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THE CRYSTAL STRUCTURE OF GOLD
(III) CHLORIDE

BERKELEY, CALIFORNIA

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UNIVERSITY OF CALIFORNIA

Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

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(Thesis)

November 8, 1955

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ABSTRACT

Gold (III) chloride is a monoclinic, space group $P2_1/c$, with cell dimensions $a = 6.57 \text{ \AA}$, $b = 11.04 \text{ \AA}$, $c = 6.44 \text{ \AA}$, $\beta = 113^\circ 19'$. The structure consists of planar molecules Au_2Cl_6 , in which each gold atom is surrounded by four chlorine atoms at the corners of a slightly distorted square.

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INTRODUCTION

In the course of my research in crystallography, I was studying methods for the preparation and handling of single crystals of trichloride compounds. The crystal structures of many of the trichlorides have been determined, and an interesting variation is found in structure types, in ionic and molecular nature, in closeness of packing of chloride atoms, etc. The explanation of these variations and prediction of structures and properties of new trichlorides create an interest in determining as many trichloride structures as possible. Crystals of gold chloride were prepared with little difficulty and x-ray diffraction photographs indicated that this trichloride possessed a new type of structure. Therefore an investigation was begun to determine the structure of this new addition to the series of trichloride structures.

This research was performed over a two-year period at the University of California in Berkeley under auspices of the Atomic Energy Commission and the Municipal University of Amsterdam under a Fulbright grant.

I. PREPARATION OF GOLD CHLORIDE

A. Preparation from the Elements

In a study of methods of preparation of metal trihalides, direct combination of the elements proved simple for chlorides, bromides, and iodides, yielding products of high purity. This method was found to be especially satisfactory for the preparation of gold chloride. Freshly snipped gold foil was placed in a glass tube resting in a furnace. After chlorine had been introduced into a sidearm and frozen with liquid nitrogen, the system was evacuated with high-speed mercury diffusion pumps and sealed. The pressure of the chlorine was raised to about four atmospheres by replacing the nitrogen bath with ice water. The gold metal was then heated and crystals of gold chloride grew by sublimation at the cool ends of the furnace. When a suitable quantity of crystals had been collected, the nitrogen bath was again placed about the chlorine

and the portion of the system containing the crystals was sealed off. The tube containing the very hygroscopic gold chloride crystals was subsequently broken open inside a drybox. Crystals of suitable size and morphology were selected and sealed in very thin-walled glass capillary tubes for x-ray photography.

B. Preparation from the Hydrate

A method for the preparation of single crystals of gold chloride from the hydrate was devised and executed by Mr. A. Krueger of the Netherlands Organization for Pure Research (Z. W. O.). Gold chloride hydrate was dried under vacuum at room temperature for 24 hours. The temperature was then raised to 100°C and the evolved water was distilled into a sidearm immersed in a liquid air bath. Following removal of water, the remaining crystalline material was kept at slightly above 100°C for several days. Minute crystals of gold chloride were observed growing slowly by sublimation in a cool part of the system. When the desired number of crystals had been prepared, heating was discontinued. Under a positive pressure of very dry nitrogen, some of the tiny crystals were coaxed into thin-walled glass capillary tubes attached to the system and these tubes containing the crystals were sealed off for mounting on a goniometer.

C. Morphology

At 200°C , growth by sublimation was slow, with the formation of thin "cellophane-like" crystals in the (100) Bragg plane. At 280°C , growth was more rapid with the formation of [100] needles. A preparation which remained at 200°C for 24 hours and was then raised to 250°C for several hours consisted of a lacy network of needles within thin plates. The needle preparations would sometimes appear fibrous when broken with a probe. The thin plates are orange; the needles are wine red. This is probably due to differences in light absorption with crystals of different thicknesses since x-ray diffraction patterns of needles and plates were identical. Cases of twinning were not observed morphologically or in diffraction patterns.

Gravimetric analysis of the trichloride by decomposition with heat followed by absorption of the chlorine gave 35.20% chlorine against a theoretical 35.04%. I wish to thank Mr. V. H. Tashinian of the microanalytical laboratory of the University of California for analyses of the chlorides.

D. Aurous Chloride, AuCl

Aurous chloride was prepared by heating auric chloride with an excess of gold in a system all parts of which were kept at 270°C to prevent preferential sublimation of auric chloride to a cool area. The reaction proceeded slowly, giving bright yellow crystals of aurous chloride. Analysis gave 14.08% chlorine against a theoretical 15.24%. No evidence was found for the formation of chlorides of intermediate composition, e. g., Au_2Cl_4 , etc.

II. INTENSITY DATA

All diffraction data were recorded photographically. From direct combination of the elements, a prismatic needle crystal of dimensions 0.072 by 0.11 by 2.2 mm was grown, and with this [001] needle, a series of 3-film Weissenberg photographs was made. Layers (hk0), (hk1), (hk2), and (hk3) were photographed with copper radiation. Layers (hk4), (hk5), (hk6), and (hk7) were photographed with molybdenum radiation. The wavelengths assigned for unresolved $k\alpha$ radiation were $1.5418 \text{ \AA}$ for copper and $0.7107 \text{ \AA}$ for molybdenum. From a small crystal roughly 0.066 by 0.09 by 0.25 mm prepared by dehydration of the hydrate, a zero-layer Weissenberg pattern with [101] axis rotation was photographed with copper radiation. A thin plate (100) crystal prepared from direct union of the elements was used, and an (0k ℓ) precession pattern was photographed with molybdenum radiation. Three-film intensity standards were obtained from 3° oscillations about a strongly diffracting Bragg plane in the needle crystal, one set of standards with copper radiation, and one set with molybdenum radiation.

The intensities of the diffraction spots of the precession photograph and the (hk0) - (hk3) Weissenberg patterns were estimated by visual comparison with three-film standards. Intensity measurements on the (hk4) - (hk7) Weissenberg patterns and on the zero-layer Weissenberg film with [101] rotation were made photometrically with a nonintegrating photometer. The ratios of the absorption of the photometer light beam by a diffraction spot to the absorption by the immediate background were measured for spots on the standard-intensity films, and the logarithms of these ratios were plotted against intensity values (the number of oscillations contributing to the blackening of a spot on the film). A linear relationship was found except at very high intensity values. Corresponding ratios for diffraction spots of unknown

intensity were determined and compared with the standard plot to obtain intensity values. Second- and third-film intensity estimates were compared against first-film standards and adjusted to first-film values by normalization. The correction of the measured intensities for absorption and distortion is discussed later.

III. PRELIMINARY INVESTIGATION OF STRUCTURE

A. Investigation of x and y Parameters

A needle crystal was aligned about the needle axis on the Weissenberg goniometer and a series of photographs was made. These were interpreted to give the following information concerning the unit cell:

Space group $P2_1/c$,

$a = 6.57 \text{ \AA}$,

$b = 11.04 \text{ \AA}$,

$c = 6.44 \text{ \AA}$,

$\beta = 113^\circ 19'$.

The axial lengths a and b were measured on quartz-calibrated films. The c axial length was determined from a noncalibrated rotation photograph. The monoclinic angle β was determined as 113.3° from an equiinclination (hkl) Weissenberg photograph superimposed on an antiequiinclination $(hk0)$ Weissenberg photograph according to a method described by Buerger (1942). Direct measurement on a $[010]$ precession photograph gave $113^\circ 20'$. On the assumption of four gold atoms and twelve chlorine atoms per unit cell, a density of 4.72 was calculated, which compared favorably with the experimental value 4.67 reported by Fischer and Biltz (1928). From a zero-layer Weissenberg photograph, intensities of the $(hk0)$ Bragg planes were estimated and a Patterson projection parallel to the $[001]$ axis was made photographically with Huggins masks. This projection was interpreted to give the parameters $x = 0.042$, $y = 0.084$ for a gold atom, and with these parameters phase angles for the $(hk0)$ Bragg planes were calculated. These phase angles were used with the observed structure factors, and a Fourier projection parallel to the $[001]$ axis was made and the expected 12 chlorine peaks appeared. After a check of phase angles and correction of the projection, the following parameters were derived:

	x	y
Au	0.043	0.088
Cl ₁	0.263	0.004
Cl ₂	0.338	0.168
Cl ₃	0.793	0.158

This projection is shown in Fig. 1. A discussion of the probable structure of gold chloride has been made by Wells (1950), who states that a square-bonded molecule Au_2Cl_6 is to be expected:

An examination of Fig. 1 shows what appears to be a projection of such a molecule. With this information, experimentation was continued to determine z parameters.

B. Investigation of z Parameters

1. Precession Technique

When x and y parameters had been obtained from $(hk0)$ Weissenberg data, additional data were desired for z -parameter information. This could best be accomplished with photography of a crystal aligned about an axis other than $[001]$. When either a needle crystal wedged cross-wise within a capillary tube or a thin plate crystal was used to obtain Weissenberg photographs with rotation about an axis other than $[001]$, extreme absorption effects were observed and these were judged to be beyond practical correction in all but a few small areas of the films.

As described previously, thin plate (100) crystals were prepared and although very thin plates do not lend themselves to the Weissenberg technique, good data can often be obtained by employing the Buerger precession technique. Through the courtesy of Professor A. Pabst and the Department of Geological Sciences of the University of California, precession equipment was made available. With a (100) plate crystal sealed in a glass capillary, an $(0kl)$ precession pattern was photographed with a precession angle of 30° and molybdenum radiation. From the relative values of the intensities of the diffraction spots corrected for Lorentz and polarization effects, a photographic Patterson projection was made with Huggins masks. This projection was interpreted to

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Fig. 1. [001] projection. Contours drawn at equal arbitrary intervals. Zero contour omitted.

give a gold parameter of $z = 0.25$ corresponding to $y = 0.088$. Phase angles for the observed structure factors were calculated on the basis of this gold parameter. When a gold atom is placed at $z = 0.25$, diffraction contributions to $(0kl)$ Bragg planes with odd values of k are nil. Using only $(0kl)$ structure factors with even values of k , a Fourier projection parallel to $[100]$ was calculated and is shown in Fig. 2. It is seen that because of exclusion of structure factors for odd values of k , a false mirror line is introduced into the projection at $z = 0.25$. The fact that there are 12 chlorine atoms per unit cell requires that there be 12 chlorine peaks in a projection. Therefore this projection with 24 chlorine peaks can be interpreted to give the following parameters:

	y	z
Au	0.088	0.250
Cl ₁	0.996	0.534 or 0.967
Cl ₂	0.169	0.000 or 0.500
Cl ₃	0.164	0.125 or 0.375

An inspection of the data derived from this precession pattern reveals the interesting fact that only the Bragg plane (031) for which the diffraction contribution from gold atoms is nil is found to be of strong intensity. It can be assumed that the diffraction contributions to this plane are from the chlorine atoms. The phase angle for this plane is according to space-group symmetry either zero or $1/2$. A zero-phase angle for (031) was assumed, and the contribution to the projection from this plane was calculated and added to the projection. The results show suppression of 12 peaks and sharpening of 12 peaks, indicating choice A for chlorine parameters. (See below.). If a phase angle of $1/2$ is chosen for (031), it is found that the peaks suppressed by a zero-angle assumption are sharpened and, correspondingly, the formerly sharpened peaks are suppressed. This indicates choice B for chlorine parameters. It appeared at first glance as if a knowledge of the structure would depend on a choice between A and B for z parameters.

		Choice A	Choice B
	y	z	z
Cl ₁	0.996	0.967	0.534
Cl ₂	0.169	0.500	0.000
Cl ₃	0.164	0.375	0.125

Fig. 2. [100] projection, using only $(Ok\ell)$ construction factors with even values of k . Contours drawn at equal arbitrary intervals. Chlorine peaks accented; gold peaks reduced.

However, the choice is found not to be between structures but between locations of cell origin. The parameters of choice A are structurally equivalent to the choice B parameters with a shift of origin on the projection of one-half unit in the y direction. Since the phase angle for the Bragg plane (031) determines location of origin and does not alter the structure, the phase angle is arbitrarily assigned a zero value. With this assumption (choice A), phase angles for all (0kl) Bragg planes were calculated and a Fourier projection parallel to [100] using all (0kl) data was made. The results shown in Fig. 3 give the parameters:

	y	z
Au	0.088	0.242
Cl ₁	0.006	0.006
Cl ₂	0.139	0.528
Cl ₃	0.150	0.375

The bumpiness of the projection, the lack of close agreement between observed and calculated structure factors, and the change in chlorine y parameters from those previously obtained with (hk0) data, cause the accuracy of the derived parameters to be considered as low and indicate the necessity for further study.

When x and y parameters from (hk0) Weissenberg data were used with the above z parameters, and a square-bonded planar Au₂Cl₆ molecule was assumed with the Au-Cl distance taken as 2.5 Å, a "best compromise" set of parameters was devised to be used as a guide for further work in obtaining accurate structure parameters.

"Best compromise parameters"

	x	y	z
Au	0.043	0.088	0.248
Cl ₁	0.263	0.004	0.052
Cl ₂	0.338	0.168	0.518
Cl ₃	0.815	0.167	0.428

2. Weissenberg Technique

Since greater accuracy in z parameters than was obtained from precession data was desired, a new approach was made, employing the Weissenberg technique. Examination of the "best compromise structure" (see Section III-B-1) showed that a zero-layer Weissenberg photograph with rotation about

Fig. 3. [100] projection. Contours drawn at equal arbitrary intervals. Chlorine peaks accented; gold peaks reduced.

the [101] axis would give the best resolution of chlorine atoms for determination of z parameters. The awkward problem of securing a small crystal in the required skew orientation while sealed within a capillary tube was solved by admitting a minute quantity of water vapor into the tube, "gluing" the crystal to the tube wall by a sludge of gold chloride and water.

The skew orientation of the crystal plus the presence of noncrystalline sludge and glass gives rise to significant absorption effects for which accurate correction was impossible. From rough observation and measurements of the crystal, an assumption that the crystal had a rectangular cross section of constant dimensions was made. This admittedly crude approximation proved useful in deriving corrections for absorption by the crystalline portion of the diffracting material. A regularly spaced net of 105 points was constructed over the cross section, and by use of this, measurements of distances traversed by the x-ray beam from entry of the cross section to a point of the net to exit from the cross section were made, one set of measurements for each Bragg plane. The absorption of an x-ray beam was assumed to follow the exponential form,

$$I = I_0 \exp(-us),$$

where I is the intensity of the diffracted radiation, I_0 that of the incident radiation, u the linear absorption coefficient, and s the distance traversed by the beam through the crystal. Values for atomic absorption coefficients are taken from work of E. L. Eichorn (with C. H. MacGillavry) for the yet unpublished Volume II of the "International Tables for X-ray Crystallography." For copper radiation, the coefficient for gold is 7364×10^{-23} and for chlorine, 620.6×10^{-23} . Thus

$$u_{\text{atomic}} = \frac{4 \times (7364 + 3 \times 620.6) \times 10^{-23}}{427.4 \times 10^{-24}} = 864.$$

Corrections for absorption from noncrystalline material were assumed to follow some smooth function of the Bragg angle. From ratios of these intensity data corrected for crystalline absorption to corresponding data from an (hkn) series of Weissenberg photographs (the series used for final refinement of structure), a smooth curve was derived for noncrystalline absorption corrections as a function of the Bragg angle. Phase angles calculated from the "best compromise structure" were used, and a Fourier projection parallel

to the [101] axis was made by use of the corrected data. The results of this summation (see Fig. 4) show that the overwhelming effect of the diffraction from gold atoms makes observation of chlorine peaks difficult. From this projection the following parameters were assigned:

	y	z'
Au	0.086	0.194
Cl ₁	0.004	0.822
Cl ₂	0.170	0.192
Cl ₃	0.173	0.589

In this projection, parameters perpendicular to the y direction are designated as z'. The transformation to z parameters of the unit cell is

$$z = z' + x$$

To increase accuracy of observation of chlorine peaks, a subtraction Fourier projection with the coefficients ($F_0 - F_{Au}$) was made. From a plot of $\log(F_c/F_0)$ versus $\sin^2 \theta$, a scaling factor and a temperature factor were derived to correct and adjust the calculated structure factor for gold. The results of this subtraction Fourier projection (Fig. 5) give the following chlorine parameters:

	y	z'
Cl ₁	0.011	0.815
Cl ₂	0.181	0.180
Cl ₃	0.172	0.578

Using x and y parameters obtained from previous work and transforming z' to z, one obtains the complete parameters:

	x	y	z
Au	0.0425	0.0876	0.236
Cl ₁	0.236	0.004	0.078
Cl ₂	0.338	0.168	0.518
Cl ₃	0.815	0.167	0.393

Because of the awkward and inaccurate absorption corrections applied, it is felt that these (hkh) data should not be used for temperature-effect discussions and that these intensity data should not be used in a direct sense for correlation of (hkn) layers of Weissenberg photographs.

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Fig. 4. [101] projection. Contours drawn at equal arbitrary intervals.

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Fig. 5. [101] projection, difference synthesis; gold atoms removed. Contours drawn at equal arbitrary intervals.

IV. REFINEMENT OF PARAMETERS

A. Preparation of Three-Dimensional Data

The data used for the final refinement of parameters was taken from a series of Weissenberg photographs photographed with rotation about [001]. These are (hkn) layers with n ranging from 0 through 7. The crystal used for these photographs was a needle prism rotated about the needle axis. (See section I-C.) It was assumed for purposes of absorption correction that the crystal was cylindrical with a radius of 5×10^{-3} cm. Corrections for absorption derived by Bradley (1935) were applied to these diffraction data, using $u_r = 4.3$ for copper radiation and $u_r = 2.0$ for molybdenum radiation where u is the linear absorption coefficient and r the radius of the cylinder.

Because of the geometry of the Weissenberg mechanism, beam divergence, mosaic nature of the crystal, etc., diffraction spots on nonzero-layer films are elongated on one half of the film and foreshortened on the other half. Corrections of nonintegrated intensity estimations were necessary to obtain an integrated intensity value for each Bragg plane. This correction was especially awkward for these (hkn) data since the majority of the ($\bar{h}$ kn) Bragg planes appeared as elongated spots on one half of the film and the (hkn) Bragg planes were foreshortened spots on the other half. By symmetry $F_{(hkn)} \neq F_{(\bar{h}kn)}$, making any simple method of averaging intensities of elongated and foreshortened spots of equivalent intensity impossible. With the aid of the calibrated film transport mechanism and optical system of the photometer, the length of each spot was measured as accurately as possible. The difficulty of measurement increased with the distance g of a spot from the center streak (trace of the beam catcher) of the Weissenberg film, since the ends of the spots trailed into the background. Strong thermal atomic vibration coupled with Lorentz and polarization effects causes intensity of spots to diminish rapidly with increasing Bragg angle, especially with molybdenum radiation. It was judged that the measured length of a spot with a high g value was too small relative to the measured length of stronger spots of low g . Since these errors of measurement for both elongated and foreshortened spots should be symmetrical with the central streak line, the ratio of the lengths of elongated and foreshortened spots as a function of g would be expected to be of greater significance than the lengths of the spots alone. From measurements of spot lengths and g values within an (hkn) layer, this ratio was calculated as a

function of g , and a treatment for correction of intensity data was derived. With the assumptions that the total integrated intensity of a spot is the same whether a spot is elongated or foreshortened, and that density is uniform within spot area, the following approximation was made:

$$I_0 A = I_e (A + v) = I_f (A - v) ,$$

where I_0 represents integrated intensity; I_e and I_f , nonintegrated intensity estimates for elongated and foreshortened spots; A , the undistorted area of a spot; and v , the amount of distortion. Within a layer, v is assumed to be a function of g . Assuming the width of spots to be constant within a layer, we find

$$I_0 S = I_e (S + w) = I_f (S - w) ,$$

where S represents spot length and w the amount of distortion of length, a function of g . If H represents the ratio of length of an elongated spot to the length of a foreshortened spot (H being a function of g), then

$$H = \frac{(S + w)}{(S - w)} ,$$

and, with substitution,

$$I_0 = \frac{2I_f}{(1 + H)} = \frac{2I_e}{(1 + H^{-1})} .$$

These formulae are equivalent to taking the harmonic mean of I_e and I_f for the case in which both elongated and foreshortened spots are observed for equivalent Bragg planes.

From a plot of H versus g for each layer and of g measurements for each spot, these (hkn) data were corrected to integrated intensity values.

A major problem in preparation of intensity data was the scaling of relative data from one (hkn) layer to another (hkn) layer. The intensity data previously used for the determination of the structure were not considered accurate enough to be used for direct correlation of layers. However, the structure parameters derived from these data were considered to be reasonably accurate, and by use of calculated structure factors from these parameters, scaling factors were derived. Comparison of observed and calculated structure factors for the purpose of scaling relative data was made at values of the Bragg angle as low as possible to minimize errors resulting from inaccurate

correction of the calculated structure factors for temperature effects. The correction for temperature effects (resulting from thermal vibrations in the crystal) that was applied was derived from zero-layer data by plotting $\log (F_0/F_c)$ versus $\sin^2 \theta$. A value of $B = 3.90$ was derived where B is defined by

$$F_{c(\text{corrected})} = F_c \exp (-B \sin^2 \theta) / \lambda^2 .$$

B was assumed to be isotropic and the same for all atoms.

B. Three-Dimensional Fourier Calculations

On the basis of these corrected intensity data and phase angles calculated with the best available parameters (see the end of section III-B-2), three-dimensional Fourier calculations were made. Three sections parallel to (010) were calculated:

- a section at $y = 0.088$ for Au,
- a section at $y = 0.333$ for Cl_2 and Cl_3 ,
- a section at $y = 0.000$ for Cl_1 .

These sections gave x and z parameters for each atom and at these x and z coordinates a line Fourier summation to determine the y parameter was calculated for each atom (four lines). The results of these three-dimensional calculations give the following parameters:

	x	y	z
Au	0.0414	0.0868	0.2336
Cl_1	0.254	0.006	0.060
Cl_2	0.334	0.170	0.508
Cl_3	0.819	0.162	0.385

C. Refinement by the Method of Least Squares

At the time that this structure determination was in the final stages of refinement, work was being completed by Michael E. Senko and David H. Templeton in programming the International Business Machines 650 computer to handle refinement of structure parameters by the method of least squares. The method of approach followed in general the procedure discussed by Lipson and Cochran (1953). For gold chloride, an extra variable was introduced--a scaling factor for each n layer correlating the (hkn) structure

factors. In actual practice it was found that in this least-squares method, the atomic parameters were insensitive to variation in these scaling factors. Atomic scattering factors for gold were derived by David H. Templeton, taking account of dispersion effects. (Templeton, 1955; Dauben and Templeton, 1955.) Atomic scattering factors for chlorine were taken from work of Berghuis, Haanappel, et al. (1955). The observed structure factors were weighted by the factor $w^{1/2} = 1/F_0$ for values above 10 and $w^{1/2} = 1/10$ for F_0 less than 10. This tends to minimize errors in observation of high-intensity spots. The criterion of refinement was minimization of the quantity

$$P = \frac{\sum w |F_0 - F_c|^2}{\sum w |F_0|^2}$$

The following parameters were derived from this least-squares method:

	x	y	z
Au	0.0415	0.0868	0.2337
Cl ₁	0.258	0.003	0.059
Cl ₂	0.335	0.169	0.509
Cl ₃	0.820	0.162	0.395

These parameters should be taken as the final and most accurate values.

The standard deviations of the least-squares fit determined by the usual statistical methods by Senko, Dauben, and Templeton are:

	σ_x	σ_y	σ_z
Au	0.00024	0.00014	0.00029
Cl ₁	0.0017	0.0010	0.0021
Cl ₂	0.0020	0.0011	0.0026
Cl ₃	0.0020	0.0012	0.0026

An isotropic thermal vibration coefficient, B, for each atom was also derived from the least-squares refinement by using temperature factors of the form

$$\exp - (B_i/\lambda^2) \sin^2 \theta$$

The values obtained were: $B_{Au} = 3.31$, $B_{Cl_1} = 4.14$, $B_{Cl_2} = 4.80$, $B_{Cl_3} = 4.91$. The factor "P" in the final refinement was 0.061. The conventional "reliability factor",

$$R = \frac{\sum |F_0 - F_c|}{\sum |F_0|},$$

was 0.15 excluding the structure factors observed as zero (about 20% of the total number of structure factors) and 0.20 if all structure factors were included. Observed and calculated structure factors are tabulated in Table III. A calculated powder pattern based on these values is given in Table IV.

V. DISCUSSION OF STRUCTURE

A. Interatomic Distances

1. Neighboring Atoms Within the Molecule

Considering the atoms within the Au_2Cl_6 molecular unit to be labeled as follows,

we have the interatomic distances

$$\begin{array}{ll} \text{Au}_1 - \text{Cl}_a = \text{Au}_2 - \text{Cl}_f = 2.23 \text{ \AA} & \text{Cl}_a - \text{Cl}_b = \text{Cl}_e - \text{Cl}_f = 3.16 \text{ \AA} \\ \text{Au}_1 - \text{Cl}_b = \text{Au}_2 - \text{Cl}_e = 2.25 & \text{Cl}_b - \text{Cl}_d = \text{Cl}_c - \text{Cl}_e = 3.30 \\ \text{Au}_1 - \text{Cl}_c = \text{Au}_2 - \text{Cl}_d = 2.33 & \text{Cl}_a - \text{Cl}_c = \text{Cl}_d - \text{Cl}_f = 3.30 \\ \text{Au}_1 - \text{Cl}_d = \text{Au}_2 - \text{Cl}_c = 2.34 & \text{Cl}_c - \text{Cl}_d = 3.17 \\ & \text{Au}_1 - \text{Au}_2 = 3.42 \end{array}$$

(Note: The atoms Au_1 , Cl_d , Cl_b , Cl_a represent the atoms designated previously as Au , Cl_1 , Cl_2 , Cl_3 .)

2. Planarity

If the plane containing the atoms Cl_a , Cl_b , Cl_e , Cl_f is taken as the plane of the molecule, then Au_1 is calculated to be 0.01 $\text{\AA}$ below the plane, Au_2 is 0.01 $\text{\AA}$ above the plane, Cl_c is 0.01 $\text{\AA}$ above, and Cl_d 0.01 $\text{\AA}$ below. (The center of the molecule is a center of symmetry.) Thus the molecule is planar within the limits of experimental error.

3. Interatomic Distances Between Molecules

Closest chlorine neighbors to gold are; one at 3.47 $\text{\AA}$, one at 3.52 $\text{\AA}$, one at 3.91 $\text{\AA}$, and one at 4.48 $\text{\AA}$. Closest gold-gold neighbors are 4.15 $\text{\AA}$.

Closest chlorine-chlorine neighbors are at the distances 3.55 Å, 3.68 Å, and 3.83 Å.

B. Bonding

One of the more interesting features of this structure is the square planar bonding of the chlorine atoms about gold. This type of bonding is expected for trivalent gold, and is explained by Pauling (1942) on the basis of the formation of dsp^2 square planar bonds. In particular, the molecule Au_2Cl_6 has been discussed by Wells (1950), who predicts a planar structure

with the electronic structure in the gold atom

Since the chlorine atoms c and d are bonded to two gold atoms, it might be expected that these bonds would be less strong than those between gold and chlorines a and b. It is found that the bond distances between Cl_c or Cl_d and gold are about one-tenth Angstrom longer than the bond distances between Cl_a or Cl_b and gold. (See section V-A.) This square bonding about trivalent gold has been observed previously in crystalline gold compounds, including $Cs_2Au^I Au^{III}Cl_6$ (Elliott and Pauling, 1938), $KAuBr_4$ (Cox and Webster, 1936), and $Au_2Br_2(C_2H_5)_4$ (Burawoy, Gibson, Hampson, and Powell, 1937).

C. Arrangement of Molecules

The stacking of the planar Au_2Cl_6 molecules within the crystal lattice is shown in Figs. 6 and 7. The stacking follows a general scheme exhibited in the crystal structures of many planar organic molecules such as naphthalene (Abrahams, Robertson, and White, 1949) and durene (tetramethyl benzene) (Robertson, 1933). In Fig. 7 it can be seen that a layer of chlorine atoms is directly adjacent to another chlorine layer parallel to (100). In section I-C a strong tendency of the crystals to form (100) plates was noted.

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Fig. 6. Projection on (100).

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Fig. 7. Projection on (001).

ACKNOWLEDGMENTS

I wish to express my thanks to Professor David H. Templeton and to Professor C. H. MacGillavry for their guidance in this research. The assistance of Professor A. Pabst, especially in use of the precession technique, is appreciated. Appreciation is expressed also to Dr. R. Douglass for help in the precession photography. I wish to thank Mr. A. Kreuger of the Netherlands Organization for Pure Research (Z.W.O.) for a crystal preparation and x-ray photography discussed in Section III-B-2 and for construction of an Au_2Cl_6 crystal model. Special acknowledgment is given to Mr. Michael E. Senko and Professor David H. Templeton for designing and executing the program for least-squares refinement, outlined in Section IV-C. These calculations were performed on equipment at the University of California Radiation Laboratory at Livermore. I wish to thank the personnel of the Mathematical Center in Amsterdam, the Computer Laboratory at the University of California, and to Mrs. Carol H. Dauben and Mrs. H. W. Ruben for help in Fourier calculations. The aid of Mr. A. L. Veenendaal and Mr. K. Stom in using facilities at the crystallographic laboratory in Amsterdam is greatly appreciated.

This research was supported by the U. S. Atomic Energy Commission and a grant under the Fulbright Act, 79th Congress, P.L. 584.

Table I

(0kℓ) Precession Data							
k	ℓ	F ₀	F _c	k	ℓ	F ₀	F _c
2	0	54.1	41.2	1	3	17.4	6.7
4	0	61.5	-49.1	2	3	48.4	-51.0
6	0	38.0	-35.6	3	3	14.7	10.0
8	0	19.5	1.9	4	3	49.5	-46.8
10	0	22.1	27.4	5	3	17.9	12.8
12	0	26.3	43.9	6	3	0.0	9.4
1	1	0.0	0.0	7	3	13.4	7.5
2	1	75.2	70.8	8	3	32.6	47.8
3	1	39.0	32.7	9	3	0.0	3.4
4	1	62.6	53.5	10	3	20.8	27.3
5	1	0.0	13.0	11	3	0.0	7.6
6	1	0.0	-12.5	12	3	0.0	-15.0
7	1	0.0	-6.5	0	4	56.3	60.2
8	1	43.6	-44.8	1	4	12.1	2.8
9	1	11.6	10.7	2	4	24.7	33.5
10	1	24.7	-32.1	3	4	21.0	0.3
11	1	0.0	16.9	4	4	25.2	-21.6
12	1	0.0	10.8	5	4	0.0	-6.3
0	2	51.0	-43.0	6	4	39.2	-42.6
1	2	0.0	-5.8	7	4	8.7	1.0
2	2	32.4	-19.6	8	4	12.6	-3.8
3	2	16.0	0.2	9	4	8.9	6.8
4	2	40.2	37.5	10	4	17.9	38.7
5	2	16.0	7.0	11	4	0.0	0.0
6	2	75.1	67.0	1	5	17.1	10.1
7	2	0.0	-3.8	2	5	28.9	32.6
8	2	21.0	27.3	3	5	0.0	6.0
9	2	0.0	-4.4	4	5	29.4	41.8
10	2	21.5	-30.8	5	5	22.6	5.9
11	2	0.0	5.2	6	5	0.0	0.5
12	2	20.5	-35.6	7	5	0.0	4.8

k	l	F ₀	F _c	k	l	F ₀	F _c
8	5	25.7	-46.6	5	6	0.0	-10.8
9	5	0.0	4.1	6	6	22.4	47.3
10	5	13.9	-29.5	7	6	0.0	-0.6
0	6	32.1	-32.5	1	7	20.0	-0.8
1	6	16.0	12.2	2	7	20.0	-45.4
2	6	19.7	-18.3	3	7	0.0	12.0
3	6	22.9	8.5	4	7	11.6	-26.4
4	6	14.5	28.3				

F₀ is not corrected for absorption effects

F_c is not corrected for temperature effects

F₀ is scaled to F_c by normalization

$$\left(\text{Reliability factor} = \frac{\sum |F_0| - |F_c|}{\sum |F_0|} = 0.34 \right)$$

Table II

(hkh) Data						
h	k	A	B	C	corrected $ F_0 $	$ F_c $
0	2	22.9	2.55	10.5	61.3	51.1
0	4	34.6	2.27	6.6	51.8	45.4
0	6	33.1	2.05	4.4	29.8	28.3
0	8	20.0	1.94	3.0	11.6	15.1
0	10	29.3	1.85	2.2	11.9	13.1
0	12	51.3	1.79	1.8	16.1	12.8
0	14	5.2	1.73	1.5	1.4	0.7
1	1	17.0	2.73	10.0	46.4	37.6
1	2	34.9	2.52	8.6	76.0	90.9
1	3	7.6	2.63	7.2	14.4	12.3
1	4	34.6	2.72	6.0	56.5	54.0
1	5	15.8	2.84	5.0	22.2	18.5
1	6	8.1	2.20	4.1	7.3	5.8
1	7	18.0	2.04	3.4	12.5	9.8
1	8	44.0	1.97	2.8	24.7	27.5
1	9	8.9	1.88	2.4	4.0	4.1
1	10	38.0	1.82	2.1	14.5	14.3
1	11	19.2	1.82	1.9	6.6	4.2
1	12	10.5	1.77	1.7	3.1	1.4
1	13	7.8	1.76	1.6	2.1	1.7
2	0	32.5	2.81	6.6	60.3	70.2
2	1	25.3	3.01	6.4	48.7	49.3
2	2	23.1	2.63	6.0	36.4	38.5
2	3	29.2	2.53	5.3	39.2	42.7
2	4	14.0	2.57	4.7	16.9	18.4
2	5	0.0	--	--	0.0	2.1
2	6	28.6	2.68	3.4	26.0	29.7
2	7	12.9	2.30	2.9	8.6	5.3

h	k	A	B	C	corrected $ F_0 $	$ F_c $
2	8	10.1	2.03	2.6	5.2	4.3
2	9	26.9	1.91	2.2	11.3	14.2
2	10	28.2	1.86	2.0	10.5	8.5
2	11	15.7	1.82	1.8	5.0	4.3
2	12	28.0	1.78	1.6	8.0	5.6
2	13	17.1	1.75	1.5	4.5	3.1
3	1	34.2	2.50	4.2	35.9	53.9
3	2	23.2	2.66	4.0	25.0	28.4
3	3	0.0	--	--	0.0	3.6
3	4	10.7	2.69	3.4	9.8	12.3
3	5	22.8	2.63	3.0	18.0	19.0
3	6	0.0	--	--	0.0	0.8
3	7	19.7	2.64	2.4	12.5	11.5
3	8	11.4	2.12	2.2	5.2	7.0
3	9	0.0	--	--	0.0	1.4
3	10	20.2	1.88	1.8	6.8	5.2
3	11	33.6	1.83	1.6	10.2	8.1
4	0	0.0	--	--	0.0	0.4
4	1	16.2	2.31	2.8	10.7	15.6
4	2	0.0	--	--	0.0	5.8
4	3	29.7	2.36	2.6	18.6	28.0
4	4	0.0	--	--	0.0	1.4
4	5	14.4	2.47	2.4	8.4	9.5
4	6	6.3	2.52	2.2	3.4	6.2
4	7	21.9	2.54	2.0	11.1	9.6
4	8	0.0	--	--	0.0	--
4	9	33.0	1.91	1.7	10.7	2.0
5	1	26.2	2.17	2.2	12.2	18.8
5	2	11.3	2.18	2.1	5.2	6.4
5	3	0.0	--	--	0.0	0.8

h	k	A	B	C	corrected $ F_0 $	$ F_c $
5	4	0.0	--	--	0.0	1.4
5	5	18.4	2.24	1.9	7.8	8.2
5	6	0.0	--	--	0.0	0.1
5	7	13.7	2.00	1.7	4.6	5.1
6	0	11.9	2.09	1.7	4.2	5.7
6	1	9.8	2.10	1.7	3.5	3.7
6	2	0.0	--	--	0.0	3.1
6	3	16.7	2.09	1.6	5.8	6.3
6	4	0.0	--	--	0.0	1.0
6	5	0.0	--	--	0.0	2.0
6	6	12.0	1.85	1.5	3.4	1.7

*A - $|F_0|$ uncorrected for absorption

B - correction for crystalline absorption

C - correction for non-crystalline absorption

Note: $|F_c|$ is scaled to the relative values of $|F_0|$ and a temperature correction is applied which was derived from a plot of $\log (F_c/F_0)$ versus $\sin^2 \theta$.

Table III

Observed and calculated structure factors

The following tabulation of data has been reproduced by a photographic process from pages printed automatically by the IBM 405 tabulator from cards punched by the IBM 650 computer as a result of the least-squares refinement calculations. By virtue of the mechanism of the automatic printer, some of the zero values for " h ", " F_0 ", and " F_c ", appear as blank spaces. A minus sign to the right of the F_c values indicates that the value has been calculated as negative.

OBSERVED AND CALCULATED
STRUCTURE FACTORS

H	K	L	F _O	F _C	H	K	L	F _O	F _C
0	2	00	34.1	31.5	1	09	00	7.7	6.0
0	4	00	38.6	31.2-	1	10	00	12.5	11.1
0	6	00	25.8	20.6-	1	11	00		.2
0	8	00	11.8	8.7-	1	12	00	14.2	10.1
0	10	00	13.9	12.5	1	13	00	2.7	2.1-
0	12	00	19.8	14.8	1	14	00	1.6	1.5
0	14	00	1.9	1.7	2	00	00	35.4	26.0
1	00	00	58.8	64.4	2	01	00		1.1
1	01	00	13.9	9.1-	2	02	00	19.3	17.0
1	02	00	33.1	28.7	2	03	00	25.3	24.6-
1	03	00	18.0	14.1-	2	04	00	25.3	25.9-
1	04	00	27.6	29.5-	2	05	00	17.1	16.8-
1	05	00	8.0	6.4-	2	06	00	31.5	40.7-
1	06	00	38.9	37.7-	2	07	00	14.6	14.7
1	07	00	4.9	3.8	2	08	00	10.4	9.2-
1	08	00	10.7	8.3-	2	09	00	10.0	9.9

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H	K	L	F _O	F _C	H	K	L	F _O	F _C
2	10	00	10.5	8.3	4	02	00	18.0	14.8
2	11	00		.1-	4	03	00	25.6	27.3-
2	12	00	8.3	6.3	4	04	00		2.6-
2	13	00	2.3	1.7-	4	05	00	2.7	3.4-
3	00	00	42.2	34.5	4	06	00	7.4	10.1-
3	01	00	22.5	18.3-	4	07	00	4.2	6.7
3	02	00	16.2	14.8	4	08	00		.1
3	03	00	23.4	28.5-	4	09	00	11.7	11.3
3	04	00	11.7	13.4-	4	10	00	5.6	5.6
3	05	00	6.2	7.7-	4	11	00	3.9	3.5
3	06	00	15.8	19.3-	4	12	00	4.1	3.8
3	07	00	8.6	10.6	5	00	00	7.0	6.8
3	08	00	5.5	5.4-	5	01	00	11.6	11.7-
3	09	00	11.6	12.1	5	02	00		1.6
3	10	00	8.1	7.4	5	03	00	21.1	22.8-
3	11	00	3.1	2.8	5	04	00	4.3	4.7-
3	12	00	7.6	6.2	5	05	00	6.3	8.2-
3	13	00	3.5	3.3-	5	06	00	4.8	4.4-
4	00	00	22.6	19.7	5	07	00	8.7	9.2
4	01	00	25.5	23.7-	5	08	00		1.4-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
5	09	00	10.6	9.3	2	01	53.8	62.8-	
6	00	00		1.8	3	01	32.1	30.5	
6	01	00	9.2	8.3-	4	01	42.6	38.2-	
6	02	00	4.7	4.2-	5	01	4.5	3.4-	
6	03	00	16.5	16.0-	6	01	6.9	5.2	
6	04	00	3.4	3.8-	7	01	3.8	2.1-	
6	05	00	5.8	6.1-	8	01	26.0	22.8	
6	06	00		.7	9	01	9.8	8.4	
6	07	00	6.7	7.0	10	01	16.9	13.6	
6	08	00	3.0	1.9-	11	01		1.8	
6	09	00	6.1	7.6	12	01	2.9	2.6-	
7	00	00	3.0	3.2-	13	01	4.1	.8	
7	01	00	5.3	5.8-	14	01	11.5	6.6-	
7	02	00		.4-	1	01	01	11.6	8.6-
7	03	00	9.2	10.3-	1	02	01	53.4	52.7-
7	04	00	2.4	2.2	1	03	01	16.5	11.0-
7	05	00	3.2	3.7-	1	04	01	34.1	38.8-
7	06	00	1.3	1.9	1	05	01	6.6	5.8
					1	06	01	5.9	5.2
					1	07	01	4.6	3.4
	1	01	13.6	6.5					

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
1	08	1	22.0	21.9	3	01	1	23.0	19.2-
1	09	1	4.3	3.8-	3	02	1	23.7	21.6-
1	10	1	14.6	11.5	3	03	1	7.2	6.4
1	11	1	2.8	2.1-	3	04	1	19.1	23.7-
1	12	1	2.8	2.4-	3	05	1	14.9	17.6
1	13	1	1.7	1.0-	3	06	1		2.4
1	14	1		6.2-	3	07	1	8.9	12.4
2	01	1	23.7	19.4-	3	08	1	14.8	15.7
2	02	1	39.6	47.1-	3	09	1		-
2	03	1	18.3	16.2-	3	10	1	7.7	6.6
2	04	1	24.2	23.8-	3	11	1	6.5	5.9-
2	05	1	11.3	11.5	4	01	1	18.0	16.5-
2	06	1	3.2	3.6	4	02	1	10.2	9.1-
2	07	1	7.4	7.8	4	03	1	4.4	4.4
2	08	1	16.0	16.7	4	04	1	10.9	17.0-
2	09	1	7.2	6.8-	4	05	1	16.9	19.8
2	10	1	14.9	12.0	4	06	1		1.1
2	11	1	6.2	5.4-	4	07	1	12.2	12.6
2	12	1	2.4	2.1-	4	08	1	10.1	10.3
2	13	1	2.3	2.2-	4	09	1		.6-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
4	10	1	3.4	2.7	7	02	1	4.6	1.3
4	11	1	6.1	5.1-	1	01	-1	30.2	21.0
5	01	1	18.8	19.9-	1	02	-1	54.5	56.1
5	02	1	9.2	8.9-	1	03	-1	12.0	6.9
5	03	1		.8	1	04	-1	38.3	34.3
5	04	1	4.4	3.7-	1	05	-1	17.5	12.4-
5	05	1	13.3	12.3	1	06	-1	5.3	4.2-
5	06	1		.3	1	07	-1	11.8	9.2-
5	07	1	7.3	7.4	1	08	-1	25.4	23.1-
5	08	1		2.6	1	09	-1	4.4	3.5
5	09	1	2.4	1.8-	1	10	-1	16.3	13.8-
5	10	1	2.2	2.4	1	11	-1	7.3	5.5
6	01	1	16.2	15.4-	1	12	-1	2.9	2.6
6	02	1		2.5-	1	13	-1		1.9
6	03	1		1.5	2	01	-1	23.1	21.3
6	04	1		.1-	2	02	-1	25.8	22.9
6	05	1	7.2	8.3	2	03	-1	20.7	16.5-
6	06	1		.4	2	04	-1	40.0	42.8
6	07	1	4.9	5.4	2	05	-1	25.6	26.3-
7	01	1	15.4	6.8-	2	06	-1		3.3-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	07	-1	17.8	17.0-	4	01	-1	43.8	39.3
2	08	-1	23.7	24.4-	4	02	-1	22.7	20.6
2	09	-1		2.0-	4	03	-1		2.8-
2	10	-1	9.6	7.1-	4	04	-1	4.6	4.6
2	11	-1	7.4	5.1	4	05	-1	11.9	16.8-
2	12	-1		2.2	4	06	-1		1.2-
2	13	-1	2.8	2.4	4	07	-1	7.0	10.0-
3	01	-1	36.6	30.4	4	08	-1	4.3	3.9-
3	02	-1	22.9	23.5	4	09	-1		2.5
3	03	-1	4.8	3.1-	4	10	-1	5.2	5.2-
3	04	-1	23.0	23.0	4	11	-1	10.6	10.1
3	05	-1	23.6	27.0-	5	01	-1	24.3	24.7
3	06	-1		1.6-	5	02	-1	4.1	4.2
3	07	-1	12.3	15.5-	5	03	-1	4.0	2.1-
3	08	-1	12.0	13.5-	5	04	-1	4.0	2.9
3	09	-1		2.3	5	05	-1	15.5	18.2-
3	10	-1	6.9	5.9-	5	06	-1		1.3-
3	11	-1	8.4	7.6	5	07	-1	10.9	12.1-
3	12	-1		1.9	5	08	-1		2.1-
3	13	-1	3.8	3.8	5	09	-1		1.9

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
5	10	-1		12-					
5	11	-1	7.2	7.4			2	40.7	34.0-
6	01	-1	10.5	11.5	1	2		1.7	
6	02	-1		13-	2	2	28.8	23.2-	
6	03	-1		.5	3	2	13.1	9.6-	
6	04	-1	11.9	15-	4	2	26.6	26.7	
6	05	-1	17.9	17.8-	5	2	9.8	8.6-	
6	06	-1		.1	6	2	43.6	43.4	
6	07	-1	11.7	12.1-	7	2	7.5	5.7	
6	08	-1		1.0	8	2	10.4	8.5	
6	09	-1	1.9	2.1	9	2	4.6	4.2	
7	01	-1	9.6	10.9	10	2	14.0	9.9-	
7	02	-1	3.4	3.9-	11	2		.7-	
7	03	-1		.7-	12	2	10.2	7.3-	
7	04	-1	2.0	3.3-	13	2	1.6	.9-	
7	05	-1	7.5	9.0-	1	00	2	70.0	70.6-
7	06	-1		.8	1	01	2		.2-
7	07	-1	4.5	6.2-	1	02	2	25.0	22.9-
8	01	-1	5.6	7.9	1	03	2	3.7	2.7
8	02	-1	3.0	5.7-	1	04	2	25.1	23.1

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
1	05	2		.7	2	12	2	10.6	9.1-
1	06	2	19.3	21.3	3	00	2	20.5	18.6-
1	07	2	3.7	2.2-	3	01	2	5.9	4.6
1	08	2	7.3	6.9	3	02	2	12.5	10.6-
1	09	2		.6-	3	03	2	16.4	15.7
1	10	2	11.2	10.1-	3	04	2	12.5	14.5
1	11	2		.4-	3	05	2	7.3	6.8
1	12	2	13.9	11.0-	3	06	2	18.4	22.8
2	00	2	55.3	53.6-	3	07	2	6.5	7.9-
2	01	2	13.2	9.7	3	08	2	5.3	5.0
2	02	2	18.5	18.1-	3	09	2	7.0	7.0-
2	03	2	10.7	11.3	3	10	2	5.8	5.2-
2	04	2	6.9	18.5	4	00	2	14.8	13.2-
2	05	2		2.6	4	01	2	6.5	5.8
2	06	2	15.4	17.6	4	02	2	5.0	5.3-
2	07	2		2.4-	4	03	2	15.9	16.1
2	08	2	5.7	5.5	4	04	2	9.0	6.8
2	09	2	4.9	5.0-	4	05	2	7.5	7.6
2	10	2	9.1	8.3-	4	06	2	12.4	12.5
2	11	2		.9-	4	07	2	8.7	8.4-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
4	08	2	4.6	3.8	1	04	-2	31.7	25.6
4	09	2	7.9	7.5-	1	05	-2	17.4	12.8
4	10	2	3.6	3.4-	1	06	-2	41.6	37.3
5	00	2	10.8	9.2-	1	07	-2	17.4	12.9-
5	01	2	12.1	10.6	1	08	-2	11.9	9.8
5	02	2	6.7	5.7-	1	09	-2	10.1	9.1-
5	03	2	15.6	13.8	1	10	-2	13.1	9.4-
5	04	2		1.6	1	11	-2	5.0	.6-
5	05	2		2.6	1	12	-2	9.6	7.4-
5	06	2	4.1	4.4	1	13	-2	2.0	1.5
5	07	2	5.0	4.3-	2	00	-2	56.0	50.5-
6	00	2	2.4	2.3-	2	01	-2	37.2	33.1
6	01	2	5.9	6.7	2	02	-2	32.4	25.5-
6	02	2	2.7	2.3-	2	03	-2	34.8	32.0
6	03	2	9.6	10.6	2	04	-2	14.9	12.0
6	04	2		.2	2	05	-2		1.6
6	05	2	2.8	3.0	2	06	-2	22.8	20.3
1	01	-2		2.2	2	07	-2	9.0	6.7-
1	02	-2	24.7	18.4-	2	08	-2	5.3	3.8
1	03	-2	29.8	23.0	2	09	-2	13.2	12.7-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	10	-2	11.4	10.1-	4	02	-2	3.8	3.4
2	11	-2	4.2	4.4-	4	03	-2	24.8	32.7
2	12	-2	9.8	8.1-	4	04	-2	11.1	13.4
2	13	-2	4.8	4.3	4	05	-2	10.6	14.0
3	00	-2	38.5	26.7-	4	06	-2	4.5	6.3
3	01	-2	29.8	27.2	4	07	-2	9.3	14.6-
3	02	-2	20.3	13.1-	4	08	-2	5.3	5.3
3	03	-2	34.2	35.9	4	09	-2	13.4	13.3-
3	04	-2	8.1	7.6	4	10	-2		-
3	05	-2	7.3	7.5	4	11	-2		1.7-
3	06	-2	14.2	15.7	4	12	-2	3.1	2.4-
3	07	-2	9.6	10.2-	5	00	-2	3.8	3.7-
3	08	-2		.9	5	01	-2	16.0	14.6
3	09	-2	12.9	13.4-	5	02	-2	3.5	2.9
3	10	-2	6.4	6.3-	5	03	-2	23.1	25.5
3	11	-2	3.5	3.4-	5	04	-2	3.7	4.1
3	12	-2	5.7	4.8-	5	05	-2	7.3	9.0
3	13	-2	5.0	4.7	5	06	-2		.2
4	00	-2	20.6	15.2-	5	07	-2	9.0	10.5-
4	01	-2	17.9	13.8	5	08	-2		1.9

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
5	09	-2	12.8	12.3-	7	07	-2	4.0	5.4-
5	10	-2		.6	8	00	-2	6.2	7.4
5	11	-2	2.0	2.2-	8	01	-2	4.3	5.4
6	00	-2	5.1	5.9	8	02	-2	3.1	4.3
6	01	-2	9.1	9.2	8	03	-2	4.4	6.9
6	02	-2	4.1	3.0-					
6	03	-2	19.3	18.7	1	3	12.3	10.0-	
6	04	-2	7.5	6.2-	2	3	32.9	31.6	
6	05	-2	7.5	7.5	3	3	9.3	7.5	
6	06	-2		1.9-	4	3	30.5	31.3	
6	07	-2	7.8	8.4-	5	3	9.4	9.2	
6	08	-2		2.9-	6	3	3.6	3.2-	
6	09	-2	8.2	8.8-	7	3	7.1	6.9	
7	00	-2	6.3	6.5	8	3	19.7	20.6-	
7	01	-2	5.2	6.0	9	3		1.3	
7	02	-2		1.8	10	3	12.3	9.3-	
7	03	-2	11.9	12.4	11	3	4.7	3.1-	
7	04	-2	3.9	4.3-	12	3	2.7	2.1	
7	05	-2	4.4	4.9	1	01	3	2.2	2.4-
7	06	-2	3.5	4.4-	1	02	3	29.4	37.0

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
1	03	3	14.0	13.7-	2	11	3	2.2	1.5
1	04	3	19.8	23.1	3	01	3	12.1	10.6
1	05	3		.1	3	02	3	21.3	21.7
1	06	3	3.2	3.1-	3	03	3	7.6	7.2
1	07	3		.4	3	04	3	14.2	13.1
1	08	3	18.2	16.0-	3	05	3	7.7	7.1-
1	09	3	5.7	4.8-	3	06	3	2.3	2.0-
1	10	3	13.7	10.2-	3	07	3	4.3	4.5-
1	11	3		1.0-	3	08	3	9.7	9.0-
1	12	3	2.2	2.0	3	09	3	5.1	3.8
2	01	3	6.5	5.8	3	10	3	7.5	6.0-
2	02	3	24.5	27.0	4	01	3	13.8	10.7
2	03	3	4.6	5.2-	4	02	3	15.0	12.5
2	04	3	16.9	22.2	4	03	3		.4
2	05	3	3.9	4.7-	4	04	3	9.8	8.3
2	06	3	2.7	2.9-	4	05	3	8.6	8.0-
2	07	3	2.8	2.9-	4	06	3		1.2-
2	08	3	15.3	13.7-	4	07	3	5.7	5.7-
2	09	3		1.1-	4	08	3	7.2	6.3-
2	10	3	8.3	7.0-	5	01	3	7.6	7.5

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H	K	L	F _O	F _C	H	K	L	F _O	F _C
5	02	3	3.3	3.6	2	03	-3		.3
5	03	3	2.7	2.3-	2	04	-3	18.2	16.1-
5	04	3	6.9	6.7	2	05	-3	21.4	19.7
5	05	3	6.9	8.8-	2	06	-3	2.7	1.9
6	01	3	3.7	6.8	2	07	-3	12.7	10.9
1	01	-3	15.4	16.1-	2	08	-3	12.2	10.5
1	02	-3	25.7	23.1-	2	09	-3	4.2	3.1-
1	03	-3	13.4	9.8	2	10	-3	10.9	8.1
1	04	-3	40.1	35.5-	2	11	-3	10.7	8.4-
1	05	-3	26.4	21.4	2	12	-3		1.8-
1	06	-3	2.6	2.7	2	13	-3	4.2	4.2-
1	07	-3	14.1	13.0	3	01	-3	34.3	41.6-
1	08	-3	22.0	20.6	3	02	-3	24.2	22.7-
1	09	-3		.9	3	03	-3	4.4	3.8
1	10	-3	8.5	6.4	3	04	-3	9.5	8.0-
1	11	-3	5.8	4.4-	3	05	-3	17.9	18.1
1	12	-3	2.6	2.1-	3	06	-3		2.4
1	13	-3	2.9	2.1-	3	07	-3	12.3	11.5
2	01	-3	37.4	35.5-	3	08	-3	7.5	6.1
2	02	-3	36.1	33.8-	3	09	-3	3.4	2.3-

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H	K	L	F _O	F _C	H	K	L	F _O	F _C
3	10	-3	7.9	5.8	5	08	-3		.9-
3	11	-3	12.4	10.7-	5	09	-3	2.8	2.7-
4	01	-3	25.4	22.7-	5	10	-3		-
4	02	-3	5.3	5.0-	5	11	-3	6.0	6.1-
4	03	-3		.2-	6	01	-3	22.5	20.7-
4	04	-3	6.0	6.5-	6	02	-3	8.3	7.1
4	05	-3	20.2	27.6	6	03	-3		1.8
4	06	-3	2.2	1.5	6	04	-3		2.6
4	07	-3	15.2	13.3	6	05	-3	11.9	11.2
4	08	-3	2.9	4.1	6	06	-3		1.0-
4	09	-3	4.0	3.1-	6	07	-3	6.7	7.4
4	10	-3	2.5	1.4	6	08	-3		2.1-
4	11	-3	7.9	7.4-	6	09	-3	1.5	1.4-
5	01	-3	19.5	17.7-	7	01	-3	14.0	12.8-
5	02	-3			7	02	-3	8.7	8.7
5	03	-3		.4-	7	03	-3		.2
5	04	-3		1.5	7	04	-3	3.9	4.1
5	05	-3	17.0	23.3	7	05	-3	6.6	7.7
5	06	-3		.7-	7	06	-3		.5-
5	07	-3	13.2	15.7	7	07	-3	4.1	4.7

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
8	01	-3	3.7	5.0-	1	01	4		2.3-
8	02	-3	4.1	5.1	1	02	4	11.9	12.0
8	03	-3	1.4	1.4	1	03	4	4.6	4.0
8	04	-3	4.2	6.4	1	04	4	16.0	15.8-
					1	05	4	5.4	4.6
		4	25.3	34.3	1	06	4	28.2	26.6-
1	4		7.8	8.2	1	07	4	29.5	3.8-
2	4		16.0	14.5	1	08	4	8.8	6.0-
3	4		13.9	12.9	1	09	4		1.9-
4	4		16.6	14.8-	1	10	4	9.6	6.5
5	4		5.3	3.0	1	11	4		.4
6	4		23.6	20.7-	1	12	4	8.6	4.9
7	4		6.8	5.1-	2	00	4	23.6	24.9
8	4		7.8	5.8-	2	01	4		1.2-
9	4		8.6	5.7-	2	02	4	10.5	11.3
10	4		10.5	7.7	2	03	4		2.7-
11	4			1.5-	2	04	4	13.1	12.0-
12	4		10.8	6.8	2	05	4		3-
13	4			1.5	2	06	4	18.8	16.8-
1	00	4	18.2	20.0	2	07	4		1.5

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	08	4		4.1-	5	01	4		2.4-
2	09	4		.9	5	02	4		1.9
2	10	4		5.8	5	03	4	9.6	7.0-
2	11	4		.5	1	02	-4	21.0	19.9
2	12	4	6.8	5.3	1	03	-4	24.2	21.9-
3	00	4	22.9	25.2	1	04	-4	11.5	9.3-
3	01	4	6.4	4.5-	1	05	-4		.8-
3	02	4	7.9	8.5	1	06	-4	20.0	16.9-
3	03	4	6.1	6.4-	1	07	-4	5.5	4.1
3	04	4	8.5	8.4-	1	08	-4		2.1-
3	05	4		1.5-	1	09	-4	11.0	9.1
3	06	4	9.0	7.9-	1	10	-4	9.1	8.3
4	00	4	10.3	11.2	1	11	-4	6.3	3.3
4	01	4	6.5	4.3-	1	12	-4	10.2	6.8
4	02	4	6.6	5.0	1	13	-4	8.7	3.5-
4	03	4	8.7	7.6-	2	02	-4		8.9
4	04	4		5.8-	2	03	-4	28.5	29.0-
4	05	4		2.9-	2	04	-4	14.4	13.1-
4	06	4	8.7	8.1-	2	05	-4	11.9	10.8-
5	00	4		4.4	2	06	-4	17.0	15.0-

MU-10299

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	07	-4	13.6	11.7	4	03	-4	25.7	28.1-
2	08	-4	6.2	3.9-	4	04	-4		.4
2	09	-4	14.4	11.4	4	05	-4	11.3	9.7-
2	10	-4	7.3	4.2	4	06	-4		3.1-
2	11	-4		1.8	4	07	-4	13.6	11.4
2	12	-4	8.4	4.5	4	08	-4		.4
2	13	-4		3.5-	4	09	-4	15.2	13.6
3	00	-4	14.1	17.3	5	00	-4	6.2	5.7-
3	01	-4	12.4	13.7-	5	01	-4	9.6	10.9-
3	02	-4		3.3-	5	02	-4	6.6	4.2
3	03	-4	27.4	30.4-	5	03	-4	20.2	24.0-
3	04	-4	14.2	14.3-	5	04	-4	8.8	7.0
3	05	-4	13.9	12.9-	5	05	-4	10.2	9.9-
3	06	-4	9.7	7.0-	5	06	-4		1.4
3	07	-4	15.3	13.8	5	07	-4	10.9	10.8
3	08	-4	8.4	6.1-	5	08	-4		3.1
3	09	-4	17.0	13.7	5	09	-4	12.8	10.6
4	00	-4		2.5	6	00	-4	7.9	8.2-
4	01	-4	12.9	16.5-	6	01	-4	9.6	11.1-
4	02	-4	5.3	4.2	6	02	-4	5.9	5.3-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
6	03	-4	14.5	17.5-	9	5			.6
6	04	-4		2.7	10	5		7.2	5.2
6	05	-4		5.0-	1	01	5		3.1
6	06	-4	7.7	5.4	1	02	5	14.3	14.6-
6	07	-4		6.3	1	03	5	5.5	5.3-
6	08	-4		.4	1	04	5	19.4	17.7-
6	09	-4	7.0	7.5	1	05	5	6.0	5.0-
7	00	-4	9.9	11.0-	1	06	5		1.7
7	01	-4	7.5	6.7-	1	07	5		3.5-
7	02	-4	6.4	6.0-	1	08	5	37.6	11.9
7	03	-4	10.0	11.0-	1	09	5		1.4-
					1	10	5	6.4	4.7
	1	5	8.8	10.0	1	11	5		1.1
	2	5	17.5	13.3-	2	01	5		.1
	3	5		1.6-	2	02	5	14.7	15.6-
	4	5	19.5	15.8-	2	03	5		1.7
	5	5	12.1	10.0-	2	04	5	11.4	11.5-
	6	5		1.6	2	05	5		.5
	7	5	7.3	5.9-	2	06	5		1.4
	8	5	13.2	10.9	2	07	5		.1

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	08	5	9.9	8.6	1	05	-5	11.5	10.0-
2	09	5		.6	1	06	-5		1.7-
2	10	5	8.5	5.1	1	07	-5	7.9	6.0-
2	11	5	7.8	.1	1	08	-5	9.6	7.2-
3	01	5		2.7-	1	09	-5		2.1
3	02	5	9.9	11.3-	1	10	-5	10.3	6.4-
3	03	5		3.9	1	11	-5	9.6	6.4
3	04	5	8.2	9.1-	2	02	-5	10.1	13.4
3	05	5		2.8	2	03	-5		1.6-
3	06	5		1.1	2	04	-5	11.3	9.9
3	07	5		1.8	2	05	-5	18.2	16.5-
3	08	5	9.0	6.2	2	06	-5		2.1-
4	01	5		4.4-	2	07	-5	14.1	11.2-
4	02	5	7.3	7.5-	2	08	-5	8.3	6.9-
4	03	5		.7-	2	09	-5		1.9
4	04	5	7.0	5.8-	2	10	-5	6.5	4.0-
1	01	-5	17.1	22.9	2	11	-5	10.3	7.1
1	02	-5	20.3	23.1	3	02	-5	6.1	5.7
1	03	-5		.2-	3	03	-5		1.1
1	04	-5	11.0	9.6	3	04	-5	8.6	6.3

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
3	05	-5	24.1	24.6-	5	01	-5	17.4	23.5
3	06	-5		.7-	5	02	-5	8.7	7.7-
3	07	-5	17.7	16.7-	5	03	-5		1.8-
3	08	-5		4.1-	5	04	-5		1.0-
3	09	-5		2.9	5	05	-5	11.7	11.6-
3	10	-5		1.7-	5	06	-5		.5
3	11	-5	8.5	5.8	5	07	-5	10.5	7.3-
4	01	-5	16.4	21.9	5	08	-5		1.1
4	02	-5		.4	5	09	-5		1.7
4	03	-5	4.9	1.5-	5	10	-5		2.1
4	04	-5		.1	5	11	-5	7.6	6.9
4	05	-5	18.7	18.2-	6	01	-5	11.6	13.3
4	06	-5		.7	6	02	-5	6.9	7.3-
4	07	-5	13.6	12.3-	6	03	-5		.9-
4	08	-5		-	6	04	-5		6.2-
4	09	-5	4.8	2.0	6	05	-5	11.2	11.4-
4	10	-5		.1-	6	06	-5		.4
4	11	-5	10.5	7.0	6	07	-5	7.4	7.1-
4	12	-5		.4	6	08	-5		4.1
4	13	-5	6.9	3.0	6	09	-5		1.3

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
6	10	-5		2.1	1	02	6	6.6	7.4-
6	11	-5	8.8	4.1	1	03	6	4.8	4.8-
7	01	-5	8.1	6.9	1	04	6	6.6	5.8
					1	05	6		
	6	13.4	15.8-		1	06	6	9.4	6.3
1	6	6.8	7.2-		1	07	6		1.0
2	6	8.8	8.4-		1	08	6	3.3	2.0
3	6	10.5	9.7-		1	09	6	3.2	2.2
4	6	6.8	5.9		1	10	6	4.6	3.9-
5	6		2.0-		1	11	6		.9
6	6	11.7	9.5		1	12	6	5.4	3.5-
7	6	3.1	2.8		2	00	6	9.9	10.0-
8	6	2.9	1.6		2	01	6		.4
9	6	4.8	4.2		2	02	6	4.6	4.7-
10	6	5.1	3.9-		2	03	6		1.0-
11	6		1.1		2	04	6	5.7	6.2
12	6	5.7	3.4-		2	05	6		.9-
13	6		1.5-		2	06	6	10.0	9.5
1	00	6	15.3	16.5-	2	07	6		1.0
1	01	6	4.4	4.8-	2	08	6	3.5	2.5

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	09	6		.5	1	01	-6	4.5	5.4
2	10	6	3.4	2.8-	1	02	-6	3.2	2.3-
2	11	6		-	1	03	-6	14.9	14.4
2	12	6	4.5	2.4-	1	04	-6	9.7	9.5
3	00	6	7.1	7.0-	1	05	-6	7.3	6.8
3	01	6		1.0	1	06	-6	10.3	8.7
3	02	6	4.6	3.8-	1	07	-6	8.2	7.1-
3	03	6		1.4	1	08	-6	5.0	3.7
3	04	6	4.0	4.5	1	09	-6	8.5	6.4-
3	05	6		.1	1	10	-6	3.9	1.9-
3	06	6	7.5	7.3	1	11	-6		.7-
4	00	6	7.5	7.1-	1	12	-6	5.4	2.8-
4	01	6		1.4	1	13	-6	2.6	1.7
4	02	6	3.3	2.3-	1	14	-6		.1-
4	03	6		2.4	2	02	-6	1.5	1.4-
4	04	6	2.6	2.7	2	03	-6	15.4	17.4
4	05	6		.7	2	04	-6	6.3	6.5
4	06	6	3.7	3.3	2	05	-6	7.0	6.5
5	00	6	4.8	4.0-	2	06	-6	6.6	5.7
1	00	-6	8.5	13.5-	2	07	-6	9.1	7.6-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
2	08	-6	4.6	2.8	3	14	-6		.4-
2	09	-6	11.5	8.7-	4	00	-6	2.7	2.0
2	10	-6		1.4-	4	01	-6	8.6	9.3
2	11	-6		1.4-	4	02	-6		.9-
2	12	-6	3.6	2.0-	4	03	-6	18.1	18.6
2	13	-6	4.8	2.4	4	04	-6	3.9	2.5-
2	14	-6		-	4	05	-6	7.0	7.0
3	00	-6		1.7-	4	06	-6		1.0-
3	02	-6	5.4	6.3-	4	07	-6	8.1	7.9-
3	03	-6	18.5	19.0	4	08	-6		.9-
3	04	-6	3.1	2.2-	4	09	-6	8.3	8.0-
3	05	-6	7.4	6.9	4	10	-6		.2-
3	06	-6	4.8	3.5	4	11	-6		1.3-
3	07	-6	9.4	8.1-	4	12	-6		.3
3	08	-6		1.4-	4	13	-6	1.5	2.5
3	09	-6	11.0	9.1-	4	14	-6		-
3	10	-6	4.5	2.2-	5	00	-6	5.8	6.6
3	11	-6		1.6-	5	01	-6	9.3	11.4
3	12	-6		.6-	5	02	-6	4.5	5.6
3	13	-6	4.8	2.6	5	03	-6	13.8	15.3

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
5	04	-6		.4-	7	02	-6	2.5	3.0
5	05	-6	4.3	3.2	7	03	-6	5.2	6.8
5	06	-6	4.2	3.7-	7	04	-6	4.6	5.0-
5	07	-6	4.9	4.8-	7	05	-6	4.3	3.5
5	08	-6		.3	7	06	-6	7.2	7.6-
5	09	-6	8.4	6.9-	7	07	-6		3.7-
5	10	-6		2.2	7	08	-6		2.0-
6	00	-6	7.1	9.1	7	09	-6	4.0	3.2-
6	01	-6	5.9	7.0	8	00	-6	6.0	7.3
6	02	-6	3.8	4.1	8	01	-6		1.8
6	03	-6	9.1	10.9	8	02	-6		3.4
6	04	-6	1.2	3.4-	8	03	-6	3.7	3.3
6	05	-6	3.9	3.0	8	04	-6	4.5	3.9-
6	06	-6	6.4	5.3-	8	05	-6		1.4
6	07	-6	4.2	4.3-	8	06	-6	5.1	5.7-
6	08	-6		1.4-					
6	09	-6	7.1	5.3-	1	7	-	7.2	8.6-
6	10	-6	4.7	2.3	2	7	-	9.1	9.1
7	00	-6	5.5	6.4	3	7	-		.2
7	01	-6		2.1	4	7	-	6.0	5.2

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
	5	7	4.8	4.2	2	04	7	6.4	6.1
	6	7		.9-	2	05	7		1.5
	7	7	3.7	2.8	2	06	7		.6-
	8	7	5.2	3.9-	2	07	7		1.0
	9	7		.8-	2	08	7	5.2	4.1-
	10	7	4.4	2.8-	3	01	7		.4
	11	7	4.3	2.7-	3	02	7	5.4	4.6
1	01	7	4.1	4.4-	3	03	7		.5
1	02	7	7.9	8.5	3	04	7	4.2	4.1
1	03	7		.2-	3	05	7		.2-
1	04	7	6.0	5.6	3	06	7		.5-
1	05	7	3.2	2.7	3	07	7		.1-
1	06	7		.7-	3	08	7	3.1	3.0-
1	07	7		1.6	4	01	7		.9
1	08	7	5.3	3.9-	4	02	7	4.1	3.3
1	09	7		.5-	1	01	-7	6.9	8.0-
1	10	7	4.0	2.5-	1	02	-7	5.9	5.8-
2	01	7		.7-	1	03	-7		.2
2	02	7	5.7	5.6	1	04	-7	7.5	6.0-
2	03	7		1.2	1	05	-7	10.8	9.3

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
1	06	-7		.9	3	03	-7	1.5	1.5
1	07	-7	7.6	6.5	3	04	-7	2.6	1.4-
1	08	-7	5.2	4.2	3	05	-7	11.0	9.0
1	09	-7		1.0-	3	06	-7		.2-
1	10	-7		1.9	3	07	-7	7.7	5.9
1	11	-7	4.7	2.5-	3	08	-7		.8
2	01	-7	4.8	9.3-	3	09	-7		1.0-
2	02	-7	3.1	4.0-	3	10	-7		
2	03	-7		.	3	11	-7	7.0	4.8-
2	04	-7	4.5	3.4-	3	12	-7		.2-
2	05	-7	13.4	12.0	3	13	-7	4.4	2.1-
2	06	-7		.1	4	01	-7	12.1	14.3-
2	07	-7	9.6	8.2	4	02	-7	4.2	3.8
2	08	-7	2.8	2.3	4	03	-7		.7
2	09	-7	2.3	1.3-	4	04	-7		.7
2	10	-7	3.4	1.2	4	05	-7	10.2	8.9
2	11	-7	5.6	3.4-	4	06	-7		-
2	12	-7	2.5	.4-	4	07	-7	6.4	5.5
2	13	-7	3.8	1.4-	4	08	-7	3.7	.6-
3	02	-7		.1-	4	09	-7		1.3-

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H	K	L	F ₀	F _C	H	K	L	F ₀	F _C
4	10	-7		1.0-	6	05	-7	6.2	6.3
4	11	-7	6.3	4.4-	6	06	-7		.6-
4	12	-7		.2	6	07	-7	5.7	4.6
4	13	-7	4.1	2.1-	6	08	-7	4.4	4.2-
5	01	-7	7.7	8.8-	6	09	-7		.2-
5	02	-7	3.3	3.3	6	10	-7		1.8-
5	03	-7		1.5	6	11	-7	3.7	2.3-
5	04	-7	5.3	5.4	6	12	-7		.4
5	05	-7	9.7	9.7	7	01	-7	4.1	4.8-
5	06	-7		.3-	7	02	-7	5.4	7.2
5	07	-7	7.6	6.3	7	03	-7		1.3-
5	08	-7	4.6	3.5-	7	04	-7	5.2	4.5
5	09	-7		.6-	7	05	-7	3.0	3.3
5	10	-7		1.0-	7	06	-7		.6-
5	11	-7	3.9	3.0-	7	07	-7	2.8	2.3
5	12	-7		.4	7	08	-7	3.8	3.5-
6	01	-7	5.6	6.6-	8	01	-7		2.1-
6	02	-7	4.6	5.1	8	02	-7	5.3	5.8
6	03	-7		1.7	8	03	-7		.8-
6	04	-7	5.6	5.9	8	04	-7	4.5	4.6

MU-10310

Table IV

Powder pattern from calculated data											
h	k	l	$\sin^2 \theta$	d	pF^2	h	k	l	$\sin^2 \theta$	d	pF^2
1	0	0	0.0163	6.04	95	3	1	-1	0.130	2.14	41
1	1	0	0.0221	5.18	3	2	2	1	0.132	2.12	99
0	1	1	0.0228	5.10	2	2	3	-2	0.133	2.12	46
0	2	0	0.0231	5.07	22	3	0	-2	0.136	2.09	16
1	1	-1	0.0259	4.78	20	1	1	4	0.139	2.07	69
1	2	0	0.0394	3.88	38	3	1	-2	0.142	2.04	32
0	2	1	0.0401	3.85	179	2	1	-3	0.145	2.02	57
1	2	-1	0.0432	3.71	142	3	0	0	0.147	2.01	27
1	1	1	0.0523	3.37	3	2	4	-1	0.148	2.00	80
2	0	0	0.0653	3.02	17	2	4	0	0.158	1.94	30
0	0	2	0.0680	2.96	28	0	4	2	0.160	1.92	32
0	3	1	0.0690	2.93	37	2	2	-3	0.162	1.91	50
1	2	1	0.0696	2.92	126	0	2	3	0.176	1.84	45
2	0	-2	0.0805	2.72	56	2	0	2	0.186	1.79	64
2	1	-2	0.0863	2.63	48	3	1	-3	0.187	1.78	76
0	4	0	0.0925	2.53	22	3	3	-2	0.188	1.78	58
1	4	0	0.109	2.34	39	3	3	0	0.199	1.73	36
0	4	1	0.110	2.33	66	1	4	-3	0.222	1.63	54
1	0	2	0.111	2.32	108	1	6	0	0.224	1.63	63
1	4	-1	0.113	2.30	54	4	1	-1	0.231	1.60	67
1	2	3	0.232	1.60	60	0	6	2	0.276	1.47	82
0	4	3	0.245	1.56	43	2	3	-4	0.284	1.45	34
1	6	-2	0.266	1.50	60	3	3	-4	0.313	1.38	37
3	5	-1	0.269	1.49	32	4	3	0	0.313	1.38	33
0	0	4	0.272	1.48	24	2	3	3	0.320	1.37	32
2	6	0	0.273	1.48	71	4	3	-4	0.374	1.26	30
4	3	-2	0.276	1.47	47	4	5	-3	0.400	1.22	33

$\sin^2 \theta$ is for copper radiation, $\lambda = 1.5418 \text{ \AA}$

pF^2 values are relative using $F_{\text{calculated}}$

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