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DETERMINATION OF LATTICE PARAMETERS WITH
THE AID OF A COMPUTER

by

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TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	5
I. INTRODUCTION	5
II. METHOD OF SOLUTION AND PROGRAM	6
III. INPUT AND OUTPUT DATA	10
IV. DISCUSSION OF RESULTS	11
V. EXAMPLES	11
Cubic - Au	12
Cubic - UN	14
Cubic - AuBe	15
Cubic - UO ₂	16
Cubic - Si	17
Hexagonal - Ni ₃ Ti	20
Hexagonal - Os	23
Orthorhombic - α U	24
VI. DATA FOR TEST PROBLEM	25
VII. ACKNOWLEDGEMENTS	29
REFERENCES	29

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
I.	Systematic Error Correction Functions	8
II.	Formulas for Lattice Parameter Determination and Their Errors.	9
III.	Lattice Parameters Obtained for Cubic Au Using Various Correction Terms and Weights	13
IV.	Results Obtained by a Change in the Starting Value A_0 (Weyerer Au Data)	14
V.	Lattice Parameters Obtained for Cubic UN Using Various Correction Terms and Weights	15
VI.	Lattice Parameters Obtained for Cubic AuBe Using Various Correction Terms and Weights	16
VII.	Lattice Parameters Obtained for Cubic UO_2 Using Various Correction Terms and Weights.	17
VIII.	Lattice Parameters Obtained for Cubic Si Using Various Correction Terms and Weights	18
IX.	A Comparision of v 's for the Individual Si Reflections for Angles Expressed in Radians to Six and Eight Significant Figures (First and Second Calculation).	19
X.	Lattice Parameters Obtained for Cubic Si Using Various Correction Terms and Weights	20
XIA.	Lattice Parameters Obtained for Hexagonal Ni_3Ti Using Various Correction Terms and Weights (Taylor and Floyd Data ⁽⁵⁾).	21
XIB.	Lattice Parameters Obtained for Hexagonal Ni_3Ti Using Various Correction Terms and Weights (Taylor and Floyd Data ⁽⁵⁾).	22
XII.	Comparison of the Σv_i both plus and minus for the Taylor and Floyd Solution and the Present Determination	23
XIII.	Lattice Parameters Obtained for Hexagonal Os Using Various Correction Terms and Weights	24
XIV.	Lattice Parameters Obtained for Orthorhombic Uranium Using Various Correction Terms and Weights	25

LIST OF FIGURES

<u>No.</u>	<u>Title</u>	<u>Page</u>
1.	Plot of v Versus θ for Cubic Gold Pattern.	13
2.	Plot of v Versus θ for Cubic UN Pattern.	14
3.	Plot of v Versus θ for Cubic AuBe.	16
4.	Plot of v Versus θ for Cubic UO_2	17
5.	Plot of v Versus θ for Cubic Silicon.	18
6.	Plot of v Versus θ for Hexagonal Ni_3Ti	21
7.	Plot of v Versus θ for Hexagonal Osmium.	23
8.	Plot of v Versus θ for Orthorhombic Uranium.	24
9.	Met 124 704 Data Sheet I - Test Problem	26
10.	Met 124 704 Data Sheet II - Test Problem.	27
11.	Met 124 704 Lattice Parameter Results for Test Problem. .	28

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ABSTRACT

The determination of precision lattice parameters using a least-squares analytical treatment has been programmed into a computer. Although it was originally coded for the Argonne AVIDAC and GEORGE computers, it is now programmed for the IBM 704. The present program permits the determination of lattice parameters and standard errors for the orthorhombic system and for all other crystal systems of higher symmetry. The angular measurements of line positions from a Debye-Scherrer or symmetrical focussing camera or a diffractometer may be given in degrees or radians from several different wavelengths. Provision has been made for using as many as three separate correction terms for eccentricity, absorption, divergence, etc.; however, one, two, three, or none at all, may be used. The exact trigonometric function or functions used in these correction terms may be selected from several of those previously suggested. If desired, a weighting factor may also be used for each reflection which may include an observation weight or trigonometric function or both. Examples will be given of lattice parameters obtained for various crystal systems using different correction terms with and without weighting.

I. INTRODUCTION

It has been recognized for some time in the determination of more reliable lattice parameters that graphical extrapolation methods could be used to eliminate, or at least minimize, some of the systematic errors occurring in the position of X-ray diffraction lines. Later it was shown that extrapolation could be carried out analytically by the method of least squares. Important advantages of the later method were: the elimination of subjective errors which occur when a curve or straight line is fitted to a set of points, and the possible use of more of the observed data for the determination of lattice parameters, especially for the nonisometric systems. One of the chief limitations of this method is the elimination of the observer's judgment in deciding which of the measurements are most reliable. It has been pointed out, however, that this objection can be overcome by a procedure in which the lines at higher angle are given more weight.

Since there is a large amount of computation necessary in the analytical extrapolation method using weighting factors, especially for the nonisometric systems, it becomes desirable to use computer techniques. Such a technique makes it possible to try a number of different systematic error-correcting functions which have been suggested over a period of years and thus to observe the effect of each.

Although a brief write-up of the determination of lattice parameters with the aid of a computer has appeared in *Acta Crystallographica*⁽¹⁾ and an oral presentation made at the International Union of Crystallography Conference on Precision Lattice Parameter Determination, Stockholm, Sweden, June 1959, a more detailed description is given in this report.

This report has been written with several objectives in mind:

(1) to briefly describe the general approach to the problem and technique used in the solution, (2) to describe in detail the input data necessary for use with the IBM-704 and GEORGE computers, together with the output data obtained, (3) to illustrate the use of the program with a number of examples, and (4) to give sufficient information on the program so that it can be added to or otherwise modified.

II. METHOD OF SOLUTION AND PROGRAM

The determination of precision lattice parameters was originally coded for the Argonne AVIDAC computer; however, it is now programmed for the Argonne GEORGE digital computer and for IBM-704. The present program permits the determination by a method of least squares of lattice parameters and standard errors for the orthorhombic system and all other crystal systems of higher symmetry. The angular measurements of lines or spots for several different wave lengths obtained from various types of cameras or a diffractometer may be used.

Provision has been made for using as many as three separate correction terms for eccentricity, absorption, divergence, etc.; however, one, two, three or none at all, may be used. The exact trigonometric function or functions used in these correction terms may be selected from a number of those previously suggested, for example, $\sin^2 2\theta$, $\phi \sin 2\phi$, $\cos^2 \theta \sin 2\theta$, $\sin^2 2\theta [(1/\sin \theta) + (1/\theta)]$, $\cos^2 \theta \sin^2 2\theta$, or $\cos 2\theta$. If desired, a weighting factor as suggested by Hess⁽²⁾ may also be used for each reflection, which may include an observation weight and/or a trigonometric function appropriate for the particular instrument, such as $1/\sin^2 2\theta$ for a Debye-Scherrer camera, and in addition a refraction correction may also be used.

The program as written has been made flexible in order to provide for easy modification, and although it makes use of a least-squares analytical treatment, it was possible to incorporate some of the advantages of the graphical methods.

For convenience in defining the problem, the difference, v , between the computed $\sin^2\theta$ and the observed $\sin^2\theta$ for each reflection, i , may be defined as

$$v_i = \sin^2\theta_i \text{ (computed)} - \sin^2\theta_i \text{ (observed)}.$$

The computed $\sin^2\theta_i$ may be written as

$$\sin^2\theta_i \text{ (computed)} = [A g \alpha_i + B \beta_i + C \gamma_i] \lambda_i^2 \text{ (read)} / \lambda^2 \text{ (used in computing parameters)},$$

where

$A, B, C = \lambda^2 \text{ (used)} / 4a_0^2$; $\lambda^2 \text{ (used)} / 4b_0^2$; and $\lambda^2 \text{ (used)} / 4c_0^2$, respectively;

$g = 4/3$ for hexagonal, and 1 for all other systems;

and α_i, β_i and γ_i have the usual meaning related to the Miller indices, that is, for

<u>Cubic</u>	<u>Tetragonal</u>	<u>Hexagonal</u>	<u>Orthorhombic</u>
$\alpha = h^2 + k^2 + l^2$	$h^2 + k^2$	$h^2 + hk + k^2$	h^2
$\beta =$ -	-	-	k^2
$\gamma =$ -	l^2	l^2	l^2

If, however, approximate values of A_0, B_0 and C_0 are adopted, then

$$\sin^2\theta_i \text{ (computed)} = [(A_0 + \Delta A) g \alpha_i + (B_0 + \Delta B) \beta_i + (C_0 + \Delta C) \gamma_i] \lambda_i^2 \text{ (read)} / \lambda^2 \text{ (used)}.$$

If it is assumed that there are systematic errors in θ as measured, then

$$\sin^2\theta_i \text{ (observed)} = \sin^2(\theta_i + \Delta\theta_i) .$$

By squaring and expanding the equation

$$\lambda/2d = \sin(\theta + \Delta\theta)$$

according to the Taylor theorem, and neglecting second-order powers of the error, we obtain

$$(\lambda/2d)^2 = \sin^2\theta + (\Delta\theta) \sin 2\theta .$$

Therefore we may write

$$v_i = \left\{ [(A_0 + \Delta A)g\alpha_i + (B_0 + \Delta B)\beta_i + (C_0 + \Delta C)\gamma_i]\lambda_i^2(\text{read})/\lambda^2(\text{used}) \right\} \\ -\sin^2\theta + (\Delta\theta)\sin 2\theta,$$

where

$$\Delta\theta_i \sin 2\theta_i = \Delta D \delta_j(\theta_i) + \Delta E \epsilon_k(\theta_i) + \Delta F \zeta_\ell(\theta_i)$$

and ΔD , ΔE and ΔF are drift constants associated with $\delta_j(\theta_i)$, $\epsilon_k(\theta_i)$, and $\zeta_\ell(\theta_i)$, which are the various trigonometric functions used in correcting for systematic errors.

The problem is then to minimize the following:

$$\sum_n W_i v_i^2 (\Delta A, \Delta B, \Delta C, \Delta D, \Delta E, \Delta F),$$

where W_i is the weighting factor.

The best values for the particular delta terms used are determined from a set of normal equations which are solved by matrix methods using the computers. The presently included trigonometric systematic error correction functions, $\delta_j(\theta_i)$, $\epsilon_k(\theta_i)$, and $\zeta_\ell(\theta_i)$, which are associated with the ΔD , ΔE , and ΔF drift constants, are summarized in Table I; however, other functions may be conveniently added to the program.

Table I

SYSTEMATIC ERROR CORRECTION FUNCTIONS*

$\delta_j(\theta_i)$	$\epsilon_k(\theta_i)$	$\zeta_\ell(\theta_i)$
$D^1 = \sin^2 2\theta$	$E^1 = \cos^2 \theta \sin^2 \theta$	$F^1 = \cos 2\theta$
$D^2 = \phi \sin 2\phi$	$E^2 = \sin^2 2\theta [(1/\sin \theta) + (1/\theta)]$	
	$E^3 = \sin^2 2\theta / 2\theta$	
	$E^4 = \cos^2 \theta \sin \theta$	
	$E^5 = \cos^2 \theta \sin^2 2\theta$	

* Capital letters with superscript numbers are shorthand notation for these correction terms.

As indicated above, the program is also designed to accommodate a weighting factor W , if desired, where

$$W_i = \frac{w_i}{\text{trig. function of } \theta_i}$$

and w_i is an observation weight for each observation. Each line may be assigned a number varying from 1 to 10, with the larger number indicating more weight. The trigonometric function may change, as suggested by Hess,⁽²⁾ according to the type of instrument used for obtaining the angular positions of the lines or peaks. Provision has been made to use the observational weight, w , and the trigonometric function independently. For convenience in designating the weighting used, a W^1 has been used to indicate no observational or trigonometric weighting, or in other words a weight of one for each line. The term W^2 indicates a weight of $1/\sin^2 2\theta_i$ for each observation, which is the usual weighting for the Debye-Scherrer type camera, and W^3 , W^4 , etc., may be used for other weighting functions.

A refraction correction may be applied, if desired, using the following correction⁽³⁾:

$$\Delta \sin^2 \theta = - \frac{19.58 \rho Z}{M} \frac{\lambda^2}{4} \times 10^{-6} ,$$

where ρ is density, Z is the total number of electrons in the molecule, and M is the molecular weight.

After the best value for the particular delta term or terms used are determined, the lattice parameters and their errors are then calculated with the computer as shown in Table II.

Table II

FORMULAS FOR LATTICE PARAMETER
DETERMINATION AND THEIR ERRORS

Lattice Parameter		Errors		
		50% Confidence Limit (Probable Error)		95% Confidence Limit
$a_0 =$	$\left[\frac{\lambda^2}{4(A_0 + \Delta A)} g \right]^{1/2}$	$a_0 =$	$\frac{0.6745 a_0}{2A} g \sigma_{\Delta A}$	2.9 P.E.
$b_0 =$	$\left[\frac{\lambda^2}{4(B_0 + \Delta B)} \right]^{1/2}$	$S_{b_0} =$	$\frac{0.6745 b_0}{2B} \sigma_{\Delta B}$	2.9 P.E.
$c_0 =$	$\left[\frac{\lambda^2}{4(C_0 + \Delta C)} \right]^{1/2}$	$S_{c_0} =$	$\frac{0.6745 c_0}{2C} \sigma_{\Delta C}$	2.9 P.E.

III. INPUT AND OUTPUT DATA

The input data necessary for a solution of a lattice parameter problem is shown below. In addition, a problem for illustration is given in Section VI. The required data are:

- (1) the number of lattice parameters to be determined - one, two, or three, together with the number of drift constants, ΔD , ΔE , ΔF , to be used, ranging from zero to three;
- (2) type of trigonometric function, $\delta_j(\theta_i)$, $\epsilon_k(\theta_i)$, $\zeta_l(\theta_i)$, to be used with each drift constant;
- (3) α_i , β_i , γ_i , which are related to the Miller indices as indicated above;
- (4) θ_i in degrees or radians;
- (5) value of g ;
- (6) type of trigonometric weighting factor, if used;
- (7) value for w , the observation weight, which may range in value from one to ten, if used;
- (8) starting values for A_0 , B_0 and C_0 as appropriate, together with λ_0 , which is the reference wavelength for the determination;
- (9) λ , the wavelength for each observation;
- (10) the refraction correction, if used;
- (11) the number of observations, n , and
- (12) values for M , Z and ρ if a refraction connection is to be made.

The present program calls for a print out of the following:

- (1) the input data which makes it possible to check for errors;
- (2) ΔA , ΔB , ΔC , and drift constants together with their standard deviations, σ^2 ;
- (3) lattice parameters and standard errors;
- (4) the v for each observation;
- (5) $\sum_n W_i v_i^2 / (n - k - 1) \sum_n W_i$, where n is the number of observations and k the number of degrees of freedom. This last term, the σ^2 of the v_i , is useful in evaluating the fit of the lattice parameters to the observed data.

IV. DISCUSSION OF RESULTS

In the use of this program it has been found advantageous to carry out a number of different solutions to the problem by means of various combinations of systematic correction terms and weights, including a solution using no systematic correction and with equal weight for each observation. From these solutions, a plot of v versus θ for each set of observations is then made, which incorporates some of the advantages of the graphical extrapolation method. From these plots it is possible to:

- (1) detect the degree of systematic errors and to aid in the selection of the most suitable type of systematic correction,
- (2) determine, indeed, if any systematic correction is necessary,
- (3) indicate the degree of randomness, and
- (4) pick out large deviations in individual observations which indicate errors in θ or in incorrect indexing.

Although the plot described above may serve as an excellent guide and in some cases a sufficient one for the determination of the lattice parameters which best fit the data, there are also other ways of judging the fit. Since the solution of this problem was set up on the basis of minimizing the $\sum_n W_i v_i^2$, the size of this term can be observed - the smaller the sum the better the fit.

It should be kept in mind, however, that comparisons between different solutions are comparable only if the same type of weighting has been used for the various solutions and if the same number of systematic correction terms are used. A considerable difference in the numerical value of $\sum_n W_i$ may be obtained for different weighting, depending upon whether it is equal to W^1 , W^2 , W^3 , etc. This will be shown in the examples. Therefore another expression has been used to assist in evaluating the fit. In this expression, $\sum_n W_i v_i^2 / (n-k-1) \sum_n W_i$, the former term, $\sum_n W_i v_i^2$, is divided by the $\sum_n W_i$ and, in addition, compensation is made for a variable number of correction terms by dividing by $(n-k-1)$, where n is the number of observations and k is the number of degrees of freedom.

V. EXAMPLES

The examples given below illustrate the use of the program for crystal systems ranging from cubic to orthorhombic. The results obtained illustrate a number of different features, such as:

- (1) in some cases no systematic correction term is warranted and no benefit is derived from its use;
- (2) in most cases an analytical weighting, such as a Hess type, gives a better set of lattice parameters; however, this is not always true;
- (3) different solutions using the same data but different systematic correction terms in many cases give essentially the same lattice parameters.

All lattice parameters are given in terms of $\overset{\circ}{\text{\AA}}$, using a value of $1.54051 \overset{\circ}{\text{\AA}}$ for the wavelength of Cu K_{α_1} . In some cases the parameters are carried out to more significant numbers than is warranted by the accuracy of the wavelength and/or the angular positions of the lines. This was necessary in order to show variations in the solutions.

Cubic - Au

Figure 1 is a plot of v versus θ using the θ values obtained by Weyerer⁽⁴⁾ from a gold pattern. This pattern was obtained with Cu K_{α} radiation, and the lines with the following values for $h^2 + k^2 + \ell^2$ were used in the solution of the problem: $20\alpha_1$, $24\alpha_1$ and α_2 , and $27\alpha_1$ and α_2 . This figure shows the change in the plot as a result of three different solutions: no systematic correction with equal weight for all observations (AW^1), a $\sin^2 2\theta$ correction with equal weight (AD^1W^1), and a separate two-term correction ($\text{AD}^1\text{E}^5\text{W}^1$), using a $\sin^2 2\theta$ term plus a $\cos^2 \theta \sin^2 2\theta$ with equal weight for all reflections. It is interesting to note that the solution with no systematic correction indeed shows the need for such a correction. The other two solutions indicate a more acceptable solution, as evidenced by the minimization of the v 's. In this particular set of data the two separate correction terms appear to give the best solution.

In Table III the numerical values for the lattice parameters are shown for the Au data together with their probable errors based on a 50% probability. In addition, the values for $\sum W_i v_i^2$ and $\sum W_i v_i^2 / (n-k-1) \sum W_i$ for each solution are given. The considerable difference in the numerical value of $\sum W_i$ as discussed previously is shown in Table III, where the sum is 5 or 20.4.

It is indicated in Table III that the best fit for this particular set of data has been obtained with the $\text{D}^1\text{E}^1\text{W}^1$ solution, which does not involve a Hess-type weighting. It should be noted that the $\text{D}^1\text{E}^5\text{W}^1$ solution gives an almost equally good fit; however, the lattice parameter is slightly different. It is realized that more numbers are used for the parameters and errors than are significant, but in many cases they were necessary to show up significant differences in the solutions. It is also realized that 95% confidence limits are more acceptable which it is possible to use in the program.

Figure 1
Plot of v Versus θ for Cubic Gold Pattern
(Weyerer Data)

Table III

LATTICE PARAMETERS OBTAINED FOR CUBIC Au USING VARIOUS CORRECTION TERMS AND WEIGHTS

Correction Term and Weight

	AW^1	AD^1W^1	AD^1W^2	$AD^1E^1W^1$	$AD^1E^1W^2$	$AD^1E^2W^1$	$AD^1E^2W^2$	$AD^1E^5W^1$	$AD^1E^5W^2$
a_0	4 077 773	4 078 546	4 078 449	4 078 212	4 078 209	4 078 254	4 078 251	4 078 251	4 078 248
$PE a_0$	$\pm 0 000 109$	$\pm 0 000 047$	$\pm 0 000 013$	$\pm 0 000 008$	$\pm 0 000 004$	$\pm 0 000 008$	$\pm 0 000 003$	$\pm 0 000 006$	$\pm 0 000 003$
$\Sigma W_i v_i^2$	$3 65 \times 10^{-7}$	$2 53 \times 10^{-8}$	$4 94 \times 10^{-8}$	$9 84 \times 10^{-11}$	$7 03 \times 10^{-10}$	$1 17 \times 10^{-10}$	$8 49 \times 10^{-10}$	$1 12 \times 10^{-10}$	$8 03 \times 10^{-10}$
$\frac{\Sigma W_i v_i^2}{(n-k-1)\Sigma W_i}$	$2 43 \times 10^{-8}$	$2 53 \times 10^{-9}$	$1 24 \times 10^{-9}$	$1 97 \times 10^{-11}$	$3 51 \times 10^{-11}$	$2 34 \times 10^{-11}$	$4 24 \times 10^{-11}$	$2 22 \times 10^{-11}$	$4 02 \times 10^{-11}$

$$D^1 \sin^2 2\theta \quad \Sigma W_i^1 \quad 5 \quad n \quad E^1 \cos^2 \theta \sin 2\theta$$

$$\Sigma W_i^2 \quad 20.4 \quad E^2 \sin^2 2\theta \left(\frac{1}{\sin \theta} + 1/\theta \right)$$

$$E^5 \cos^2 \theta \sin^2 2\theta$$

Table IV is included to show the rapid convergence of the program. The upper set of values are those taken from Table III, in which a starting value of 0.035662 was used for A_0 . The seven solutions indicated in the table using this value resulted in a rather small ΔA value for each; however, when the starting value for A_0 was changed by a factor of ten, there was a tremendous increase in the ΔA . It should be noted that the a_0 's did not change at all and the standard errors only very slightly, beyond the point of significance. The results shown here and obtained with other sets of data indicate that the convergence is very rapid and hence reiteration is not necessary.

Table IV
RESULTS OBTAINED BY A CHANGE IN THE STARTING VALUE A_0
(Weyerer Au Data)

Correction Term and Weight								
A_0		AW^1	AD^1W^1	AD^1W^2	$AD^1E^1W^2$	$AD^1E^2W^2$	$AD^1E^5W^1$	$AD^1E^5W^2$
0 035662	a_0	4 077 773	4 078 546	4 078 449	4 078 212	4 078 251	4 078 251	4 078 248
	$P E a_0$	$\pm 0 000 109$	$\pm 0 000 047$	$\pm 0 000 013$	$\pm 0 000 008$	$\pm 0 000 003$	$\pm 0 000 006$	$\pm 0 000 003$
	ΔA	+0 000 017	+0 000 004	+0 000 006	+0 000 010	+0 000 009	+0 000 009	+0 000 009
0 356624	a_0	4 077 773	4 078 546	4 078 449	4 078 212	4 078 251	4 078 251	4 078 248
	$P E a_0$	$\pm 0 000 109$	$\pm 0 000 047$	$\pm 0 000 013$	$\pm 0 000 004$	$\pm 0 000 004$	$\pm 0 000 006$	$\pm 0 000 003$
	ΔA	-0 320 944	-0 320 958	0 320 956	-0 320 952	-0 320 953	-0 320 953	-0 320 952

$$D^1 \sin^2 2\theta \quad \Sigma W_i^1 \quad 5 \quad n \quad E^1 \cos^2 \theta \sin 2\theta$$

$$\Sigma W_i^2 - 20.4 \quad E^2 \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

$$E^5 \cos^2 \theta \sin^2 2\theta$$

Cubic - UN

Figure 2 is a plot showing the v 's versus θ for several solutions for data obtained from a diffraction pattern of cubic UN. The diffraction pattern was obtained with a 114.59-mm diameter camera, using Cu $K\alpha$ radiation, and the lattice parameters were obtained from measurements on all the face-centered cubic lines with an $h^2 + k^2 + l^2$ equal to 27 to 40 inclusive. The open circles, which are a plot of the results obtained using no systematic correction term, indicate that such a systematic correction is needed. It is also obvious that the solution $AD^1E^2W^2$ is minimizing the v 's; however, there is considerably more variation in this data than in the previously discussed data for Au. This is indicated by the bumping around of the plotted points.

Figure 2
Plot of v Versus θ for Cubic UN Pattern

A glance at Table V indicates that the degree of precision with the UN data is less than that for the Au data. However, from experience with a number of sets of data, the UN results are very acceptable and quite typical, much more so than the previous Au data. Values for both $\sum W_i v_i^2$ and $\sum W_i v_i^2 / (n-k-1) \sum W_i$ are given, and it can be noted that it is difficult to judge the fit on the basis of the first of these two terms due to the difference in weighting factor of 10 to 146; however, the second term indicates that the $D^1 W^2$ solution gives the best fit. The $E^2 W^2$ and $D^1 E^2 W^2$ solutions also seem to give about the same fit and, indeed, have very nearly the same lattice parameters. Although the best fits for the previous Au data (Table III) were obtained using an equal weight for all lines (W^1), the UN data indicate that the weighted solutions (W^2) give the best fit.

Table V

LATTICE PARAMETERS OBTAINED FOR CUBIC UN USING VARIOUS CORRECTION TERMS AND WEIGHTS

	Correction Term and Weight						
	AW ¹	AD ¹ W ¹	AD ¹ W ²	AE ² W ¹	AE ² W ²	AD ¹ E ² W ¹	AD ¹ E ² W ²
a_0	4.889 08	4.890 00	4.889 98	4.889 90	4.889 97	4.890 08	4.889 98
P.E. a_0	$\pm 0.000 06$	$\pm 0.000 03$	$\pm 0.000 00$	$\pm 0.000 03$	$\pm 0.000 00$	$\pm 0.000 04$	$\pm 0.000 00$
$\sum W_i v_i^2$	7.26×10^{-7}	7.84×10^{-8}	4.21×10^{-7}	9.50×10^{-8}	4.35×10^{-7}	7.27×10^{-8}	4.21×10^{-7}
$\frac{\sum W_i v_i^2}{(n-k-1) \sum W_i}$	9.08×10^{-9}	1.12×10^{-9}	4.13×10^{-10}	1.36×10^{-9}	4.26×10^{-10}	1.21×10^{-9}	4.81×10^{-10}

$$D^1 = \sin^2 2\theta \quad \sum_i W_i^1 = 10 = n \quad E^2 = \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

$$\sum_i W_i^2 = 146$$

Cubic - AuBe

The results obtained from another cubic set of data, which illustrates a different type of result, is shown in Figure 3 and Table VI. These data were obtained from a cubic AuBe X-ray diffraction pattern using Cu K α radiation with a 114.59-mm diameter camera. It is evident from the plot of open circles shown in Figure 3 that (1) there is considerable scatter in the data, and (2) there is no evidence for the need for a systematic correction, since all the open circles in the plot seem to be rather randomly distributed above and below the zero line. It is also evident from the AE²W² solution that the use of a systematic correction did not help. By looking at Table VI it can also be observed from the lattice parameters and the values for the $\sum W_i v_i^2 / (n-k-1) \sum W_i$ that the use of the combination of various weights and systematic correction terms did not appreciably improve the fit nor change the values of the lattice parameters.

Figure 3
Plot of v Versus θ for Cubic AuBe

Table VI
LATTICE PARAMETERS OBTAINED FOR CUBIC AuBe USING VARIOUS CORRECTION TERMS AND WEIGHTS

	Correction Term and Weight							
	AW^1	AE^2W^1	AE^2W^2	AE^3W^2	AD^2W^1	AD^2W^2	$AD^1E^2W^2$	$AD^1E^3W^2$
a_0	4 668 70	4 668 73	4 668 56	4 668 56	4 668 53	4 668 56	4 668 61	4 668 61
P E a_0	$\pm 0.000\ 03$	$\pm 0.000\ 05$	$\pm 0.000\ 01$	$\pm 0.000\ 01$	$\pm 0.000\ 05$	$\pm 0.000\ 01$	$\pm 0.000\ 02$	$\pm 0.000\ 02$
$\Sigma W_i v_i^2$	1.35×10^{-6}	1.31×10^{-6}	2.92×10^{-6}	2.91×10^{-6}	1.31×10^{-6}	2.92×10^{-6}	2.90×10^{-6}	2.90×10^{-6}
$\frac{\Sigma W_i v_i^2}{(n-k) \Sigma W_i}$	4.70×10^{-9}	4.84×10^{-9}	2.86×10^{-9}	2.86×10^{-9}	4.84×10^{-9}	2.86×10^{-9}	3.05×10^{-9}	3.05×10^{-9}

$$D^1 - \sin^2 2\theta \quad \Sigma W_i^1 \quad 18 - n \quad E^2 - \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

$$D^2 - \phi \sin 2\phi \quad \Sigma W_i^2 \quad 68 \quad E^3 - \sin^2 2\theta / 2\theta$$

Cubic - UO_2

Another rather typical set of data is shown in Figure 4 and Table VII, which are the results obtained from a cubic UO_2 pattern. The UO_2 is probably of a composition near $UO_{2.03}$. This pattern was obtained using $Cu K\alpha$ radiation with a 114.59-mm diameter camera. It is evident from the plot shown in Figure 4 that a systematic correction term is necessary. The improvement obtained from the AD^1W^2 solution is shown graphically on this same figure. After applying various correction terms the value of the lattice parameter changes considerably, as shown in Table VII.

Figure 4
Plot of v Versus θ for Cubic UO_2

Table VII

LATTICE PARAMETERS OBTAINED FOR CUBIC UO_2 USING VARIOUS CORRECTION TERMS AND WEIGHTS

	Correction Term and Weight						
	AW^1	AD^1W^1	AD^1W^2	$AD^1E^2W^1$	$AD^1E^2W^2$	AE^2W^1	AE^2W^2
a_0	5.467 422	5.469 081	5.469 110	5.469 508	5.469 231	5.468 888	5.468 977
P.E. a_0	$\pm 0.000\ 064$	$\pm 0.000\ 071$	$\pm 0.000\ 030$	$\pm 0.000\ 128$	$\pm 0.000\ 055$	$\pm 0.000\ 068$	$\pm 0.000\ 029$
$\Sigma W_i v_i^2$	1.17×10^{-6}	2.96×10^{-7}	5.22×10^{-7}	2.74×10^{-7}	5.14×10^{-7}	3.17×10^{-7}	5.46×10^{-7}
$\frac{\Sigma W_i v_i^2}{(n-k-1)\Sigma W_i}$	9.75×10^{-9}	2.74×10^{-9}	2.06×10^{-9}	2.86×10^{-9}	2.29×10^{-9}	2.93×10^{-9}	2.16×10^{-9}

$$D^1 = \sin^2 2\theta \quad \Sigma W_i^1 = 12 = n \quad E^2 = \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

$$\Sigma W_i^2 = 28.1$$

Cubic - Si

In order to make a rather severe test of the program it was decided to use calculated angles as input data which would therefore not need any correction. Angles were then calculated for Si using $\text{Cu } K\alpha_1$ and $K\alpha_2$ radiations over the range from 27 to 48 for the value of $h^2 + k^2 + l^2$. A value of $5.43062 \text{ \AA}$ was used for the value of a_0 for Si, and angles were first calculated in degrees to 6 significant numbers. The results obtained for these calculations are shown in Figure 5 and Table VIII.

Figure 5

Plot of v Versus θ for Cubic Silicon

Table VIII (First Calculation)

LATTICE PARAMETERS OBTAINED FOR CUBIC Si USING VARIOUS CORRECTION TERMS AND WEIGHTS

Correction Term and Weight

	AW ¹	AD ¹ W ¹	AD ¹ W ²	AE ² W ¹	AE ² W ²	AD ¹ E ¹ W ¹	AD ¹ E ¹ W ²	AD ¹ E ¹ FW ¹	AD ¹ E ¹ FW ²
a_0	5 4306 163	5 4306 157	5 4306 157	5 4306 154	5 4306 157	5 4306 199	5 4306 161	5 4305 962	5 4314 728
P E a_0	$\pm 0.0000\ 023$	$\pm 0.0000\ 043$	$\pm 0.0000\ 022$	$\pm 0.0000\ 039$	$\pm 0.0000\ 020$	$\pm 0.0000\ 065$	$\pm 0.0000\ 032$	$\pm 0.0005\ 490$	$\pm 0.0005\ 367$
$\Sigma W_i v_i^2$	1.37×10^{-9}	1.37×10^{-9}	4.96×10^{-9}	1.37×10^{-9}	4.96×10^{-9}	1.36×10^{-9}	4.96×10^{-9}	1.36×10^{-9}	4.93×10^{-9}
$\frac{\Sigma W_i v_i^2}{(n-k-1)\Sigma W_i}$	1.14×10^{-11}	1.26×10^{-11}	1.8×10^{-11}	1.26×10^{-11}	1.81×10^{-11}	1.42×10^{-11}	2.04×10^{-11}	1.62×10^{-11}	2.32×10^{-11}

$$\Sigma W_i^1 = 12 - n \quad D^1 - \sin^2 2\theta \quad E^1 - \cos^2 \theta \sin 2\theta \quad F - \cos 2\theta$$

$$\Sigma W_i^2 = 30.4 \quad E^2 - \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

The lattice parameters as determined and shown in Table VIII are not significantly different from the starting value until the last two solutions (AD¹E¹FW¹ and AD¹E¹FW²) were carried out, in which three independent systematic correction terms are being applied. Even in these last two cases the error from the starting value of the parameter was only 1 part in 250,000 and 8 parts in 50,000, respectively.

There were two rather significant variations noted in the above solutions for Si. First, even in the case where no systematic correction was applied (the AW¹ solution shown in Table VIII), there was some slight

variation in the lattice parameter between calculated and the starting value. Secondly, it was noticed, as shown in Table IX, first calculation, that there was a very periodic change of sign of the v 's depending upon whether it was an α_1 or an α_2 line. As a result of these observations, it was decided to recalculate the lattice parameters for Si using calculated angles with more significant numbers. For this purpose, the same starting a_0 for Si was used, but the angles were determined in radians to eight significant numbers. The results obtained from the program with this set of data are shown in Table X. The determined lattice parameters for the first seven solutions are much closer to the starting value of 5.43062 Å, and as shown in Table IX, second calculation, there was a degree of magnitude reduction in the size of the v 's; however, the periodic change of sign was still present.

Table IX

A Comparison of v 's* for the Individual
Si Reflections for Angles Expressed in
Radians to Six and Eight Significant Figures
(First and Second Calculation)

	v 's for AW^1 Solution	
	First Calculation	Second Calculation
$27\alpha_1$	+8.0	-0.6
$27\alpha_2$	-7.0	+0.7
$32\alpha_1$	+8.0	-0.8
$32\alpha_2$	-2.0	+0.8
$35\alpha_1$	+6.0	-0.9
$35\alpha_2$	-13.0	+0.9
$40\alpha_1$	+8.0	-1.0
$40\alpha_2$	-7.0	+1.0
$43\alpha_1$	+13.0	-1.0
$43\alpha_2$	-16.0	+1.1
$48\alpha_1$	+16.0	-1.2
$48\alpha_2$	-13.0	+1.2

*Numbers shown in table are $v(x 10^6)$

Table X (Second Calculation)
LATTICE PARAMETERS OBTAINED FOR CUBIC Si USING VARIOUS CORRECTION TERMS AND WEIGHTS

Correction Term and Weight									
	AW ¹	AD ¹ W ¹	AD ¹ W ²	AE ² W ¹	AE ² W ²	AD ¹ E ¹ W ¹	AD ¹ E ¹ W ²	AD ¹ E ¹ FW ¹	AD ¹ E ¹ FW ²
a ₀	5 4306 193	5 4306 193	5 4306 192	5 4306 193	5 4306 192	5 4306 193	5 4306 192	5 4306 270	5 4306 422
P E a ₀	±0 0000 000	±0 0000 000	±0 0000 000	±0 0000 001	±0 0000 000	±0 0000 001	±0 0000 001	±0 0000 107	±0 0000 098
$\Sigma W_i v_i^2$	5 18 x 10 ⁻¹³	5 18 x 10 ⁻¹³	1 67 x 10 ⁻¹²	5 18 x 10 ⁻¹³	1 67 x 10 ⁻¹²	5 17 x 10 ⁻¹³	1 67 x 10 ⁻¹²	5 17 x 10 ⁻¹³	1 65 x 10 ⁻¹²
$\frac{\Sigma W_i v_i^2}{(n-k-1) \Sigma W_i}$	4 32 x 10 ⁻¹⁵	4 80 x 10 ⁻¹⁵	6 11 x 10 ⁻¹⁵	4 80 x 10 ⁻¹⁵	6 12 x 10 ⁻¹⁵	5 40 x 10 ⁻¹⁵	6 87 x 10 ⁻¹⁵	6 15 x 10 ⁻¹⁵	7 76 x 10 ⁻¹⁵

$$\Sigma W_i^1 = 12 \cdot n \quad D^1 = \sin^2 2\theta \quad E^1 = \cos^2 \theta \sin 2\theta \quad F = \cos 2\theta$$

$$\Sigma W_i^2 = 30.4 \quad E^2 = \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

Again, as in the first set of calculations, there is a greater change in the lattice parameter when attempting three independent systematic corrections. The last two calculated parameters of this second calculation show a deviation of approximately one part in a million and 1 part in 250,000, respectively.

A plot of v versus θ is not included for this second calculation since, as indicated in Table IX, the v 's become smaller by a factor of ten for this second calculation which, as plotted, would show the points closer to the zero line.

Hexagonal - Ni₃Ti

Although the examples used so far have been of cubic systems, the program is equally useful, as indicated previously, for the less symmetrical crystal systems thru the orthorhombic. Figure 6 and Table XIA are the results obtained for hexagonal Ni₃Ti using the observed values of $\sin^2 \theta$ reported by Taylor and Floyd⁽⁵⁾ using Cu K α radiation with a 19-cm diameter powder camera. The plot of open circles resulting from the ACW¹ solution as shown in Figure 6 show considerable scatter, but definitely indicates the need for a systematic correction term. The plot of closed circles indicates the improvement obtained with the ACE²W¹ solution. A further summary of the results obtained with a number of different solutions is given in Table XIA. It should be noted that these solutions have used the same trigonometric correction terms as discussed by Taylor and Floyd. These solutions indicate that the ones involving weighting seem to be slightly better; however, the lattice parameters are not much different with or without weighting. It can also be noted that the lattice parameters as determined with the various corrections applied are not very much different.

The values reported by Taylor and Floyd⁽⁵⁾ from this set of data were as follows, after correcting for refraction: $a_0 = 2.5505 \text{ \AA}$ and $c_0 = 8.3067 \text{ \AA}$. It is to be noted that the presently determined parameters shown in Table XIA are in very good agreement with these results. The parameters reported by Taylor and Floyd were obtained by a graphical extrapolation using the function $1/2 \left(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right)$.

Figure 6
Plot of v Versus θ for Hexagonal Ni_3Ti

Table XIA
LATTICE PARAMETERS OBTAINED FOR HEXAGONAL Ni_3Ti USING VARIOUS CORRECTION TERMS AND WEIGHTS
(Taylor and Floyd Data⁽⁵⁾)
Correction Term and Weight

	ACW ¹	ACE ² W ¹ Taylor and Floyd	ACE ² W ²	ACE ³ W ¹ Bradley and Jay	ACE ³ W ²	ACD ¹ W ¹ Cohen	ACD ¹ W ²	ACE ¹ W ¹ Hadding	ACE ¹ W ²
a_0	2 549 31	2 550 16	2 550 15	2 550 12	2 550 11	2 550 38	2 550 39	2 549 93	2 549 91
P.E. a_0	$\pm 0.000 04$	$\pm 0.000 02$	$\pm 0.000 01$	$\pm 0.000 02$	$\pm 0.000 01$	$\pm 0.000 03$	$\pm 0.000 02$	$\pm 0.000 02$	$\pm 0.000 01$
c_0	8 304 28	8 306 65	8 306 57	8 306 54	8 306 53	8 307 27	8 306 75	8 306 04	8 306 38
P.E. c_0	$\pm 0.000 10$	$\pm 0.000 07$	$\pm 0.000 02$	$\pm 0.000 06$	$\pm 0.000 02$	$\pm 0.000 09$	$\pm 0.000 03$	$\pm 0.000 06$	$\pm 0.000 02$
$\sum W_i v_i^2$	1.30×10^{-5}	2.71×10^{-6}	5.04×10^{-6}	2.63×10^{-6}	4.96×10^{-6}	4.81×10^{-6}	8.52×10^{-6}	2.40×10^{-6}	4.91×10^{-6}
$\frac{\sum W_i v_i^2}{(n-k-1)(\sum W_i)}$	9.80×10^{-9}	2.10×10^{-9}	1.51×10^{-9}	2.04×10^{-9}	1.49×10^{-9}	3.73×10^{-9}	2.55×10^{-9}	1.86×10^{-9}	1.47×10^{-9}

$$\begin{aligned} \sum_1 W_1^1 &= 38 - n & E^1 &= \cos^2 \theta \sin 2\theta \\ \sum_1 W_1^2 &= 98 & E^2 &= \sin^2 2\theta (1/\sin \theta + 1/\theta) \\ & & E^3 &= \sin^2 2\theta / 2\theta \end{aligned}$$

These parameters as obtained were used to calculate a set of $\sin^2 \theta$. Then, after correcting the observed $\sin^2 \theta$ by $\Delta \sin^2 \theta$, in which $\Delta \sin^2 \theta = D \sin^2 2\theta [(1/\sin \theta) + (1/\theta)]$, the difference between calculated and observed was tabulated for all hkl's (our v term). A procedure similar to the latter was carried out for the other three correction terms considered, namely, by Bradley and Jay,⁽⁶⁾ by Cohen,⁽⁷⁾ and by Hadding.⁽⁸⁾

We have already pointed out the good agreement between the lattice parameters as reported by Taylor and Floyd and the present results. It is also interesting to make a comparison of the v 's reported by Taylor and

Floyd with those presently determined. This can be most rapidly done by comparing the $\sum +v_i$ and $\sum -v_i$ for each solution as shown in Table XIA. The summation of the $+v$'s and $-v$'s are almost identical for the two solutions using the Taylor and Floyd correction (ACE^2W^1). The other three sets of solutions are also similar, except it was found especially in the Cohen and Hadding cases that there was a better balance of plus and minus sums for the present determination. This is probably due to a different drift constant (D) for the two different types of solutions. After looking at these results, shown in Table XII, it is not surprising that approximately the same lattice parameters were obtained for all solutions in the present determination.

A set of solutions was also obtained using the same starting data; however, a refraction correction was applied, according to the previously discussed correction:

$$\Delta \sin^2 \theta = - \frac{19.58 \rho Z}{M} \frac{\lambda^2}{4} \times 10^{-6} .$$

The results obtained are summarized in Table XIB. It should be noted that as the lattice parameters changed in the fourth and fifth decimal places, no significant changes occurred in the probable errors and a very slight improvement was indicated in most cases, as shown by a very small decrease in the term $\sum W_i v_i^2 / (n-k-1) \sum W_i$.

Table XIB

LATTICE PARAMETERS OBTAINED FOR HEXAGONAL Ni_3Ti USING VARIOUS CORRECTION TERMS AND WEIGHTS(Taylor and Floyd Data⁽⁵⁾)

Correction Term and Weight

	ACW ¹	ACE ² W ¹ Taylor and Floyd	ACE ² W ²	ACE ³ W ¹ Bradley and Jay	ACE ³ W ²	ACD ¹ W ¹ Cohen	ACD ¹ W ²	ACE ¹ W ¹ Hadding	ACE ¹ W ²
a_0	2.549 38	2.550 20	2.550 19	2.550 16	2.550 15	2.550 42	2.550 43	2.549 98	2.549 96
P.E. a_0	± 0.000 04	± 0.000 02	± 0.000 01	± 0.000 02	± 0.000 01	± 0.000 03	± 0.000 02	± 0.000 02	± 0.000 01
c_0	8.304 50	8.306 80	8.306 73	8.306 69	8.306 70	8.307 40	8.306 91	8.306 20	8.306 55
P.E. c_0	± 0.000 10	± 0.000 07	± 0.000 02	± 0.000 06	± 0.000 02	± 0.000 09	± 0.000 03	± 0.000 06	± 0.000 02
$\frac{\sum W_i v_i^2}{(n-k-1) \sum W_i}$	9.30×10^{-9}	2.08×10^{-9}	1.51×10^{-9}	2.03×10^{-9}	1.49×10^{-9}	3.60×10^{-9}	2.47×10^{-9}	1.86×10^{-9}	1.48×10^{-9}

$$\sum_i W_i^1 = 38 = n \quad E^1 = \cos^2 \theta \sin 2\theta$$

$$\sum_i W_i^2 = 98 \quad E^2 = \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

$$E^3 = \sin^2 2\theta / 2\theta$$

Table XII

Comparison of the Σv_i^* , Both Plus and Minus,
for The Taylor and Floyd Solution
and The Present Determination

		ACE ² W ¹ Taylor and Floyd	ACE ³ W ¹ Bradley and Jay	ACD ¹ W ¹ Cohen	ACE ¹ W ¹ Hadding
Taylor and Floyd Determination	$\Sigma +v_i$	405	419	334	651
	$\Sigma -v_i$	393	386	818	445
Present Determination	$\Sigma +v_i$	406	420	497	396
	$\Sigma -v_i$	441	430	696	402

* All Σv 's have been multiplied $\times 10^5$.

Hexagonal - Os

The results obtained from hexagonal osmium shown in Figure 7 and Table XIII are included to show indications of a lack of a need for a systematic correction. The open circles shown in Figure 7 appear to show a rather random distribution of plotted points. The results summarized in Table XIII indeed show little change in the lattice parameters with or without a systematic correction term or weights.

Figure 7

Plot of v Versus θ for Hexagonal Osmium

Table XIII
LATTICE PARAMETERS OBTAINED FOR HEXAGONAL Os USING VARIOUS CORRECTION TERMS AND WEIGHTS

Correction Term and Weight								
	ACW ¹	ACE ² W ¹	ACE ² W ²	ACE ³ W ²	ACD ² W ¹	ACD ² W ²	ACD ¹ E ² W ²	ACD ¹ E ³ W ²
a ₀	2.73 451	2.73 442	2.73 434	2.73 435	2.73 441	2.73 434	2.73 380	2.73 375
P.E. a ₀	±0.00 005	±0.00 008	±0.00 003	±0.00 003	±0.00 008	±0.00 003	±0.00 011	±0.00 012
c ₀	4.31 994	4.31 969	4.31 974	4.31 975	4.31 969	4.31 969	4.31 857	4.31 849
P.E. c ₀	±0.00 007	±0.00 013	±0.00 007	±0.00 007	±0.00 013	±0.00 007	±0.00 018	±0.00 019
$\sum W_i v_i^2$	4.00 x 10 ⁻⁷	3.86 x 10 ⁻⁷	1.03 x 10 ⁻⁶	1.03 x 10 ⁻⁶	3.86 x 10 ⁻⁷	1.03 x 10 ⁻⁶	9.28 x 10 ⁻⁷	9.28 x 10 ⁻⁷
$\frac{\sum W_i v_i^2}{(n-k-1)\sum W_i}$	5.71 x 10 ⁻⁹	6.43 x 10 ⁻⁹	5.16 x 10 ⁻⁹	5.16 x 10 ⁻⁹	6.43 x 10 ⁻⁹	5.16 x 10 ⁻⁹	5.57 x 10 ⁻⁹	5.57 x 10 ⁻⁹

$D^1 = \sin^2 2\theta \quad \sum W_i^1 = 10 = n \quad E^2 = \sin^2 2\theta (1/\sin \theta + 1/\theta)$

$D^2 = \phi \sin 2\phi \quad \sum W_i^2 = 33.3 \quad E^3 = \sin^2 2\theta / 2\theta$

Orthorhombic - Alpha U

The results obtained with an orthorhombic test case, namely, alpha uranium, are summarized in Figure 8 and Table XIV. In many ways these results are similar to those for the hexagonal Ni₃Ti case, in that the open circles shown in Figure 8 indicate a need for a systematic correction in spite of their scatter. The closed circles indicate the improvement shown by the D¹E²W² solution, which appears to be about the best solution, although several of the others, as indicated in Table XIV, are perhaps equally as good.

Figure 8
Plot of v Versus θ for Orthorhombic Uranium Pattern

Table XIV

LATTICE PARAMETERS OBTAINED FOR ORTHORHOMBIC URANIUM USING VARIOUS CORRECTION TERMS AND WEIGHTS

	Correction Term and Weight							
	ABCW ¹	ABCE ² W ¹	ABCE ² W ²	ABCE ³ W ²	ABCD ² W ¹	ABCD ² W ²	ABCD ¹ E ² W ²	ABCD ¹ E ³ W ²
a ₀	2.85 255	2.85 396	2.85 404	2.85 402	2.85 397	2.85 404	2.85 386	2.85 385
P.E. a ₀	±0.00 006	±0.00 004	±0.00 002	±0.00 002	±0.00 004	±0.00 002	±0.00 003	±0.00 003
b ₀	5.87 064	5.87 055	5.86 969	5.86 962	5.87 055	5.86 970	5.86 914	5.86 910
P.E. b ₀	±0.00 041	±0.00 020	±0.00 011	±0.00 011	±0.00 020	±0.00 011	±0.00 012	±0.00 012
c ₀	4.95 408	4.95 581	4.95 566	4.95 564	4.95 583	4.95 568	4.95 541	4.95 539
P.E. c ₀	±0.00 009	±0.00 006	±0.00 003	±0.00 003	±0.00 006	±0.00 003	±0.00 003	±0.00 003
$\sum W_i v_i^2$	2.20×10^{-6}	4.81×10^{-7}	7.83×10^{-7}	7.64×10^{-7}	4.80×10^{-7}	7.82×10^{-7}	6.86×10^{-7}	6.87×10^{-7}
$\frac{\sum W_i v_i^2}{(n-k-1)\sum W_i}$	8.73×10^{-9}	2.05×10^{-9}	1.42×10^{-9}	1.38×10^{-9}	2.05×10^{-9}	1.42×10^{-9}	1.36×10^{-9}	1.47×10^{-9}

$$D^1 = \sin^2 2\theta \quad \sum_i W_i^1 = 18 = n \quad E^2 = \sin^2 2\theta (1/\sin \theta + 1/\theta)$$

$$D^2 = \phi \sin 2\phi \quad \sum_i W_i^2 = 98 \quad E^3 = \sin^2 2\theta / 2\theta$$

VI. DATA FOR TEST PROBLEM

A set of data is included in order to test this program on the GEORGE or IBM-704 computers. This is especially desirable for someone using the program for the first time. Since the GEORGE computer is available only at Argonne, the test data have been written in terms of the IBM-704, which is more generally available.

The starting data and results are given for the ABCD¹E²W² solution for orthorhombic uranium previously discussed. Sheet I (Figure 9) contains the necessary information for the particular solution, and Sheet II (Figure 10) contains the general data which is necessary for all solutions. The output data are also shown in Figure 11, which is a reproduction of the IBM-704 output data sheet.

The necessary decks for use of this program on the IBM-704 may be obtained, together with a copy of this report, by contacting one of the authors. The program has been written in Fortran by W. G. Greenhow of the Applied Mathematics Division with the object in mind of making modifications and additions from time to time. Therefore, by also obtaining a copy of the print-out of Fortran statements for this program together with a word of explanation from Mr. Greenhow, it should be possible to obtain a good deal of flexibility.

		1	2	3
A B C D E	X	0	0	1
A B C D		0	0	2
A B C E		0	0	3
A B C		0	0	4
A C D E		0	0	5
A C D		0	0	6
A C E		0	0	7
A C		0	0	8
A D E		0	0	9
A D		0	1	0
A E		0	1	1
A		0	1	2
A B C D E F		0	1	3
A B C D F		0	1	4
A B C E F		0	1	5
A B C F		0	1	6
A C D E F		0	1	7
A C D F		0	1	8
A C E F		0	1	9
A C F		0	2	0
A D E F		0	2	1
A D F		0	2	2
A E F		0	2	3
A F		0	2	4

		1	2	3	
2	θ IN RADIANS	X	0	2	5
	θ IN DEGREES		0	2	6
3	$W_1 = \omega$		0	2	7
	$W_2 = \omega / \sin^2 2\theta$	X	0	2	8
	$W_3 = \omega / \sin^2 (\pi - 2\theta) \cos^4 (\pi - 2\theta)$		0	2	9
4	$\delta_1 = \sin^2 2\theta$	X	0	3	0
	$\delta_2 = (\pi/2 - \theta) \sin (\pi - 2\theta)$		0	3	1
	$\delta_3 = \cos^2 \theta$		0	3	2
	$\epsilon_1 = \cos^2 \theta \sin 2\theta$		0	3	3
5	$\epsilon_2 = (1/\sin \theta + 1/\theta) \sin^2 2\theta$	X	0	3	4
	$\epsilon_3 = (\sin^2 2\theta)/2\theta$		0	3	5
	$\epsilon_4 = \cos^2 \theta \sin \theta$		0	3	6
	$\epsilon_5 = \cos^2 \theta \sin^2 2\theta$		0	3	7
	$\epsilon_6 = \sin 2\theta$		0	3	8
	$\zeta = \cos 2\theta$		0	3	9
7	USE REFRACTION CORR.		0	4	0
8	$g = 1$	X	0	4	1
	$g = 4/3$		0	4	2
9	STOP (USE AFTER LAST COMPLETE SET OF DATA)		0	4	3

Figure 9

Met 124 704 Data Sheet I - Test Problem

1												2												3												4												5												6												7											
1 2 3 4 5 6 7 8 9 0 1 2												3 4 5 6 7 8 9 0 1 2 3 4												5 6 7 8 9 0 1 2 3 4 5 6												7 8 9 0 1 2 3 4 5 6 7 8												9 0 1 2 3 4 5 6 7 8 9 0												1 2 3 4 5 6 7 8 9 0 1 2																							

DATE and MESSAGE

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M																Z																P															
+																+																+															

I																A ₀																B ₀																C ₀																v ₀															
+ 1 8 0 0																+ 0 0 7 2 8 3 9 2																+ 0 0 1 7 2 1 5 2																+ 0 0 2 4 1 5 6 8																+ 1 5 4 0 5 1															

0 θ																1 α																2 β																3 γ																3 LAMBDA																3 ω															
+																+																+																+																+																+															
0 9 8 5 6 7 6																1 0																1 0																2 5 10																1 5 4 0 5 1																1 0															
0 9 9 3 0 9 7																9 0																1 0																1 0																1 5 4 4 3 3																1 0															
1 0 4 3 9 9 6																4 0																4 0																1 6 10																1 5 4 0 5 1																1 0															
1 0 4 8 8 8 5																4 0																4 0																1 6 10																1 5 4 4 3 3																1 0															
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1 0 7 5 3 3 9																9 0																1 0																4 0																1 5 4 4 3 3																1 0															
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1 0 9 3 5 8 6																4 0																1 6 10																9 10																1 5 4 4 3 3																1 0															
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1												2												3												4												5												6												7											
1 2 3 4 5 6 7 8 9 0 1 2												3 4 5 6 7 8 9 0 1 2 3 4												5 6 7 8 9 0 1 2 3 4 5 6												7 8 9 0 1 2 3 4 5 6 7 8												9 0 1 2 3 4 5 6 7 8 9 0												1 2 3 4 5 6 7 8 9 0 1 2																							

Figure 10

Met 124 704 Data Sheet II - Test Problem

MET-124 LATTICE PARAMETER DETERMINATION

FILM TEST CASE ORTHORHOMBIC URANIUM

THETA IS IN RADIAN.

SUM W

4.2377155E 01

SWVSQ/(P-K-1)SUMW	A ZERO	B ZERO	C ZERO	LAMBDA ZERO	D1 E2 F0 W2	
1.3610350E-09	7.2839199E-02	1.7215200E-02	2.4156800E-02	1.5405100E 00		
V	THETA	ALPHA	BETA	GAMMA	LAMBDA	W
1.6847873E-04	9.8567599E-01	1.0000000E 00	1.0000000E 00	2.5000000E 01	1.5405100E 00	1.1793085E 00
-3.0849315E-04	9.9309700E-01	9.0000000E 00	1.0000000E 00	1.0000000E 00	1.5443300E 00	1.1945372E 00
4.1653553E-04	1.0439960E 00	4.0000000E 00	4.0000000E 00	1.6000000E 01	1.5405100E 00	1.3235837E 00
-1.3238223E-04	1.0488850E 00	4.0000000E 00	4.0000000E 00	1.6000000E 01	1.5443300E 00	1.3385598E 00
-1.3771580E-04	1.0709740E 00	9.0000000E 00	1.0000000E 00	4.0000000E 00	1.5405100E 00	1.4129278E 00
5.0331582E-06	1.0753390E 00	9.0000000E 00	1.0000000E 00	4.0000000E 00	1.5443300E 00	1.4290242E 00
1.3138349E-04	1.0885220E 00	4.0000000E 00	1.6000000E 01	9.0000000E 00	1.5405100E 00	1.4807317E 00
-1.3835204E-04	1.0935860E 00	4.0000000E 00	1.6000000E 01	9.0000000E 00	1.5443300E 00	1.5019037E 00
1.6980422E-04	1.1210000E 00	9.0000000E 00	9.0000000E 00	0.	1.5405100E 00	1.6307779E 00
-1.1027623E-04	1.1265000E 00	9.0000000E 00	9.0000000E 00	0.	1.5443300E 00	1.6598518E 00
2.3360553E-05	1.1488500E 00	1.0000000E 00	9.0000000E 00	2.5000000E 01	1.5405100E 00	1.7909556E 00
-6.4484746E-05	1.1584540E 00	9.0000000E 00	9.0000000E 00	1.0000000E 00	1.5443300E 00	1.8544410E 00
-9.5482217E-05	1.2021930E 00	0.	0.	3.6000000E 01	1.5405100E 00	2.2129619E 00
-4.5109001E-05	1.2085670E 00	0.	0.	3.6000000E 01	1.5443300E 00	2.2768088E 00
1.6316715E-04	1.2613860E 00	9.0000000E 00	9.0000000E 00	4.0000000E 00	1.5405100E 00	2.9718840E 00
-9.1995752E-07	1.2695060E 00	9.0000000E 00	9.0000000E 00	4.0000000E 00	1.5443300E 00	3.1130461E 00
-6.8121178E-05	1.3538430E 00	4.0000000E 00	1.6000000E 01	1.6000000E 01	1.5405100E 00	5.6576504E 00
2.3573297E-05	1.3940900E 00	4.0000000E 00	4.0000000E 00	2.5000000E 01	1.5443300E 00	8.3482021E 00

I	DELTA(I)	SIGMASQ(I)
A	2.7532029E-06	7.2714663E-13
B	3.4698626E-06	1.9592296E-13
C	1.6541319E-06	4.0105849E-14
D	-2.9436117E-03	1.2060815E-07
E	1.8867592E-03	2.5701220E-08

LATTICE PARAMETERS	PROBABLE ERRORS
ASUB0 = 2.8538587E 00	PASUB0 = 2.6737471E-05
BSUB0 = 5.8691424E 00	PBSUB0 = 1.2071981E-04
CSUB0 = 4.9554094E 00	PCSUB0 = 3.2874142E-05

Figure 11

Met 124 704 Output Sheet - Test Problem

VII. ACKNOWLEDGEMENTS

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