OAK RIDGE NATIONAL LABORATORY
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

ORNL-TM-229

OR ABS

A FORTRAN PROGRAM FOR CALCULATING SINGLE CRYSTAL ABSORPTION CORRECTIONS

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ABSTRACT

This memorandum describes a Fortran program for calculating the absorption correction to be applied to single crystal x-ray or neutron diffraction intensity measurements. Instructions are included for using the program which is available from the authors in the form of symbolic punched cards.

INTRODUCTION

The derivation of structure factors from integrated intensity measurements in X-ray or neutron diffraction usually requires a correction for absorption of radiation in the specimen. Tabulated values of this correction, expressed as the ratio of integrated intensity yielded by an absorbing specimen to that yielded by an hypothetical non-absorbing specimen of equal volume, are available for cylindrical (Bradley, 1935) and spherical (Evans and Ekstein, 1952) sample shapes. For accurate measurement of structure factors, the specimen is often reduced to one of these simple forms.

However, for a number of reasons, it frequently proves to be undesirable or difficult to shape a sample. The size and shape of available crystals may not permit cutting a sphere or cylinder large enough to give satisfactory intensities. Physical properties such as anisotropic resistance to grinding, or ease of cleavage or fracture may make shaping difficult. Furthermore, a cylindrical specimen may be used in only one orientation; while a spherical specimen obviates this difficulty, it may not permit optimum use of a beam with a long narrow cross section such as is usual in neutron diffraction spectrometers.

Several methods of correcting for absorption in samples of other shapes have been reported by Hendershot (1937), Albrecht (1939), Howells (1950) and Evans (1952), but all of them appear to be rather laborious. The availability of high-speed computers now makes possible the rapid calculation of the absorption correction factor for each reflection from a crystal of essentially arbitrary shape. The program to be described is similar to one prepared for the Oak Ridge computer, the Oracle (Busing and Levy, 1956).

MATHEMATICAL METHOD

It is assumed that the crystal is bounded by n plane surfaces and thus is described by a set of inequalities

$$a_s x + b_s y + c_s z - d_s \geq 0, \qquad s = 1, 2, \ldots, n, \tag{1}$$

with coefficients a_s, b_s, c_s, d_s chosen so that the inequalities are all satisfied only if the point x, y, z lies inside or on the surface of the crystal. This is a satisfactory description if there are no re-entrant angles between bounding planes, a condition which is assumed for this treatment. Cartesian coordinate axes for this description are those used to describe the angles which give the directions of the primary and diffracted beam. Two configurations are discussed under the subroutine ANGLE.

The factor to be computed is given by

$$A = \int (1/V)\exp[-\mu(r_\alpha + r_\beta)]dV, \tag{2}$$

where the integration is over the volume of the crystal, V, and where μ is the linear absorption coefficient, r_α the path length along the primary beam direction, and r_β that along the diffracted beam direction. In this program the integral is evaluated numerically using the method of Gauss (see, for example, Margenau and Murphy, 1943, p. 462) which will be described first for a one-dimensional integration. The method approximates the integral by a weighted sum of m terms:

$$\int_a^b g(x)dx \approx (b-a) \sum_{i=1}^{m} R_i g(x_i) \ ,$$

where

$$x_i = a+(b-a)u_i$$

and where the u_i's and R_i's are fractional constants which depend only on m, and their values are available for $m \leq 16$ (Lowan, Davids, and Levenson, 1942). The u_i's determine the points, x_i, at which the integrand

is evaluated, while the R_i's are the relative weights of the terms in the sum.

For triple integration, the approximation becomes

$$\int_a^b dx \int_{c(x)}^{d(x)} dy \int_{e(x,y)}^{f(x,y)} g(x,y,z)dz \approx$$

$$\sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{k=1}^{m} (b-a)[d(x_i)-c(x_i)][f(x_i,y_j)-e(x_i,y_j)]R_iR_jR_k g(x_i,y_j,z_k),$$

where

$$x_i = a+(b-a)u_i, \tag{3}$$

$$y_j = c(x_i)+[d(x_i)-c(x_i)]u_j, \tag{4}$$

$$z_k = e(x_i,y_j)+[f(x_i,y_j)-e(x_i,y_j)]u_k \ . \tag{5}$$

Tests of the method for conditions typical of neutron diffraction studies indicate that an m of 8 is satisfactory. The problem of determining A then reduces to finding the limits of integration, a, b, $c(x_i)$, $d(x_i)$, $e(x_i,y_j)$, and $f(x_i,y_i)$ and evaluating $g(x_i,y_j,z_k) = (1/V)\exp[-\mu(r_\alpha+r_\beta)]$.

In order to find a and b, the lower and upper limits on x, the routine first takes all possible combinations of three of the n planes which bound the crystal and solves for the coordinates of their intersections. Because there are no re-entrant angles between the faces, those intersections which are not corners of the crystal must lie outside of it. These are distinguished from the corners by rejecting points which fail to satisfy any one of the inequalities (1). The smallest and largest x values in the remaining set are then taken as a and b, respectively.

For a given value of x_i, the limits on y are found in a similar way by solving the equations of all possible pairs of faces, subject to the condition that $x = x_i$. Points outside the crystal are again rejected

and the smallest and largest y values remaining are taken as $c(x_i)$ and $d(x_i)$, respectively. The limits on z are determined in an analogous way for given values of x_i and y_j.

For a point x_i, y_j, z_k, the function $\exp[-\mu(r_\alpha+r_\beta)]$ is evaluated as follows. The distance from this point to the intersection of the primary beam with a face s of the crystal (or its extension) specified by one of the inequalities (1) is given by

$$r_{\alpha s} = \frac{d_s - a_s x_i - b_s y_j - c_s z_k}{a_s \gamma_{\alpha x} + b_s \gamma_{\alpha y} + c_s \gamma_{\alpha z}} \tag{6}$$

where the γ_α's are the direction cosines of a vector parallel to the primary beam and directed toward its source. This quantity is positive if the intersection lies toward the source of the primary beam from (x_i, y_j, z_k) and negative if it lies away from the source. The desired path length, r_α, is the smallest positive quantity of the set $r_{\alpha s}$. Similarly, the path length r_β is the smallest positive quantity in the set

$$r_{\beta s} = \frac{d_s - a_s x_i - b_s y_j - c_s z_k}{a_s \gamma_{\beta x} + b_s \gamma_{\beta y} + c_s \gamma_{\beta z}} \tag{7}$$

where the γ_β's are the direction cosines of the diffracted beam. The exponential is then evaluated in a straightforward way.

OUTLINE OF PROGRAM

It is usually necessary to determine the values of A for many reflections from a given crystal, and, sometimes, for several values of μ. The program avoids much repetition by calculating only once the limits of integration a, b, c, d, e, and f and the points of integration x_i, y_i, z_i. These determine the nm^3 numerators of Equations (6) and (7) and the m^3 weights of integration

$$R_{ijk} = (b-a)(d-c)(f-e)R_iR_jR_k \ ,$$

which are saved in a block of core, or on magnetic tape, if necessary. In the second part of the program the numerators are used to determine A for each reflection.

The amount of core available for data storage is determined by a subroutine (which must be the last one loaded) which determines the length of the code, size of machine, and amount of upper core unavailable. The size of the numerator block is then computed as the largest factor of m^2 possible, considering the number of faces, number of points of integration, and number of μ. In some cases, all numbers can be stored in fast storage, and no magnetic tape is used.

The majority of the input is read by two subroutines, one of which describes the shape of the crystal (FACE) and the other of which describes the angles of the reflection (ANGLE). Thus the user may describe his crystal and reflections in any convenient manner and supply a subroutine which will convert his input into the desired data.

The calculations begin with the determination of the limits a and b as described earlier, and the values of x_i are then found from (3), using the tabulated u's. For each x_i the limits c and d are then calculated and the values of y_j found from (4). Finally, for each combination x_i, y_j the limits e and f are determined and the values z_k taken from (5). Given the coordinates x_i, y_j, and z_k the n numerators of (6) and (7) may be calculated and stored, together with the weight which is determined using the tabulated values of R. The crystal volume, which is simply the sum of all the weights, is also determined in this part of the code.

In the second part of the program remaining storage is used for reflection data for several reflections. By performing the calculation

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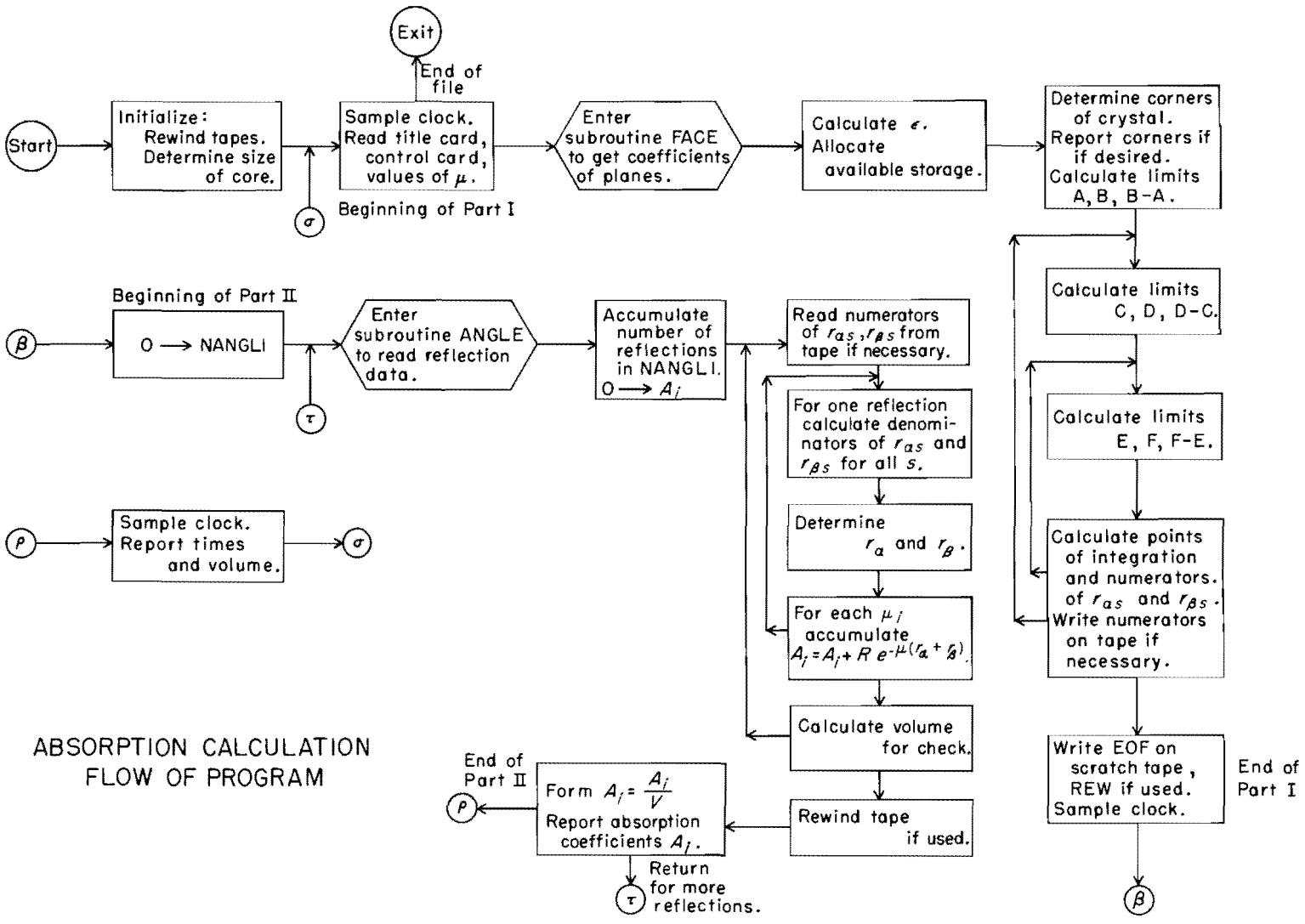

ABSORPTION CALCULATION
FLOW OF PROGRAM

for several reflections at a time, magnetic tape handling is minimized. As each block of numerators is read from magnetic tape, the 2n denominators of (6) and (7) are calculated. The distances r_α and r_β are determined, and appropriate contribution added to the sums for each reflection in core.

An on-line clock helps the user to estimate the time required for each run. The clock is sampled at the beginning of the program, at the end of the first part, and at the end of the problem. The last page of output for any crystal is a log giving the crystal identification, date, n, m, number of blocks of magnetic tape used, the number of values of μ, the number of reflections, and the time required for the two parts of the program. The volume of the crystal is also reported at this time for checking purposes.

Several checks are made during the calculations. Should the program fail a check, a notation is made on the output as to the nature of the error and the extent of the calculation before the run is terminated.

PREPARATION OF THE PROGRAM DECK

There are many features of this program which depend either on the arrangement of the diffraction equipment used or on the requirements of the computing installation. For this reason it is expected that in most cases minor modifications will have to be made before the program can be used. The program is therefore being transmitted in the form of symbolic cards, although column-binary cards are also available on request.

The following is a list of the subprograms which should be included in the assembled program deck. Several of them are discussed in more

detail in the next section.

Subprogram	Identification of Symbolic Cards	Remarks
1. Fortran II BSS loader		
2. Main program	P1 000-336	
3. Fortran II library subroutines		Not punched automatically on compiling
4. GAUSØL	G 337-384	
5. IDØUT	ID 385-391	
6. ØCØR	ØC 392-407	
7. EPSR	E1 408-413	
8. CLØCK	C1 414-421 C2 422-488	Alternative versions
9. ANGLE	A1 489-533 A2 534-591	Alternative versions
10. FACE	F1 592-630	
11. SIZE	S 631-659	Must be last subprogram
12. Fortran II transfer card		
13. Gaussian constants		
(a) Number of points	M 660	
(b) Gaussian weights	R1-2 661-662	These constants are read by the program as data cards.
(c) Gaussian points	U1-2 663-664	

DETAILS OF THE SUBPROGRAMS

Subroutines ERRØR and EXIT

The Oak Ridge installation requires that a run be terminated in one of three ways. The Fortran input routine has been modified to recognize an end of file on the input tape as the normal end of the run. An entrance

into EXIT subroutine terminates the problem in a similar fashion. An entrance into ERRØR implies that an octal dump of core is desired. The user must supply EXIT and ERRØR routines which conform to local standards.

Subroutine SIZE

This subroutine determines the number of cells available in core for storage of data.

The routine labelled S in columns 77-78 should be usable on a IBM 704, 709, or 7090 of any size. In the decrement of SIZE + 5 is the amount of upper core not available to the program (205 for Oak Ridge). The routine uses the fact that it is the last subprogram loaded to determine the length of the code and the part of lower core not available to the program.

If a new routine is written it must use the calling sequence

CALL SIZE (NS)

and place the number of cells available for data storage in the decrement of NS as an integer. The main program will subtract from this the number of cells used by variables and fixed arrays in CØMMØN, thus determining the length of the array DATA.

Subroutine CLØCK

The routine CLØCK is entered three times for each crystal to provide the user with the date of the run and the time required for Parts I and II of the program.

Two subroutines are provided. CLØCK with the identification C1 in columns 77-78 is a dummy which places blanks in DATE and gives zero for the time in T. It may be used when no on line clock is available.

The second routine, identified by C2 in columns 77-78, reads a Chrono-log digital clock model 2704-1, which has been connected to the 716 on-line printer control panel according to drawing 2704-9 which is furnished with the clock by the Chrono-log Corporation of Philadelphia 31, Pennsylvania. In addition to the wiring shown on the drawing, a wire is run from the load switching circuit (clock cable wire 50) through a filter into the sense entry hub. The read out of the clock is under control of printer sense exit six. The date of the run is given in BCD in DATE in the form mmddyy, mm being the month, dd, the day, and yy, the year. The time of the run in 10^8s of seconds is placed in the decrement of IT.

The calling sequence is CALL CLØCK (IT, DATE). The routine, in general, must place 6 BCD characters in DATE and an integer in the decrement of IT. The main program will report elapsed time as $IT-IT_1$ (IT_1 obtained on an earlier entry).

Subroutine EPSR

When determining the corners of the crystal, it is necessary, because of rounding errors, to accept a point as on the crystal surface if

$$a_s x + b_s y + c_s z - d_s + \epsilon \geq 0$$

for some small $\epsilon > 0$. If the program is not giving correct results, it is possible that an examination of the corners of the crystal that were found would indicate that an adjustment of the tolerance ϵ is required.

The main program reads an input parameter EPS. The subroutine EPSR must calculate EPS1 which is to be used as ϵ in the above inequality. The subprogram identified by E1 in columns 77-78 simply sets EPS1 equal to EPS.

Subroutine FACE

This subroutine provides the program with the 4n coefficients a_s, b_s, c_s, and d_s defined in Equation (1). The subroutine includes

the reading of input, the calculation of coefficients, and the reporting of input or coefficients, if desired.

The subroutine identified by F1 in columns 77-78 reads the following input cards via tape 10:

Card 1: Columns 1-5: N, the number of faces of the crystal, $N < 100$

6-10: NØP. A number other than zero implies that the input is to be reported.

Cards 2, ..., N + 1:	Columns 1-10	a_s	As defined in Equation (1)
	11-20	b_s	
	21-30	c_s	
	31-40	d_s	

The coefficients a_s, b_s, c_s, d_s must be given with references to a coordinate system which is consistent with the angle description (see below). If NØP is not zero, the title card read in the main program and a list of the coefficients a, b, c, and d are reported on tape 9.

To write a different subroutine FACE, the following conventions should be observed:

(1) The subroutine is entered with the statement CALL FACE (IDENT, N, DATA, NCØF, DATE).

(2) The subroutine should include the reading and reporting of all data needed to define the crystal faces. Output on tape K may be headed with the title and date of run by using the statement CALL IDØUT (IDENT, DATE, K).

(3) The number of faces is stored by the subroutine as an integer in the decrement of N.

(4) The 4n coefficients are stored in DATA (NCØF) through DATA (NCØF + 4N - 1) in the order a_1, b_1, c_1, d_1, a_2, etc. At least

2N cells beyond DATA (NCØF + 4N - 1) are available to the subroutine for temporary storage.

(5) If sense lights 1 and 2 are used, they must be turned off before returning to the main program.

Subroutine ANGLE

This subroutine gives the main program an identification for each reflection and calculates the direction cosines $\gamma_{\alpha x}$, $\gamma_{\alpha y}$, $\gamma_{\alpha z}$, $\gamma_{\beta x}$, $\gamma_{\beta y}$, and $\gamma_{\beta z}$ used in Equations (6) and (7). Two versions of this subroutine have been provided.

The subprogram identified by A1 in columns 77-78 deals with reflections in one zone. Let the z-axis be parallel to the zone axis being studied, and let the x-axis lie in a crystal plane which will be used as a reference plane for all the reflections being studied. The y-axis is chosen to give a right handed coordinate system. The configuration of the crystal and the spectrometer for a given reflection is specified by Θ, the Bragg angle, and X, the interplanar angle with respect to the reference plane. (See Busing and Levy, 1957, Fig. 1.) From these the routine calculates

$$\alpha = X + \Theta + \pi$$

and

$$\beta = X - \Theta$$

which define the reverse directions of the primary beam and the forward direction of the diffracted beam. The direction cosines required by the main program are

$$\gamma_{\alpha x} = \cos \alpha \qquad \gamma_{\beta x} = \cos \beta$$

$$\gamma_{\alpha y} = \sin \alpha \qquad \gamma_{\beta y} = \sin \beta$$

$$\gamma_{\alpha z} = 0 \qquad \gamma_{\beta z} = 0.$$

Input for each reflection consists of a BCD identification and the angles Θ and X. This input will be reported as BCD output on tape 6 if desired.

The subprogram identified A2 in columns 77-78 is for use with the Oak Ridge automatic neutron diffractometer or with the General Electric single crystal orienter. The geometry for each reflection is defined by three angles: Θ, the Bragg angle, and X and ϕ, the orienter settings.

The crystal may be mounted on the orienter in an arbitrary way (but the values of X and ϕ depend on the way in which it is mounted). The coordinate system to which the crystal faces are referred is chosen as shown in Fig. 1. Assume the instrument to be in position for a hypothetical reflection for which $X = \phi = 0$ and Θ has a small positive value. The x-axis is then chosen as the normal to this hypothetical reflecting plane, and the z-axis is taken parallel to the ϕ-axis in the direction away from the goniometer mount. The y-axis is then parallel to the X-axis in a direction chosen so that the coordinate system will be right-handed. For the Oak Ridge diffractometer (Fig. 1a) the y-axis will point in the general direction of the primary and diffracted beams, while for the General Electric orienter (Fig. 1b) the opposite will be true. (Note that for the General Electric orienter the roles of the primary and diffracted beams are interchanged but this has no effect on the calculation.)

The subprogram evaluates the required direction cosines as follows:

$$\gamma_{\alpha x} = \cos X \cos \phi \sin \Theta + \sin \phi \cos \Theta \qquad \gamma_{\beta x} = \cos X \cos \phi \sin \Theta - \sin \phi \cos \Theta$$

$$\gamma_{\alpha y} = \cos X \sin \phi \sin \Theta - \cos \phi \cos \Theta \qquad \gamma_{\beta y} = \cos X \sin \phi \sin \Theta + \cos \phi \cos \Theta$$

$$\gamma_{\alpha z} = \sin X \sin \Theta \qquad \gamma_{\beta z} = \sin X \sin \Theta .$$

Input for the subroutine consists of a BCD identification and the angles Θ, X, and ϕ. If desired, the identification and input angles will be reported as BCD output on tape 6.

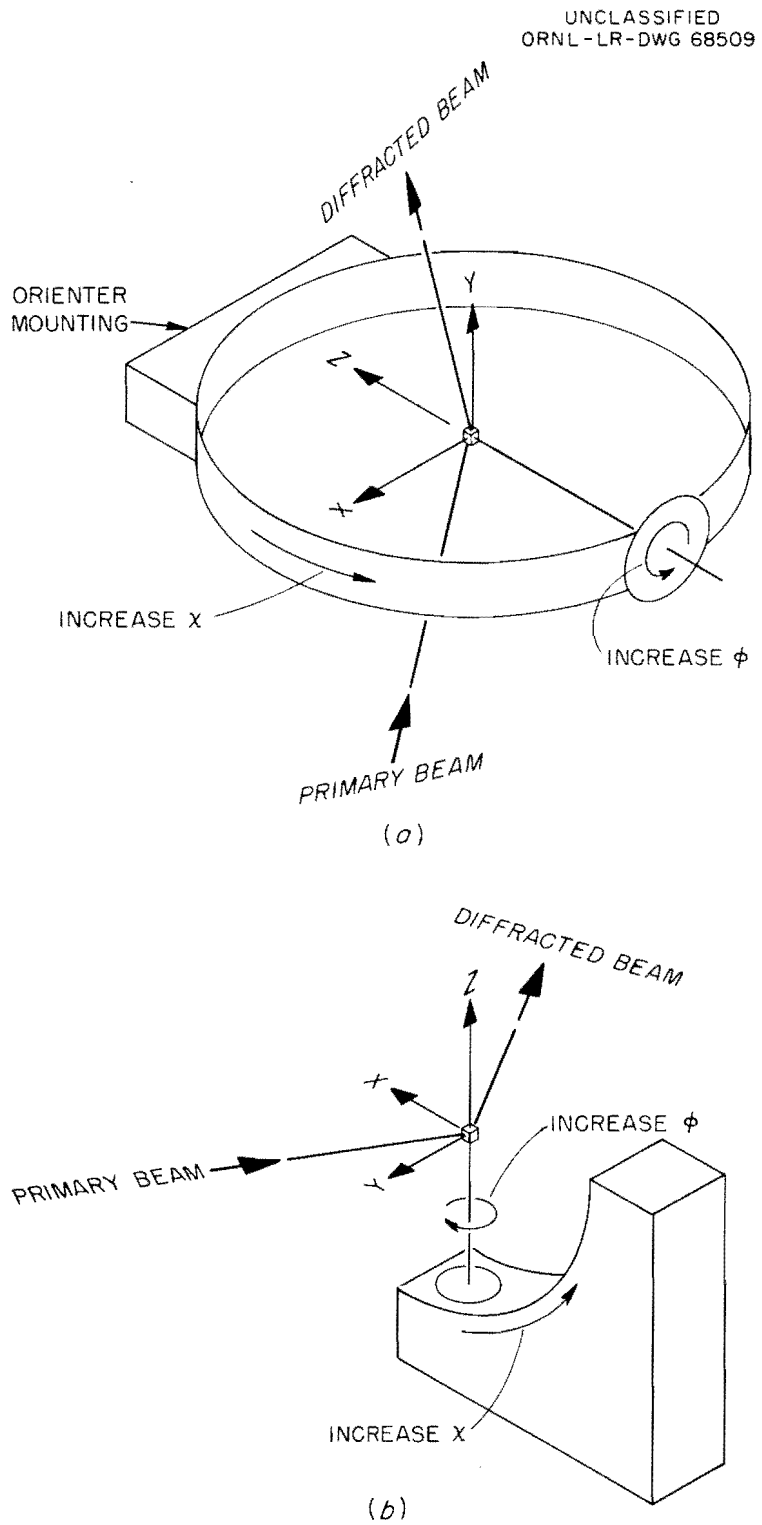

Figure 1. The angles and coordinate systems for (a) the Oak Ridge automatic diffractometer and (b) the General Electric single crystal orienter. The axes to which the crystal faces are referred are shown for $X = \phi = 0$.

To write ANGLE subroutines for other crystal orientations, the following specifications must be adhered to.

(1) Entry is by the statement

CALL ANGLE (IDENT, DATA, IANG, NANGL, DATE, NANGL1).

The arguments are defined below.

(2) The routine must read all of the input needed to define the reflections. If the user wishes to report this input or other results, this must be done within the subroutine. Tape 6 is rewound only once at the beginning of the main program and may be used for output by ANGLE.

(3) The crystal identification is found in the twelve word BCD array IDENT, and the date is in BCD in DATE. These may be reported by the subroutine on tape K, together with a skip to Channel 1, by the statement

CALL IDOUT (IDENT, DATE, K)

(4) The first entry into ANGLE may be distinguished from subsequent entries, since NANGL1 is zero only for the first entry.

(5) The program is more efficient on small machines if the data for several reflections are in core as a group. The maximum number of reflections that can be processed in such a group is found in NANGL on the first entry only. The subroutine should set NANGL to the actual number of reflections for which the angle data has been stored in core.

(6) Data for the reflections must be stored in the one-dimensional array DATA beginning at DATA (IANG). At exit, the data should be stored in groups of seven words in the following order:

1st word: Six BCD characters to identify the following reflection

2nd word: γ_{0x}

3rd word:	$\gamma_{\alpha y}$	direction cosines for primary beam
4th word:	$\gamma_{\alpha z}$	
5th word:	$\gamma_{\beta x}$	direction cosines for diffracted beam
6th word:	$\gamma_{\beta y}$	
7th word:	$\gamma_{\beta z}$	

NANGL words of storage in DATA following the reflection data may be used as temporary storage.

(7) When the data for the last reflection has been read into core, the subroutine must turn on sense light 1.

RESTRICTIONS AND MACHINE REQUIREMENTS

The following restrictions and requirements apply to the program as written. Most of them can be changed by making the appropriate modification. Equipment needed:

(1) The source program may be assembled and run on an IBM 704, 709, or 7090. At least 8,192 words of storage are required.

(2) At most 4 tape units are required. One for scratch (tape 2), one for input (tape 10), and two for output. (Main output is on tape 9, but reflection angles are put out via tape 6, if desired).

(3) A card-to-tape unit is used to prepare the input tape.

(4) All output is printed off-line.

(5) An on-line clock is used for timing.

Program restrictions:

(1) Uses sense lights 1 and 2.

(2) Does not use sense switches.

(3) Output gives 56 lines per page. It should be listed under program control. Automatic overflow switch should be off if the carriage tape has less than 56 lines.

(4) Program does not rewind input or output tapes. No end of file is written on the main output tape by the program at the end of a run.

TIMING

The machine time for a problem may be estimated from the expression

$$T = (C_1 N + C_2)R .$$

Here T is the time in seconds, N is the number of crystal faces, and R is the number of reflections for which the correction is to be calculated. Preliminary tests on an IBM 704 computer show that $C_1 = 1.1$ seconds per face per reflection, and $C_2 = 2.0$ seconds per reflection if intermediate magnetic tape storage is used, or $C_2 = 0$ when magnetic storage is not needed. Usually magnetic storage will be needed with an 8K memory but not with a 32 K memory.

DATA INPUT

1. Title card. FORMAT (12A6)

cols.
1-72 Any 72 Hollerith characters. This title will head each section of the output.

2. Card control. FORMAT (I5, E15.8, I5)

cols.
1-5 NMU, the number of absorption coefficients. $1 \leq NMU \leq 6$.

6-20 EPS, the increment used to compensate for round-off error in determining the limits of integration. For crystals of dimensions of the order of 0.1 and face equations with coefficients of the order of 1 an EPS of 10^{-6} (i.e. 1.0E-6) will usually be satisfactory.

21-25 KØ = 0 if output of coordinates of crystal corners is not desired. KØ = 1 to obtain this output.

3. Absorption coefficients. FORMAT (6E10.8)

cols.	
1-10	MU(K), the absorption coefficients to be used in calculating
11-20 etc.	A for each reflection. The number of MU(K) must be NMU given on the control card above.

4. Input for FACE routine F1.

a. Face control card. FØRMAT (2I5)

col.	
1-5	N, the number of faces of the crystal. $4 \leq N < 100$
6-10	NØP = 0 if output of the coefficients a, b, c, d are not desired; NØP = 1 if this output is desired.

b. Coefficients of planes describing faces of crystal. FØRMAT (4E10.8)

The number of cards is equal to N, the number of faces of the crystal.

col.	
1-10	a.
11-20	b.
21-30	c.
31-40	d.

Note that the coordinate system to which these equations refer must be consistent with the angle description used below.

5. Input for ANGLE routine A1. (Used for zero level reflections).

a. Angle control card FØRMAT (I1)

Column 1 = 1 if the input angles are to be reported.

Column 1 = 0 or blank, if this output is not desired.

b. Reflection angles and identification. FØRMAT (2(A6, 2F8.3))

Two reflections are placed on each card. For a definition of the reference system used in measuring the angles, see the discussion of the subroutine.

col.	
1-6	6 BCD characters to identify the following reflection
7-14	θ, the Bragg angle
15-22	χ, the interplanar angle
23-28	6 BCD characters to identify the following reflection
29-36	θ, the Bragg angle
37-44	χ, the interplanar angle

Angles are given in degrees. The list of reflections is terminated with six zeros in the identification field following the last χ.

6. Input for ANGLE routine A2. (Used with three-dimensional orienter).

a. Angle control card FØRMAT(I1)

Column 1 = 1 if the input angles are to be reported.

Column 1 = 0 or blank if this output is not desired.

b. Reflection angles and identification FØRMAT (2(A6, 3F8.3))

Two reflections are placed on each card. For a definition of the reference system used in measuring the angles, see the discussion of the subroutine.

col.		
1-6	6 BCD characters identifying the following reflection.	
7-14	θ, the Bragg angle	
15-22	χ	orienter angles
23-30	ϕ	orienter angles
31-36	6 BCD characters identifying the following reflection.	
37-44	θ, the Bragg angle	
45-52	χ	orienter angles
53-60	ϕ	orienter angles

Angles are given in degrees. The list of reflections is terminated with six zeros in the identification field following the last ϕ.

CARD DECK FOR OAK RIDGE INSTALLATION

1. Monitor control cards
2. Program deck
3. Data
   a. Title card
   b. Control card
   c. Absorption coefficients
   d. Input for FACE routine
   e. Input for ANGLE routine
4. Repeat (3) if absorption coefficients are to be calculated for more than one crystal in a single monitor job.

OPERATING PROCEDURE FOR OAK RIDGE INSTALLATION

When preparing the monitor control cards the user should call for tapes on units 2 and 6. If either ANGLE routines A1 or A2 are used and the angle output is called for, the number of the files on tape 6 to be printed is equal to the number of crystals run. If the angle output has not been called for, there will be nothing on tape 6. The program rewinds tape 6 regardless of which ANGLE routine is being used.

SYMBOLS USED

EPS	input parameter. It is used in the calculation of ϵ, the tolerance used in the determination of the corners.
NS	amount of core storage available in data block.
NP	NP * M * (N+1) words are written in each block of magnetic tape in the first part of the program.
NANGL	number of reflections to be processed at one time.
N	number of planes bounding crystal.
V	volume of crystal.

V1	volume of crystal computed with weights read from magnetic tape; used as a check.
IDENT	BCD array containing crystal identification.
IT1	clock time at beginning of program; time for part I.
IT2	clock time at end of part I of program; time for part II.
IT3	clock time at end of program.
NANGL1	total number of reflections processed.
NMU	number of values of μ to be used.
NCØF	DATA subscript of first coefficient a_1 of planes describing crystal.
NEND	DATA subscript of last coefficient d_N of planes describing crystal.
NUM	DATA subscript of first numerator of $r_{\alpha s}$ in core.
NUMED	DATA subscript of last numerator of $r_{\alpha s}$ in core.
JCØR	the number of words to be reported in one line crystal corner output.
IANG	DATA subscript of first angle identification.
ISUM	DATA subscript of first absorption correction factor.
IDIF1	DATA subscript of the first of the N differences $d_s - a_s x_i$ (Part 1); DATA subscript of the first of the N denominators $a\gamma_{\alpha s} + b\gamma_{\alpha s} + c\gamma_{\alpha s}$ (Part 2).
IDIF2	DATA subscript of the first of the N differences $d_s - a_s x_i - b_s y_j$ (Part 1); DATA subscript of the first of the N denominators $a\gamma_{\beta s} + b\gamma_{\beta s} + c\gamma_{\beta s}$ (Part 2).
T	temporary storage used by Gaussian elimination routine.
TA	current value of $r_{\alpha s}$.
TB	current value of $r_{\beta s}$.
X	current value of x coordinate of point of integration.
RA	r_α
RB	r_β
WX	$(b-a)\ x_i$

Y	current value of y coordinate of point of integration.
WY	$(c-d)\ (a-b)\ x_i y_j$
Z	equivalent to I6, current value of z coordinate of point of integration.
A	a, lower limit of integration on x axis.
B	b, upper limit of integration on x axis.
DIF1	b-a; equivalent to B.
C	$c(x_i)$, lower limit of integration on y axis.
D	$d(x_i)$, upper limit of integration on y axis.
DIF2	$d(x_i) - c(x_i)$, equivalent to D.
E	$e(x_i, y_j)$ lower limit of integration on z axis.
F	$f(x_i, y_j)$ upper limit of integration on z axis.
VMU	equivalent to DATA; storage for values of μ.
DATA	name of block of storage which contains coefficients of faces, direction cosines of angles, values of $d_s - a_s x_i - b_s y_j - c_s z_k$, etc. The subscripts for each block are calculated.
NDATA	equivalent to DATA; fixed point name for DATA.
IX	DATA subscript for first index of corners of crystal.
R	Gaussian weights.
U	Gaussian points.
IP	
IQ	DATA subscripts used in determining corners of crystal.
IR	
I	IP1 and IQ1
I1, I2, I3, I4, I5, I6, I7, J, K, K1	Dummy subscripts for DATA.
EPS1	tolerance ϵ used in determining corners of crystal.
KØ	output option on the reporting of the corners of the crystal.
M	number of Gaussian points used in integration.

KØNST	number of words of CØMMØN storage used excepting DATA block.
NP1	number of blocks on magnetic tape.

STORAGE TABLE FOR THE ARRAY DATA*

Number of words		Subscript
NMU ≤ 6	$\mu_1, \ldots, \mu_{NMU}$	1 | NMU
4 * N	$a_s, b_s, c_s, d_s, (s = 1, \ldots, n)$	NCØF | NEND
NP*M*(N+1)	$d_s - a_s x_i - b_s y_j - c_s z_k$ $(b-a)(d-c)(f-e)R_i R_j R_k$ for $s = 1, \ldots, n$ $i, j, k = 1, \ldots, m$	NUM | NUMED
N	(Part 1) $d_s - a_s x_i$ $(s = 1, \ldots, n)$ (Part 2) $a_s \gamma_{\alpha x} + b_s \gamma_{\alpha y} + c_s \gamma_{\alpha z}$	IDIF1 | IDIF2-1
N	(Part 1) $d_s - a_s x_i - b_s y_j$ $(s = 1, \ldots, n)$ (Part 2) $a_s \gamma_{\beta x} + b_s \gamma_{\beta y} + c_x \gamma_{\beta z}$	IDIF2 | IX-1
12	(Part 1) Indices of planes and coordinates of corners	IX | IX+11
7*NANGL	(Part 2) Id, $\gamma_{\alpha x}, \gamma_{\alpha y}, \gamma_{\alpha z}, \gamma_{\beta x}, \gamma_{\beta y}, \gamma_{\beta z}$ for each reflection	IANG | ISUM-1
NMU*NANGL	(Part 2) $A_1 (\mu_k), A_2 (\mu_k) \ldots$	ISUM |

*DATA is equivalent to VMU and NDATA.

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C        ABSORPTION CALCULATION,  3-DIMENSIONAL                          P1   000
      COMMON EPS,NS,NB,NP,NANGL,N,V,V1,IDENT,IT1,IT2,IT3,NANGL1,NMU,      P1   001
     2NCOF,NEND,NUM,NUMED,IDIF1,IDIF2,IANG,ISUM,JCOR,                     P1   002
     3T,X,WX,Y,WY,Z,A,B,C,D,E,F,DIF1,DIF2,DIF3,TA,TB,RA,RB,               P1   003
     4VMU,DATA                                                            P1   004
      DIMENSIONIDENT(12),T(12),R(16),U(16),VMU(1),DATA(1),NDATA(1)        P1   005
      EQUIVALENCE(EPS,DUM4),(NS,DUM5),                                    P1   006
     1(NB,DUM6),(NP,DUM7),(NANGL,DUM8),(N,DUM9),(V,DUM10),(V1,DUM11),     P1   007
     2(IDENT,DUM12),(IT1,DUM13),(IT2,DUM14),(IT3,DUM15),(NANGL1,DUM16),   P1   008
     3(NMU,DUM17),(IANG,DU33),(ISUM,DU34),                                P1   009
     4(NCOF,DUM19),(NEND,DUM20),(NUM,DUM21),(NUMED,DUM22),(JCOR,DUM23),   P1   010
     5(IDIF1,DU31),(IDIF2,DU32),(T(3),X),(T(6),WX),(T(9),Y),(T(12),WY),   P1   011
     6(Z,I6),(A,DUM24),(B,DIF1),(C,DUM25),(D,DIF2),(E,DUM26),(F,DIF3),    P1   012
     7(IP1,IQ1,I),(T(1),TA),(T(2),TB),(T(4),RA),(T(5),RB),                P1   013
     8(DATA,VMU,NDATA)                                                    P1   014
      READINPUTTAPE10,1003,M                                              P1   015
      IF(M-16)9001,9001,9002                                              P1   016
 9001 READINPUTTAPE10,1005,(U(I),I=1,M),(R(I),I=1,M)                      P1   017
      REWIND 6                                                            P1   018
      LINES =50                                                           P1   019
      SENSELIGHT0                                                         P1   020
      CALLSIZE(NS)                                                        P1   021
 3213 CALLCLOCK(IT1,DATE)                                                 P1   022
      READINPUTTAPE10,1001,(IDENT(I),I=1,12)                              P1   023
      READINPUTTAPE10,1003,NMU,EPS,KO                                     P1   024
      IF(NMU-6)314,314,315                                                P1   025
  314 NCOF=NMU+1                                                          P1   026
      READINPUTTAPE10,1004,(VMU(I),I=1,NMU)                               P1   027
      CALLFACE(IDENT,N,DATA,NCOF,DATE)                                    P1   028
 9020 CALLEPSR(EPS,EPS1)                                                  P1   029
      I1=NS-KONST-NMU-6*N-12                                              P1   030
      NP=I1/(M*(N+1))                                                     P1   031
      I2=M**2                                                             P1   032
  316 IF(XMODF(I2,NP))318,312,318                                         P1   033
  318 NP=NP-1                                                             P1   034
      GO TO316                                                            P1   035
  312 IF(NP)8313,8313,311                                                 P1   036
  311 NANGL=(I1-NP*M*(N+1)+12)/(7+NMU)                                    P1   037
      IF(NANGL-2)317,317,313                                              P1   038
  317 IF(NP-1)8313,8313,318                                               P1   039
  313 NB=I2/NP                                                            P1   040
      NEND=NCOF+4*N-1                                                     P1   041
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      NUM=NEND+1                                                        P1   042
      NUMED=NP*M*(N+1)+NEND                                             P1   043
      IDIF1=NUMED+1                                                     P1   044
      IDIF2=IDIF1+N                                                     P1   045
      IX=IDIF2+N                                                        P1   046
      IANG=IX                                                           P1   047
      ISUM=NANGL*7+IANG                                                 P1   048
C        DETERMINE COEFFICIENTS OF CORNERS AND REPORT                   P1   049
C        CALCULATE A, B, B-A                                            P1   050
      IF(NB-1)7006,7006,7007                                            P1   051
 7007 REWIND2                                                           P1   052
 7006 IF(KO)60,60,61                                                    P1   053
   61 CALLIDOUT(IDENT,DATE,9)                                           P1   054
      WRITEOUTPUTTAPE 9,2001                                            P1   055
      NLINES=LINES                                                      P1   056
   60 A=10.0E37                                                         P1   057
      B=-A                                                              P1   058
      JCOR=0                                                            P1   059
      I1=N-2                                                            P1   060
      DO27IP=1,I1                                                       P1   061
      IP1=IP+1                                                          P1   062
      I1=N-1                                                            P1   063
      DO26IQ=IP1,I1                                                     P1   064
      IQ1=IQ+1                                                          P1   065
      DO54IR=IQ1,N                                                      P1   066
      I1=NCOF+4*(IP-1)                                                  P1   067
      DO24K=1,12,3                                                      P1   068
      T(K)=DATA(I1)                                                     P1   069
   24 I1=I1+1                                                           P1   070
      I1=NCOF+4*(IQ-1)                                                  P1   071
      DO23K=1,12,3                                                      P1   072
      T(K+1)=DATA(I1)                                                   P1   073
   23 I1=I1+1                                                           P1   074
      I1=NCOF+4*(IR-1)                                                  P1   075
      DO22K=1,12,3                                                      P1   076
      T(K+2)=DATA(I1)                                                   P1   077
   22 I1=I1+1                                                           P1   078
      CALLGAUSOL(T,3)                                                   P1   079
      IF(SENSELIGHT2)54,69                                              P1   080
   69 DO28K=NCOF,NEND,4                                                 P1   081
      IF(DATA(K)*T(10)+DATA(K+1)*T(11)+DATA(K+2)*T(12)-DATA(K+3)+EPS1)5 P1   082
     14,28,28                                                           P1   083
   28 CONTINUE                                                          P1   084
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      IF(A-T(10))50,50,51                                               P1   085
   51 A=T(10)                                                           P1   086
   50 IF(T(10)-B)52,52,53                                               P1   087
   53 B=T(10)                                                           P1   088
   52 IF(KO)54,54,62                                                    P1   089
   62 I1=IX+JCOR                                                        P1   090
      NDATA(I1)=IP                                                      P1   091
      NDATA(I1+1)=IQ                                                    P1   092
      NDATA(I1+2)=IR                                                    P1   093
      DO20K=3,5                                                         P1   094
      I1=JCOR+K+IX                                                      P1   095
   20 DATA(I1)=T(K+7)                                                   P1   096
      JCOR=JCOR+6                                                       P1   097
      IF(JCOR-12)54,29,29                                               P1   098
   29 CALLOCOR(DATA,IX,JCOR)                                            P1   099
   54 CONTINUE                                                          P1   100
   26 CONTINUE                                                          P1   101
   27 CONTINUE                                                          P1   102
      IF(KO)57,57,64                                                    P1   103
   64 IF(JCOR)57,57,58                                                  P1   104
   58 CALLOCOR(DATA,IX,JCOR)                                            P1   105
   57 DIF1=B-A                                                          P1   106
      IF(DIF1)56,56,55                                                  P1   107
   55 CONTINUE                                                          P1   108
      V =0.0                                                            P1   109
      NP1=NP                                                            P1   110
      K1=NUM                                                            P1   111
      DO107I=1,M                                                        P1   112
      X=A+DIF1*U(I)                                                     P1   113
      WX=R(I)*DIF1                                                      P1   114
      I2=IDIF1                                                          P1   115
      DO70I1=NCOF,NEND,4                                                P1   116
      DATA(I2)=DATA(I1+3)-DATA(I1)*X                                    P1   117
   70 I2=I2+1                                                           P1   118
C        CALCULATE C, D, D-C                                            P1   119
      C=10.0E37                                                         P1   120
      D=-C                                                              P1   121
      I20=N-1                                                           P1   122
      DO71IP=1,I20                                                      P1   123
      IP1=IP+1                                                          P1   124
      DO76IQ=IP1,N                                                      P1   125
      I1=NCOF+1+4*(IP-1)                                                P1   126
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      DO73K=1,4,3                                                       P1   127
      T(K)=DATA(I1)                                                     P1   128
   73 I1=I1+1                                                           P1   129
      I1=NCOF+1+4*(IQ-1)                                                P1   130
      DO74K=1,4,3                                                       P1   131
      T(K+1)=DATA(I1)                                                   P1   132
   74 I1=I1+1                                                           P1   133
      I1=IDIF1+IP-1                                                     P1   134
      T(7)=DATA(I1)                                                     P1   135
      I1=IDIF1+IQ-1                                                     P1   136
      T(8)=DATA(I1)                                                     P1   137
      CALLGAUSOL(T,2)                                                   P1   138
      IF(SENSELIGHT2)76,68                                              P1   139
   68 I2=IDIF1                                                          P1   140
      DO75I1=NCOF,NEND,4                                                P1   141
      IF(DATA(I1+1)*T(7)+DATA(I1+2)*T(8)-DATA(I2)+EPS1)76,75,75         P1   142
   75 I2=I2+1                                                           P1   143
      IF(C-T(7))77,77,78                                                P1   144
   78 C=T(7)                                                            P1   145
   77 IF(T(7)-D)76,76,79                                                P1   146
   79 D=T(7)                                                            P1   147
   76 CONTINUE                                                          P1   148
   71 CONTINUE                                                          P1   149
      DIF2=D-C                                                          P1   150
      IF(DIF2)72,72,80                                                  P1   151
   80 CONTINUE                                                          P1   152
      DO91J=1,M                                                         P1   153
      Y=C+DIF2*U(J)                                                     P1   154
      WY=WX*DIF2*R(J)                                                   P1   155
      I2=IDIF1                                                          P1   156
      I3=IDIF2                                                          P1   157
      DO90I1=NCOF,NEND,4                                                P1   158
      DATA(I3)=DATA(I2)-DATA(I1+1)*Y                                    P1   159
      I2=I2+1                                                           P1   160
   90 I3=I3+1                                                           P1   161
      E=10.0E37                                                         P1   162
      F=-E                                                              P1   163
      I3=IDIF2                                                          P1   164
      DO93I1=NCOF,NEND,4                                                P1   165
      Z=DATA(I3)/DATA(I1+2)                                             P1   166
      I4=IDIF2                                                          P1   167
      DO94I2=NCOF,NEND,4                                                P1   168
      IF(DATA(I2+2)*Z-DATA(I4)+EPS1)93,94,94                            P1   169
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   94 I4=I4+1                                                          P1   170
      IF(E-Z)96,96,97                                                  P1   171
   97 E=Z                                                              P1   172
   96 IF(Z-F)93,93,98                                                  P1   173
   98 F=Z                                                              P1   174
   93 I3=I3+1                                                          P1   175
      DIF3=F-E                                                         P1   176
      IF(DIF3)99,99,100                                                P1   177
  100 CONTINUE                                                         P1   178
      DO101K=1,M                                                       P1   179
      Z=E+DIF3*U(K)                                                    P1   180
      I2=IDIF2                                                         P1   181
      DO102I1=NCOF,NEND,4                                              P1   182
      DATA(K1)=DATA(I2)-DATA(I1+2)*Z                                   P1   183
      IF(DATA(K1))103,103,104                                          P1   184
  104 DATA(K1)=0.0                                                     P1   185
  103 K1=K1+1                                                          P1   186
  102 I2=I2+1                                                          P1   187
      DATA(K1)=WY*DIF3*R(K)                                            P1   188
      V=V+DATA(K1)                                                     P1   189
  101 K1=K1+1                                                          P1   190
      IF(NB-1)91,91,7002                                               P1   191
 7002 NP1=NP1-1                                                        P1   192
      IF(NP1)105,105,91                                                P1   193
  105 WRITETAPE2,(DATA(I1),I1=NUM,NUMED)                               P1   194
      K1=NUM                                                           P1   195
      NP1=NP                                                           P1   196
   91 CONTINUE                                                         P1   197
  107 CONTINUE                                                         P1   198
      IF(NB-1)7004,7004,7005                                           P1   199
 7005 ENDFILE2                                                         P1   200
      REWIND2                                                          P1   201
 7004 CALLCLOCK(IT2,DATE)                                              P1   202
C     END OF PART I,  BEGINNING OF PART II                             P1   204
      CALLIDOUT(IDENT,DATE,9)                                          P1   205
      WRITEOUTPUTTAPE9,2003,(VMU(I),I=1,NMU)                           P1   206
      NANGL1=0                                                         P1   207
  211 CALLANGLE(IDENT,DATA,IANG,NANGL,DATE,NANGL1)                     P1   208
      V1=0.0                                                           P1   209
      NANGL1=NANGL1+NANGL                                              P1   210
      K1 =N+1                                                          P1   211
      I3=NANGL*7-1+IANG                                                P1   212
```

```
      I2=ISUM+NMU*NANGL-1                                               P1   213
      DO200I1=ISUM,I2                                                   P1   214
  200 DATA(I1)=0.0                                                      P1   215
      DO201I1=1,NB                                                      P1   216
      IF(NB-1)7001,7001,7003                                            P1   217
 7003 READTAPE2,(DATA(I2),I2=NUM,NUMED)                                 P1   218
 7001 I6=ISUM                                                           P1   219
      DO202I2=IANG,I3,7                                                 P1   220
      I9=IDIF1                                                          P1   221
      I8=IDIF2                                                          P1   222
      DO203I4=NCOF,NEND,4                                               P1   223
      DATA(I9)=DATA(I4)*DATA(I2+1)+DATA(I4+1)*DATA(I2+2)+DATA(I4+2)*DATAP1   224
     1(I2+3)                                                            P1   225
      DATA(I8)=DATA(I4)*DATA(I2+4)+DATA(I4+1)*DATA(I2+5)+DATA(I4+2)*DATAP1   226
     1(I2+6)                                                            P1   227
      I9=I9+1                                                           P1   228
  203 I8=I8+1                                                           P1   229
      DO215I7=NUM,NUMED,K1                                              P1   230
      I5=I7                                                             P1   231
      RA=10.0E37                                                        P1   232
      RB=RA                                                             P1   233
      I9=IDIF2-1                                                        P1   234
      I8=IDIF2                                                          P1   235
      DO208I4=IDIF1,I9                                                  P1   236
      IF(DATA(I4))911,213,213                                           P1   237
  911 TA=DATA(I5)/DATA(I4)                                              P1   238
      IF(RA-TA)213,213,205                                              P1   239
  205 RA=TA                                                             P1   240
  213 IF(DATA(I8))216,217,217                                           P1   241
  216 TB=DATA(I5)/DATA(I8)                                              P1   242
      IF(RB-TB)217,217,207                                              P1   243
  207 RB=TB                                                             P1   244
  217 I5=I5+1                                                           P1   245
      I8=I8+1                                                           P1   246
  208 CONTINUE                                                          P1   247
      RA=RA+RB                                                          P1   248
      I10=I6                                                            P1   249
      DO206I4=1,NMU                                                     P1   250
      DATA(I10)=DATA(I10)+EXPF(-VMU(I4)*RA)*DATA(I5)                    P1   251
  206 I10=I10+1                                                         P1   252
  215 CONTINUE                                                          P1   253
      I6=I6+NMU                                                         P1   254
  202 CONTINUE                                                          P1   255
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      DO8204I4=NUM,NUMED,K1                                             P1   256
      I5=I4+N                                                           P1   257
 8204 V1=VI+DATA(I5)                                                    P1   258
  201 CONTINUE                                                          P1   259
      IF(NB-1)7009,7009,7010                                            P1   260
 7010 REWIND2                                                           P1   261
 7009 I6=ISUM+NANGL*NMU-1                                               P1   262
      DO8021I4=ISUM,I6                                                  P1   263
 8021 DATA(I4)=DATA(I4)/V                                               P1   264
      IF(V-V1)209,210,209                                               P1   265
  210 I2=ISUM                                                           P1   266
      I5=IANG+7*NANGL-1                                                 P1   267
      DO400I1=IANG,I5,7                                                 P1   268
      I3=I2+NMU-1                                                       P1   269
      NLINES=NLINES-1                                                   P1   270
      IF(NLINES)240,240,241                                             P1   271
  240 NLINES=LINES                                                      P1   272
      CALLIDOUT(IDENT,DATE,9)                                           P1   273
      WRITEOUTPUTTAPE9,2003,(VMU(I),I=1,NMU)                            P1   274
  241 WRITE OUTPUT TAPE9,2008,DATA(I1),(DATA(I4),I4=I2,I3)              P1   275
  400 I2=I3+1                                                           P1   276
      IF(SENSELIGHT1)212,211                                            P1   277
  212 CALLCLOCK(IT3,DATE)                                               P1   278
      IT1=IT2-IT1                                                       P1   279
      IT2=IT3-IT2                                                       P1   280
      CALLIDOUT(IDENT,DATE,9)                                           P1   281
      WRITEOUTPUTTAPE9,2093,V                                           P1   282
      WRITEOUTPUTTAPE9,2004,N,NANGL1,NMU,IT1,IT2                        P1   283
      GOTO8213                                                          P1   284
C     ERROR RETURNS                                                     P1   285
  315 CALLIDOUT(IDENT,DATE,9)                                           P1   286
      WRITEOUTPUTTAPE9,2010,NMU                                         P1   287
      CALLEXIT                                                          P1   288
   56 CALLIDOUT(IDENT,DATE,9)                                           P1   289
      WRITEOUTPUTTAPE9,2011,A,DIF1                                      P1   290
      CALLERROR                                                         P1   291
   72 CALLIDOUT(IDENT,DATE,9)                                           P1   292
      WRITEOUTPUTTAPE9,2012,C,DIF2                                      P1   293
      CALLERROR                                                         P1   294
   99 CALLIDOUT(IDENT,DATE,9)                                           P1   295
      WRITEOUTPUTTAPE9,2013,E,DIF3                                      P1   296
      CALLERROR                                                         P1   297
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  209 CALLIDOUT(IDENT,DATE,9)                                           P1   298
      WRITE OUTPUTTAPE9,2020,V,V1                                       P1   299
      CALL ERROR                                                        P1   300
 9021 CALLIDOUT(IDENT,DATE,9)                                           P1   301
      WRITEOUTPUTTAPE9,2092,N                                           P1   302
      CALLEXIT                                                          P1   303
 9002 WRITEOUTPUTTAPE9,2090,M                                           P1   304
      CALLEXIT                                                          P1   305
 3313 CALLIDOUT(IDENT,DATE,9)                                           P1   306
      WRITEOUTPUTTAPE9,2313,N,M,NMU,NS,NP                               P1   307
      CALLEXIT                                                          P1   308
 2313 FORMAT(36H0MEMORY IS TOO SMALL FOR PARAMETERS./4H0N =I3,3HM =I3,5HP1   309
     1NMU =I2,19HAVAILABLE STORAGE =I6,4HNP =I5)                        P1   310
 2090 FORMAT(21H1M IS TOO LARGE.  M = I5)                               P1   311
 2092 FORMAT(5H0N = I5,15H  IS TOO LARGE.)                              P1   312
 2093 FORMAT(10H0VOLUME = F15.8)                                        P1   313
 1001 FORMAT(12A6)                                                      P1   314
 1002 FORMAT(1I1)                                                       P1   315
 1003 FORMAT(I5,E15.8,I5)                                               P1   316
 1004 FORMAT(6E10.8)                                                    P1   317
 1005 FORMAT(4F10.8)                                                    P1   318
 2001 FORMAT(34H0COORDINATES OF CORNERS OF CRYSTAL/52H0INDEX OF PLANES FP1   319
     1ORMING CORNER, FOLLOWED BY X, Y, Z//)                             P1   320
 2003 FORMAT(33H0ABSORPTION CORRECTION FACTOR,  A/6H0MU = 6(E10.5)//)   P1   321
 2004 FORMAT(5H0N = I5,3X,19HNUMBER OF ANGLES = I5,3X,15HNUMBER OF MU = P1   322
     1I2//29H TIME USED IN PARTS 1 AND 2 = 2I10,3X,18HIN 10S OF SECONDS.P1   323
     2)                                                                 P1   324
 2008 FORMAT(1H01A6,3X,6F12.8)                                          P1   325
 2010 FORMAT(29H0INPUT ERROR.  NUMBER OF MU =I5,24HWHICH IS GREATER THANP1   326
     1 6.)                                                              P1   327
 2011 FORMAT(62H0ERROR IN CALCULATION OF UPPER AND LOWER LIMITS (B, A,).P1   328
     1  A = E15.8,8H, B-A = E15.8/19H0CORE DUMPS FOLLOW.)               P1   329
 2012 FORMAT(62H0ERROR IN CALCULATION OF UPPER AND LOWER LIMITS (D, C). P1   330
     1  C = E15.8,8H, D-C = E15.8/19H0CORE DUMPS FOLLOW.)               P1   331
 2013 FORMAT(62H0ERROR IN CALCULATION OF UPPER AND LOWER LIMITS (F, E). P1   332
     1  E = E15.8,8H, F-E = E15.8/19H0CORE DUMPS FOLLOW.)               P1   333
 2020 FORMAT(58H0ERROR.  VOLUME FROM CORE IS NOT EQUAL TO VOLUME FROM TAP1   334
     1PE/11H0V(CORE) = E15.8,10HV(TAPE) = E15.8/14H0DUMP FOLLOWS.)      P1   335
      END (0,1,0,0,0)                                                   P1   336
```

```
C        SUBROUTINE GAUSOL(A,N)                                          G   337
      SUBROUTINE GAUSOL(A,N)                                             G   338
      DIMENSION A(3,4)                                                   G   339
C        SOLUTION OF SYSTEM OF EQUATIONS BY GAUSSIAN ELIMINATION         G   340
C             USING INTERCHANGES                                         G   341
C             A = NAME OF MATRIX (ORIGINAL MATRIX IS DESTROYED)          G   342
C                 MATRIX IS STORED BY COLUMNS, VECTOR FOLLOWS            G   343
C             N = ORDER OF MATRIX                                        G   344
C                 (N MUST BE LESS THAN OR EQUAL DIMENSION STATEMENT)     G   345
C        SOLUTION IS FOUND IN A(1,N+1) THROUGH A(N,N+1)                  G   346
      IF(SENSELIGHT2)20,20                                               G   347
 20   N2=N-1                                                             G   348
      N1=N+1                                                             G   349
      DO9I1=1,N2                                                         G   350
      L=0                                                                G   351
      R=A(I1,I1)                                                         G   352
      I11=I1+1                                                           G   353
      DO2IR=I11,N                                                        G   354
      IF(ABSF(R)-ABSF(A(IR,I1)))3,2,2                                    G   355
    3 R=A(IR,I1)                                                         G   356
      L=IR                                                               G   357
    2 CONTINUE                                                           G   358
      IF(L)4,4,5                                                         G   359
    5 DO6IJ=I1,N1                                                        G   360
      X=A(L,IJ)                                                          G   361
      A(L,IJ)=A(I1,IJ)                                                   G   362
    6 A(I1,IJ)=X                                                         G   363
    4 DO8I2=I11,N                                                        G   364
      T=A(I2,I1)/A(I1,I1)                                                G   365
      DO7I3=I11,N1                                                       G   366
    7 A(I2,I3)=A(I2,I3)-A(I1,I3)*T                                       G   367
    8 CONTINUE                                                           G   368
    9 CONTINUE                                                           G   369
      A(N,N1)=A(N,N1)/A(N,N)                                             G   370
      DO11I=1,N2                                                         G   371
      I1=N-I                                                             G   372
      I2=I1+1                                                            G   373
      DO10I3=I2,N                                                        G   374
   10 A(I1,N1)=A(I1,N1)-A(I1,I3)*A(I3,N1)                                G   375
   11 A(I1,N1)=A(I1,N1)/A(I1,I1)                                         G   376
      IFDIVIDECHECK15,14                                                 G   377
   15 SENSELIGHT2                                                        G   378
```

```
   14 IF ACCUMULATOR OVERFLOW12,17                                    G   379
   12 SENSELIGHT2                                                     G   380
   17 IFQUOTIENTOVERFLOW16,13                                         G   381
   16 SENSELIGHT2                                                     G   382
   13 RETURN                                                          G   383
      END(0,1,0,0,1)                                                  G   384

C        REPORT CRYSTAL IDENTIFICATION                               ID   385
      SUBROUTINE IDOUT(IDENT,DATE,N)                                 ID   386
      DIMENSION IDENT(12)                                            ID   387
      WRITEOUTPUTTAPEN,2001,(IDENT(I),I=1,12),DATE                   ID   388
 2001 FORMAT(1H112A6,41X,1A6)                                        ID   389
      RETURN                                                         ID   390
      END(0,1,0,0,0)                                                 ID   391

C        REPORT ONE LINE OF ONE OR TWO CORNERS OF A CRYSTAL          OC   392
C           FOR 3-DIMENSIONAL PROBLEM                                OC   393
C        FIRST THREE NUMBERS REPORTED ARE INTEGERS WHICH DESIGNATE   OC   394
C           THE PLANES WHICH FORM CORNERS,                           OC   395
C        SECOND THREE NUMBERS ARE THE X, Y, Z COORDINATES OF THE CORNER.OC 396
C        NOTATION  X = LOCATION OF ARRAY OF 12 NUMBERS               OC   397
C                 IX = SUBSCRIPT OF FIRST NUMBER OF ARRAY X          OC   398
C               JCOR = 6*I, WHERE I IS THE NUMBER OF CORNERS TO REPORT OC 399
      SUBROUTINEOCOR(X,IX,JCOR)                                      OC   400
      DIMENSION X(1)                                                 OC   401
      JCOR =JCOR+IX-1                                                OC   402
      WRITE OUTPUT TAPE9,2002,(X(K),K=IX,JCOR)                       OC   403
      JCOR=0                                                         OC   404
 2002 FORMAT(1H 2(3I3.0,3F13.9,4X))                                  OC   405
      RETURN                                                         OC   406
      END(0,1,0,0,0)                                                 OC   407

C           DUMMY EPSR SUBROUTINE                                    E1   408
C        TO CALCULATE EPS1 = TOLERANCE FOR CORNERS OF CRYSTAL        E1   409
      SUBROUTINEEPSR(EPS,EPS1)                                       E1   410
      EPS1=EPS                                                       E1   411
      RETURN                                                         E1   412
      END(0,1,0,1,0)                                                 E1   413
```

```
C       DUMMY CLOCK SUBROUTINE                                          C1   414
C       PLACES 0 IN TIME, BLANKS IN DATE                                C1   415
       SUBROUTINE CLOCK(IT,DATE)                                        C1   416
S BLK  ALF                                                              C1   417
       IT =0                                                            C1   418
       DATE=BLK                                                         C1   419
       RETURN                                                           C1   420
       END(0,1,0,0,0)                                                   C1   421


*        CLOCK SUBROUTINE                                               C2   422
        FUL                     PROGRAM CARD                            C2   423
        ORG 0                   PROGRAM CARD                            C2   424
        MZE 0,0,4               9L                                      C2   425
        PZE 0                   9R                                      C2   426
        PZE T+1                 8L                                      C2   427
        PZE 0                   8R                                      C2   428
        BCD 1CLOCK              7L                                      C2   429
        PZE 0                   7R                                      C2   430
        ORG 0                                                           C2   431
        REL                                                             C2   432
        CLA 1,4                                                         C2   433
        STA ADD                                                         C2   434
        CLA 2,4                                                         C2   435
        STA ADD+2                                                       C2   436
        SXD T,4                                                         C2   437
        TSX CLOCK,4                                                     C2   438
        HTR *+1                                                         C2   439
        ALS 18                                                          C2   440
 ADD    STO 0                                                           C2   441
        CLA DATE                                                        C2   442
        STO 0                                                           C2   443
        LXD T,4                                                         C2   444
        TRA 3,4                                                         C2   445
 DATE   BSS 1                                                           C2   446
ORCLK5  REM                                                             C2   447
        REM READ CHRONO-LOG CLOCK ROUTINE.  ERROR RETURN IF CLOCK FAILS C2   448
        REM BINARY TIME (10 SEC.=1 UNIT) IN AC. FOR USE WITH CHRONO-LOG C2   449
        REM DIGITAL CLOCK MODEL 2704-1 WIRED TO 716 PRINT ECHO ENTRIES. C2   450
 CLOCK  RPR                                                             C2   451
        SPR 6                   SENSE THE CLOCK                         C2   452
        STZ DATE                                                        C2   453
```

```
        SXD *+35,2                                                      C2   454
        STZ COMMON                                                      C2   455
        SXD COMMON+1,1                                                  C2   456
        LXD *+13,1                                                      C2   457
        TNX *+15,1,2                                                    C2   458
        CPY DATE                                                        C2   459
        CPY COMMON                                                      C2   460
        TQP *-3                                                         C2   461
        LXD *+15,2                                                      C2   462
        LXA *+1,1                                                       C2   463
        PXD 3                                                           C2   464
        RQL 1                                                           C2   465
        TQP *+5                                                         C2   466
        RQL 1                                                           C2   467
        TNX *+6,1,1                                                     C2   468
        TQP *-2                ERROR IF MQ MINUS                        C2   469
        TXL *+3,,47                                                     C2   470
        ADD *+14,2                                                      C2   471
        TIX *-7,1,1                                                     C2   472
        TXI *+12,4,1           ERROR RETURN                             C2   473
        TNX *+11,2,1                                                    C2   474
        TRA *+5,2                                                       C2   475
        TXI *-10,1,9                                                    C2   476
        TXI *-11,1,5                                                    C2   477
        TXI *-12,1,9                                                    C2   478
        TXI *-13,1,5                                                    C2   479
        DEC 3600,360,60,6,1                                             C2   480
        LXD COMMON+1,1                                                  C2   481
        LXD *+3,2                                                       C2   482
        SPT                                                             C2   483
        TRA 2,4                                                         C2   484
        TXL *-2                                                         C2   485
COMMON  BSS 2                                                           C2   486
 T      HTR 0                                                           C2   487
        END 0                                                           C2   488


C         SUBROUTINE ANGLE (IDENT,DATA,IANG,NANGL,DATE,NANGL1)          A1   489
C         USING ONLY TWO ANGLES, THETA AND CHI                          A1   490
C         ZERO IS STORED FOR REMAINING DIRECTION COSINES                A1   491
      SUBROUTINEANGLE(IDENT,DATA,IANG,NANGL,DATE,NANGL1)                A1   492
      DIMENSIONIDENT(12),DATA(1)                                        A1   493
      K1=0                                                              A1   494
```

```
      I3=IANG+7*NANGL-1                                                 A1   495
      IF(NANGL1)30,31,30                                                A1   496
   31 READINPUTTAPE10,1002,NOP                                          A1   497
   30 DO10I2=IANG,I3,14                                                 A1   498
      I4=I2+13                                                          A1   499
      READINPUTTAPE10,1001,(DATA(I1),DATA(I1+1),DATA(I1+2),I1=I2,I4,7)  A1   500
      DO13I5=I2,I4,7                                                    A1   501
      IF(DATA(I5)) 13,12,13                                             A1   502
   13 K1=K1+1                                                           A1   503
      IF(NANGL-K1-2) 11,10,10                                           A1   504
   12 SENSELIGHT1                                                       A1   505
      NANGL=K1                                                          A1   506
      GOTO11                                                            A1   507
   10 CONTINUE                                                          A1   508
   11 I3=IANG+7*NANGL-1                                                 A1   509
      IF(NOP)17,16,15                                                   A1   510
   15 NOP=-1                                                            A1   511
      CALLIDOUT(IDENT,DATE,6)                                           A1   512
      WRITEOUTPUTTAPE6,2001                                             A1   513
   17 WRITEOUTPUTTAPE6,2002,(DATA(I1),DATA(I1+1),DATA(I1+2),I1=IANG,I3,7A1   514
     1)                                                                 A1   515
       IF(SENSELIGHT1)20,16                                             A1   516
   20 SENSELIGHT1                                                       A1   517
       END FILE 6                                                       A1   518
   16 DO14I2=IANG,I3,7                                                  A1   519
      DATA(I2+6)=(DATA(I2+2)-DATA(I2+1))*0.0174533                      A1   520
      DATA(I2+3)=(DATA(I2+2)+DATA(I2+1))*0.0174533+3.1415926            A1   521
      DATA(I2+1)=COSF(DATA(I2+3))                                       A1   522
      DATA(I2+2)=SINF(DATA(I2+3))                                       A1   523
      DATA(I2+3)=0                                                      A1   524
      DATA(I2+4)=COSF(DATA(I2+6))                                       A1   525
      DATA(I2+5)=SINF(DATA(I2+6))                                       A1   526
   14 DATA(I2+6)=0                                                      A1   527
 1001 FORMAT(2(1A6,2F8.3))                                              A1   528
 1002 FORMAT(1I1)                                                       A1   529
 2001 FORMAT(12H0ANGLE INPUT/1H0,9X,14HTHETA       CHI//)               A1   530
 2002 FORMAT(1H (2(1A6,2F10.3,5X)))                                     A1   531
      RETURN                                                            A1   532
      END (0,1,0,0,0)                                                   A1   533
```

```
C        SUBROUTINE ANGLE(2),  FOR 3-D ORIENTING EQUIPMENT                A2   534
C     WRITTEN 9-9-60                                                      A2   535
      SUBROUTINEANGLE(IDENT,DATA,IANG,NANGL,DATE,NANGL1)                  A2   536
      DIMENSION IDENT(12),DATA(1)                                         A2   537
      K1#0                                                                A2   538
      I3#IANG+7*NANGL-1                                                   A2   539
      IF(NANGL1)30,31,30                                                  A2   540
   31 READINPUTTAPE10,1002,NOP                                            A2   541
   30 DO10I2#IANG,I3,14                                                   A2   542
      CONTINUE                                                            A2   543
      CONTINUE                                                            A2   544
      I4#I2+13                                                            A2   545
      READINPUTTAPE10,1001,(DATA(I1),DATA(I1+1),DATA(I1+2),DATA(I1*3)     A2   546
     1,I1#I2,I4,7)                                                        A2   547
      DO13I5#I2,I4,7                                                      A2   548
      IF(DATA(I5)) 13,12,13                                               A2   549
   13 K1#K1+1                                                             A2   550
      IF(NANGL-K1-2) 11,10,10                                             A2   551
   12 SENSELIGHT1                                                         A2   552
      NANGL#K1                                                            A2   553
      GOTO11                                                              A2   554
   10 CONTINUE                                                            A2   555
   11 I3#IANG+7*NANGL-1                                                   A2   556
      IF(NOP)17,16,15                                                     A2   557
   15 NOP#-1                                                              A2   558
      CALLIDOUT(IDENT,DATE,6)                                             A2   559
      WRITEOUTPUTTAPE6,2001                                               A2   560
   17 WRITEOUTPUTTAPE6,2002,(DATA(I1),DATA(I1+1),DATA(I1+2), DATA(I1+3),A2 561
     1I1#IANG,I3,7)                                                       A2   562
       IF(SENSELIGHT1)20,16                                               A2   563
   20 SENSELIGHT1                                                         A2   564
       END FILE 6                                                         A2   565
   16 DO14I2#IANG,I3,7                                                    A2   566
      DATA(I2+1)#DATA(I2+1)*0.174532925E-1                                A2   567
      DATA(I2+2)#DATA(I2+2)*0.174532925E-1                                A2   568
      DATA(I2+3)#DATA(I2+3)*0.174532925E-1                                A2   569
      T1#SINF(DATA(I2+1))                                                 A2   570
      T2#COSF(DATA(I2+1))                                                 A2   571
      T3#VINF(DATA(I2+3))                                                 A2   572
      T4#COSF(DATA(I2+3))                                                 A2   573
      DATA(I2+6)#SINF(DATA(I2+2))*T1                                      A2   574
      DATA(I2+3)#COSF(DATA(I2+2))*T1                                      A2   575
      DATA(I2+4)#DATA(I2+3)*T4                                            A2   576
```

```
      DATA(I2+5)=T3*T2                                                  A2   577
      DATA(I2+1)=DATA(I2+4)+DATA(I2+5)                                  A2   578
      DATA(I2+4)=DATA(I2+4)-DATA(I2+5)                                  A2   579
      DATA(I2+5)=T4*T2                                                  A2   580
      DATA(I2+3)=DATA(I2+3)*T3                                          A2   581
      DATA(I2+2)=DATA(I2+3)-DATA(I2+5)                                  A2   582
      DATA(I2+5)=DATA(I2+3)+DATA(I2+5)                                  A2   583
      DATA(I2+3)=DATA(I2+6)                                             A2   584
   14 CONTINUE                                                          A2   585
 1001 FORMAT(2(1A6,3F8.3))                                              A2   586
 1002 FORMAT(1I1)                                                       A2   587
 2001 FORMAT(1H016X,11HANGLE INPUT/1H010X,5HTHETA,8X,3HCHI,8X,3HPHI//)  A2   588
 2002 FORMAT(1H (2(A6,3F11.3,6X)))                                      A2   589
      RETURN                                                            A2   590
      END (0,1,0,0,0)                                                   A2   591


C       SUBROUTINE FACE(IDENT,N,DATA,NCOF,DATE), 3 DIMENSIONAL PROBLEM  F1   592
C        BEFORE ENTRY, IDENT, NCOF ARE SET                              F1   593
C        UPON EXIT, SUBROUTINE SUPPLIES N AND COEFFICIENTS WHICH        F1   594
C                   DESCRIBE PLANES FORMING FACES OF CRYSTAL            F1   595
C        NOTATION   IDENT = IDENTIFICATION OF CRYSTAL                   F1   596
C                       N = NUMBER OF FACES                             F1   597
C                    DATA = BLOCK OF GENERAL STORAGE                    F1   598
C                    NCOF = ELEMENT OF DATA CONTAINING FIRST            F1   599
C                           COEFFICIENT DESCRIBING PLANES,  OR FIRST    F1   600
C                           AVAILABLE CELL OF STORAGE UPON ENTRY        F1   601
C                     NOP = 0  IMPLIES DO NOT REPORT INPUT              F1   602
C                         = 1  IMPLIES REPORT INPUT                     F1   603
C                    DATE = BCD DATE                                    F1   604
      SUBROUTINEFACE(IDENT,N,DATA,NCOF,DATE)                            F1   605
      DIMENSION IDENT(12),DATA(1)                                       F1   606
      READINPUTTAPE10,1001,N,NOP                                        F1   607
      NEND=4*N+NCOF-1                                                   F1   608
      READINPUTTAPE10,1002,(DATA(I1),I1=NCOF,NEND)                      F1   609
      IF(NOP)2,2,3                                                      F1   610
    3 NBEG=NCOF                                                         F1   611
      K3=0                                                              F1   612
    7 CALLIDOUT(IDENT,DATE,9)                                           F1   613
      WRITEOUTPUTTAPE9,2001,N                                           F1   614
      DO4K1=NBEG,NEND,4                                                 F1   615
      K2=K1+3                                                           F1   616
```

```
      K3=K3+1                                                           F1   617
      WRITEOUTPUTTAPE9,2002,K3,(DATA(I1),I1=K1,K2)                      F1   618
      IF(50-K3)5,5,4                                                    F1   619
    5 NBEG=K1                                                           F1   620
      GOTO7                                                             F1   621
    4 CONTINUE                                                          F1   622
 1001 FORMAT(2I5)                                                       F1   623
 1002 FORMAT(4E10.8)                                                    F1   624
 2001 FORMAT(1H+,70X,17HNUMBER OF FACES =I5/75HOCOEFFICIENTS A, B, C, D F1   625
     1WHERE  AX + BY + CZ = D  DESCRIBES FACE OF CRYSTAL/1HO,2X,1HN,7X,1F1   626
     2HA,9X,1HB,9X,1HC,9X,1HD//)                                        F1   627
 2002 FORMAT(1H I3,2X,4F10.5)                                           F1   628
    2 RETURN                                                            F1   629
      END(0,1,0,0,0)                                                    F1   630


*       SUBROUTINE SIZE                                                  S   631
       REM TO DETERMINE AMOUNT OF STORAGE AVAILABLE FOR DATA             S   632
       REM MAKE DECREMENT OF SIZE + 5 =PART OF UPPER CORE NOT AVAILABLE  S   633
       REM ENTER WITH  TSX SIZE,4                                        S   634
       REM             HTR NS                                            S   635
       REM EXIT WITH   TRA 2,4                                           S   636
       REM NS WILL CONTAIN AMOUNT OF AVAILABLE STORAGE IN DECREMENT.     S   637
       REM THIS SUBROUTINE MUST BE THE LAST SUBROUTINE LOADED.           S   638
       FUL                                                               S   639
       ORG 0                  PROGRAM CARD                               S   640
       MZE 0,0,4              9L                                         S   641
       PZE 0                  9R                                         S   642
       PZE END+1              8L                                         S   643
       PZE 0                  8R                                         S   644
       BCD 1SIZE              7L                                         S   645
       PZE 0                  7R                                         S   646
       ORG 0                                                             S   647
       REL                                                               S   648
 SIZE  SXD END,4                                                         S   649
       CLA 1,4                                                           S   650
       STA SIZE+6                                                        S   651
       LXA END,4                                                         S   652
       TIX *+1,4,END                                                     S   653
       TIX *+1,4,205                                                     S   654
       SXD 0,4                NS                                         S   655
       LXD END,4                                                         S   656
       TRA 2,4                                                           S   657
 END   HTR -1                                                            S   658
       END 0                                                             S   659
```

```
   8                                                          M     660
.019855072.101666761.237233795.408282679                      U1    661
.591717321.762766205.898333239.980144928                      U2    662
.050614268.111190517.156853323.181341892                       R1   663
.181341892.156853323.111190517.050614268                      R2    664
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