used in this determination is related to theirs by the transformation :

$$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

The results of the two crystal structures are the same within the limits of the combined errors. The main differences are (1) the alternation of bonds in the C₇ ring of ligand 2 (their ligand 4) is not so pronounced, and (2), the reduced thermal motion of the tropolonate ligands involved in the hydrogen bond is not so apparent from their rigid body analysis.

A paper describing this structure was presented at the 57th C.I.C. Conference, held in Regina in June, 1974.

The crystal structure of (NbT₄)₂(H₃OCl₃). (CH₃CN) is to be submitted for publication.

APPENDIX A.

THE INCIDENT BEAM MONOCHROMATOR

The use of crystal-monochromatized X-radiation has the great advantage over the use of filters in that background scattering due to non-characteristic radiation is virtually eliminated. By suitable choice of the monochromator crystal and X-radiation, the loss of intensity in the diffracted beam can be minimized. An incident beam monochromator, fitted with a graphite crystal, was used in the collection of diffraction data from the $(\text{NbTe}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})$ crystal, and since the crystal-monochromatized radiation is itself partially polarized, this must be included in the polarization correction to the intensity data. If $2\theta_m$ is the reflection angle for the beam incident to the graphite crystal, and 2θ is the reflection angle at the specimen, the expression for the polarization correction p (as derived originally by Azaroff²⁴) is :

$$p = (\cos^2 2\theta_m + \cos^2 2\theta) / (1 + \cos^2 2\theta_m).$$

The program used in this laboratory to apply Lorentz and polarization corrections to 'raw' intensity data was modified by me so that the correction necessary for either monochromatized or filtered radiation can be used.

The polarization effect arises because the efficiency with which an X-ray beam is reflected by a plane in a crystal is dependent on the electron density in the plane, and on the reflection angle. The waves of the non-polarized beam can be resolved into components parallel and perpendicular to the reflection plane; the reflection of the parallel component depends only on the electron density, but the reflection of

the perpendicular component depends on the electron density in the plane and on $\cos^2 2\theta$, the intensity of this component decreasing to zero as $2\theta \rightarrow 90^\circ$.

APPENDIX B : STRUCTURE FACTOR TABLES (X10) FOR (HSC_{T1})₂.

L	FL	FC	L	FL	FC	L	FL	FC	L	FL	FC
H=	0, K=	0	0	6*	-42	0	295	-306	0	63	42
1	1003	944	H=	0, K=	4	1	357	-368	H=	1, K=	12
2	343	346	0	224	214	2	69	-59	2	134	142
3	197	194	1	52	69	3	51	30	1	106	122
4	175	-167	2	162	156	4	166	-160	0	85	78
5	57	-34	3	9	4	5	13*	-5	H=	1, K=	11
6	11*	12	4	223	222	6	127	-125	0	57	66
7	26	230	5	135	139	H=	0, K=	9	1	58*	73
8	101	-105	6	72	71	6	77	-87	2	60	44
9	109	-115	7	67	48	7	94	105	3	76	71
10	63	-27	8	144	166	4	13*	-17	H=	1, K=	10
H=	0, K=	1	9	14	34	3	121	-132	4	75	53
10	14*	-22	H=	0, K=	5	2	104	-92	3	42*	47
9	13*	-46	8	43*	-9	1	133	-142	2	40*	32
8	37*	-31	7	120	94	0	257	-261	1	129	139
7	71	74	6	83	92	H=	0, K=	10	0	53*	-27
6	1*	-33	5	243	252	0	12*	22	H=	1, K=	9
5	102	-93	4	144	143	1	12*	16	0	50*	-41
4	532	-521	3	192	207	2	110	-99	1	36*	-27
3	287	282	2	355	357	3	13*	-7	2	38*	-47
2	473	464	1	70	95	4	13*	9	3	125	-121
1	83	85	0	3*	18	5	44*	18	4	92	-79
0	617	566	H=	0, K=	6	H=	0, K=	11	5	61	-43
0	138	-131	0	531	580	4	77	-82	H=	1, K=	8
1	18*	-8	1	391	396	3	128	-114	6	107	-114
2	255	236	2	224	220	2	101	94	5	249	-260
3	24*	-33	3	119	133	1	13*	29	4	147	-169
4	110	-103	4	11	-27	0	142	144	3	91	-68
5	31*	-50	5	81	82	H=	0, K=	12	2	71	71
6	36*	-356	6	57	-71	0	110	103	1	11*	-5
7	38*	58	7	42	-14	1	42*	28	0	128	-125
8	12*	-24	8	41	-8	2	62	50	H=	1, K=	7
9	43*	32	H=	0, K=	7	3	78	74	0	213	207
H=	0, K=	3	7	14*	-19	H=	0, K=	13	1	153	153
9	157	154	6	91	-102	1	45*	-6	2	177	183
8	222	216	5	171	-189	0	14*	43	3	70	55
7	12*	-6	4	130	-186	H=	1, K=	13	4	112	122
6	143	-134	3	11	-33	0	14*	43	5	97	-105
5	95	-32	2	10	-9	H=	1, K=	13	6	59	-53
4	122	-127	1	53	-56	0	14*	43	0	213	207
3	50	47	0	186	180	1	45*	-6	1	153	153
2	135	173	H=	0, K=	8	2	62	50	2	177	183
1	224	212	7	14*	-19	3	78	74	3	70	55

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	2, K=	10	1	65	36	4	84	-103	7	125	121
			0	81	66	5	105	107	8	14	27
0	96	-91				6	80	-30			
1	13*	42	H=	3, K=	7	7	86	-76	H=	4, K=	1
2	13*	-27				8	46*	-50			
3	114	-103	0	34*	23				8	14*	49
4	45*	30	1	141	146	H=	3, K=	2	7	74	111
			2	152	157				6	224	217
H=	2, K=	11	3	209	298	8	77	-56	5	110	111
			4	123	147	7	42*	-60	4	193	200
3	91	82	5	14	22	5	55	-14	3	109	120
2	62	-40	5	65	39	5	36*	32	2	50	65
1	153	-140				4	47*	-47	1	128	114
0	191	-195	H=	3, K=	6	3	269	274	0	25	4
						2	122	130			
H=	2, K=	12	6	44*	70	1	137	153	H=	4, K=	2
			5	93	89	0	392	396			
0	14*	-10	4	78	95				0	150	151
1	14*	-5	3	117	124	H=	3, K=	1	1	377	378
			2	35	55				2	125	144
H=	3, K=	12	1	100	-98	0	259	263	3	302	313
			0	10	-27	1	162	157	4	276	285
0	78	-65				2	257	258	5	156	153
			H=	3, K=	5	3	369	384	6	41	4
H=	3, K=	11				4	347	357	7	14*	43
			0	30*	-11	5	234	228			
0	201	-205	1	31*	-50	6	38*	20	H=	4, K=	3
1	76	-101	2	57	-53	7	41*	-4			
2	144	-121	3	145	-141	8	14*	4	7	63	55
			4	154	-178				6	59	-26
H=	3, K=	10	5	89	-78	H=	3, K=	0	5	55	-30
			6	60*	103				4	73	61
3	63*	-77	7	14*	-24	3	96	80	3	200	200
2	137	-109				7	150	147	2	192	198
1	138	-125	H=	3, K=	4	6	313	306	1	281	281
0	107	-113				5	181	174	0	213	214
			7	44*	-50	4	496	499			
H=	3, K=	9	6	92	67	3	153	154	H=	4, K=	4
			5	32*	-29	2	8*	-8			
0	60	67	4	152	-150	1	141	-152	0	42*	-10
1	131	123	3	123	-149	0	542	-541	1	76	73
2	13*	-5	2	171	-177				2	47*	33
3	18*	15	1	27*	-15	H=	4, K=	0	3	141	-138
4	39	-108	0	160	182				4	146	-143
						0	508	-507	5	57	64
H=	3, K=	8	H=	3, K=	3	1	34	-336	6	114	-121
						2	371	-380			
5	45*	-49				3	31*	-22	H=	4, K=	5
4	14*	3	1	274	267	4	221	227			
3	41*	58	2	275	255	5	125	130	6	14*	-56
2	74	73	3	10*	2	6	12*	36	5	13	15

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
4	79	-53				0	106	97	H=	5, K=	0
3	152	-148	1	45	14				0	211	-228
2	297	-299	2	98	102	H=	5, K=	3	1	303	297
1	57	-74				0	136	131	2	156	162
0	175	-181	H=	5, K=	9	1	166	169	3	133	-123
H=	4, K=	6	0	42	48	2	204	208	4	38	-29
0	279	-196	1	14	20	3	145	152	5	107	-135
1	204	-210	2	77	77	4	77	60	6	156	-161
2	73	-70	H=	5, K=	8	5	13	29			
3	55	63				5	44	26	H=	5, K=	1
4	55	6	3	63	30	H=	5, K=	2	6	76	-81
5	130	115	2	43	26				5	230	-228
H=	4, K=	7	1	13	-11	7	46	23	4	102	112
0	45	21	0	56	-67	6	14	23	3	11	-39
4	6	-83	H=	5, K=	7	5	41	42	2	59	-50
3	57	52				4	12	9	1	208	-206
2	67	61	0	12	-43	H=	5, K=	3	H=	5, K=	2
1	37	51	1	12	47				0	181	-198
0	5	-45	2	13	20	2	167	208	0	197	-198
H=	4, K=	3	3	43	-80	H=	5, K=	2	1	172	-171
0	53	45	4	40	-40				2	70	75
1	146	142	H=	5, K=	5	2	176	-178	3	12	21
2	146	152				1	249	-232	4	13	12
3	104	78	5	14	23	0	50	-15	5	60	66
4	89	59	4	61	14	H=	5, K=	1	6	127	133
H=	4, K=	9	3	41	-50				H=	5, K=	3
0	53	13	2	55	-29	H=	5, K=	1	0	381	-375
1	12	-31	1	117	-127				1	472	-472
2	40	-8	0	94	-95	2	256	-250	2	274	259
H=	4, K=	11	H=	5, K=	5	3	144	-146	3	231	247
0	53	13				4	12	-26	2	89	84
1	12	-31	0	220	-233	5	39	6	1	77	74
2	40	-8	1	291	-283	6	13	-24	0	57	48
H=	4, K=	10	2	240	-249	7	14	-5	H=	5, K=	4
0	53	13	3	117	-143	H=	5, K=	0	0	191	188
1	12	-31	4	171	39				1	62	-60
2	40	-8	5	1	-20	H=	5, K=	0	2	93	71
H=	4, K=	11	H=	5, K=	4	7	14	-30	3	144	164
0	53	13				6	188	-181	4	127	113
1	12	-31	6	119	-114	5	54	-28	5	89	79
2	40	-8	5	60	-42	4	128	-129	H=	5, K=	5
H=	4, K=	10	4	59	55	3	57	12	0	283	-281
0	53	13	3	12	-7	2	141	-154	4	14	26
1	43	-57	2	137	130	1	223	-234			
2	40	-8	1	49	78	0	283	-281			
H=	5, K=	10									

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	6, K=	5	H=	7, K=	5	H=	8, K=	0			
3	13*	7	0	55	-30	0	93	-78	0	62	52
2	12*	-29	1	49*	40	1	12*	7	H=	9, K=	6
1	105	-98	2	110	115	2	102	99			
0	51*	-69	3	44*	52	3	13*	26	0	14*	49
H=	6, K=	6	H=	7, K=	4	4	113	-127	H=	9, K=	5
0	65	-60	4	134	147	5	14*	0			
1	12*	13	3	42*	63	H=	8, K=	1	0	43*	-40
2	71	-60	2	57	36	4	145	-147	1	45*	11
3	43*	-69	1	102	-104	3	155	-164	H=	9, K=	4
4	14*	7	0	52*	-26	2	136	-122			
H=	6, K=	7	H=	7, K=	3	1	140	148	2	64	-15
3	126	-115	0	162	-168	0	11*	-16	1	14*	-16
2	160	-172	1	155	-158	H=	8, K=	2	0	84	-106
1	213	-221	2	39*	-41				H=	9, K=	3
0	112	-119	3	82	90	0	82	-86	0	57	48
H=	6, K=	8	4	114	114	1	203	-213	1	42*	-51
			H=	7, K=	2	2	228	-239	2	96	-83
1	131	-140	5	39	-72	3	112	-120	H=	9, K=	2
1	114	-114	4	50	31	4	109	-136			
2	115	-119	3	93	-123	H=	8, K=	3	3	216	-213
H=	6, K=	9	2	131	-130	3	14*	-36	2	74	-100
1	14*	30	1	179	-182	2	203	-180	1	13*	11
0	41*	44	0	269	-271	1	119	-102	0	39*	62
H=	7, K=	8	H=	7, K=	1	0	126	-121	H=	9, K=	1
						H=	8, K=	4			
1	75	-73	0	113	-118	0	152	-156	0	77	86
0	75	-54	1	110	100	1	58	-30	1	59	48
H=	7, K=	7	2	113	122	2	14*	-14	2	13*	23
0			3	110	-96	3	45*	47	3	62	-64
1	13*	17	4	101	-115	H=	8, K=	5	H=	9, K=	0
1	43*	-75	5	44*	-82						
2	101	-118	H=	7, K=	0	2	99	119	4	45*	80
						1	73	52	3	106	96
H=	7, K=	6	6	14*	-6	0	58*	26	2	116	120
			5	74	75	H=	8, K=	6	1	239	238
3	45*	-17	4	57	-24				0	164	160
2	51	-34	3	103	102	H=	9, K=	7	H=	10, K=	0
1	33	70	2	156	153						
0	4*	75	1	122	142	0	95	87	0	242	242
			0	165	160	1	116	106	1	73	34
						H=	8, K=	7	2	62	30

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
			3	45	57	H= -13, K= 7	6	95	-116		
H= 1, K= 1			2	14	7		7	43	-17		
						5	46	33			
2	45	54	H= -13, K= 2			5	14	18	8	14	14
1	105	101				4	14	-6	9	46	19
0	170	182	2	14	6	3	14	-6	H= -12, K= 4		
			3	62	95						
H= 1, K= 2			4	62	52	H= -12, K= 9			9	14	-60
			5	131	125				9	98	-100
0	146	132	6	75	82	2	78	82	7	204	-201
1	14	69	7	75	36	3	64	53	6	13	-30
			8	14	14	4	45	28	5	125	-132
H= 1, K= 3						5	45	6	4	59	-91
			H= -13, K= 3						3	111	-106
1	14	3				H= -12, K= 6			2	42	-10
0	61	72	8	78	-68				1	61	65
			7	33	-84	5	100	102			
H= 1, K= 4			6	62	-77	5	147	146	H= -12, K= 3		
			5	87	-73	4	170	197			
0	44	-33	4	14	-16	3	108	127	1	14	31
			3	44	61	2	126	127	2	112	98
H= 11, K= 2			2	45	30	1	14	28	3	204	191
									4	58	35
0	14	49	H= -13, K= 4			H= -12, K= 7			5	58	45
									6	59	64
H= 11, K= 1			2	53	-12	1	63	-60	7	13	-50
			3	130	-141	2	62	-14	8	106	-92
0	132	142	4	76	-87	3	14	-15	9	14	-39
1	64	7	5	37	-98	4	14	15			
			6	14	-54	5	61	49	H= -12, K= 2		
H= 11, K= 0			7	77	-71	6	124	167			
			8	14	-20	7	59	68	9	177	196
1	45	-18							8	43	58
0	1	14	H= -13, K= 5			H= -12, K= 6			7	60	-41
									6	72	55
H= -13, K= 0			7	157	158	1	78	55	5	101	82
			6	44	-1	7	44	-3	4	234	226
3	45	22	5	14	-29	6	14	47	3	156	159
4	14	11	4	14	-14	5	141	-137	2	60	38
5	62	58	3	63	-39	4	42	-17	1	62	77
6	85	104	2	14	-77	3	60	43			
7	125	119				2	143	-126	H= -12, K= 1		
8	45	54	H= -13, K= 6			1	14	-38			
									1	62	-27
H= -13, K= 1			2	45	-25	H= -12, K= 5			2	96	72
			3	45	34				3	13	-53
2	14	-9	4	14	44	1	43	53	4	59	-48
7	3	7	5	53	55	2	154	-179	5	59	-43
6	12	137	6	152	138	3	163	-158	6	42	65
5	62	36	7	102	82	4	132	-139	7	13	47
4	14	32				5	178	-168	8	136	118

L	F	FC	L	F	FC	L	F	FC	L	F	FC	
H= -12, K= 1			4	13	39	5	115	-116	4	45*	18	
			9	36	109	5	72	-72	5	45*	-22	
	9	193	210	10	77	63	7	60*	70			
H= -12, K= 0			H= -11, K= 3			8	14*	-34	H= -10, K= 10			
						9	14*	-11				
9	14*	-5	4	53*	3	H= -11, K= 7			6	63*	-93	
3	137	150							5	14*	61	
7	43*	57	H= -11, K= 3			3	77	73	4	61*	47	
6	13*	42				7	61*	42	3	61*	81	
5	73	-55	10	110	-93	6	84	101	2	74	53	
4	73	-50	9	51	-17	5	137	5	1	162	153	
3	95	-107	8	13*	-5	4	82	-66	H= -10, K= 9			
2	14*	-46	7	121	-123	3	41*	-46				
1	4*	-28	6	195	-98	2	199	-202	1	126	118	
			5	96	95	1	193	-204	2	171	175	
H= -11, K= 0			3	55*	55				3	72	64	
			2	105	106	H= -11, K= 8			4	13*	-63	
1	42*	31	1	70	.58				5	60*	43	
2	91	-80				1	61	-30	6	14*	54	
3	219	-222	H= -11, K= 4			2	73	103	7	14*	71	
4	199	-215				3	140	155				
5	153	-157	1	13*	-8	4	152	162	H= -10, K= 8			
6	199	-190	2	133	177	5	165	163				
7	81	-176	3	39*	21	6	14*	45	8	14*	39	
8	102	107	4	39	-46	7	14*	26	7	97	122	
9	14*	1	5	134	-108	3	46*	14	6	73	56	
10	14*	37	6	149	-150				5	101	105	
			7	245	-243	H= -11, K= 9			4	70	-103	
H= -11, K= 1			8	157	-160				3	13*	15	
			9	87	-88	7	14*	4	2	57*	16	
10	133	142	10	91	-93	6	14*	68	1	200	-210	
9	14*	-13				5	44*	49				
8	124	105	H= -11, K= 5			4	43*	25	H= -10, K= 7			
7	4*	10				3	51*	73				
6	181	-175	9	93	-93	2	87	83	1	355	-357	
5	111	-104	8	166	-163	1	152	142	1	355	-357	
4	12*	-22	7	133	-133				2	294	-288	
3	10*	-91	6	145	-136	H= -11, K= 10			3	55*	-62	
2	175	-175	5	57	37				4	88	-72	
1	5*	-65	4	14*	6	1	135	137	5	13*	-64	
			3	93	-93	2	14*	53	6	58*	-8	
H= -11, K= 2			2	4*	70	3	44*	-69	7	59*	-32	
			1	13*	22	4	100	-119	8	14*	-17	
1	50*	-21				5	14*	-7	9	45*	34	
2	12*	129	H= -11, K= 6									
3	111	104				H= -10, K= 11			H= -10, K= 6			
4	12*	24	1	59	15							
5	37*	-13	2	141	-131	1	45*	4	9	14*	-12	
6	12*	17	3	90	-86	2	44*	-8	8	112	-113	
7	4*	-28	4	101	-157	3	63	26	7	159	-178	

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
6	300	-296	8	13	22				9	58*	68
5	12*	-7	7	225	229	11	63	-26	10	43*	-15
4	163	-163	6	24	74	10	13*	-2			
3	143	-140	5	52	51	9	13*	-13	H=	-9, K=	5
2	122	-106	4	63	54	8	54*	72			
1	55*	34	3	104	94	7	64*	-99	10	89	-90
			2	65	67	5	94	-103	9	103	-77
H=	-10, K=	5				5	120	-136	8	40*	21
			H=	-10, K=	1	4	103	-98	7	12*	-9
1	55*	61				3	182	-182	6	12*	-14
2	294	202	1	247	-240	2	35*	-21	5	11*	-4
3	75	74	2	206	-190	1	72	-69	4	239*	241
4	12*	42	3	12*	-18				3	150	155
5	12*	36	4	12*	-12	H=	-9, K=	2	2	391	399
6	34*	-41	5	93	-115				1	321	322
7	155	-150	5	105	-122	1	233	-220			
8	59*	-48	7	12*	-17	2	147	-153	H=	-9, K=	6
9	86	-95	8	47*	-34	3	48*	52			
10	45*	-58	9	71	-55	4	128	144	1	152	166
			10	95	74	5	35*	-42	2	11*	22
H=	-10, K=	4	11	78	99	6	62	37	3	81	81
						7	209	215	4	219	227
1	77	-65	H=	-10, K=	0	8	12*	-23	5	12*	60
9	13*	-46				9	40*	25	6	233	-250
8	153	163	11	14*	28	10	164	178	7	168	-174
7	12*	18	10	61*	69	11	89	90	8	58*	-83
5	12*	-23	9	13*	33				9	61	-27
5	159	148	8	113	-97	H=	-9, K=	3	10	91	74
4	52*	64	7	164	-161						
3	215	216	6	251	-269	11	14*	39	H=	-9, K=	7
2	113	116	5	182	-181	10	128	133			
1	103	96	4	74	-75	9	173	158	9	44*	10
			3	65	-54	8	12*	-14	8	13*	-41
H=	-10, K=	3	2	55	-31	7	197	192	7	173	-161
			1	55*	64	5	130	126	6	136	-139
1	293	306				5	35*	-39	5	171	-178
2	23*	249	H=	-9, K=	0	4	69	64	4	12*	42
3	33*	357				3	11*	41	3	53*	-63
4	155	138	1	81	83	2	125	131	2	230	-233
5	153	158	2	153	151	1	11*	-4	1	12*	-45
6	12*	20	3	217	213						
7	37*	45	4	51	-58	H=	-9, K=	4	H=	-9, K=	8
8	127	132	5	70	33						
9	126	116	6	95	-103	1	115	115	1	78	-69
10	62*	50	7	157	-159	2	61	55	2	67	37
			8	153	-177	3	67	67	3	109	-95
H=	-10, K=	2	9	90	-81	4	11*	-13	4	110	-125
			10	59*	23	5	61	18	5	158	-171
11	64*	64	11	63*	-69	6	36*	43	6	13*	28
10	115	97				7	211	215	7	60*	-14
9	51*	12	H=	-9, K=	1	8	142	157	8	14*	46

L	FJ	FC	L	FJ	FC	L	FJ	FC	L	FJ	FC
H= -9, K= 9						9	107	-105	8	12*	-36
			1	155	155				9	113	106
8	14*	7	2	161	180	H= -8, K= 6			10	103	115
7	75	74	3	173	161				11	14*	33
6	9*	108	4	209	210	10	100	-103			
5	135	135	5	157	150	9	104	-69	H= -8, K= 2		
4	99	94	6	14*	65	8	141	-138			
3	13*	5				7	39*	4	11	44*	4
2	14*	150	H= -8, K= 10			6	98	-95	10	13*	-55
1	57	22				5	36*	-45	9	12*	-21
			7	43*	-7	4	14*	-141	8	53*	52
H= -9, K= 10			6	177	167	3	34*	54	7	171	-170
			5	177	179	2	271	269	6	177	-178
1	59*	13	4	203	216	1	35*	13	5	235	-238
2	101	108	3	13*	11				4	157	-160
3	143	148	2	23	76	H= -5, K= 5			3	163	-163
4	172	159	1	13*	25				2	208	-205
5	104	87				1	11*	26	1	233	-236
6	14*	25	H= -8, K= 9			2	146	151			
7	14*	-44				3	88	78	H= -8, K= 1		
			1	265	-272	4	251	252			
H= -9, K= 11			2	77	-36	5	35*	46	1	88	-85
			3	39*	-20	6	51*	42	2	65	-62
6	91	-76	4	78	83	7	38*	39	3	298	-294
5	4*	59	5	163	169	8	12*	-25	4	318	-323
4	107	111	6	41*	77	9	42*	-40	5	334	-338
3	1*	52	7	14*	14	10	14*	-12	6	198	-205
2	96	103	8	63	-20				7	296	-295
1	114	102				H= -8, K= 4			8	111	-100
			H= -8, K= 3						9	124	-142
H= -9, K= 12						11	14*	2	10	155	-171
			9	64	35	10	14*	13	11	44*	-38
1	63	41	8	14*	-12	9	150	152			
2	14*	23	7	72	-60	8	96	57	H= -8, K= 0		
3	45*	7	6	132	-129	7	12*	-15			
4	45*	33	5	258	-281	6	211	214	11	44*	-55
			4	12*	9	5	68	55	10	202	-219
H= -8, K= 13			3	64	-55	4	104	-117	9	103	-119
			2	64	-44	3	10*	41	8	170	-164
1	6*	-39	1	37*	-36	2	167	160	7	94	-105
2	1*	-11				1	33*	-16	6	11*	-30
			H= -8, K= 7						5	136	134
H= -8, K= 12						H= -8, K= 3			4	10*	9
			1	162	195				3	10*	-10
5	91	68	2	155	137	1	209	-201	2	150	149
4	141	134	3	94	99	2	79	-77	1	207	203
3	63*	62	4	11*	26	3	56	-35			
2	43*	75	5	196	-191	4	183	-193	H= -7, K= 0		
1	43*	64	6	438	-447	5	262	-259			
			7	174	-158	6	91	113	1	266	277
H= -8, K= 11			8	172	-171	7	108	109	2	128	124

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
3	24*	246				1	312	318			
4	417	419	H= -7, K= 4						H= -7, K= 13		
5	293	298				H= -7, K= 8					
6	223	222	1	274	-281				3	14*	36
7	102	117	2	219	-229	1	71	-51	2	63	41
8	143	-132	3	13*	46	2	159	-167	1	89	82
9	94	-80	4	44*	-51	3	95	86			
10	191	-204	5	13*	41	4	37*	-11	H= -5, K= 13		
11	14*	-33	6	199	188	5	262	-266			
			7	72	-64	6	124	-121	1	108	133
H= -7, K= 1			8	152	-160	7	71	-79	2	44*	49
			9	57*	47	8	114	-85	3	14*	54
11	75	-61	10	74	36	9	45*	-28			
12	142	-134	11	14*	46				H= -5, K= 12		
4	185	-179				H= -7, K= 9					
8	192	-191	H= -7, K= 5						5	162	162
7	137	-135				3	14*	-3	4	158	164
5	32*	-33	10	14*	80	7	43*	-26	3	210	200
5	164	165	9	124	130	5	82*	-70	2	126	109
4	115	122	8	55*	51	5	39*	-75	1	126	105
3	7*	19	7	155	-174	4	94	-92			
2	143	158	6	139	191	3	12*	31	H= -5, K= 11		
1	167	170	5	204	213	2	166	-170			
			4	11*	14	1	310	-306	1	59	-74
H= -7, K= 2			3	213	211				2	139	-134
			2	31*	-41	H= -7, K= 10			3	13	-26
			1	45*	30				4	93	83
1	297	301				1	288	-297	5	43*	62
2	18	169				2	258	-256	6	14*	71
3	229	-221	H= -7, K= 6			3	12*	-44			
4	121	-128				4	57*	20	H= -6, K= 10		
5	297	-308	1	159	179	5	137	149			
6	154	-154	2	254	293	6	74	64	7	44*	-5
7	11*	-32	3	240	246	7	14*	36	6	74	-66
8	12*	30	4	257	252				5	116	-117
9	39*	9	5	35	105	H= -7, K= 11			4	206	-219
10	12*	-125	6	233	248				3	67	-69
11	14*	12	7	54*	79	5	53*	85	2	126	-132
			8	13*	35	6	106	105	1	278	-297
H= -7, K= 3			9	13*	-65	4	60	34			
			10	110	-122	3	52*	15	H= -5, K= 9		
11	1*	-4				2	82	-111			
12	42*	-4	H= -7, K= 7			1	13*	-21	1	120	-118
7	8*	106							2	177	-161
6	53*	65	9	124	-126	H= -7, K= 12			3	37*	-38
5	141	133	8	132	-91				4	85	-83
4	147	-157	7	55*	-28				5	290	-290
3	191	-209	6	110	-131	1	13*	51			
2	253	-258	5	36	-89	2	14*	-7	H= -9, K= 9		
1	153	-154	4	51*	-61	3	61*	57			
			3	297	286	4	62*	56			
			2	156	175	5	78	57	6	60	108

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= -5, K= 9			8	232	232	4	195	201	H= -5, K= 2		
7	43*	-40	9	159	174	5	392	393			
8	63	-17	10	93	136	6	44*	31	1	8*	19
H= -6, K= 8			H= -6, K= 4			7	82	-56	2	8*	28
9	101	-117	11	45*	31	8	11*	11	3	276	291
8	96	-108	10	123	110	9	163	-138	4	429	429
7	115	-127	9	13	-43	10	71	27	5	111	116
6	12*	23	8	135	-135	11	97	-85	6	10*	-24
5	12*	7	7	137	87	H= -6, K= 0			7	125	-128
4	51*	21	6	81	100	11	14*	-5	8	36*	-33
3	7	51	5	160	152	10	13*	38	9	150	-171
2	77	-59	4	9*	-39	9	131	133	10	58*	-45
1	225	207	3	9*	-29	8	100	114	11	14*	5
H= -6, K= 7			2	164	-166	7	176	175	H= -5, K= 3		
1	224	217	1	410	-417	6	347	362			
2	143	146	H= -6, K= 3			5	543	532	11	64	51
3	12	111	1	298	293	4	359	370	10	94	-79
4	84	-74	2	301	-299	3	315	320	9	201	-222
5	107	96	4	50	-57	2	28*	10	8	279	-282
6	106	107	3	249	-251	1	40*	-45	7	208	-215
7	12*	4*	5	10*	17	H= -5, K= 0			6	191	201
8	43*	-3*	6	123	-123	1	421	-418	5	132	133
9	124	-117	7	210	202	2	56	-53	4	68	55
H= -6, K= 6			8	97	96	3	84	-89	3	197	-194
10	45*	-10	9	244	-211	4	132	133	2	425	-409
9	43*	57	10	13*	-27	5	49*	-64	1	92	-83
8	227	213	11	45*	18	6	96	-82	H= -5, K= 4		
7	10*	114	H= -6, K= 2			7	103	105			
6	95	110	1	298	293	8	94	95	1	390	-363
5	29*	296	2	301	-299	9	280	276	2	799	-796
4	257	279	4	50	-57	10	99	100	3	500	-510
3	16*	186	3	249	-251	11	73	64	4	271	-275
2	312	315	5	10*	17	H= -5, K= 1			5	223	-226
1	91	95	6	123	-123	1	421	-418	6	205	-204
H= -5, K= 5			7	210	202	2	56	-53	7	105	-80
1	73	-96	8	97	96	3	84	-89	8	136	-126
2	73	95	9	244	-211	4	132	133	9	209	-215
3	43*	70	10	13*	-27	5	49*	-64	10	43*	-51
4	1*	-6	11	45*	18	6	96	-82	H= -5, K= 5		
5	390	393	H= -6, K= 1			7	103	105			
6	160	160	1	298	293	8	94	95	1	14*	-54
7	60	53	2	301	-299	9	280	276	9	58	6
			4	50	-57	10	99	100	8	39*	64
			3	249	-251	11	73	64	7	39	88
			5	10*	17	H= -5, K= 1			6	226	227
			6	123	-123	1	76	-79	5	169	-171
			7	210	202	1	115	-114	4	235	-231
			8	97	96	1	12*	31	3	161	-178
			9	244	-211	2	11*	-4			
			10	13*	-27	3	33*	-8			
			11	45*	18	4	30*	14			
			H= -6, K= 2			5	344	338			
			1	298	293	6	167	168			
			2	301	-299	7	363	361			
			4	50	-57	8	253	259			
			3	249	-251	9	150	-136			
			5	10*	17	1	150	-136			
			6	123	-123						
			7	210	202						
			8	97	96						
			9	244	-211						
			10	13*	-27						
			11	45*	18						



L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC	
2	393	-391	H= -5, K= 10	H= -4, K= 11	9	77	106					
1	55	-551										
H= -5, K= 6			1	74	-84	1	134	-137	H= -4, K= 6			
			2	105	105	2	12	-20				
1	53	53	3	12	-13	3	98	-91	9	74	71	
2	335	330	4	256	-261	4	251	-252	8	40	16	
3	7	74	5	129	-134	5	86	-92	7	84	92	
4	6	59	6	74	-63	6	100	-108	6	281	276	
5	154	149	7	14	-15				5	74	78	
6	38	28	H= -5, K= 11	H= -4, K= 10	4	122	-118	4	122	-118		
7	53	14			3	267	-264	3	267	-264		
8	231	229	6	14	58	7	100	-105	2	144	-148	
9	80	72	5	61	-2	6	135	-136	1	40	-47	
10	48	-50	4	13	-21	5	108	-117				
H= -5, K= 7			3	77	-91	4	215	-209	H= -4, K= 5			
			2	55	-25	3	156	-179				
9	14	16	1	244	-245	2	91	-100	1	618	-621	
8	72	61	H= -5, K= 12	H= -4, K= 9	1	103	-110	2	357	-357		
7	111	113						3	181	-173		
6	6	57	1	53	7	1	161	179	4	129	-132	
5	269	286	2	117	115	2	70	69	5	233	-230	
4	168	163	3	121	121	3	11	-22	6	68	62	
3	134	-141	4	123	126	4	162	161	7	202	211	
2	125	139	5	43	33	5	67	52	8	110	-93	
1	77	-86	H= -5, K= 13	H= -4, K= 8	6	13	-26	9	72	56		
H= -5, K= 8					7	60	-44	10	63	14		
			3	89	82	3	64	-92	H= -4, K= 4			
1	172	174	2	3	35				10	14	-43	
2	34	-7	1	14	-9	H= -4, K= 6				9	57	-56
3	11	17							8	229	-219	
4	11	-12	H= -4, K= 14			3	87	70	7	61	68	
5	262	261				7	201	194	6	329	-324	
6	12	47	1	48	-13	5	55	60	5	216	-212	
7	9	64	H= -4, K= 13			5	64	70	4	173	-193	
8	4	-6				4	70	64	3	341	-336	
9	6	-55	1	176	-94	3	11	-16	2	492	-486	
H= -5, K= 9			2	14	-55	2	33	-38	1	174	-178	
			3	45	-2	1	137	140				
4	53	-74	H= -4, K= 12	H= -4, K= 7				H= -4, K= 3				
7	13	-43			1	30	-21	1	218	-202		
5	13	12			2	150	-144	2	245	251		
5	70	-59	5	45	-9	3	300	-316	3	109	-104	
4	37	11	4	14	-40	4	199	199	4	792	777	
3	11	-1	3	13	-16	5	35	36	5	395	406	
2	18	191	2	59	37	6	37	15	6	95	-95	
1	111	114	1	53	-34	7	176	176	7	181	-194	
						8	167	166	8	363	-384	
									9	149	-166	

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= -4, K= 3			3	175	158	H= -3, K= 4					
			4	132	-164				1	10*	32
10	181	-137	5	54	36	1	7*	16	2	131	-127
11	45*	-64	6	0*	5	2	211	212	3	59	-11
			7	33*	-42	3	266	259	4	87	94
H= -4, K= 2			8	11*	22	4	49	49	5	53*	56
			9	66	59	5	91	-29	6	68	39
11	89	-95	10*	72	78	6	276	-266	7	167	173
10	7*	-85	11	53	23	7	129	-130	8	88	86
9	11	-109				8	54*	20			
3	91*	-45	H= -3, K= 1			9	13*	55	H= -3, K= 9		
7	125	116				10	14*	33			
6	215	229	11	99	59				7	14*	41
5	200	278	12	102	89	H= -3, K= 5			6	83	68
4	73	68	9	236	235				5	56*	37
3	34*	-10	8	51*	-43	10	14*	53	4	113	126
2	23*	10	7	174	152	9	60*	-42	3	114	123
1	492	-473	6	116	-120	8	97	-84	2	35*	49
			5	112	-103	7	12*	-24	1	326	328
H= -4, K= 1			4	294	-283	6	172	-169			
			3	49	51	5	120	-118	H= -3, K= 10		
1	209	-201	2	305	301	4	188	-196			
2	84	91	1	145	-152	3	68	-32	1	109	105
3	143	-145				2	268	-261	2	37*	7
4	255	271	H= -3, K= 2			1	308	-308	3	12*	-30
5	106	-92							4	173	167
6	69	-67	1	369	369	H= -3, K= 6			5	101	-112
7	272	278	2	450	-439				6	75	-83
8	35*	37	3	138	-129	1	393	-378	7	46*	-32
9	175	174	4	331	339	2	468	-471			
10	5*	-30	5	834	851	3	275	-271	H= -3, K= 11		
11	44*	-26	6	695	676	4	264	-270			
			7	333	335	5	11*	37	6	45*	-77
H= -4, K= 0			8	305	312	6	165	177	5	62*	-83
			9	12*	21	7	38*	-9	4	119	-124
11	14*	43	10	13	9	8	58*	-59	3	41*	-6
10	141	139	11	14*	-13	9	14*	32	2	12*	3
9	107	110							1	39*	-25
8	7*	70	H= -3, K= 3			H= -3, K= 7					
7	4*	32							H= -3, K= 12		
6	67	72	10	14*	-22	9	45*	38			
5	5*	-42	9	40*	-22	8	95	98	1	13*	-15
4	93	72	8	134	208	7	57*	75	2	116	-130
3	24	74	7	162	-172	6	53*	47	3	297	-310
2	166	152	6	318	320	5	61	67	4	159	-144
1	7*	-26	5	164	168	4	225	-229			
			4	722	703	3	278	-270	H= -3, K= 13		
H= -3, K= 0			3	693	688	2	86	-98			
			2	517	522	1	143	-143	3	119	-127
1	217	-210	1	376	380				2	171	-167
2	9*	-92				H= -3, K= 8			1	14*	-55

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= -2, K= 13			H= -2, K= 7			2 180 185			1 531 496		
1	14*	-8	1	215	-225	3	192	200	2	111	-111
2	63*	-61	2	257	-264	4	134	-122	3	790	-784
H= -2, K= 12			3	207	-218	5	66	-60	4	613	-597
4	100	-108	4	184	-183	6	133	123	5	441	-434
3	15*	-155	5	11*	47	7	61	-54	6	171	-165
2	61*	-83	6	135	188	8	202	206	7	59	38
1	101	101	7	153	-168	9	58*	54	8	12*	53
H= -2, K= 11			8	14*	-16	H= -2, K= 2			9	233	-234
1	87	107	H= -2, K= 6			10	97	111	10	129	-118
2	56*	-38	9	14*	23	9	251	244	H= -1, K= 1		
3	13*	38	8	42*	-46	3	123	128	10	14*	-17
4	13*	-7	7	130	-149	7	174	162	9	99	-108
5	44*	-26	6	12*	-10	6	174	174	8	12*	32
H= -2, K= 10			5	373	-358	5	9*	-30	7	137	-147
6	77	184	4	79	-83	4	335	-327	6	190	-179
5	50	-24	3	10*	-5	3	311	-301	5	596	-589
4	107	99	2	132	-178	2	1038	-1049	4	823	-810
3	173	169	1	131	-121	1	709	-711	3	1071	-1071
2	99	94	H= -2, K= 5			H= -2, K= 1			2	1197	-1207
1	12*	14	1	523	517	1	97	-95	1	146	158
H= -2, K= 9			2	162	-158	2	832	-838	H= -1, K= 2		
1	259*	273	3	84	73	3	1239	-1248	1	17*	10
2	11*	20	4	91	-85	4	594	-579	2	708	711
3	276	259	5	193	-181	5	87	79	3	195	-203
4	94	90	6	157	-158	6	61	50	4	160	-159
5	57*	64	7	207	-217	7	58	-48	5	197	-195
6	134	111	8	81	-85	8	12*	22	6	328	-326
7	109	99	9	51*	-72	9	185	167	7	153	-142
H= -2, K= 8			H= -2, K= 4			10	74	56	8	12*	38
3	45*	57	10	14*	-73	H= -2, K= 0			9	179	189
7	43*	64	9	73	-34	11	45*	-42	10	14*	73
5	121	121	8	55*	-53	10	42*	-17	H= -1, K= 3		
5	183	192	7	81	-76	9	12*	-25	10	135	117
4	96	91	6	34*	-35	3	72	69	9	152	138
3	6	-45	5	15*	-178	7	203	-203	8	268	264
2	47*	-42	4	245*	253	6	95	78	7	63	-41
1	89	-73	3	357	351	5	293	-291	6	58	16
H= -2, K= 3			2	251	267	4	314	-310	5	61	70
1	324	325	1	215	217	3	667	676	4	103	114
H= -1, K= 0			H= -2, K= 3			2	273	270	3	156	159
H= -1, K= 0			H= -2, K= 3			1	305	-297	2	73	65
H= -1, K= 0			H= -2, K= 3			H= -1, K= 0			1	52	53

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= -1, K= 4			4	12	-3	5	45*	11	1	11*	13
1	7*	42	5	117	123	4	14*	-13	0	127	-119
2	312	325	6	13*	-26	3	43*	72	H= 1, K= -8		
3	141	-129	7	7	-63	2	96	106	0	378	-386
4	59	72	H= -1, K= 9			1	14*	2	1	319	-324
5	153	167				0	43*	-56	2	220	-207
6	9*	91	7	46*	78	H= 1, K= -12			3	237	-253
7	140	124	6	43*	12	0	153	150	4	336	-337
8	4*	6	5	71	50	1	172	181	5	11*	-1
9	61	-6	4	95	105	2	81	67	6	37*	-14
H= -1, K= 5			3	53*	66	3	41*	-50	7	68	75
9	99	-99	2	35*	-33	4	110	102	8	118	100
3	131	-151	1	121	-117	5	74	59	9	88	61
7	12*	-33	H= -1, K= 10			6	76	56	H= 1, K= -7		
5	231	-220	1	53*	72	7	111	129	9	14*	8
5	11*	3	2	35	82	H= 1, K= -11			8	115	109
4	1*	-20	3	4*	13	7	14*	-21	7	12*	-12
3	344	340	4	41*	37	6	178	-155	6	95	-63
2	326	328	5	122	98	5	186	-190	5	11*	-31
1	333	343	6	169	166	4	40*	-42	4	56*	82
H= -1, K= 6			H= -1, K= 11			3	12*	-55	3	97	92
1	243	235	5	45*	-14	2	66	-27	2	273	282
2	195	205	4	51	-27	1	101	92	1	113	124
3	75	30	3	50*	34	0	376	379	0	304	-310
4	104	-107	2	57*	50	H= 1, K= -10			H= 1, K= -6		
5	179	-177	1	112	124	0	36*	57	0	372	371
6	172	-138	H= -1, K= 12			1	11*	32	1	120	128
7	81	-55	1	42*	-3	2	108	118	2	402	403
8	114	-103	2	14*	-40	3	52	-88	3	128	152
H= -1, K= 7			3	11*	23	4	99	-94	4	30*	68
8	77	-47	H= -1, K= 13			5	110	-112	5	166	161
7	34	-73	2	54*	-69	5	133	-193	6	126	-118
6	56*	-31	1	63*	-48	7	103	-109	7	12*	12
5	153	-140	H= 1, K= -14			3	117	-102	8	69	-50
4	187	-103	0	64*	63	H= 1, K= -9			9	43*	16
3	235	-252	1	143	-128	10	14*	-18	H= 1, K= -5		
2	284	-290	2	5*	-28	3	43*	-11	10	101	-102
1	451	-453	3	14*	-35	7	13*	-26	9	152	-140
H= -1, K= 8			H= 1, K= -13			6	239	-252	8	124	-137
1	305	-314	0	80	-71	5	117	-108	7	37*	10
2	121	-132	3	109	-105	4	80	-71	6	254	-272
3	244	-250	2	11*	-40	2	11*	-40	5	44*	-55

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
4	133	117	9	59	39				H=	2	K= -8
3	273	-258	3	67	44	9	14	-50			
2	247	-241	7	185	193	3	90	-94	9	45	63
1	117	113	6	303	298	7	312	-327	8	43	25
5	267	275	5	115	108	6	134	-124	7	107	93
H=	1	K= -4	4	219	219	5	153	-161	6	56	-54
0	432	436	3	106	114	4	314	305	5	96	-95
1	525	-521	2	31	91	3	599	577	4	114	-135
2	142	-139	1	847	874	2	8	-11	3	155	-173
3	12	-133	0	417	-396	1	133	-132	2	236	-229
4	153	-150	H=	2	K= -1	0	397	-380	1	95	-89
5	193	-187							0	70	55
6	165	-175	0	645	-650	H=	2	K= -5	H=	2	K= -9
7	72	-83	1	127	-137	0	252	255	0	237	235
8	325	-348	2	7	-12	1	522	517	1	182	174
9	72	-54	3	433	-430	2	87	-88	2	59	57
10	45	71	4	218	-228	3	291	314	3	126	-116
H=	1	K= -3	5	113	107	4	52	50	4	89	-91
10	10	108	6	49	6	5	92	-88	5	250	-253
9	182	169	7	112	112	6	79	-79	6	168	-161
8	12	-38	8	13	1	7	12	-34	7	72	-45
7	164	-176	9	14	-5	8	57	68	8	62	-77
6	279	-280	H=	2	K= -2	9	14	-11	H=	2	K= -10
5	15	-146	9	14	-6	H=	2	K= -6	H=	2	K= -10
4	259	-271	8	57	78	9	105	105	8	64	-87
3	205	-212	7	53	-60	8	297	293	7	96	-86
2	660	638	6	193	-193	7	144	139	6	82	-59
1	14	-150	5	155	-169	6	72	80	5	39	-17
0	225	-233	4	405	-429	5	218	225	4	170	189
H=	1	K= -2	3	667	-574	4	189	200	3	234	278
0	730	-742	2	425	-434	3	196	197	2	103	107
1	216	-227	1	229	-232	2	434	425	1	36	-38
2	347	-349	0	201	-211	1	640	625	0	51	67
3	45	-447	H=	2	K= -3	0	180	180	H=	2	K= -11
4	323	-316	0	28	-20	H=	2	K= -7	0	243	227
5	178	175	1	14	-187	0	226	-222	1	157	158
6	35	-106	2	216	214	1	134	133	2	109	125
7	205	205	3	35	-52	2	235	232	3	161	165
8	208	193	4	113	-124	3	31	24	4	80	78
9	11	127	5	213	-216	4	47	29	5	41	-29
10	63	47	6	153	-138	5	97	96	6	13	67
H=	1	K= -1	7	315	-325	6	277	273	7	44	43
10	1	15	8	93	-100	7	118	115	H=	2	K= -12
H=	1	K= -4	9	43	-2	8	183	202	6	172	158
						9	134	128			

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	2, K= -12		H=	3, K= -11		5	165	-164	6	36*	-35
5	136	131	7	14*	5	4	140	-145	5	305	-315
4	59	22	6	123	108	3	361	-377	4	101	98
3	92	81	5	113	125	2	356	-359	3	474	466
2	135	127	4	114	112	1	95	-101	2	260	257
1	28*	239	3	56*	-85	0	59	-95	1	179	182
0	223	224	2	57	-76	H=	3, K= -6		0	469	477
H=	2, K= -13		1	54*	28	0	137	140	H=	3, K= -2	
0	43*	-69	0	65	-74	1	322	313	0	249	-248
1	14*	-24	H=	3, K= -10		2	237	237	1	324	311
2	14*	21	0	153	149	3	10*	-20	2	288	274
3	61	-16	1	114	126	4	176	175	3	55	-66
4	44*	-57	2	127	129	5	78	-59	4	121	-123
5	64	60	3	311	319	6	135	142	5	100	-107
H=	2, K= -14		4	116	94	7	164	160	6	51*	45
3	79	-47	5	13*	-19	8	74	57	7	256	-278
2	45*	-32	6	94	80	9	14*	46	8	119	-112
1	135	-145	7	62	-30	H=	3, K= -5		9	45*	-25
0	79	-65	H=	3, K= -9		0	78	75	H=	3, K= -1	
H=	3, K= -14		8	45*	-77	1	42*	-25	9	101	87
0	64*	-73	7	74	-56	2	39*	18	8	85	70
1	78	-61	6	13*	15	3	73	-94	7	12*	33
2	64*	-76	5	145	-144	4	113	129	6	51*	-41
3	112	-90	4	37*	-38	3	239	245	5	11*	34
H=	3, K= -13		3	138	146	2	198	219	4	143	137
5	14*	-10	2	155	160	1	341	336	3	161	-162
4	44*	-25	1	248	249	0	324	328	2	482	-481
3	151	-145	0	113	138	H=	3, K= -4		1	402	385
2	7*	-90	H=	3, K= -8		0	36*	41	0	56	-57
1	95	-94	0	63	-71	H=	3, K= -4		H=	4, K= -1	
0	113	-93	1	72	-63	1	186	-170	0	512	-521
H=	3, K= -12		2	222	-215	2	486	485	1	474	-465
0	162	-157	3	83	-92	3	336	337	2	324	-322
1	81	55	4	250	-248	4	435	420	3	67	-61
2	75*	84	5	293	-290	5	383	384	4	179	-182
3	13*	6	6	37*	-60	6	212	-205	5	36*	6
4	42*	2	7	54	-43	7	185	-179	6	323	-322
5	52*	90	8	14*	-32	8	76	-70	7	130	-135
6	101	94	H=	3, K= -7		9	42*	-33	8	62	-17
			3	114	125	H=	3, K= -3		H=	4, K= -2	
			7	13*	31	0	45*	-25	0	164	-160
			6	33*	34	1	151	-143	1	163	-154
						2	145	-158	2	211	-212

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
5	11*	12	2	101	-114				5	45*	-14
4	125	-126	1	265	-267	0	193	-196			
3	67	62	0	300	-306	1	140	-135	H=	5, K=	-11
2	24	241				2	68	-53			
1	238	-230	H=	4, K=	-7	3	13*	-50	6	46*	-8
0	62	-52				4	124	133	5	76	60
			0	43	46	5	148	157	4	13*	17
H=	4, K=	-3	1	167	-167	6	44*	22	3	82	89
0	372	384	2	205	-217				2	98	-90
1	203	220	3	11*	-23	H=	4, K=	-12	1	88	-90
2	536	529	4	381	-379				0	290	-286
3	317	303	5	287	-289	5	14*	48			
4	1*	-22	6	97	-103	4	43*	17	H=	5, K=	-10
5	11*	-36	7	103	-84	3	59	-44			
6	38	-5	8	14*	-50	2	109	-103	0	134	128
7	163	163				1	91	-99	1	124	124
8	4*	-10	H=	4, K=	-8	0	178	-187	2	38	-12
									3	79	52
H=	4, K=	-4	8	144	-145	H=	4, K=	-13	4	153	146
			7	177	-179				5	141	142
			6	240	-264	0	86	-87	6	63	39
8	62	9	5	213	-220	1	122	-132			
7	71	84	4	345	-327	2	106	-83	H=	5, K=	-9
6	5*	-88	3	185	-133	3	76	-60			
5	11*	16	2	117	112	4	45*	-79	7	64	63
4	167	164	1	135	143				6	75	71
3	312	321	0	32*	42	H=	4, K=	-14	5	226	229
2	383	375							4	236	232
1	530	525	H=	4, K=	-9	2	14*	-23	3	242	244
0	414	402				1	64*	60	2	155	153
			0	109	115	0	45*	75	1	296	301
H=	4, K=	-5	1	60	-61				0	384	370
			2	170	170	H=	5, K=	-14			
0	20	-204	3	52*	68				H=	5, K=	-8
1	127	-119	4	125	-137	0	120	128			
2	0*	-43	5	13*	-14	1	79	83	0	256	254
3	21-	217	6	42*	4				1	176	172
4	203	212	7	75	-51	H=	5, K=	-13	2	299	297
5	199	199							3	131	142
6	86	-82	H=	4, K=	-10	3	14*	3	4	12*	18
7	5-	39				2	62	29	5	80	70
8	44*	34	7	45*	19	1	14*	8	6	13*	-4
			6	14*	59	0	87	96	7	45*	7
H=	4, K=	-6	5	32	97						
			4	07	96	H=	5, K=	-12	H=	5, K=	-7
3	14*	58	3	77	-52						
7	102	-75	2	37*	55	0	92	-69	7	88	-92
6	117	138	1	52*	70	1	166	-179	6	72	-69
5	73	81	0	163	159	2	151	-158	5	12*	38
4	11*	-33				3	14*	-8	4	264	-273
3	112	-117	H=	4, K=	-11	4	14*	-25	3	93	-90

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	5, K=	-7	0	347	363	3	216	212	6	88	81
2	171	163	H=	5, K=	-2	4	353	358	5	125	116
1	97	103	0	304	275	5	209	197	4	138	117
0	89	94	1	134	-120	6	140	137	3	85	96
H=	5, K=	-6	2	85	102	7	100	105	2	52	44
0	112	-122	3	280	281	H=	5, K=	-4	1	50	59
1	377	-381	4	92	-71	7	190	180	0	35	-32
2	129	-136	5	130	-154	6	60	43	H=	5, K=	-9
3	63	-65	6	13	-44	5	119	113	0	73	86
4	11	-39	7	129	-118	4	91	-90	1	74	62
5	12	27	H=	5, K=	-1	3	110	-122	2	12	-53
6	13	-30	0	144	-155	2	46	14	3	215	211
7	61	-70	7	121	-123	0	10	-5	4	292	300
H=	5, K=	-5	6	121	-123	H=	5, K=	-5	5	105	100
8	14	21	5	12	-23	0	389	-394	6	110	105
7	61	32	4	214	-210	1	282	-279	H=	5, K=	-10
6	90	79	3	93	-86	2	33	32	5	14	51
5	16	162	2	60	-59	3	314	-312	4	126	143
4	35	46	1	323	-310	4	124	-114	3	13	23
3	165	149	0	405	-481	5	40	-25	2	68	65
2	113	-122	H=	6, K=	-1	5	42	8	1	39	-64
1	441	-441	0	58	-63	7	75	63	0	213	-226
0	463	-469	1	44	-50	H=	6, K=	-6	H=	6, K=	-11
H=	5, K=	-4	2	93	102	7	90	-67	0	187	-174
0	123	-122	3	35	-47	6	43	16	1	81	-101
1	81	91	4	112	-99	5	57	-25	2	13	7
2	31	-35	5	93	-138	4	12	12	3	60	-32
3	181	180	6	43	28	3	102	-115	4	52	-23
4	75	-53	7	45	-59	2	90	-87	5	14	-13
5	97	99	H=	6, K=	-2	1	73	-84	H=	5, K=	-12
6	144	127	7	54	61	0	135	-112	4	45	-46
7	121	122	6	85	94	H=	6, K=	-7	3	52	-71
8	91	76	5	40	-42	0	33	-7	2	14	19
H=	5, K=	-3	4	111	95	1	180	191	1	94	-113
3	40	57	3	60	69	2	35	-47	0	13	3
7	72	73	2	108	106	3	82	-86	H=	5, K=	-13
6	200	202	1	137	138	4	155	167	0	164	145
5	53	-15	0	410	411	5	91	85	1	44	44
4	63	81	H=	6, K=	-3	6	43	-56	2	14	60
3	79	84	0	215	227	7	129	-111	3	91	55
2	52	28	1	110	110	H=	6, K=	-8			
1	507	503	2	203	211						

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= 11, K= -4			H= 0, K= 1			-10	14*	-14	-9	144	144
0	4*	77	-10	14*	-54	H= 0, K= 5			H= 0, K= 9		
1	123	112	-9	13*	-6	-10	98	-89	-9	141	155
2	14*	80	-8	12*	-34	-9	130	-149	-8	13*	20
H= 11, K= -3			-7	59*	8*	-8	268	-273	-7	40*	-36
2	1*	43	-6	241	245	-7	147	-140	-6	77	-94
1	14*	10	-5	339	343	-5	66	-53	-5	82	-84
0	59	23	-4	432	409	-5	181	-178	-4	128	-127
H= 11, K= -2			-3	62	89	-4	271	-259	-3	85	76
0	162	-177	-2	329	335	-3	116	-129	-2	48*	58
1	107	-104	-1	653	652	-2	423	-414	-1	216	-220
2	102	-102	H= 0, K= 2			-1	190	-181	H= 0, K= 10		
H= 11, K= -1			-1	837	-874	H= 0, K= 6			-1	12*	-36
1	216	-205	-2	42	-38	-1	276	279	-2	250	-255
0	147	-139	-3	402	404	-2	47*	89	-3	349	-357
H= 12, K= -1			-4	174	-166	-3	40*	-22	-4	316	-313
0	91	-122	-5	159	169	-4	172	165	-5	208	-228
H= 12, K= -2			-6	77	86	-5	10*	49	-6	98	-90
0	14*	29	-7	155	153	-6	132	-145	-7	13*	18
H= 12, K= -3			-8	105	113	-7	89	83	-8	52*	79
0	118	109	-9	152	153	-8	68*	-79	H= 0, K= 11		
H= 12, K= -4			-10	62*	42	-9	13*	-4*	-10	63*	-64
0	14*	-23	H= 0, K= 3			H= 1, K= 7			-3	64*	-75
H= 12, K= -5			-10	123	119	-7	130	-127	-6	111	-114
0	45*	4	-9	190	178	-10	14*	4	-5	13*	-47
H= 12, K= -6			-8	219	229	-9	74*	97	-4	213	-220
0	64*	-71	-7	11*	-43	-8	40*	31	-3	199	-198
H= 12, K= -7			-6	10*	35	-7	65	8	-2	39*	-56
0	45*	-46	-5	41*	5	-6	141	123	-1	87	89
H= 0, K= 4			-4	173	-176	-5	227	232	H= 0, K= 12		
0	253	-254	-3	46*	40	-4	314	323	-1	148	140
H= 0, K= 5			-2	69	-77	-3	133	141	-2	100	82
0	222	-231	-1	365	-372	-2	280	278	-3	92	97
H= 0, K= 6			H= 0, K= 4			-1	9*	-8	-4	59*	72
0	419	-430	-1	253	-254	H= 0, K= 8			-5	43*	-24
H= 0, K= 7			-2	222	-231	-1	119	-115	-6	14*	-67
0	535	-535	-3	419	-430	-2	175	163	-7	64	-8
H= 0, K= 8			-4	535	-535	-3	153	155	H= 0, K= 13		
0	115	-136	-5	115	-136	-4	95	89	-5	14*	19
H= 0, K= 9			-6	10*	52	-5	11*	-42	-6	14*	38
0	135	-132	-7	135	-132	-6	52*	-10	-7	14*	30
H= 0, K= 10			-8	12*	-48	-7	12*	-32	-8	14*	30
0	13*	16	-9	13*	16	-8	92	89	-9	14*	30

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	1, K=	13	-4	129	140	-4	409	-416	-1	397	390
			-5	180	172	-5	300	-322	-2	135	-135
-2	14*	37	-6	195	200	-6	65	51	-3	151	-141
-1	123	122	-7	137	203	-7	70	-28	-4	120	129
			-8	151	142	-8	37*	-48	-5	228	-209
H=	1, K=	13	-9	146	142	-9	98	-82	-6	58	-50
						-10	86	83	-7	100	111
-1	133	137	H=	1, K=	3				-8	63*	35
-2	14*	31				H=	1, K=	4	-9	112	-120
-3	14*	45	-10	111	123				-10	60*	-70
-4	99	101	-9	113	124	-10	120	124			
-5	111	111	-8	123	129	-9	186	192	H=	2, K=	1
			-7	163	-166	-8	165	159			
H=	1, K=	12	-6	37	-24	-7	34*	-18	-11	100	-125
			-5	11*	16	-6	283	291	-10	110	-108
-7	45*	-49	-4	101	98	-5	29*	-35	-9	55*	-36
-6	14*	-48	-3	291	295	-4	270	-266	-8	217	220
-5	96	-90	-2	258	249	-3	273	-291	-7	57*	40
-4	13*	-53	-1	150	153	-2	7*	-32	-6	198	-204
-3	59*	74				-1	554	-562	-5	670	-657
-2	13*	54	H=	1, K=	7				-4	150	-159
-1	8*	68				H=	1, K=	3	-3	147	-146
			-1	203	211				-2	223	-221
H=	1, K=	11	-2	60	63	-1	335	-324	-1	521	519
			-3	115	121	-2	454	-461			
-1	40*	43	-4	155	154	-3	247	-242	H=	2, K=	2
-2	88	80	-5	256	251	-4	240	239			
-3	112	-89	-6	73	55	-5	493	495	-1	1459	1490
-4	256	-261	-7	64	-25	-6	263	266	-2	662	-651
-5	158	-163	-8	39*	45	-7	306	316	-3	72	-64
-6	13*	-47	-9	84	-94	-8	190	178	-4	244	247
-7	115	-94	-10	14	-13	-9	12*	37	-5	9*	-24
-8	14*	5				-10	60*	80	-6	30*	33
			H=	1, K=	6	-11	14*	70	-7	154	-142
H=	1, K=	10							-8	80	88
			-10	44*	-62	H=	1, K=	2	-9	145	-136
-9	111	120	-9	196	-215				-10	132	-125
-8	97	121	-8	33*	-33	-11	45*	-4	-11	14*	-46
-7	110	95	-7	62*	-66	-10	60*	35			
-6	130	140	-6	11*	7	-9	56*	24	H=	2, K=	3
-5	39*	42	-5	95	91	-8	11*	3			
-4	12*	-49	-4	42*	33	-7	173	173	-11	14*	-24
-3	204	-187	-3	169	166	-6	30*	7	-10	93	-44
-2	162	-162	-2	7*	-18	-5	48*	69	-9	116	-103
-1	53*	-35*	-1	431	434	-4	176	192	-8	72	44
						-3	71	92	-7	248	250
H=	1, K=	9	H=	1, K=	5	-2	53	71	-6	343	362
						-1	506	514	-5	485	492
-1	135	-136	-1	91	-109				-4	150	157
-2	6*	-25	-2	292	-307	H=	1, K=	1	-3	173	185
-3	235	233	-3	3*	-25				-2	112	-114

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
-1	493	493	-4	65	-70	-1	178	-174			
H=	P, K=	4	-3	70	-59	H=	2, K=	12	H=	3, K=	9
			-2	132	188						
			-1	83	69						
-1	241	-244	H=	2, K=	8	-1	61*	-59	-1	12*	-82
-2	709	-705				-2	14*	16	-2	74	-74
-3	367	-357				-3	13*	-13	-3	83	-83
-4	89	39	-1	153	169	-4	105	-99	-4	54	12
-5	29*	24	-2	11*	-8	-5	115	-108	-5	137	138
-6	25*	271	-3	43*	74	-5	89	-70	-6	252	274
-7	21*	216	-4	84	72	-7	45*	-58	-7	13*	33
-8	168	164	-5	11*	11	H=	2, K=	13	-8	42*	-70
-9	12*	21*	-6	64*	48				-9	14*	-16
-10	73	47	-7	54*	-69				H=	3, K=	8
-11	16*	23	-8	13*	-7	-5	46*	-12			
H=	2, K=	5	-9	35	-80	-4	78	36	-10	210	-225
			-10	90	-44	-3	45*	43	-9	141	-152
-11	6*	19	H=	2, K=	9	-2	14*	38	-8	134	-134
-10	13*	32				-1	14*	44	-7	87	-119
-9	105	110	-9	14*	-15	H=	3, K=	12	-6	53*	-51
-8	105	-108	-5	13*	11				-5	36	33
-7	9*	-93	-7	57	49	-6	76	-86	-4	11*	12
-6	45*	-56	-6	172	179	-5	62*	-64	-3	297	-305
-5	383	-383	-5	313	325	-4	76	-71	-2	110	-98
-4	52*	-532	-4	136	141	-3	44*	-76	-1	100	-105
-3	547	-544	-3	51*	-6	-2	44*	-60	H=	3, K=	7
-2	589	-580	-2	71	-77	-1	99	-110			
-1	399	-390	-1	51*	58				-1	201	-202
H=	2, K=	6	H=	2, K=	10	H=	3, K=	11	-2	250	-255
									-3	108	-107
-1	29*	-2	-1	195	-194	-1	206	-205	-4	47*	-44
-2	255	-257	-2	173	-193	-2	155	-148	-5	365	-360
-3	66	59	-3	38*	-56	-3	41*	-57	-6	256	-261
-4	1*	10	-4	66	-67	-4	72	67	-7	37*	42
-5	293	-308	-5	12*	34	-5	13*	-2	-8	55*	-88
-6	82	-123	-6	106	114	-6	14*	4	-9	72*	-61
-7	5*	-75	-7	133	112	-7	14*	23	-10	62*	-61
-8	255	-264	-8	43*	-5	-8	14*	38	H=	3, K=	6
-9	121	-137	-9	6*	75	H=	3, K=	10			
-10	1*	-3							-11	14*	37
H=	2, K=	7	H=	2, K=	11	-1	64*	52	-10	61*	65
						-3	14*	28	-9	13*	58
-10	4*	-77	-8	90	68	-7	163	171	-8	38*	-34
-9	5*	-6	-7	4*	31	-5	123	134	-7	62*	53
-8	12*	32	-6	80*	-79	-5	126	101	-6	83	-89
-7	12*	12	-4	185	-179	-4	118	120	-5	200	207
-6	140	-120	-4	3*	-102	-3	12*	39	-4	248	-248
-5	134	-119	-3	134	-125	-2	12*	19	-3	43*	-42
			-2	131	-174	-1	56*	-66	-2	158	-167

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
-7	86	89	-6	135	-129	-5	10*	40			
-3	14*	17	-7	145	-144	-6	231	230	-1	481	-487
-9	14*	28	-8	43*	-8	-7	160	156	-2	246	-253
			-9	117	-122	-8	150	134	-3	186	-193
H=	4, K=	11				-9	40*	-14	-4	391	-386
			H=	5, K=	8	-10	13*	-71	-5	111	-115
-8	65*	28				-11	194	-181	-6	43*	22
-7	45*	69	-10	64*	-90				-7	10*	10
-6	37	96	-9	232	-228	H=	5, K=	4	-8	79	85
-5	86	75	-8	131	-140				-9	12*	-37
-4	43*	84	-7	57*	-73	-11	116	-110	-10	195	200
-3	74	32	-6	115	-110	-10	58*	54	-11	106	117
-2	43*	-6	-5	12*	-16	-9	39*	41			
-1	41*	-55	-4	53*	28	-8	37*	-18	H=	5, K=	1
			-3	225	-244	-7	115	-93			
H=	4, K=	12	-2	240	-248	-6	73	-69	-11	14*	43
			-1	95	-95	-5	122	107	-10	147	173
-2	101	-82				-4	110	-97	-9	54*	78
-3	45*	-39	H=	5, K=	7	-3	240	245	-8	303	284
-4	45*	60				-2	228	226	-7	106	129
-5	64*	61	-1	53	-74	-1	98	90	-6	71	77
-6	14*	31	-2	51*	-66				-5	242	244
			-3	50*	-42	H=	5, K=	3	-4	153	150
H=	5, K=	11	-4	163	-152	-1	302	312	-3	360	357
			-5	53*	63	-2	556	-552	-2	90	-96
-1	14*	4	-6	145	151	-3	90	78	-1	72	-75
-2	77	72	-7	12*	-5						
-3	132	127	-8	120	-90	-4	50*	-32	H=	5, K=	2
-4	76	75	-9	42*	33	-5	43*	-65			
-5	85	71	-10	62*	65	-6	10*	-55	-1	302	-300
-6	14*	37				-7	165	-160	-2	51	-41
-7	14*	56	H=	5, K=	6	-8	95	-102	-3	263	-262
						-9	180	-166	-4	126	-136
H=	5, K=	10	-11	64*	-57	-10	58*	-26	-5	53*	63
			-10	14*	-53	-11	44*	-101	-6	10*	-32
-2	14*	-6	-9	182	174				-7	83	-67
-7	40*	6	-8	239	248	H=	5, K=	2	-8	125	-111
-5	14*	24	-7	165	151				-9	86	-72
-5	42*	75	-6	241	221	-11	14*	19	-10	13*	59
-4	20	58	-5	235	241	-10	13*	-26	-11	123	102
-3	126	125	-4	57*	45	-9	166	-167			
-2	73	65	-3	11*	19	-8	198	-190	H=	5, K=	3
-1	155	151	-2	11*	-23	-7	120	-113			
			-1	77	-63	-6	132	-131	-11	14*	47
H=	5, K=	9				-5	338	-335	-10	58*	-52
			H=	5, K=	5	-4	118	-136	-9	110	-116
-1	92	92				-3	244	-236	-8	12*	-46
-2	114	104	-1	86	-86	-2	562	-540	-7	49*	31
-3	13*	9	-2	320	320	-1	734	-732	-6	57*	-53
-4	56*	-57	-3	512	506				-5	55*	-46
-5	4*	-11	-4	55*	57	H=	5, K=	1	-4	69	57

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	6, K=	3	-8	58*	-35				-6	76	51
			-7	63*	39	H=	7, K=	10	-5	84	82
-3	1*	13	-6	33*	61				-4	439	441
-2	323	-332	-5	32	103	-7	79	-80	-3	345	341
-1	102	-183	-4	37*	7	-5	14*	-54	-2	165	155
			-3	65	80	-5	14*	-35	-1	95	93
H=	6, K=	4	-2	170	-178	-4	14*	-19			
			-1	190	-200	-3	45*	51	H=	7, K=	5
-1	394	403									
-2	134	130	H=	6, K=	8	H=	7, K=	9	-1	37*	-11
-3	116	126							-2	120	124
-4	56*	84	-1	13*	-40	-1	14*	-30	-3	124	-120
-5	60	-35	-2	40*	-40	-2	62	9	-4	133	137
-6	202	-157	-3	150	-162	-3	87	-62	-5	80	88
-7	57*	-80	-4	291	-297	-4	74	-82	-6	52*	-22
-8	106	-91	-5	163	-156	-5	136	-123	-7	113	-109
-9	153	-142	-6	40	-44	-5	51*	-43	-8	166	-148
-10	72*	-69	-7	13*	-32	-7	14*	-2	-9	13*	-9
-11	14*	-67	-8	73	-20	-8	64*	-4	-10	43*	-34
			-9	44*	4				-11	14*	4
H=	6, K=	5	-10	14*	20	H=	7, K=	8			
									H=	7, K=	4
-11	170	-172	H=	6, K=	9	-9	142	140			
-10	112	-86				-8	97	80	-11	14*	27
-9	139	-150	-7	79	-60	-7	127	132	-10	133	-136
-8	77	-81	-8	14*	-44	-6	42*	27	-9	98	-103
-7	11*	-125	-7	123	-128	-5	210	-193	-8	12*	12
-6	141	-139	-6	125	-137	-4	109	-102	-7	97	-96
-5	34*	40	-5	131	-114	-3	41*	-5	-6	292	-285
-3	265	274	-4	41*	-98	-2	13*	-55	-5	196	-189
-2	334	335	-3	23	-79	-1	14*	-14	-4	11*	-7
-1	11*	-13	-2	42*	29				-3	34*	69
			-1	1*	-2	H=	7, K=	7	-2	11*	2
H=	6, K=	6							-1	295	306
			H=	6, K=	10	-1	82	84			
-1	164	-176				-2	69*	98	H=	7, K=	3
-2	72	-70	-1	45*	55	-3	147	161			
-3	216	231	-2	62*	44	-4	202	232	-1	84*	-88
-4	57*	-13*	-3	62*	12	-5	166	155	-2	11*	-60
-5	35*	55	-4	43*	-36	-6	159	177	-3	33*	8
-6	147	149	-5	43*	8	-7	70*	103	-4	10*	-12
-7	12*	-58	-6	14*	-25	-8	102	85	-5	186	-181
-8	13*	-22	-7	107	-114	-7	129	114	-6	59*	-65
-9	13*	-21	-8	1*	-38	-10	14*	38	-7	36*	-56
-10	43*	8							-8	84	-89
-11	65*	-64	H=	6, K=	11	H=	7, K=	6	-9	56*	5
									-10	13*	-22
H=	6, K=	7	-5	70	-14	-10	76*	75	-11	98	99
			-5	45*	22	-9	42*	-57			
-1	14*	69	-4	64*	61	-8	81	-57	H=	7, K=	2
-2	6*	32	-3	65	28	-7	39*	-28			

L	F1	FC	L	F0	FC	L	F0	FC	L	F0	FC
-11	14*	53	-10	94	106	-5	98	-99	-4	14*	8
-10	116	121	-11	63	35	-7	256	-241	-5	75	64
-9	39*	9				-8	133	-134	-6	14*	-10
-8	12*	24	H=	8, K=	3	-9	87	-62	-7	14*	-47
-7	61*	-77				-10	64*	-30	-8	45*	3
-6	89	89	-11	155	167				-9	65*	-49
-5	137	131	-10	86	82	H=	8, K=	7			
-4	64	45	-9	168	149				H=	9, K=	6
-3	77	75	-8	87	67	-9	14*	-5			
-2	189	-193	-7	65	-5	-8	87	71	-9	63*	-75
-1	35*	-355	-6	52	-19	-7	120	124	-8	87	-119
			-5	199	-203	-6	110	97	-7	60*	-69
H=	7, K=	1	-4	128	-120	-5	13*	33	-6	13*	-38
			-3	133	-139	-4	59*	96	-5	42*	-40
-1	84	-123	-2	125	125	-3	110	131	-4	83	-84
-2	124	-123	-1	74	-57	-2	13*	50	-3	94	-104
-3	1*	4				-1	87	70	-2	113	106
-4	317	315	H=	8, K=	4				-1	14*	38
-5	349	346				H=	8, K=	8			
-6	283	289	-1	116	-95				H=	9, K=	5
-7	78	61	-2	75	-69	-1	14*	-2			
-8	82	55	-3	181	186	-2	14*	-17	-1	95	-93
-9	110	106	-4	12*	55	-3	14*	8	-2	180	-175
-10	83	86	-5	12*	-30	-4	97	102	-3	162	-159
-11	14*	21	-6	38*	-18	-5	86	57	-4	120	-129
			-7	122	-93	-5	14*	17	-5	160	-161
H=	8, K=	1	-5	56*	-42	-7	76*	72	-6	277	-284
			-9	41*	14	-8	90	72	-7	225	-213
-11	14*	46	-10	14*	2	-9	122	98	-8	94	-82
-10	151	-152	-11	14*	45				-9	14*	17
-9	69*	-50				H=	8, K=	9	-10	14*	39
-8	174	-169	H=	8, K=	5						
-7	11*	30				-7	14*	64	H=	9, K=	4
-6	32*	324	-10	14*	-34	-5	45*	-40			
-5	223	234	-9	73*	-84	-5	135	-139	-10	76*	80
-4	329	327	-8	10	-104	-4	45*	18	-9	13*	-6
-3	3*	46	-7	164	-163	-3	64	26	-8	116	-141
-2	113	94	-6	205	-217				-7	89	-74
-1	92	-99	-5	12*	-32	H=	9, K=	8	-6	79	-69
			-4	51*	69				-5	78	-43
H=	8, K=	2	-3	54*	-63	-7	45*	16	-4	67	64
			-2	30*	-38	-5	14*	-43	-3	55*	25
-1	157	-160	-1	40*	40	-5	45*	29	-2	132	-133
-2	8*	-103				-4	14*	26	-1	212	-193
-3	63*	-46	H=	8, K=	6	-3	46*	48			
-4	179	175							H=	9, K=	3
-5	14*	127	-1	157	189	H=	9, K=	7			
-6	62*	74	-2	247	259				-1	13*	35
-7	12*	-7	-3	80	43	-1	79	90	-2	102	93
-8	12*	15	-4	13*	36	-2	134	149	-3	66	-8
-9	57*	32	-5	89	72	-3	124	121	-4	53*	-35

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	9, K=	3	-4	181	195	-6	96	71	-8	147	146
			-5	107	111	-7	105	88	-9	195	193
-5	12*	22	-6	12	-12	-8	41*	28	-10	128	137
-6	5**	8	-7	12*	-57	-9	84	-43			
-7	63*	37	-8	95	-103	-10	116	-104	H=	10, K=	5
-8	13*	27	-9	99	-71						
-9	13*	63	-10	104	-96	H=	10, K=	3	-9	45*	-10
-10	14*	67							-8	14*	-57
-11	45*	20	H=	10, K=	1	-10	77*	103	-7	60*	26
						-9	43*	5	-6	13*	-5
H=	9, K=	2	-11	64	-73	-3	59*	-49	-5	73	-35
			-10	75	-64	-7	70	61	-4	103	-101
-11	100	-38	-9	13*	-13	-5	40*	13	-3	14*	-16
-10	14*	-6	-3	121	-125	-5	97	109	-2	138	-150
-9	13*	-33	-7	88	-56	-4	56*	56	-1	77	-77
-8	96	117	-6	35	-70	-3	106*	125			
-7	178	191	-5	85	-77	-2	58*	66	H=	10, K=	6
-6	162	162	-4	93	-97	-1	13*	14			
-5	146	142	-3	127	135				-2	14*	-21
-4	63*	-75	-2	233	227	H=	10, K=	4	-3	63*	-105
-3	37*	-34	-1	236	237				-4	14*	-14
-2	144	132				-1	43*	-46	-5	43*	-51
-1	132	113	H=	10, K=	2	-2	73	-54	-6	107	-113
						-3	41*	-48	-7	44*	-52
H=	9, K=	1	-1	129	122	-4	13*	-5	-8	14*	-37
			-2	173	159	-5	115	120			
-1	349	358	-3	12	48	-6	108	101	H=	10, K=	7
-2	251	278	-4	95	-111	-7	110	90			
-3	247	251	-5	95	-104						

L	FJ	FC	L	FJ	FC	L	FJ	FC	L	FJ	FC
-7	70	-54	-2	14*	-2				-4	44*	-53
-6	14*	-7				-1	60*	105	-5	115	-127
-5	45*	-47	H=	11, K=	3	-2	72*	-97	-6	163	-171
-4	14*	-74				-3	91	-105	-7	164	-160
			-1	14*	6	-4	210	-209	-8	63*	-76
H=	11, K=	6	-2	62*	93	-5	127	-134	-9	45*	-39
			-3	121	124	-6	70	-56			
-6	14*	-23	-4	119	132	-7	13*	38	H=	12, K=	3
-5	46*	-54	-5	126	88	-8	13*	-27			
			-6	73	53	-9	14*	-26	-8	78	-62
H=	11, K=	5	-7	43*	30	-10	14*	-31	-7	45*	-32
			-8	61*	53				-6	14*	-21
-3	64*	-53	-9	14*	-6	H=	12, K=	1	-5	14*	-9
-4	125	-105							-4	77	71
-5	14*	-36	F=	11, K=	2	-9	14*	57	-3	45*	55
-6	63*	43				-8	116	128			
-7	14*	37	-10	14*	4	-7	61*	43	H=	12, K=	4
-8	14*	38	-9	14*	-5	-5	14*	-43			
			-3	13*	-28	-5	85	-64	-5	45*	56
H=	11, K=	4	-7	42*	-70	-4	142	-137	-6	45*	53
			-6	117	-104	-3	162	-165	-7	112	96
-9	78	94	-5	192	-194	-2	77	-67			
-8	99	99	-4	41*	-14	-1	45*	41	H=	13, K=	1
-7	123	104	-3	42*	40						
-6	156	167	-2	13*	63	H=	12, K=	2	-4	45*	-35
-5	61*	53	-1	57	99				-5	14*	-16
-4	14*	10				-2	45*	-46	-6	14*	-24
-3	14*	-4	H=	11, K=	1	-3	14*	-36	-7	14*	5

APPENDIX C : STRUCTURE FACTOR TABLES FOR $(\text{NbT}_4)_2(\text{H}_3\text{OCl}_3) \cdot (\text{CH}_3\text{CN})_2$.

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	0, K=	0				15	52	-56	4	41	-40
			H=	0, K=	4	16	4*	13	5	4*	-1
2	119	115				17	74	-75	6	13*	-2
4	212	-195				18	4*	0	7	51	-51
6	110	-105	1	95	-95	19	16*	11	8	13*	-20
8	75	67	2	112	114	20	4*	-15	9	26	-18
10	31	-35	3	53	77	21	25*	32	10	32	29
12	73	71	4	24	23	22	5*	-5	11	39	38
14	135	-131	5	35	36	23	43	42	12	22*	-5
16	56	-53	6	114	-120	24	5*	9	13	17*	15
18	12*	13	7	114	112	25	9*	-22	14	16*	10
20	43	43	8	3*	-5	26	5*	19	15	5*	-13
22	4*	-2	9	55	59	27	16*	-3*	16	9*	-4
24	55	-57	10	49	93	28	8*	-7	17	45*	-47
26	65	-55	11	27	-26				18	25*	23
28	29*	36	12	36	28	H=	0, K=	8	19	5*	-7
30	36	46	13	121	-114				20	17*	17
			14	37	-36	0	46	53	21	21*	37
H=	0, K=	2	15	14*	13	1	34	-35	22	32	26
			16	20*	-24	2	25	18	23	27*	34
0	197	-184	17	44	36	3	52	-20	24	20*	-8
1	73	72	18	4*	19	4	10*	-5			
2	16*	-11	19	33	27	5	9*	7	H=	0, K=	12
3	16*	-29	20	52	73	6	4*	5			
4	176	171	21	21*	-24	7	17	86	0	60	-63
5	42	-45	22	4*	-6	8	4*	5	1	17*	-10
6	72	75	23	35	-46	9	36	33	2	17*	-11
7	3*	-4	24	43	-49	10	17*	-2	3	15*	-18
8	25	19	25	7*	-12	11	75	-75	4	31	34
9	14*	16	26	5*	-14	12	11*	-12	5	29	15
10	85	-82	27	16*	37	13	60*	-66	6	15*	16
11	4*	-19	28	22*	19	14	8*	-10	7	39	40
12	61	-59	29	11*	12	15	26	23	8	26*	-19
13	44	44				16	13*	6	9	16*	29
14	82	77	H=	0, K=	6	17	30	31	10	22*	-20
15	29	-29				18	17*	19	11	19*	9
16	79	31				19	9*	12	12	5*	-10
17	53	-77	1	11*	-15	20	23*	-14	13	24*	-22
18	31	-23	2	4*	-1	21	13*	-14	14	44	36
19	25	-27	3	73	171	22	16*	-6	15	24*	-17
20	52	-40	4	21	-20	23	3*	-3*	16	17*	23
21	19*	9	5	3*	-12	24	23*	10	17	26*	19
22	5*	-1	6	34	30	25	5*	-1	18	5*	-6
23	50	51	7	64	-67	26	18*	-4	19	20*	19
24	65	67	8	13*	7				20	18*	-17
25	34	20	9	129	-130	H=	0, K=	10			
26	14*	29	10	3*	-5				H=	0, K=	14
27	14*	-13	11	111	113	0	5*	-11			
28	5*	-24	12	30	34	1	32	36	0	24*	23
29	5*	-16	13	64	63	2	4*	-1	1	14*	19
30	20*	-43	14	13*	9	3	52	61	2	5*	7

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
3	19*	21	11	5*	9	H=	1, K=	7	21*	16*	11
4	40	-36	12	5*	15				22	26	-6
5	14*	-10	13	22*	-21	0	98	-101	23	16*	25
6	5*	-15				1	3*	21	24	30*	-43
7	20*	-21	H=	1, K=	11	2	28	-30	25	5*	5
8	21*	20				3	37	-29			
9	7*	-4	0	25*	-31	4	87	-93	H=	1, K=	3
10	47	43	1	20*	-6	5	55	-57			
11	14*	-8	2	4*	-14	6	42	44	0	79	-79
12	15*	13	3	53	51	7	8*	-6	1	13*	-7
13	20*	1	4	21*	-22	8	17*	10	2	84	82
14	37	-34	5	13*	3	9	29	-27	3	117	-110
15	13*	-6	6	54	63	10	73	-82	4	26	26
16	31*	-37	7	23	-27	11	21*	17	5	15*	-1
			8	40	-30	12	57	-55	6	106	-101
H=	0, K=	15	9	25*	-34	13	4*	14	7	20	-15
			10	48	-49	14	65	65	8	29	29
0	46	-45	11	4*	-2	15	4*	-0	9	34	33
1	21*	-1	12	25*	-24	16	43	44	10	124	-112
2	5*	-12	13	28	23	17	4*	-1	11	55	-50
3	7*	0	14	3*	15	18	39	-42	12	50	-46
4	14*	29	15	13*	8	19	4*	0	13	110	-109
5	5*	2	16	17*	20	20	36	-37	14	36	37
5	16*	29	17	30	-24	21	5*	-7			
7	3*	0	18	5*	-2	22	5*	-9	H=	1, K=	1
						23	5*	4			
H=	1, K=	15	H=	1, K=	9	24	5*	17	0	59	66
0	12*	-15	0	52	54	H=	1, K=	5	H=	1, K=	3
1	5*	15	1	34	-36						
2	5*	-3	2	13*	25	0	97	100	15	17*	-23
3	13*	34	3	20*	18	1	35	-31	16	12*	10
4	5*	-4	4	51	-53	2	3*	-0	17	39	39
5	5*	11	5	11*	-3	3	56	70	18	27	15
6	7*	7	6	39	-43	4	35	-42	19	20	24
7	19*	-30	7	14*	9	5	7*	9	20	51	-51
8	5*	-7	8	19*	-5	6	117	-115	21	26*	-27
			9	4*	1	7	41	43	22	59	-63
H=	1, K=	13	10	54	54	8	36	-31	23	39	-41
			11	15*	1	9	85	-83	24	41	35
0	45*	-1	12	14*	-2	10	100	104	25	5*	-4
1	1*	-7	13	36	-26	11	3*	6	26	7*	26
2	1*	17	14	51	-57	12	105	100			
3	47	-36	15	4*	-4	13	35	37	H=	1, K=	1
4	25*	-29	16	34	-41	14	63	-65			
5	5*	5	17	12*	-14	15	36	-33	1	75	78
6	3*	-33	18	23*	23	16	55	-64	2	15	-16
7	34	25	19	5*	0	17	75	-64	3	225	204
8	10*	-1	20	25*	39	18	41	40	4	38	38
9	21*	29	21	5*	10	19	4*	-7	5	79	73
10	41	34				20	49	4*	6	65	-64

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	1, K=	1	3	30	31				22	5*	0
			9	53	-56	0	13*	-13			
7	102	-100	10	35	-34	1	63	63	H=	2, K=	10
8	31	31	11	3*	-4	2	97	-8*			
9	11*	-23	12	13*	-16	3	87	95	0	15*	-12
10	25	20	13	62	62	4	54	-55	1	8*	-26
11	97	89	14	77	75	5	64	66	2	40	38
12	25	-23	15	12*	10	6	52	49	3	71	74
13	73	76	16	95	90	7	55	-55	4	4*	-19
14	62	-50	17	54	-56	8	24	-23	5	29	37
15	11*	-19	18	17*	15	9	120	-122	6	46	-45
16	42	38	19	25	-22	10	3*	4	7	16*	-9
17	77	-74	20	50	-47	11	4*	1	8	13*	-25
18	27	-24	21	21*	16	12	4*	5	9	63	-52
19	64	-35	22	25*	-37	13	65	63	10	21*	16
20	37	37	23	25	19	14	4*	-5	11	19*	9
21	4*	17	24	37	39	15	41	40	12	4*	-9
22	34	33	25	54	15	16	13*	16	13	63	56
23	79	84	26	29*	37	17	45	-35	14	16*	10
24	28	-23				18	20	26	15	29	19
25	5*	-8	H=	2, K=	4	19	55	-51	16	9*	-2
26	13*	-27				20	5*	1	17	44	-50
27	3*	-57	0	71	58	21	5*	6	18	11*	-16
			1	163	-168	22	33	-20	19	5*	-14
H=	2, K=	0	2	-1	44	23	62	73	20	5*	1
			3	3*	4	24	5*	-4			
0	213	200	4	21	21				H=	2, K=	12
2	154	156	5	13*	-14	H=	2, K=	1			
4	73	61	6	100	-97				0	27	-25
6	97	-3*	7	55	62	0	3*	-2	1	26	-29
8	127	105	8	3*	2	1	27	24	2	25*	-40
10	173	155	9	115	108	2	21*	34	3	13*	-15
12	71	71	10	24	24	3	90	-90	4	25	11
14	157	-144	11	67	65	4	7*	0	5	4*	15
16	124	-114	12	34	34	5	47	-46	6	32	28
18	14*	-15	13	104	-101	6	33	37	7	5*	16
20	85	67	14	35*	-39	7	90	95	8	6*	11
22	23	25	15	12*	-10	8	16*	-22	9	43	45
24	25*	-40	16	10	-30	9	75	74	10	43	-41
25	41	-60	17	45	40	10	13*	-6	11	26*	19
			18	22*	-23	11	39	-35	12	39	-35
H=	2, K=	2	19	33	37	12	4*	-7	13	26	-28
			20	45	44	13	64	-70	14	5*	2
0	113	-112	21	13*	-20	14	6*	5	15	18*	-21
1	11*	4	22	43	52	15	11*	-2	16	21*	18
2	77	-73	23	37	-47	16	35	-34			
3	105	74	24	3*	-22	17	45	35	H=	2, K=	14
4	57	52	25	13*	-26	18	19*	7			
5	59	-55	26	45	-50	19	45	46	0	38	33
6	15*	16				20	16*	0	1	5*	-4
7	153	143	H=	2, K=	6	21	5*	-4	2	12*	20

L	FJ	FC	L	FJ	FC	L	FJ	FC	L	FJ	FC
3	5*	9	4	4*	1	3	21	28	25	29	-30
4	23*	-32	5	4*	-13	4	3*	-9	26	18*	31
5	5*	13	6	50	-54	5	20	-21			
6	22*	-19	7	15*	14	6	56	-59	H=	3, K=	1
7	12*	-22	8	56	-56	7	36	39			
8	5*	-12	9	28	27	3	39	-40	0	69	-70
9	23*	-17	10	31	30	0	24	-15	1	31	-27
			11	54	51	10	54	52	2	88	86
H=	3, K=	13	12	49	50	11	25	-29	3	220	212
			13	20*	-20	12	10*	106	4	122	117
0	21*	-8	14	4*	-9	13	62	56	5	174	164
1	5*	-12	15	10*	-3	14	20*	-12	6	36	-34
2	5*	13	16	59	-61	15	63	61	7	59	-55
3	46	-49	17	5*	-14	16	45	-44	8	31	-29
4	12*	-19	18	5*	-7	17	34	-36	9	113	-108
5	25*	-28	19	13*	-11	18	35	-32	10	30	23
6	30	-22	20	7*	19	19	54	-60	11	131	116
7	23	21	21	14*	-8	20	37	50	12	6*	9
8	19*	-14				21	36	-34	13	120	110
9	30	34	H=	3, K=	7	22	55	56	14	3*	-13
10	25*	25				23	47	4*	15	4*	15
11	5*	-2	0	145	-151	24	17*	-11	16	26	-24
12	26	25	1	83	33	25	33	39	17	50	-47
			2	4*	-43				18	14*	4
H=	3, K=	11	3	3-	-3	H=	3, K=	3	19	69	-68
			4	20	29				20	51	49
0	19*	-4	5	3*	-2	0	142	139	21	28	-25
1	25	-12	6	65	67	1	24	24	22	13*	26
2	33	-29	7	41	43	2	36	28	23	34	40
3	29	29	8	67	67	3	12*	7	24	21*	18
4	4*	-2	9	4*	8	4	71	67	25	19*	6
5	37	24	10	47	-50	5	19*	-20	26	5*	-6
6	63	71	11	4*	-3	6	37	41			
7	4*	-5	12	-1	-30	7	33	32	H=	4, K=	0
8	31	37	13	57	-54	8	14*	19			
9	43	-48	14	30	33	9	97	88	0	9*	-13
10	25*	-12	15	3*	-17	10	80	-20	2	116	-117
11	15*	-10	16	48	53	11	15*	12	4	100	92
12	50	-60	17	3*	11	12	17*	-20	6	27	-32
13	37	32	18	4*	14	13	54	-79	8	21	-25
14	5*	-5	19	54	-2	14	4*	3	10	93	91
15	22*	11	20	9*	-21	15	65	-69	12	132	147
16	19*	25	21	30	17	16	59	57	14	110	-109
17	27*	-31	22	33	-32	17	4*	-6	16	91	-94
			23	22*	14	18	4*	13	13	55	-57
H=	3, K=	9				19	64	62	20	18*	19
			H=	3, K=	5	20	44	-46	22	48	48
0	70	78				21	16*	-9	24	20*	19
1	15*	-14	0	35	36	22	36	-3*	25	42	-47
2	85	87	1	25	-25	23	50	-60			
3	4*	5	2	16*	22	24	5*	13	H=	4, K=	2

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	4, K=	2	19	40	41	14	4*	-9	0	29*	33
0	163	-164	20	21*	22	15	12*	-1*	1	5*	-22
1	112	-107	21	16*	-1*	16	5*	-10	2	34	36
2	142	-144	22	60	56	17	5*	16	3	5*	-4
3	51	-49	23	23*	-27	18	12*	-9	4	5*	-1
4	17*	23	24	3*	-9	19	39	48	5	5*	12
5	66	64	25	17*	-26	20	14*	-25	6	36	-30
6	61	81	H=	4, K=	6	21	14*	17	H=	5, K=	13
7	23	31				H=	4, K=	10			
8	33	84	0	33	-31				0	5*	-15
9	75	-79	1	37	-34	0	14*	0	1	10*	27
10	103	-100	2	102	-101	1	23*	-30	2	5*	25
11	26	25	3	102	105	2	75	77	3	23*	-26
12	65	-67	4	35	-31	3	12*	14	4	5*	8
13	56	50	5	3*	8	4	17*	22	5	49	-30
14	11*	0	6	75	82	5	40	42	6	21*	-19
15	22*	16	7	3*	3	6	24*	-30	7	12*	-1
16	85	74	8	15*	9	7	4*	1	8	24*	-12
17	4*	-12	9	35	-37	8	12*	-28	9	33	37
18	45	41	10	48	-43	9	53	-47	10	5*	20
19	9*	14	11	39	-34	10	26*	-26	H=	5, K=	11
20	7*	-9	12	73	-71	11	20*	-37			
21	24	-3	13	4*	5	12	19*	12	0	17*	-13
22	56	-52	14	5*	-13	13	51	53	1	14*	-12
23	5*	-1	15	78	32	14	5*	0	2	9*	-13
24	5*	3	16	15*	19	15	35	35	3	15*	-22
25	23*	22	17	4*	-11	16	19*	-27	4	4*	-9
26	47	48	18	39	44	17	5*	-2	5	4*	20
H=	4, K=	4	19	53	-54	18	15*	-27	6	37	46
0	3*	-14	20	11*	1	H=	4, K=	12	7	32	20
1	6*	-5	21	25	-27	0	4*	-23	8	30	31
2	34	91	22	23	-35	1	4*	0	9	24*	-35
3	42	-45	23	41	47	2	20*	-21	10	21*	13
4	27	23	H=	4, K=	8	3	26	-31	11	19*	-21
5	65	-65	0	17*	17	4	20*	-30	12	29	-33
6	39	-34	1	4*	-14	5	15*	-24	13	29	29
7	10*	5	2	17*	-7	6	40	35	14	16*	-10
8	47	-45	3	43	-44	7	11*	0	15	29	28
9	79	78	4	21*	-3	8	20*	21	H=	5, K=	9
10	45	41	5	77	-77	9	34	35			
11	99	84	6	4*	2	10	21*	-19	0	7*	14
12	54	53	7	27	14	11	23*	31	1	4*	7
13	42	-41	8	10*	14	12	54	-50	2	50	60
14	33	35	9	55	65	13	7*	-19	3	29	32
15	27	-25	10	4*	8	14	5*	7	4	23	18
16	63	-60	11	27	27	H=	4, K=	14	5	4*	-9
17	1*	17	12	12*	14				6	29	-27
18	76	-80	13	36	-37				7	12*	-13

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
8	59	-54	10	31	25	5	119	-115	11	49	-53
9	29	34	11	45	-42	6	41	-36	12	50	-57
10	11*	3	12	72	59	7	7*	-1	13	15*	15
11	31	20	13	55	53	8	9*	-6	14	51	-45
12	63	63	14	35	-32	9	53	-85	15	71	73
13	28	-23	15	53	57	10	30	-29	16	23*	26
14	5*	11	16	3*	-20	11	11*	10	17	4*	-6
15	5*	1	17	14*	14	12	4*	12	18	31	34
16	40	-45	18	37	-30	13	59	59	19	8*	-3
17	10*	11	19	12*	-10	14	22*	19	20	33	33
18	39	-43	20	12*	15	15	93	52	21	22*	-29
19	11*	19	21	31	-25	16	16*	-12	22	29*	-36
			22	55	57	17	42	39	23	25*	22
H=	5, K=	7	23	3*	13	18	18*	-34	24	10*	-11
						19	56	-61			
0	65	-69	H=	5, K=	3	20	13*	15	H=	5, K=	4
1	3*	-12				21	52	-59			
2	46	-52	0	32	81	22	17*	12	0	45	41
3	20	-5	1	3*	-3	23	22*	11	1	32	34
4	21*	-19	2	123	-120	24	16*	9	2	89	87
5	33	-35	3	38	-31	25	34	31	3	17*	19
6	37	34	4	50	-46				4	94	94
7	13*	23	5	105	-103	H=	5, K=	0	5	46	-46
8	66	78	6	46	48				6	71	-72
9	35	32	7	27	-27	0	52	57	7	37	-34
10	4*	-12	8	50	53	2	53	52	8	59	-60
11	32	33	9	132	118	3	115	108	9	34	41
12	77	-44	10	2*	-12	4	40	32	10	27	-29
13	35	-34	11	104	96	5	153	-141	11	61	58
14	10*	-10	12	4*	2	10	44	-44	12	49	50
15	16*	-15	13	39	-40	12	76	76	13	24	-22
16	60	60	14	29	-29	14	39	39	14	29	38
17	3*	-15	15	52	-60	15	23	-20	15	40	-40
18	23*	27	16	23*	16	18	37	-40	16	5*	7
19	22*	37	17	12*	-4	20	50	-45	17	6*	-14
20	37	-22	18	14*	17	22	16*	16	18	58	-60
21	14*	-3	19	12*	27	23	38	40	19	48	46
22	43	-50	20	22*	-23				20	22*	1
			21	35	30	H=	5, K=	2	21	44	39
H=	5, K=	5	22	24*	-27				22	36	43
			23	25*	-31	0	2*	-24	23	24*	-28
0	47	47	24	23*	14	1	55	-85			
1	3*	-30	25	4*	-4*	2	160	-15*	H=	5, K=	6
2	36	35				3	91	-90			
3	14*	14	H=	5, K=	1	4	100	-99	0	16*	4
4	3*	-8				5	61	-56	1	50	-52
5	51	62	0	79	-59	6	34	38	2	13*	-18
6	8*	-57	1	113	-119	7	52	58	3	61	59
7	8*	68	2	17*	-25	8	100	141	4	32	-35
8	73	-72	3	77	75	9	62	-61	5	67	67
9	73	-81	4	36	36	10	4*	-4	6	20*	14

L	FC	FC	L	FC	FC	L	FC	FC	L	FC	FC
H=	6, K=	6	6	4*	12	10	19*	9			
			7	10*	15	11	23*	-20	0	36	-32
7	4*	-3	8	33	-30	12	16*	-15	1	94	-94
8	46	43	9	76	-55	13	5*	21	2	26	31
9	60	-61	10	26	29				3	50	-42
10	4*	-13	11	35	-39	H=	7, K=	9	4	4*	22
11	26	-24	12	53	54				5	39	42
12	61	-62	13	5*	2	0	28	-20	6	47	-47
13	4*	16	14	15*	15	1	4*	0	7	69	67
14	4*	-14	15	29*	+3	2	4*	13	8	52	-49
15	41	40	16	21*	-25	3	20*	28	9	57	-58
16	32	35	17	15*	-27	4	39	38	10	6*	-20
17	11*	5				5	29	-24	11	40	-39
18	27*	43	H=	6, K=	12	6	26	-20	12	36	34
19	60	-58				7	43*	-25	13	30	35
20	33	-29	0	6*	9	8	87	-86	14	51	51
21	3*	-47	1	27	26	9	14*	22	15	29	37
22	17*	-19	2	5*	-3	10	5*	3	16	4*	6
			3	5*	-11	11	21*	25	17	10*	16
H=	6, K=	8	4	13*	-26	12	50	4*	18	64	-61
0	13*	-3	5	9*	-37	13	30	-33	19	25*	-3
1	46	51	6	22*	14	14	22*	30	20	5*	-14
2	4*	12	7	13*	-12	15	16*	-2	21	16*	-3
3	19*	-25	8	23*	38	16	14*	-17	22	34	46
4	23*	9	9	41	45	17	15*	8			
5	90	-93	10	55*	-5				H=	7, K=	3
6	31	32	11	27*	29	H=	7, K=	7	0	36	34
7	11*	-11	12	33	-42				1	70	69
8	5*	2	H=	7, K=	13	1	14*	-3	2	137	-136
9	30	31				2	4*	-13	3	3*	-10
10	19*	25	3	9*	-27	3	15*	12	4	94	-88
11	64	56	4	26*	31	4	51	-50	5	125	-125
12	14*	7	5	35	37	5	29	-30	6	14*	5
13	4*	-14	6	12*	5	6	24	24	7	36	-87
14	19*	-2	7	18*	17	7	24	-21	8	33	79
15	42	-49	8	25*	-23	8	22	78	9	28	24
16	14*	-15	9	24*	-7	9	21*	-14	10	37	31
17	13*	-20				10	22*	10	11	68	63
18	5*	7	H=	7, K=	11	11	4*	12	12	45	-44
19	58	62				12	57	-54	13	12*	-13
20	1*	-1	1	13*	16	13	4*	-12	14	79	-80
			2	21*	-15	14	38	-30	15	4*	-10
H=	6, K=	10	3	4*	-42	15	14*	-21	16	10*	9
			4	25*	-24	16	5*	-1	17	4*	-24
0	23*	-31	5	29	-32	17	5*	4	18	41	39
1	33	-34	6	13*	8	18	53	54	19	15*	29
2	23*	13	7	16*	30	19	27*	26	20	11*	20
3	15*	7	8	5*	24	20	11*	10	21	30	36
4	30	29	9	31	31				22	39	-45
5	27*	26	0	38	-29	H=	7, K=	5	23	5*	-7

L	F0	FC	L	F0	FC	L	F0	FC	L	F0	FC
			6	43	-99	6	29*	0	12	5*	17
H=	7, K=	-1	7	26	31	7	68	66	H=	8, K=	12
0	15*	-8	8	75	74	8	5*	-	1	32	35
1	81	-36	9	29	-28	9	42	-38	2	23	-8
2	13*	3	10	45	44	10	17*	-18	3	22*	33
3	6*	-59	11	38	-79	11	39	-39	4	5*	-21
4	14*	14	12	44	-45	12	16*	14	5	11*	-24
5	57	57	13	15*	-16	13	33	-35	6	5*	14
6	5*	-11	14	44	-41	14	19*	-19	7	34	-32
7	98	93	15	4*	18	15	14*	28	8	26	25
8	6*	4	16	22*	32	16	19*	16	H=	9, K=	11
9	11*	-3	17	45	44	17	31	34	0	32	29
10	20*	-16	18	52	58	18	17*	31	1	24*	-16
11	61	-61	19	17*	0	19	5*	-3	2	5*	-4
12	35	26	20	35	28	20	5*	-3	3	22*	6
13	21*	-11	21	13*	-25	H=	3, K=	5	4	35	-51
14	8*	15	22	52	-48	0	14*	-9	5	15*	8
15	62	68	H=	4, K=	4	1	73	74	6	16*	-4
16	12*	-11	0	15*	-4	2	6*	3	7	23*	22
17	33	35	1	71	65	3	39	27	8	25*	26
18	39	-36	2	20	82*	4	21*	-27	9	25*	-20
19	29	-22	3	45	45	5	63	-60	H=	9, K=	9
20	37	-33	4	52	46	5	23*	1	0	42	-48
21	65	-59	5	37	-90	6	41	-45	1	4*	-3
22	14*	0	6	10*	1	7	22*	14	2	11*	4
23	11*	7	7	54	-54	8	26	22	3	12*	22
H=	3, K=	0	8	43	-43	9	21*	25	4	22*	-41
0	16*	3	9	4*	11	10	4*	46	5	23*	12
2	37	-35	10	29	-26	11	5*	-6	6	34	-34
4	123	122	11	60	69	12	5*	23	7	26	20
5	29	26	12	14*	-16	13	13*	4	8	19*	-16
8	65	-67	13	7*	10	14	19*	-24	9	10*	6
10	45	-47	14	47	41	15	21*	13	10	47	53
12	35	82	15	13*	-17	16	43	-55	H=	9, K=	7
14	27	37	16	23*	-24	17	43	-55	0	71	74
16	5*	11	17	33	-32	H=	4, K=	10	1	27	22
18	74	-75	18	33	-35	0	30	-39	2	23	20
20	45	-51	19	15*	7	1	31	-33	3	19*	26
22	3*	32	20	5*	-7	2	4*	-8	4	57	-56
H=	3, K=	2	21	47	52	3	15*	-16	H=	9, K=	7
0	78	78	H=	5, K=	6	4	5*	2	0	71	74
1	23	-15	0	43	48	5	36	35	1	27	22
2	15*	-16	1	62	-60	6	5*	1	2	23	20
3	27	-22	2	33	-29	7	31	27	3	19*	26
4	103	-107	3	4*	10	8	12*	-10	4	57	-56
5	4*	0	4	23	-33	9	24*	-30			
			5	59	62	10	15*	16			
						11	25*	-39			

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= 9, K= 7			10	28	27				1	59	-53
5	18*	12	11	46	42	H= 10, K= 2			2	20*	-14
6	13*	-25	12	24*	-27				3	35	-37
7	7*	7	13	9*	-2	0	61	5*	4	4*	-24
8	61	63	14	47	-50	1	4*	-5	5	4*	14
9	27	-30	15	37	-37	2	5*	2	6	32	-25
10	35	30	16	13*	-21	3	44	-41	7	52	55
11	23*	-24	17	54	-55	4	55	-40	8	16*	-19
12	11*	4	18	55	51	5	5*	21	9	19*	15
13	19*	-13	19	5*	9	6	63	-61	10	11*	8
14	18*	-23	20	23*	28	7	73	-68	11	27*	-23
15	1*	-18	21	44	51	8	46	46	12	5*	4
16	10*	-23	H= 9, K= 1			9	57	-52	13	37	-41
17	5*	-10				10	48	48	14	29	-31
			0	18*	6	11	38	-40	15	8*	2
H= 9, K= 5			1	40	-40	12	4*	4	16	20*	-6
			2	31	26	13	4*	7	17	35	38
0	4*	-50	3	31	-30	14	64	-70			
1	5*	-55	4	37	35	15	5*	4	H= 10, K= 9		
2	4*	1	5	12*	15	16	42	-39			
3	40	-39	6	4*	-14	17	22*	21	0	23*	-23
4	105	103	7	33	75	18	52	50	1	6*	-9
5	4*	3	8	18*	13	19	17*	16	2	22*	-17
6	21*	22	9	44	35	20	45	58	3	45	44
7	11*	21	10	8*	-4	H= 10, K= 4			4	28	-27
8	7*	-71	11	37	-91				5	11*	4
9	44	-43	12	25	23	0	33	-24	6	6*	-12
10	37	-33	13	39*	-32	1	25	26	7	29*	-21
11	4*	-11	14	29*	25	2	37	39	8	5*	6
12	9*	20	15	59	59	3	90	87	9	12*	-15
13	13*	-11	16	13*	23	4	75	79	10	5*	10
14	5*	3	17	74	80	5	35	-35	11	29	34
15	31	34	18	23	-24	6	27	21	12	15*	-7
16	17*	20	19	31	-23	7	73	-70	13	42	48
17	25*	22	20	12*	-2	8	34	-27	14	5*	10
18	5*	-13	21	47	-57	9	4*	16	H= 10, K= 10		
19	3*	0				10	24*	-24			
			H= 10, K= 0			11	45	46	0	5*	-13
H= 9, K= 3						12	9*	12	1	8*	-17
			0	30	-25	13	5*	-15	2	5*	14
0	55	50	2	49	-42	14	32	34	3	32	-32
1	55	62	4	54	50	15	5*	-1	4	5*	1
2	21	-11	5	32	38	16	17*	18	5	5*	16
3	72	80	8	45	-43	17	37	-35	6	14*	14
4	48	-48	10	63	-65	18	37	-43	7	33	40
5	65	-66	12	14*	27	19	5*	-5	8	5*	-7
6	4*	-12	14	78	76				9	5*	-3
7	81	-77	15	45	44	H= 10, K= 6			10	15*	-27
8	29	35	18	58	-62						
9	4*	7	20	44	-62	0	25	30	H= 11, K= 11		

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
			14	35	30	4	64	50	2	18*	-4
0	25*	34	15	5*	2	6	39	39	3	68	-63
			16	31	32	8	23*	-35	4	14*	-15
H=	11, K=	9				10	18*	-25	5	33	-27
			H=	11, K=	3	12	43	-41	6	17*	-14
0	40	-37				14	5*	11	7	75	77
1	5*	-2	0	22*	22	16	68	74	8	5*	-12
2	23	-23	1	32	26				9	56	51
3	13*	29	2	5*	2	H=	12, K=	2	10	36	30
4	31	33	3	68	68				11	18*	-22
5	12*	16	4	4*	2	0	49	51	12	23*	5
6	17*	27	5	15*	12	1	33	-36	13	50	-49
7	5*	3	6	21*	-19	2	15*	20			
8	1*	-15	7	45	-40	3	12*	-9	H=	12, K=	8
9	13*	-10	8	34	36	4	22*	-27			
10	48	-49	9	40	-30	5	25	24	0	13*	-6
			10	4*	6	6	32	-35	1	24*	-13
H=	11, K=	7	11	33	31	7	25	23	2	20*	18
			12	16*	-12	8	16*	31	3	42	41
0	3*	41	13	33	39	9	29	-27	4	5*	-2
1	4*	-3	14	19*	-26	10	16*	25	5	19*	14
2	56	58	15	23*	-11	11	22*	5	6	10*	2
3	37*	31	16	5*	-4	12	37	35	7	12*	-20
4	45	-46	17	51	-60	13	16*	-14	8	12*	-10
5	14*	-7				14	17*	-25	9	40	-40
6	39	-40	H=	11, K=	1	15	9*	-3			
7	10*	7				15	51	-51	H=	12, K=	10
8	30	32	0	7*	10						
9	11*	-9	1	55	-54	H=	12, K=	4	0	5*	-21
10	44	52	2	4*	9				1	22*	-20
11	10*	15	3	57	-55	0	14*	-23			
12	5*	13	4	4*	15	1	13*	-17	H=	13, K=	9
13	5*	-2	5	22*	19	2	16*	-12			
14	35	-32	6	11*	-6	3	56	59	0	41	-39
			7	66	63	4	55	55			
H=	11, K=	5	8	15*	-25	5	18*	17	H=	13, K=	7
			9	23*	15	6	54	58			
0	31	-27	10	12*	-17	7	45	-42	0	35	39
1	13*	4	11	17*	-17	8	25*	22	1	15*	15
2	21*	-17	12	24*	27	9	23*	-17	2	38	49
3	22*	-13	13	55	-55	10	47	-43	3	1*	-3
4	65	65	14	25	25	11	5*	16	4	20*	-5
5	19*	7	15	5*	-5	12	15*	-14	5	11*	-2
6	45	44	16	17*	13	13	20*	24	6	43	-46
7	27	22	17	74	76	14	37	40	7	5*	6
8	50	-50	18	5*	2	15	12*	3	8	5*	-3
9	10*	17									
10	42	-44	H=	12, K=	0	H=	12, K=	6	H=	13, K=	5
11	21*	-23									
12	2*	-3	0	55	-54	0	18*	10	0	45	-37
13	30	-30	2	45	-42	1	8*	-5	1	21*	-17

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= 13, K= 0			2	95	-13				-15	34	35
			3	96	48	H= 15, K= 3			-17	83	80
2	55	-54	4	94	53				-18	4*	-1
3	44	-51	5	27*	27	0	5*	6	-19	6*	6
4	37	20	6	35	-35	1	21*	-25	-20	4*	11
5	5*	1	7	51	-61	2	10*	14	-21	54	-51
6	45	46				3	33	33	-22	16*	15
7	51	52	H= 14, K= 2			4	12*	-2	-24	13*	-4
8	15*	15				5	28*	28	-25	43	39
9	20*	34	0	39	34	6	31	-20	-26	28*	-29
10	27*	-35	1	43	40	7	5*	2	-27	64	66
11	12*	0	2	37	42						
			3	3*	1	H= 15, K= 1			H= 1, K= 3		
H= 13, K= 3			4	25*	-21	0	5*	0	-1	198	202
			5	5*	-5	1	35*	36	-2	147	-145
0	4*	5	6	50	-53	2	23	-17	-3	69	74
1	4*	0	7	7*	-3	3	47	-50	-4	85	95
2	4*	9	8	24*	-15	4	10*	4	-5	71	-73
3	74	68	9	12*	7	5	54	-53	-6	98	100
4	14*	-9	10	22*	13	6	16*	6	-7	22*	-24
5	10*	11	11	7*	14	7	13*	2	-8	3*	1
6	17*	-27				8	20*	17	-9	26	25
7	32	-35	H= 14, K= 4						-10	61	-69
8	16*	-19				H= 15, K= 0			-11	45	52
9	27	-27	0	34	-37				-12	24*	27
10	5*	-3	1	5*	-23	0	17*	-7	-13	128	139
11	5*	3	2	20*	-29	2	53	-53	-14	26*	25
12	29	28	3	25*	22				-15	8*	-17
13	32	29	4	15*	4	H= 15, K= 2			-16	4*	25
			5	14*	6				-17	92	-87
H= 13, K= 1			6	45	51	0	5*	4	-18	4*	-15
			7	18*	9	1	11*	17	-19	23*	-14
0	4*	2	8	25*	25				-20	23*	-8
1	6*	-7	9	25*	-24	H= 11, K= 1			-21	33	26
2	22*	-7							-22	54	-63
3	45	-49	H= 14, K= 6			-1	192	-194	-23	5*	6
4	14*	-1				-2	15*	-33	-24	14*	-2
5	14*	-9	0	15*	9	-3	146	-160	-25	35	-37
6	6*	2	1	45*	2	-4	123	-146	-26	25*	24
7	3*	29	2	12*	-4	-5	61	63	-27	59	-51
8	7*	3	3	15*	-36	-6	54	-65			
9	37	35	4	21*	-7	-7	124	135	H= 1, K= 5		
10	17*	-6	5	42	-36	-8	55	55			
11	5*	5	6	5*	-11	-9	107	110	-1	81	-83
12	17*	-12				-10	36	-30	-2	42	-40
13	52	-54	H= 15, K= 5			-11	136	-134	-3	171	-114
14	5*	1				-12	22*	-16	-4	40	-38
			0	5*	-5	-13	99	-95	-5	73	78
H= -14, K= 0			1	5*	-12	-14	16*	2	-6	83	-86
			2	34	-34	-15	24*	-28	-7	3*	2
0	35	-37	3	27	-30						

L	F1	FC	L	F1	FC	L	F1	FC	L	F1	FC
-8	21*	16	-3	31	-23	-3	5*	2	-13	31*	-35
-9	26*	31	-4	10*	-10*	-7	10*	-10	-14	32	-24
-10	10*	10*	-5	43	-39	-10	10*	24	-15	35	30
-11	3*	3	-6	22*	-24	-11	31*	42	-16	30*	16
-12	37	28	-7	30	37	-12	16*	6	-17	41	36
-13	22*	-21	-8	45	51	-13	33	35	-18	27*	32
-14	90	-95	-9	51	33				-19	5*	-1
-15	19*	-19	-10	54	51	H=	2, K=	14	-20	30*	20
-16	19*	9	-11	26*	-32						
-17	54	43	-12	13*	-27	-1	10*	-14	H=	2, k=	8
-18	47	33	-13	3*	30	-2	3*	-3			
-19	29*	-31	-14	43	-46	-3	22*	6	-1	99	97
-20	21*	19	-15	22*	-4	-4	4*	-41	-2	49	50
-21	21*	-30	-16	5*	-16	-5	5*	10	-3	19*	25
-22	17*	-6	-17	32*	-36	-6	7*	3	-4	4*	-30
-23	5*	13	-18	51	52	-7	14*	22	-5	21*	19
-24	55	-54	-19	33*	-20	-8	27*	27	-6	33	-32
-25	20*	22	-20	51	52	-9	20*	4	-7	80	-84
-26	30*	-22	-21	24*	6				-8	25*	16
			-22	23*	-11	H=	2, K=	12	-9	4*	7
H=	1, K=	7							-10	4*	-6
			H=	1, K=	11	-1	10*	10	-11	56	55
-1	18*	16				-2	8*	24	-12	15*	-15
-2	3*	-3	-1	55	-55	-3	30	31	-13	37	37
-3	32	35	-2	24*	17	-4	21*	20	-14	26*	23
-4	57	56	-3	33	-35	-5	30	-29	-15	50	-52
-5	35	38	-4	23*	32	-6	21*	12	-16	18*	-1
-6	22*	11	-5	35	31	-7	27*	-30	-17	26	-34
-7	3*	2	-6	40	37	-8	11*	-19	-18	22*	-17
-8	46	-53	-7	5*	8	-9	5*	-4	-19	26*	-16
-9	11*	11	-8	45	-42	-10	12*	2	-20	9*	-5
-10	69	-71	-9	14*	12	-11	17*	32	-21	69	55
-11	19*	-2	-10	37	-33	-12	12*	19	-22	16*	-14
-12	28*	-21	-11	5*	7	-13	5*	20	-23	31*	36
-13	21*	-25	-12	10*	4	-14	51	45			
-14	85	80	-13	5*	-5	-15	16*	-10	H=	2, K=	5
-15	31	-2	-14	29*	28						
-16	37	32	-15	5*	7	H=	2, K=	10	-1	55	-60
-17	3*	-6	-16	23*	1				-2	61	60
-18	55	-51	-17	28*	27	-1	61	-60	-3	106	-112
-19	19*	-34	-18	5*	-7	-2	25*	-20	-4	6*	10
-20	63	-52				-3	4*	-24	-5	96	101
-21	25*	15	H=	1, K=	13	-4	7*	-4	-6	31	38
-22	30*	16				-5	65	62	-7	134	147
-23	31*	-3	-1	5*	7	-6	26*	22	-8	36	-35
-24	49	55	-2	3*	0	-7	53	52	-9	11*	20
			-3	5*	2	-8	4*	3	-10	9*	-12
H=	1, K=	9	-4	25*	-14	-9	12*	-10	-11	89	-82
			-5	7*	-19	-10	13*	19	-12	8*	15
-1	59	54	-6	16*	-27	-11	64	-57	-13	4*	4
-2	20*	16	-7	55	-54	-12	17*	-10	-14	34	36

	U	F	FC	L	FC	FC	L	FC	FC	L	FC	FC
H=	2	K=	5	-7	3*	-16	-12	33	30	-3	10*	14
				-4	101	-103	-13	77	-73	-4	164	-169
-15	39	42	-9	55	51	-14	15*	-3	-5	99	99	
-16	25*	-15	-10	140	-141	-15	72	75	-6	61	61	
-17	34	34	-11	5*	6	-16	19*	21	-7	18*	-19	
-18	26*	7	-12	3*	2	-17	54	60	-8	125	131	
-19	5*	-29	-13	15*	-9	-18	4*	11	-9	61	-66	
-20	46	-40	-14	121	124	-19	76	-76	-10	2*	26	
-21	26*	-32	-15	13*	-4	-20	23*	22	-11	46	-48	
-22	7*	5	-16	57	60	-21	4*	-24	-12	28	-31	
-23	33*	-33	-17	41	45	-22	9*	15	-13	19*	14	
-24	16*	23	-18	82	-81	-23	5*	-7	-14	57	-59	
-25	5*	23	-19	4*	-9	-24	15*	-4	-15	4*	16	
			-20	5*	-24	-25	41	40	-16	4*	1	
H=	2	K=	4	-21	17*	-1	-26	5*	3	-17	29*	32
			-22	2*	15	-27	35	44	-18	45	39	
			-23	33	-35				-19	5*	1	
-2	205	-201	-24	41	43	H=	3	K=	3	-20	5*	18
-3	134	144	-25	5*	-5				-21	5*	-23	
-4	23	-16	-26	15*	7	-1	68	72	-22	19*	-20	
-5	52	-60	-27	7*	10	-2	58	56	-23	5*	2	
-6	3*	-7				-3	59	56	-24	27*	-17	
-7	61	-67	H=	2	K=	0	-4	55	57	-25	34*	33
-8	93	109				-5	49	-49	-26	26*	-6	
-9	3*	-13	-2	25	-21	-6	9*	-6				
-10	75	78	-4	155	-158	-7	75	-82	H=	3	K=	7
-11	23*	8	-5	31	-34	-8	3*	12				
-12	14*	-7	-8	3*	-3	-9	35	42	-1	93	84	
-13	54	49	-10	25	-24	-10	54	-59	-2	71	72	
-14	100	-98	-12	3*	13	-11	121	125	-3	59	-65	
-15	22*	-26	-14	163	-165	-12	29	42	-4	148	154	
-16	13*	1	-16	55	-66	-13	44	51	-5	3*	-14	
-17	29*	-32	-18	69	65	-14	29	21	-6	33	-27	
-18	4*	0	-20	43	38	-15	32	-72	-7	5*	-7	
-19	4*	10	-22	53	-71	-16	22*	-4	-8	123	-122	
-20	4*	1	-24	37	-40	-17	75	-70	-9	18*	25	
-21	27*	25	-26	5*	12	-18	49	-47	-10	4*	-18	
-22	5*	-21				-19	4*	3	-11	11*	-11	
-23	11*	21	H=	3	K=	1	-20	12*	-18	-12	24*	21
-24	5*	-24				-21	34	26	-13	14*	21	
-25	24*	-12	-1	73	-53	-22	23*	-21	-14	87	86	
-26	14*	-9	-2	109	-117	-23	44	-29	-15	17*	-21	
			-3	50	-34	-24	33*	39	-16	29*	23	
H=	2	K=	2	-4	57	62	-25	36	-32	-17	23*	-26
			-5	52	54	-26	5*	5	-18	59	-58	
-1	89	-89	-6	50	-53	-27	19*	-24	-19	36	-30	
-2	23	24	-7	3*	-5				-20	32*	-40	
-3	113	-121	-8	31	-21	H=	3	K=	5	-21	25*	21
-4	113	129	-9	27	30				-22	47	49	
-5	111	121	-10	31	24	-1	67	-67	-23	19*	21	
-6	60	-62	-11	121	-121	-2	30	-27	-24	45	46	

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
			-3	21*	6	-1	22*	-32	-11	101	-37
H=	3, K=	9	-4	13*	-15	-10	10*	1*	-12	48	-45
			-5	21*	-25	-11	41	-45	-13	23*	-14
-1	43	42	-6	18*	-2	-12	30*	-21	-14	32	39
-2	75	-79	-7	37	-33	-13	13*	0	-15	53	49
-3	5*	0	-8	15*	1	-14	14*	7	-16	29*	-11
-4	95	-89	-9	23*	14	-15	21*	22	-17	15*	24
-5	4*	7	-10	17*	21	-16	24*	8	-18	18*	-20
-6	4*	-1	-11	51	48	-17	16*	1*	-19	53	-34
-7	4*	3	-12	17*	-25	-18	20*	11	-20	13*	-17
-8	77	85	-13	5*	11	-19	17*	-27	-21	46	-49
-9	6*	-2				-20	5*	-21	-22	5*	-4
-10	43	53	H=	4, K=	14				-23	30*	-27
-11	30*	-41				H=	4, K=	8	-24	26*	16
-12	18*	-10	-1	7*	-1				-25	52	44
-13	12*	8	-2	29*	-20	-1	92	95			
-14	37	-35	-3	5*	3	-2	13*	-12	H=	4, K=	4
-15	20*	-35	-4	41	-33	-3	20*	-13			
-16	6*	6	-5	14*	7	-4	25*	25	-1	60	60
-17	6*	-15	-6	12*	0	-5	92	-92	-2	104	-109
-18	54	55	-7	16*	20	-6	4*	24	-3	3*	-4
-19	5*	8	-8	29*	26	-7	53	-55	-4	32	-34
-20	37	42				-8	23*	-22	-5	60	-68
-21	25*	25	H=	4, K=	12	-9	46	38	-6	3*	4
-22	5*	-22				-10	4*	-12	-7	5*	-17
			-1	20*	26	-11	71	70	-8	109	109
H=	3, K=	11	-2	35	59	-12	4*	-8	-9	86	91
			-3	10*	-1	-13	4*	5	-10	43*	15
-1	54	-66	-4	33	35	-14	6*	-8	-11	3*	-2
-2	38	33	-5	13*	-22	-15	101	-92	-12	78	-80
-3	17*	25	-6	5*	17	-16	34	-31	-13	11*	4
-4	35	19	-7	21*	-20	-17	41	-45	-14	78	-75
-5	20	1*	-8	5*	-18	-18	5*	3	-15	71	-70
-6	40	33	-9	40	25	-19	44	48	-16	29*	31
-7	15*	-14	-10	23*	-16	-20	18*	10	-17	38	-44
-8	36	-36	-11	23*	24	-21	64	60	-18	4*	-9
-9	7*	-4	-12	9*	12	-22	5*	-3	-19	26*	1*
-10	43	-35	-13	24*	-14	-23	19*	19	-20	16*	-10
-11	30	28	-14	22*	25				-21	47	50
-12	34	21	-15	30*	-33	H=	4, K=	5	-22	5*	-2
-13	21*	12							-23	34	-25
-14	43	39	H=	4, K=	10	-1	35	-34	-24	23*	-5
-15	41	34				-2	52	47	-25	25*	-23
-16	20*	-20	-1	76	-93	-3	26	19	-26	18*	11
-17	5*	11	-2	17*	-22	-4	3*	1*			
-18	20*	-27	-3	4*	-3	-5	121	130	H=	4, K=	2
			-4	25*	-50	-6	13*	19			
H=	3, K=	13	-5	89	81	-7	29	42	-1	103	-165
			-6	25*	-2	-8	35	-28	-2	57	-67
-1	37	30	-7	35	36	-9	4*	-15	-3	63	-62
-2	5*	10	-8	4*	-3	-10	11*	-5	-4	57	65

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H=	4, K=	2	-5	3*	13	-1	42	-47	H=	5, K=	9
			-7	91	-88	-2	72	-76			
-5	161	156	-10	3*	17	-3	28	-31	-1	31	34
-6	79	-30	-11	117	-118	-4	31	-34	-2	60	-60
-7	55	-30	-12	15*	32	-5	77	84	-3	10*	15
-8	34	-85	-13	17*	13	-5	64	73	-4	69	-66
-9	18*	-26	-15	82	93	-7	55	-53	-5	39	-45
-10	24*	-32	-16	37	35	-8	55	48	-6	33	43
-11	80	73	-17	23*	14	-9	59	-62	-7	39	-36
-12	97	101	-18	4*	1-8	-10	63	-62	-8	46	50
-13	3*	13	-19	40	-40	-11	54	-61	-9	30	24
-14	107	104	-20	21*	-5	-12	44	-39	-10	34	41
-15	47	-53	-21	35	-35	-13	31	21	-11	14*	-3
-16	4*	2	-22	19*	-22	-14	27*	-31	-12	21*	-22
-17	51	45	-23	5*	13	-15	16*	24	-13	5*	-2
-18	62	-66	-24	5*	19	-16	17*	19	-14	5*	-20
-19	29*	-14	-25	33*	35	-17	71	64	-15	5*	-11
-20	21*	3	-26	5*	11	-18	48	52	-16	29*	23
-21	40	-23	-27	5*	29	-19	5*	-19	-17	5*	-3
-22	351	35				-20	25*	-7	-18	50	44
-23	5*	24	H=	5, K=	3	-21	5*	-2	-19	17*	16
-24	25*	27				-22	46	-4	-20	5*	-6
-25	26*	7	-1	129	127	-23	5*		-21	9*	10
-26	7*	-12	-2	69	70	-25	37	41			
-27	29*	-7	-3	15*	19				H=	5, K=	11
			-4	4*	3	H=	5, K=	7			
H=	4, K=	0	-5	73	-104				-1	17*	-9
			-6	54	-55	-1	19*	30	-2	56	60
-2	102	-93	-7	21*	-15	-2	67	71	-3	10*	4
-4	78	-99	-8	13*	-8	-3	28	34	-4	8*	11
-6	23	-25	-9	92	91	-4	93	101	-5	61	68
-8	54	55	-10	3*	9	-5	20*	16	-6	10*	-26
-10	21*	-24	-11	65	54	-6	42	-42	-7	39	32
-12	18*	-9	-12	4*	18	-7	21*	-32	-8	52	-56
-14	12*	-115	-13	18*	-16	-8	56	-57	-9	30*	-24
-16	17*	30	-14	19*	10	-9	22*	5	-10	5*	-3
-18	91	102	-15	81*	-81	-10	20*	9	-11	32	-34
-20	74*	17	-16	71	-69	-11	4*	-3	-12	19*	20
-22	65	-86	-17	27*	-35	-12	45	48	-13	5*	11
-24	24*	-20	-18	13	-56	-13	27*	-31	-14	17*	26
-26	13*	-1	-19	40	35	-14	21*	23	-15	23*	23
			-20	10*	13	-15	31*	-25	-16	33	-33
H=	5, K=	1	-21	22*	12	-16	33	32	-17	5*	12
			-22	55	60	-17	14*	10			
-1	31	-35	-23	5*	-8	-18	64	-74	H=	5, K=	13
-2	20	-21	-24	5*	14	-19	5*	24			
-3	7*	10	-25	5*	-30	-20	19*	3	-1	38	58
-4	34	35	-26	5*	-6	-21	37	34	-2	23*	-32
-5	41	47				-22	46	47	-3	5*	-1
-6	39	-40	H=	5, K=	5	-23	5*	0	-4	18*	-8
-7	27	22							-5	18*	-27

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
-6	27*	24	-5	75	-76	-4	19*	-20			
-7	31	-8	-6	4*	-12	-3	94	-101	H=	5, K=	0
-8	5*	18	-7	53	-60	-5	44	49			
-9	15*	16	-8	1*	-18	-7	15*	2	-2	96	-101
-10	5*	-7	-9	23*	21	-3	33	39	-4	8*	-17
-11	21*	32	-10	4*	7	-9	93	92	-6	66	69
			-11	50	55	-10	4*	-24	-3	165	164
H=	6, K=	12	-12	13*	-3	-11	17*	-20	-10	91	-79
			-13	5*	6	-12	67	-69	-12	52	-46
-1	33	32	-14	5*	-15	-13	23*	-29	-14	26*	-44
-2	39	38	-15	60	-60	-14	15*	-27	-15	58	76
-3	15*	-23	-16	5*	-14	-15	48	-51	-13	41	61
-4	5*	22	-17	17*	17	-16	43	45	-20	19*	21
-5	50	-51	-18	21*	9	-17	18*	7	-22	60	-86
-6	15*	-27	-19	50	66	-18	4*	24	-24	10*	-29
-7	5*	24	-20	10*	-2	-19	32	31	-26	27*	22
-8	34	-33	-21	5*	23	-20	19*	-6			
-9	28*	29	-22	13*	-1	-21	25*	27	H=	7, K=	1
-10	5*	10				-22	17*	-8			
-11	21*	-10	H=	5, K=	6	-23	37	-38	-1	33	-34
-12	32	29				-24	15*	-2	-2	39	-90
-13	32	-26	-1	32	-26	-25	18*	-9	-3	48	54
-14	5*	22	-2	38	39				-4	15*	19
			-3	50	48	H=	5, K=	2	-5	61	64
H=	5, K=	10	-4	12*	16				-6	21*	25
			-5	84	86	-1	3*	-3	-7	3*	-21
-1	31	-32	-6	11*	24	-2	43	49	-8	16*	19
-2	25*	-24	-7	36	-37	-3	16*	-8	-9	66	-63
-3	4*	5	-8	20*	14	-4	82	84	-10	16*	-2
-4	5*	-2	-9	43	-39	-5	37	42	-11	34	-41
-5	52	48	-10	14*	-7	-6	67	-72	-12	23*	0
-6	14*	10	-11	66	-68	-7	3*	8	-13	55	60
-7	5*	8	-12	49	38	-8	36	-35	-14	4*	-4
-8	22*	-14	-13	17*	8	-9	9*	-4	-15	55	64
-9	18*	-10	-14	30	27	-10	75	75	-16	14*	16
-10	7*	12	-15	31	30	-11	33	35	-17	4*	-19
-11	19*	-20	-16	40	-45	-12	105	105	-18	4*	-5
-12	33	-31	-17	5*	19	-13	11*	20	-19	7*	-92
-13	22*	10	-18	20*	-14	-14	25*	14	-20	5*	-26
-14	5*	-19	-19	50	-59	-15	4*	21	-21	23*	-17
-15	31*	31	-20	35	31	-16	26*	-34	-22	5*	-9
-16	24*	23	-21	19*	-16	-17	4*	2	-23	40	41
-17	24*	8	-22	5*	14	-18	46	-48	-24	5*	-1
-18	23*	26	-23	5*	17	-19	4*	-37	-25	35*	61
			-24	18*	4	-20	33	33	-26	5*	-3
H=	5, K=	8				-21	15*	-7			
			H=	6, K=	4	-22	63	65	H=	7, K=	3
-1	62	59				-23	35	36			
-2	13*	19	-1	92	88	-24	24*	27	-1	89	92
-3	45	-44	-2	42	-45	-25	19*	27	-2	122	118
-4	19*	-5	-3	74	-77	-26	39	-40	-3	25	-26

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
			24	13*	19	3	5*	-14			
10	79	-80				7	24*	26	1	4*	1
12	43	-46	H=	-5, K=	5	10	35	41	2	53	-57
14	16*	-9				11	22*	-17	3	21*	13
16	20*	14	1	4*	-4	12	17*	11	4	39	37
13	8*	-14	2	21*	28				5	44	-42
20	26*	-20	3	61	-59	H=	-9, K=	9	6	73	70
22	43	-43	4	15*	2				7	37	34
24	21*	21	5	23	-37	1	5*	2	8	16*	-4
			6	27	-30	2	23*	-11	9	35	31
H=	-5, K=	2	7	64	63	3	25	4	10	42	-44
			8	4*	-4	4	5*	7	11	37	-35
9	57	53	9	45	43	5	10*	15	12	36	-29
10	48	48	10	27*	27	6	47	53	13	54	-52
11	4*	13	11	33	25	7	5*	-8	14	5*	6
12	52	56	12	12*	7	8	29	32	15	5*	7
13	84	-35	13	39	-39	9	24*	-12	16	53	52
14	28	-28	14	13*	-6	10	33	-39	17	5*	-14
15	12*	-3	15	44	-58	11	12*	29	18	48	44
16	35	-34	16	20*	-16	12	33	-26	19	5*	10
17	9*	17	17	14*	-1	13	17*	8	20	24*	-30
18	10*	-17	18	8*	9	14	38	41	21	5*	-15
19	37	39	19	47	57	15	5*	-11	22	21*	-19
20	50	50	20	28*	23	16	43	47			
21	5*	3	21	5*	-4	17	5*	-2	H=	-9, K=	3
22	22*	23	22	17*	21						
23	34	-25	23	30	-16	H=	-9, K=	7	1	9*	-11
24	21*	-19							2	61	63
25	22*	-24	H=	-8, K=	8	1	22*	13	3	42	46
H=	-5, K=	4	1	10*	-14	2	42	32	4	5*	-7
			2	5*	6	3	46	43	5	17*	17
5	31	42	3	56	61	4	23	-22	6	45	-45
6	33	31	4	42	-46	5	4*	1	7	67	-70
7	30	-25	5	35	42	6	68	-69	8	4*	-5
8	6*	5	6	4*	3	7	25*	-5	9	59	-55
9	72	-74	7	10*	-6	8	4*	-11	10	23*	10
10	20*	-30	8	4*	-4	9	48	-47	11	15*	26
11	27	29	9	17*	-18	10	33	29	12	36	38
12	24	-35	10	8*	-10	11	17*	-6	13	40	34
13	42	45	11	5*	-2	12	20*	15	14	20*	-10
14	41	-34				13	22*	-29	15	4*	12
15	29	38	H=	-9, K=	11	14	22*	-32	16	33	-31
16	13*	35				15	14*	-1	17	16*	4
17	29	-35	1	5*	13	16	39	-34	18	22*	17
18	12*	10	2	29	22	17	9*	-14	19	5*	-17
19	46	-41	3	16*	3	18	15*	-6	20	55	55
20	39	-35	4	17*	-23	19	19*	20	21	5*	7
21	20*	-20	5	23*	-16	20	24*	31	22	5*	2
22	37	-28	6	10*	-20	21	23*	31	23	59	49
23	5*	18	7	29*	29	H=	-9, K=	5	24	5*	-16

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
H= -9, K= 1			13	22*	-25	13	56	-56	4	35	-30
			14	31	-31	14	5*	15	5	5*	-7
5	67	66	15	5*	-2	15	22*	-1			
6	13*	13	16	27*	-23	16	16*	1	H= -11, K= 9		
7	54	50	17	5*	17	17	35	34			
8	29	28	18	23*	-19	18	5*	11	1	5*	-8
9	91	81	19	25*	20	19	28*	33	2	23*	-4
10	27	-26	20	11*	23	20	26*	17	3	18*	27
11	33	25	21	38	-25				4	28*	35
12	7*	-23	22	12*	2	H= -10, K= 8			5	5*	19
13	49	-36	23	19*	-13				6	50	45
14	4*	-4				1	33	41	7	30	4
15	48	-45	H= -10, K= 4			2	5*	7	8	16*	-6
16	39	46				3	52	56	9	28*	-19
17	40	36				4	5*	-1	10	36	-36
18	5*	-9	1	7*	22	5	5*	-6	11	23*	8
19	42	40	2	11*	-32	6	12*	-11	12	14*	3
20	19*	-12	3	41	42	7	35	-32	13	26*	-7
21	24*	-29	4	32	43	8	11*	22	14	40	45
22	13*	-19	5	4*	3	9	26*	-25			
23	14*	-31	6	55	57	10	17*	6	H= -11, K= 7		
24	24*	6	7	17*	-24	11	42	39			
			8	52	-32	12	10*	-19	1	5*	-4
			9	37	-41	13	10*	23	2	22*	-5
H= -10, K= 0			10	78	-62	14	20*	2	3	17*	-1
			11	4*	7	15	5*	-6	4	36	-20
2	60	-53	12	21*	-24	16	21*	2	5	29*	-29
4	4*	20	13	3*	17	17	46	-46	6	22*	-31
6	41	42	14	7*	-1	18	23*	1	7	5*	-6
8	13*	21	15	17*	17				8	16*	-7
10	79	-84	16	24*	23	H= -10, K= 10			9	33	-36
12	44	-38	17	31	-24				10	52	57
14	21*	13	18	21*	-7	1	22*	-23	11	5*	2
16	46	46	19	13*	-20	2	32*	-43	12	16*	-14
18	21*	-3	20	35	-32	3	35	-42	13	5*	9
20	21*	-45	21	5*	13	4	5*	1	14	32*	-42
22	22*	-21	22	32	-23	5	5*	-13	15	11*	2
						6	47	41	16	29	-17
H= -10, K= 2			H= -10, K= 6			7	29*	24	17	5*	5
1	22*	-1	1	40	-41	8	5*	-4			
2	25	26	2	19*	21	9	5*	27	H= -11, K= 5		
3	29	-24	3	43	-42	10	21*	-12			
4	7*	-15	4	45	-48	11	27*	-31	1	33*	-24
5	57	-61	5	19*	-26	12	7*	2	2	19*	-5
6	95	-100	6	36	-35	13	35	-39	3	15*	-34
7	37	39	7	47	48				4	18*	14
8	15*	22	8	4*	-9	H= -11, K= 11			5	25*	14
9	26*	34	9	20*	20				6	23*	20
10	46	51	10	19*	31	1	5*	-13	7	32	38
11	4*	5	11	5*	-11	2	23*	19	8	21*	-5
12	27	32	12	21*	21	3	15*	-24	9	15*	36

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
10	42	-50	14	25	-12	4	37	30	13	25*	21
11	31	-37	15	20*	3	5	28*	15			
12	20*	4	16	19*	22	6	11*	-14	H= -13, K=	10	
13	50	-64	17	21*	-4	7	23*	-10			
14	43	43	18	5*	-9	8	44	-44	14	32*	-35
15	14*	3	19	35	22	9	33	-31	2	7*	3
16	32	-35	20	37	-25	10	56	-6*	3	21*	-35
17	34	39	21	35	-33	11	31	30	4	26*	29
18	19*	-14	22	23*	-9	12	5*	-7	5	5*	8
19	7*	10				13	23*	11	6	5*	20
20	31	-27	H= -12, K=	0		14	33	37			
						15	5*	-8	H= -13, K=	9	
H= -11, K=	3		2	21*	13	16	14*	35			
			4	42	53	17	27*	-23	1	24*	18
1	2*	12	6	22*	27	18	29*	-19	2	18*	17
2	4*	-12	8	67	-68	19	5*	-4	3	5*	-7
3	31	35	10	61	-63				4	41	43
4	11*	-8	12	37	37	H= -12, K=	6		5	5*	-4
5	27	-25	14	52	42						
6	35	-39	16	20*	28	1	17*	-13	H= -13, K=	7	
7	38	-44	18	13*	-19	2	5*	7			
8	38	44	20	25*	-22	3	28	-23	1	5*	-26
9	34	-34				4	8*	-21	2	29	-20
10	4*	2	H= -12, K=	2		5	22	-16	3	22*	17
11	35	42				6	17*	-1	4	29*	-35
12	6*	16	1	33	-33	7	41	37	5	16*	-9
13	52	44	2	32	-35	8	5*	9	6	25*	-24
14	5*	-16	3	4*	7	9	5*	1	7	22*	-5
15	32	38	4	42	-41	10	16*	25	8	5*	18
16	17*	-20	5	23*	-10	11	26*	-34	9	17*	-13
17	42	-41	6	35	-36	12	32	27	10	34	26
18	3*	-3	7	35	31	13	26*	-16	11	5*	2
19	25*	-14	8	51	53	14	22*	-10	12	9*	-11
20	42	4*	9	5*	17	15	7*	24	13	11*	13
21	5*	19	10	38	36	16	5*	1			
			11	15*	-22	17	24*	30	H= -13, K=	5	
H= -11, K=	1		12	5*	-4						
			13	7*	-11	H= -12, K=	8		1	37	-40
1	37	-43	14	45	-26				2	14*	1
2	15*	-1	15	31	31	1	51	20	3	25*	0
3	53	-73	16	5*	-2	2	27*	2	4	12*	12
4	4*	14	17	10*	1	3	51	5*	5	5*	8
5	17*	-9	18	22*	7	4	5*	-1	6	27*	25
6	4*	23	19	27*	-15	5	11*	-0	7	20*	33
7	105	109	20	43	39	6	26*	10	8	21*	-16
8	19*	-11				7	30*	-37	9	15*	7
9	22*	23	H= -12, K=	4		8	45*	2	10	27*	-23
10	19*	-11				9	31*	-29	11	5*	-1
11	32	-32	1	21*	6	10	16*	11	12	27*	30
12	11*	-10	2	11*	-3	11	36	37	13	26*	-24
13	16*	-15	3	3*	12	12	5*	-2	14	32*	37

L	FD	FC	L	FD	FC	L	FD	FC	L	FD	FC
5	34	-23	9	29*	-26	4	5*	-15	10*	13*	-2
6	5*	6	10	17*	3	5	5*	-27	11	22*	-45
7	22*	-27	11	41	-37	6	5*	3	12*	24*	9
8	24*	-27				7	5*	-16	13*	13*	-9
9	11*	-5	H = -15, K =	5		3	17*	22			
10	5*	-7				7	5*	-1	H = -16, K =	0	
11	46	55	1	9*	-17	10	5*	12			
13	16*	-3	2	24*	20	11	20*	33	2	18*	57
14	16*	17	3	5*	1				4	13*	23
			4	5*	22	H = -13, K =	1		6	26*	-34
H = -14, K =	0		5	5*	15				8	11*	-29
			6	5*	-8	1	44	-46			
1	55	-55	7	20*	17	2	5*	17	H = -16, K =	2	
2	5*	0	8	7*	-21	3	7*	18			
3	5*	1				4	5*	16	1	18*	-34
4	5*	-7	H = -15, K =	3		5	5*	27	2	20*	-43
5	32	23				6	5*	-14	3	5*	15
6	5*	-7	1	32	36	7	11*	22	4	5*	-12
7	25*	34	2	26*	-25	8	5*	-10	5	18*	17
8	37	30	3	1*	25	9	5*	-2	6	5*	13
H = -13, K =	5		13	20*	-14	15	30	17	3*	5*	3
			14	7*	8	16	7*	-13	4	5*	-11
15	32	23	17	-2	-27	17	30*	30	5	13*	18
16	10*	-4	18	5*	1	18	17*	-21	6	14*	6
						19	22*	-12	7	12*	20
H = -13, K =	3		H = -13, K =	1					8	30	27
						H = -14, K =	0		9	16*	9
1	33	33	1	21*	-27				10	23*	25
2	13*	-9	2	17*	-14	2	27*	31	11	7*	-27
3	5*	-5	3	5*	-11	4	21*	32	12	5*	-8
4	3*	-34	4	36	22	5	5*	-12	13	7*	0
5	17*	-23	5	5*	54	6	5*	-9	14	40	-32
6	44	-51	6	26	7	10	35	-30	15	15*	17
7	22*	-15	7	39	36	12	51	47	16	18*	13
8	18*	17	8	7*	-6	14	29*	24			
9	13*	-2	9	35	-25	15	22*	-22	H = -14, K =	4	
10	31*	47	10	74	-33						
11	52	54	11	55	-57	H = -14, K =	2		1	30	20
12	14*	-14	12	32	28				2	5*	-1
13	35	25	13	13*	-2	1	5*	-11	3	14*	10
14	17*	-2	14	17*	-12	2	34	-33	4	15*	17

REFERENCES

1. E.L. Muetterties and C.M. Wright, Quart. Rev., Chem. Soc., 21, 109 (1967).
2. S.J. Lippard, Prog. Inorg. Chem., 8, 109 (1967).
3. E.L. Muetterties and C.M. Wright, J. Am. Chem. Soc., 87, 4706 (1965).
4. M.A. Porai-Koshits and L.A. Aslanov. Zh. Strukt. Khim., 13, 266 (1972).
5. J.L. Hoard and J.V. Silverton, Inorg. Chem., 2, 235 (1963).
6. D.G. Blight and D.L. Kepert, ibid., 11, 1556 (1972).
7. a) D.T. Cromer and J.T. Waber, Acta Cryst., 18, 104 (1965).
b) R.F. Stewart, E.P. Davidson, and W.T. Simpson, J. Chem. Phys., 42, 3175 (1965).
8. F.W.B. Einstein and R.D.G. Jones, Inorg. Chem., 11, 395 (1972).
9. V. Schomaker and K.N. Trueblood, Acta. Cryst., B24, 63 (1968).
10. S. Geller, Acta. Cryst., 14, 1026 (1961).
11. V.W. Day and J.L. Hoard, J. Amer. Chem. Soc., 92, 3626 (1970).
12. J.T. Parks, D.M. Collins, and J.L. Hoard, ibid., 92, 3626 (1970).
13. G.L. Glen, J.V. Silverton, and J.L. Hoard, Inorg. Chem., 2, 250 (1962).
14. C.D. Garner and S.C. Wallwork, J. Chem. Soc.(A), 1496 (1966).
15. C.D. Garner, D. Sutton, and S.C. Wallwork, J. Chem. Soc.(A), 1949 (1967).

16. T.J. King, N. Logan, A. Morris and S.C. Wallwork, Chem. Comm., 11, 554 (1971).
17. N. Epiotis, J. Amer. Chem. Soc., 95, 3087 (1973).
18. L.J. Guggenburger and E.L. Muetterties, ibid., 94, 8046 (1972).
19. T.J. Anderson, M.A. Neuman and G.A. Melson, Inorg. Chem., 13, 158 (1974).
20. W.C. Hamilton and J.A. Ibers, "The Hydrogen Bond" (Benjamin), p. 53 (1968).
21. K. Nakamoto, M. Margoshes and R.E. Rundle, J. Amer. Chem. Soc., 77, 6480 (1955).
22. Y.K. Yoon and G.B. Carpenter, Acta. Cryst., 12, 17 (1959).
23. L.W. Schroeder and J.A. Ibers, J. Amer. Chem. Soc., 88, 2601 (1966).
24. L.V. Azaroff, Acta. Cryst., 8, 701 (1955).