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INDX: A Computer Program to
Aid in the Indexing of X-Ray
Powder Patterns of Crystal
Structures of Unknown Symmetry

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INDX: A COMPUTER PROGRAM TO AID IN THE INDEXING OF
X-RAY POWDER PATTERNS OF CRYSTAL STRUCTURES OF UNKNOWN SYMMETRY

by

R. B. Roof, Jr.

ABSTRACT

A computer program, INDX, has been developed that attempts to index X-ray diffraction powder patterns by finding a reduced triclinic cell whose calculated Q values ($Q = 1/d^2$) match a desired percentage of the observed Q values within a given limit of error. If a reduced triclinic cell is found, the cell constants may be used to form a rectangular array, i.e., a Niggli matrix, and reference to published tables of general and special Niggli matrices reveals whether or not the specific triclinic cell may be transformed to a cell of higher symmetry.

INTRODUCTION

INDX, the computer program described in this report has been designed to provide a means for rapidly defining and testing trial unit cells as an aid to indexing powder patterns of crystal structures of unknown symmetry. Azaroff and Buerger¹ have discussed the problem in general terms. Some of their suggestions have been added to the technique employed by Hacndler and Cooney,² and the combination has been modified by the author and his colleagues to treat more aspects of the problem in a complete package. In the interest of brevity, the detailed philosophy and equations of the above two references will not be repeated in this report. The logic of the current program, however, will be described in terms of sequential blocks of code and the checkpoint information available at the end of each block. The application of the program will be illustrated by two examples.

GENERAL DESCRIPTION OF PROGRAM

The program is composed of seven sequential blocks of code, each block having statement numbers

approximately 100 greater than those of the preceding block. Within each block the sequence of statement numbers does not deviate greatly from a linear progression. A special path is taken through these seven blocks in a particular application of the program, which will be shown in the examples. The description given below is the general logic for the normal flow of calculations. The listing of the program is given in a later section.

Block 000-100. This portion of the program contains dimension of arrays, common storage, and formats for input-output information.

Block 100-200. Evenly Spaced Pairs of Q 's (ESPQ).

In the process of reading and storing general identification information and various control numbers, and clearing and storing specific information in various arrays, this portion of the program also reads and numerically identifies M observed Q values. From every possible sum of pairs of N Q values the program subtracts each of the M observed Q values. The list of differences resulting from the subtraction from a given sum is

then searched, and storage is made in each case in which there are two differences having the same magnitude (plus or minus whatever error the investigator can tolerate) but opposite signs. The storage consists of the numerical identification of the two Q values in the sum and the two Q values forming the pair that is evenly spaced about the sum. At the end of this block the number of ESPQ formed is printed.

Block 200-300. Nine Internally Consistent Q's (NICQ). This portion of the program searches the total ESPQ set of four numbers and forms every possible internally consistent set of nine numbers. "Internally consistent" in this sense refers to the use of the two Q values forming a sum as possible lattice axes and the two Q values forming an evenly spaced pair about the sum to determine the angle between the possible lattice axes. In general, nine Q values are needed to define a unit cell. This set of nine numbers is written on Tape 7 for temporary storage, one hundred sets per record in a packed array. At the end of this block the number of NICQ formed is printed.

Block 300-400. Possible Cells (PCEL). This portion of the program, after reading back NICQ's from the packed array, computes the acute reciprocal unit cell represented by the set of nine numbers. This cell, along with the set of nine numbers and the information that it is acute, is written on Tape 8 for temporary storage. The unit cell angles are then changed from all acute to all obtuse. If the sum of the three cell angles exceeds 357 degrees the next set is processed, otherwise the obtuse cell is written on Tape 8 for temporary storage. At the end of this block the number of possible cells formed is printed.

Block 400-500. Trial Cells (TCEL). This portion of the program tests a possible triclinic reciprocal unit cell by attempting to calculate Q values that match the observed Q values (plus or minus an error term). No output occurs unless the Q's calculated for the cell under test match a desired percentage (e.g., 90%) of the observed Q's. Maximum and minimum values of hkl used for calculational purposes are determined from the

maximum value of Q, and only positive values of h are used. Reciprocal unit cell constants are obtained from the PCEL portion of the program. If a certain percentage of match (e.g., 80%) is obtained between the observed and calculated Q's, the reciprocal cell constants are subjected to a least-squares refinement. If the desired percentage of match (e.g., 90%) is not obtained after a preset number of cycles of refinement, the next unit cell is processed. If the desired percentage of match is obtained, the intermediate output consists of the refined reciprocal cell constants and cell volume written on Tape 7 for temporary storage. Also stored are the identification number of the specific cell in the linear array of PCEL's, the nine identification numbers of the Q's defining the cell, the acute or obtuse information pertaining to the cell, and the number of Q values indexed by the cell. At the end of this block the number of trial cells that pass the desired percentage of match criteria is printed. (The equation utilized for the calculation of Q values is not

$$Q = h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2 hka^* b^* \cos \gamma^* + 2 hla^* c^* \cos \beta^* + 2 klb^* c^* \cos \alpha^*,$$

the classical one involving the reciprocal cell and the hkl indices found in most references and textbooks. Instead, Q values are calculated as the sum of the squares of the three components in orthogonal space of a reciprocal lattice vector; i.e.,

$$Q = (\Delta V_1)^2 + (\Delta V_2)^2 + (\Delta V_3)^2$$

where

$$\Delta V_1 = (ha^* + kb^* \cos \gamma^* + lc^* \cos \beta^*)$$

$$\Delta V_2 = (kb^* \sin \gamma^* - lc^* \sin \beta^* \cos \alpha^*)$$

$$\Delta V_3 = (lc^* \sin \alpha^* \sin \beta^*).$$

Since the equation involves a mixture of real and reciprocal space angles, the real space angles must be calculated from the reciprocal space angles. It can be shown that this equation for Q is equivalent to the classical one. Also it can be written as

$$Q = [h^*C_{11} + k^*C_{12} + l^*C_{13}]^2 \quad (\text{component a})^2 + [k^*C_{14} - l^*C_{15}]^2 \quad (\text{component b})^2 + [l^*C_{16}]^2 \quad (\text{component c})^2.$$

After the six constants, C_{ij} , have been evaluated,

Q can be quickly calculated by adding a series of terms ranging from the minimum to the maximum value of hkl . The minimum and maximum values of hkl can be determined by sequentially solving the quadratic equations,

$$\begin{aligned}(\text{component } a)^2 - Q_{\max} &= 0 \\(\text{component } b)^2 - Q_{\max} &= 0 \\(\text{component } c)^2 - Q_{\max} &= 0,\end{aligned}$$

where the two roots when truncated to integers will be the maximum and minimum values of the desired indices.)

Block 500-600. Reciprocal to Real (RTOR). This portion of the program transforms TCEL reciprocal unit cells to the corresponding real space unit cells. These cells are written on Tape 8 for temporary storage.

Block 600-700. Reduced Cell (RCEL). This portion of the program finds the reduced cell in a given lattice by searching for the three shortest noncoplanar vectors which will yield an all-obtuse or all-acute cell. Each candidate vector can be written as the vector sum of simple integral multiples of the original cell edges. The square of the absolute length of this vector is found by forming the scalar product of the vector with itself. From a list of the squares of the absolute lengths formed by allowing the integral multiples to range from -2 to +2 in three-dimensional space, the three shortest vectors are selected. A test is made for the nonlinearity of these vectors. If the two shortest vectors are linear, the reduced cell is based on the shortest length plus the next shortest length that is non-linear with the shortest. A test is made for the nonplanarity of these vectors. If the three vectors are planar, the reduced cell is based on the two minimum lengths plus the next shortest length that is noncoplanar with the two shorter. At the end of this block the reduced cell constants are printed.

The reduced cell constants may then be used to form the Niggli matrix, namely the following scalar products:

$$\begin{array}{ccc} \underline{a} \cdot \underline{a} & \underline{b} \cdot \underline{b} & \underline{c} \cdot \underline{c} \\ \underline{b} \cdot \underline{c} & \underline{a} \cdot \underline{c} & \underline{a} \cdot \underline{b}, \end{array}$$

which are

$$\begin{array}{ccc} a^2 & b^2 & c^2 \\ bc \cos \alpha & ac \cos \beta & ab \cos \gamma. \end{array}$$

Reference to published tables of general and special Niggli matrices (Azaroff and Buerger¹) will reveal whether or not the cell generating a specific Niggli matrix may be transformed to a cell having higher than triclinic symmetry.

GLOSSARY OF PROGRAM TERMS

AA	Q(IA9) - Q(IA8), the difference between two numerically identified Q values, used in calculating $\cos \alpha^*$.
AMAX	Maximum value of component <u>a</u> of reciprocal lattice vector Q.
AMIN	Minimum value of component <u>a</u> of reciprocal lattice vector Q.
AS	Reciprocal angle α^* , in radians or degrees.
AT	Real space angle α , temporary.
A1	A TCEL <u>a</u> [*] .
A2	A TCEL <u>a</u> .
BB	Q(IA7) - Q(IA6), the difference between two numerically identified Q values, used in calculating $\cos \beta^*$.
BMAX	Maximum value of component <u>b</u> of reciprocal lattice vector Q.
BMIN	Minimum value of component <u>b</u> of reciprocal lattice vector Q.
BS	Reciprocal angle β^* , radians or degrees.
BT	Real space angle β , temporary.
B1	A TCEL <u>b</u> [*] .
B2	A TCEL <u>b</u> .
C	Estimated limit of error ($\pm$) of observed Q values.
CFA	Cosine function real space α .
CFAS	Cosine function α^* , defined from PCEL edges.
CFAL	Refined value cosine function α^* .
CFA2	CFAL transformed to real space, $\cos \alpha$.
CFBS	Cosine function β^* , defined from PCEL edges.
CFB1	Refined value cosine function β^* .
CFB2	CFB1 transformed to real space, $\cos \beta$.
CFGS	Cosine function γ^* , defined from PCEL edges.
CFG1	Refined value cosine function γ^* .

CFG2	CFG1 transformed to real space, cos γ .		trix X upon return from a least-squares cycle.
CFRCA	Cosine function of reduced cell α .	DIS	Distance (in arbitrary units) from origin in UVW space to plane passing through the three shortest non-coplanar vectors in the reduced cell.
CFRCB	Cosine function of reduced cell β .		
CFRCG	Cosine function of reduced cell γ .		
CPN	That portion of the equation for the cell volume that depends on angles alone.	D1	Distance (in arbitrary units) from origin in UV space to line passing through the two shortest nonlinear vectors in the reduced cell.
CYCLE	Number of least-squares cycles per processing block.		
C1	A TCEL c .	D2	Distance (in arbitrary units) from origin in VW space to line passing through the two shortest nonlinear vectors in the reduced cell.
C11	RA		
C12	RB*CFGS		
C13	RC*CFBS		
C14	RB*SFBS	D3	Distance (in arbitrary units) from origin in UW space to line passing through the two shortest nonlinear vectors in the reduced cell.
C15	RC*SFBS*CFA		
C16	RC* S FA* S FBS		
C2	A TCEL c .		
C20	XL*C15	E	The sum of two numerically identified Q values, $Q(I) + Q(J)$, also the difference between a calculated and observed Q.
C21	C14**2		
C22	C61*C20		
C23	C20**2 - QMAX + QC		
C24	C22**2	E1	A limit on the search for evenly spaced pairs of Q's, $2.0 * \text{SQRT}(Q(I) * Q(J))$.
C25	C63*C23		
C27	SQRT(C24-C25)		
C30	XK*C12	E2	The sum of positive and negative differences from the sum of two individual Q's.
C31	C60*C30		
C32	C30**2		
C35	C11**2	QG	$Q(IA4) - Q(IA5)$, the difference between two numerically identified Q values, used in calculating $\cos \gamma^*$.
C36	C31 + C41		
C37	C32 + C42 + C45 - QMAX + QBC		
C40	XL*C13	GS	Reciprocal angle γ^* , radians or degrees.
C41	C60*C40		
C42	C40**2	GT	Real space angle γ , temporary.
C45	$2.0 * C30 * C40$	I	A general variable.
C50	C36**2	IA1, IA2, IA3 IA4, IA5, IA6 IA7, IA8, IA9	A set of nine internally consistent numbers defining various Q values used to construct a possible trial cell.
C51	C65*C37		
C52	C50 - C51		
C53	SQRT(C52)		
C60	$2.0 * C11$	IC	Integer value of C times 5000.
C61	$-2.0 * C14$	II	General variables for packed array of the nine consistent integers IA1 to IA9.
C62	$2.0 * C21$		
C63	$2.0 * C62$		
C64	$2.0 * C35$	IM	The integer value of the maximum value allowed $Q(2.000)$ times 10,000.
C65	$2.0 * C64$		
D(100)	Storage table for differences between sums of Q's and all remaining Q's.	INQ	Integer value of $Q(I)$ minus estimated error.
DET	Contains the determinant of the ma-	INQ1	Integer value of $Q(I)$ plus estimated

	error.	MF	Number of unit cells passing least-squares test in TCEL.
ISØN(900)	Storage for <u>integer sets of nine</u> numerical values.	MG	Count of number of hkl indices calculating a Q match; includes multiple matches, limit of 2000.
I1, I2 I3, I4	Numerical set of four Q values. I1 and I2 identify Q values being summed; I3 and I4 identify Q values forming equal differences about the sum.	MZ	Integer form of Z, number of cycles of least-squares per sub-block of processing.
I5	A general variable controlling the testing of PCEL's.	M1	Number of sub-blocks of processing desired, printout obtained after each sub-block is processed.
I51, I512	Control characters governing the processing path in block 400-500.	M2	Integer form of Z3, percentage of lines to be indexed.
I61	Control character governing the processing path in block 600-700.	M3	Integer form of Z4, percentage of lines to be indexed prior to entering least-squares refinement.
I7	General variable controlling the search for reduced cells from TCEL.	N	Number of observed Q values used in generating evenly spaced pairs of Q's.
I8	General variable interchangeable with I5 when I2 > 0.	NAME	Title information for a particular job.
I10, I11	Computed variables for examination of table of observed Q's.	NC	Number of cycles of least squares performed.
J, J1, J2, J3	General variables.	NHROW	Number of h rows to be processed per given l level in a hemisphere governed by QMAX.
K	A general variable.	NKROW	Number of k rows to be processed per given l level in a hemisphere governed by QMAX.
L	A general variable, a count of the number of lines indexed.	NQ	Integer value of Q times 10,000.
IA, IB	Calculated variables used in table search for evenly spaced pairs of Q's.	NQHKL	Integer value of a calculated Q, QHKL, times 10,000.
IM(100)	Storage for general variable L in table search for evenly spaced pairs of Q's.	NQTAB(20000)	Storage table for integer values of possible Q values.
IO	A general variable	PD(6)	Partial derivative storage for the six cell constants.
LT(100)	Storage for temporary line count.	Q(100)	Storage table for 100 observed Q values.
L1	Number of lines <u>not</u> indexed.	QBC	The sum of (component b) ² and (component c) ² .
L11	Limit of number of lines not indexed; if exceeded, processing passes to next trial cell.	QC	(component c) ² .
I2	Control number designating number of unit cells to be refined in the special application of the program.	QHKL	The calculated value of Q for a particular hkl and a particular test unit cell.
M	A general variable, number of observed Q values.	QMAX	The maximum value of Q used. Needed to limit the size of the hemisphere that will be searched.
MA	Number of ESPQ's found.	RA, RB, RC	Reciprocal cell constants; a*, b*, c*.
MB	Number of NICQ's generated.		
MC	A character designating an acute or obtuse reciprocal cell; acute = 1, obtuse = 2.		
MD	Count of number of times NQTAB is searched for match between calculated and observed Q's.		
ME	Number of PCEL generated.		

RCA,RCB,RCC	Reduced cell constants; a, b, c.
RMAT(6,7)	Right-hand side of matrix solved by LSS.
SFA	Sine function of real cell angle α .
SFA1	SIN(AT)
SFBS	SQRT(TBS)
SFB1	SIN(BT)
SFGS	SQRT(TGS)
SFG1	SIN(CT)
TBS	1.0 - CFBS**2
TE(2000)	Temporary storage for E (2nd sense).
TEMP(124)	Temporary storage for 2*62 TSQ's during sorting.
TGS	1.0 - CFCS**2
TH(2000)	Temporary storage for XH.
TK(2000)	Temporary storage for XK.
TL(2000)	Temporary storage for XL.
TSQ(62)	Temporary storage for 62 candidate vectors for a reduced cell.
U	General variable in UVW space.
UT(62)	Temporary storage for U.
U1	Initial value of U.
V	General variable in UVW space.
VØL	Volume of reciprocal unit cell.
VØL1	Volume of reciprocal unit cell.
VØI2	Volume of real space unit cell.
VT(62)	Temporary storage for V.
V1	Initial value of V.
W	General variable in UVW space.
WT(62)	Temporary storage for W.
W1	Initial value of W.
X(6,6)	Left-hand side of matrix solved by LSS.
XH	Floating point value of h.
XHMAX	Maximum value of XH.
XHMIN	Minimum value of XH.
XK	Floating point value of k.
XKMAX	Maximum value of XK.
XKMIN	Minimum value of XK.
XL	Floating point value of l.
XX1	2.0*RA
XX2	XX4*CFGS
XX3	XX7*CFBS
XX4	2.0*RB
XX5	XX1*CFGS
XX6	XX7*CFAS
XX7	2.0*RC

XX8	XX1*CFBS
XX9	XX4*CFAS
XX10	XX4*RC
XX11	XX7*RA
XX12	XX1*RB
X1	A2**2
X2	B2**2
X3	C2**2
X4	2.0*A2*B2*CFG2
X5	2.0*B2*C2*CFA2
X6	2.0*C2*A2*CFB2
YY1	TH(I)**2
YY2	TK(I)**2
YY3	TL(I)**2
YY4	TH(I)*TK(I)
YY5	TH(I)*TL(I)
YY6	TK(I)*TL(I)
Z	Number of least-squares cycles performed per block.
ZERO	Equal to 0.0
Z1	FLØAT(M)*Z4/100.0
Z2	FLØAT(L)
Z3	Percentage of lines to be indexed.
Z4	Percentage of lines required to be indexed before entering least-squares procedures.
Z5	FLØAT(M)*Z3/100.0

INPUT DESCRIPTION

Input to INDX consists of punched cards containing the following information in the indicated format.

Card 1: 72 Hollerith characters for problem identification.

Card 2: col. 1-5 M, number of observed Q values, (15 field).
6-10 N, number of M used to determine ESPQ, (15 field).
11-20 C, estimated allowable error in observed Q, (F10.5 field).
21-30 QMAX, maximum value of Q (F10.5 field).
31-35 Z, number of least-squares cycles per sub-block (F5.0 field).
36-40 M1, number of sub-blocks of processing desired (15 field).
41-45 Z3, percentage of lines to be indexed (F5.0 field).

46-50 Z4, percentage of lines required to be indexed prior to entering least-squares procedures (F5.0 field).

51-55 I2, control number designating number of unit cells to be refined in special applications of the program (I5 field).

Card 3: M observed Q values, one per card in an etc. F10.5 field.

OUTPUT DESCRIPTION

Output from INDX consists of the following information presented in sequential order. A print-out composed of

1. Title information identifying the job.
2. The control information on Card 2 of the input.
3. A numbered listing of the observed Q values.
4. The number of ESPQ generated by the controls M and N.
5. The number of NICQ formed from ESPQ.
6. The number of PCEL to be tested. This number is usually something less than twice NICQ.
7. A series of sets of printed lines, two lines per set. The first line consists of two numbers; the first is the sequential number in the set of PCEL; the second is the number of lines the unit cell under investigation will index. The second line lists the nine numbers comprising one NICQ (from which the trial reciprocal cell can be determined if desired) and one number indicating whether the trial reciprocal cell is acute or obtuse.

The trial reciprocal unit cell is determined as follows: The nine numbers are the numerical identification of the observed Q values and

$$\begin{aligned} a^* &= \text{SQRT}(Q(1)) \\ b^* &= \text{SQRT}(Q(2)) \\ c^* &= \text{SQRT}(Q(3)) \\ \cos \alpha^* &= 0.25(Q(4) - Q(5))/b^* \cdot c^* \\ \cos \beta^* &= 0.25(Q(6) - Q(7))/c^* \cdot a^* \\ \cos \gamma^* &= 0.25(Q(8) - Q(9))/a^* \cdot b^* \end{aligned}$$

The tenth number is 1 if the trial reciprocal unit cell is acute or 2 if the trial reciprocal unit cell is obtuse.

8. The number of TCEL passing the desired percentage of lines to be indexed test. Equals the number of sets of two printed lines.
9. The heading A, B, C, COS ALPHA, COS BETA, COS GAMMA, CELL NO.
10. A listing, under the headings of line 9, of the real space cell constants of each individual TCEL and its position in the PCEL list.

The cell constants are also punched on cards in a 6F10.5 field for use by the investigator in any manner he wishes.

ILLUSTRATIVE EXAMPLE #1: INPUT #1

The first example of the use of INDX is the indexing of compound K ($\text{PuZr}_{\sim 3}$) in the plutonium-zirconium alloy system. Table I is a listing of the Q values obtained from the published³ d spacings. Probable second- and third-order reflections appear in this list, and, on the basis of these, Q_1 and Q_2 may be revised to 0.0521 and 0.1024. The information

Table I

Q values for PuZr_3 , compound K of Pu-Zr phase diagram. hkl indexing for hexagonal ($a=5.05$, $c=3.12$) and orthorhombic ($a=4.37$, $b=2.52$, $c=3.12$) unit cells.

N	Q	Hexagonal	Orthorhombic
1	0.0517	010	100
2	0.1017	001	001
3	0.1545	011	101
4	0.1563	110	010
5	0.2085	020	110,200
6	0.2593	111	011
7	0.3114	021	111,201
8	0.3651	120	210
9	0.4098	002	002
10	0.4690	121,030	211,300
11	0.5669	112	012
12	0.6270	220	020,310
13	0.7294	221	021,311
14	0.7818	131	121
15	0.8803	032	302
16	0.9372	041	401
17	0.9747	013	103
18	1.0364	222	312
19	1.0788	113	013
20	1.0953	231,140	411,320
21	1.1322	023	113,203
22	1.1983	141	321
23	1.2878	123	213
24	1.4075	051	501
25	1.5063	142	322
26	1.5644	241	131,421,511
27	1.6000	133	123

punched on Card 2 of the input cards allows considerable latitude in describing the conditions for beginning an INDX run. Experience has shown that initially:

M should be approximately one-half of available observed Q's;
 N should be one-fourth to one-half of M;
 a reasonable value for C is one-half or less of the minimum difference between observed Q's, but also probably not more than 0.0020;
 QMAX should be slightly larger than the maximum observed Q processed;
 a value of 10 is a reasonable number of least-squares cycles (If convergence is obtained in fewer cycles the program bypasses the remaining cycle requirement.);
 one sub-block of processing is usually sufficient (It is possible to set Z = 1 and M1 = 1 to obtain printed results after each least-squares cycle, but this will cause a deluge of numbers of questionable desirability.);
 the percentage of lines indexed should be less than 100% to allow for the presumed presence of impurity lines;
 some 60 to 75% of the lines should be indexed before least-squares refinement is attempted, so that time is not wasted in trying to refine a unit cell that won't fit;
 L2 should be zero as there are no unit cells available for refinement in the special application of the program.

With the above criteria in mind, the values on Control Card 2 are:

```

M   = 17
N   = 5
C   = 0.0020
QMAX = 0.9800
Z   = 10
M1  = 1
Z3  = 90
Z4  = 60
L2  = 0

```

Figure 1 shows the control and data cards for Example #1, Input #1.

ILLUSTRATIVE EXAMPLE #1: OUTPUT #1

Figure 2 is a listing of the output obtained. The information follows the outline previously described. With M = 17 and N = 5 there are 30 ESPQ formed. These in turn generate 257 NICQ and 429 possible cells to be tested. Of these, 54 cells will index 90% or more of the listed Q values. The real space lattice reduced cell constants are given

along with a cross-reference cell number relating the listed real space cell to its original reciprocal in the PCEL list.

ILLUSTRATIVE EXAMPLE #1: INPUT #2

For a second pass through INDX, the 15 unique cells found from the first pass (Output #1) are to be tested against all 27 observed Q values. For this application the values on Control Card 2 are:

```

M   = 27
N   = 0 (No cells are generated,
        L2 cells are tested.)
C   = 0.0015
QMAX = 1.6100
Z   = 10
M1  = 1
Z3  = 100 (Only those cells that
           will index all lines
           are desired.)
Z4  = 75 (Since the cells to be
           tested index 90% or
           more of 17 lines, it is
           reasonable that they
           will also index 75% of
           27 lines.)
L2  = 15

```

Figure 3 shows the control and data cards for Example #1, Input #2.

ILLUSTRATIVE EXAMPLE #1: OUTPUT #2

Figure 4 is a listing of the output obtained. Of 15 cells tested only cells 1 and 7 will index all 27 observed Q's. If Z3 had been set to slightly less than 100%, then the numerical identification of a Q value that the cell did not index would have appeared under the heading "LINES NOT INDEXED FOR CELL NO." This feature may be useful in eliminating impurities or spurious reflections from the list of Q values. Of the two reduced cells listed in Fig. 4, one is hexagonal and the other orthorhombic, and their Niggli matrices indicate that they cannot be transformed to cells of higher symmetry. The hkl indices generated by these cells are listed in Table I. The orthorhombic cell is a special representation of the hexagonal cell and is always an alternative solution to a hexagonal powder pattern. While single crystal information, or other physical data, may ultimately prove the hexagonal cell to be correct, the orthorhombic cell is just as

9747								
9372								
8803								
7818								
7294								
6270								
5669								
4690								
4098								
3651								
3114								
2593								
2095								
1563								
1545								
1024								
0521								
17	5	00200	98000	10	1	90	60	0
POWDER PATTERN FOR PU-ZR								
COMPOUND K								
1	2	3	4	5	6	7	8	9
00	00	00	00	00	00	00	00	00
00000	00000	00000	00000	00000	00000	00000	00000	00000
11111	11111	11111	11111	11111	11111	11111	11111	11111
22222	22222	22222	22222	22222	22222	22222	22222	22222
33333	33333	33333	33333	33333	33333	33333	33333	33333
44444	44444	44444	44444	44444	44444	44444	44444	44444
55555	55555	55555	55555	55555	55555	55555	55555	55555
66666	66666	66666	66666	66666	66666	66666	66666	66666
77777	77777	77777	77777	77777	77777	77777	77777	77777
88888	88888	88888	88888	88888	88888	88888	88888	88888
99999	99999	99999	99999	99999	99999	99999	99999	99999

1. A DATA CARD-FIVE

12420701

L. A. DATA CARD-FIVE

Fig. 1. Control and data cards for Example #1, Input #1.

POWDER PATTERN FOR PU-ZR

COMPOUND K

17 5 .00200 .98000 10 1 90 60 0

1 .0521
2 .1024
3 .1545
4 .1563
5 .2085
6 .2593
7 .3114
8 .3651
9 .4098
10 .4690
11 .5669
12 .6270
13 .7294
14 .7818
15 .8803
16 .9372
17 .9747

ESPQ = 30

NICQ = 257

PCEL = 429

10 17

1 1 2 3 3 3 3 3 1 1

11 17

1 1 2 3 3 3 3 3 1 2

12 17

1 1 2 4 3 3 3 3 1 1

13 17

1 1 2 4 3 3 3 3 1 2

14 17

1 1 2 4 3 4 3 3 1 1

15 17

1 1 2 4 3 4 3 3 1 2

17 17

1 1 3 6 3 7 2 3 1 1

20 17

1 1 3 6 3 6 3 3 1 2

23 17

1 1 4 5 5 8 1 3 1 1

Fig. 2. Information obtained for Example #1, Output #1.

			1	4	5	12	2	8	3	6	4	1
207 16												
			1	4	5	12	2	8	4	6	4	1
TCEL = 54												
A	B	C	COS ALPHA	COS BETA	COS GAMMA	CELL NO.						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	10						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	11						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	12						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	13						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	14						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	15						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	17						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	20						
5.05677	5.08498	26.78331	-.04523	-.01337	-.49660	23						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	46						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	47						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	48						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	49						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	50						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	51						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	53						
5.37490	5.37600	5.40504	-.32100	-.32210	-.32467	54						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	56						
5.36372	5.36376	5.38968	-.33316	-.32789	-.33358	58						
3.51783	5.19774	5.28950	-.39914	-.15466	-.18422	85						
3.12291	5.05264	5.05265	-.50000	-0.00000	-0.00000	100						
3.12291	5.05264	5.05265	-.50000	-0.00000	-0.00000	101						
2.63897	3.12190	4.57343	0.00000	.28851	0.00000	102						
2.63897	3.12190	4.57343	0.00000	.28851	0.00000	103						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	104						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	105						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	108						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	109						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	112						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	113						
3.12635	5.05459	5.07061	.49814	.01070	.00030	122						
3.12635	5.05459	5.07061	.49814	.01070	.00030	123						
2.63804	3.12498	4.57962	.00362	.28802	0.00000	124						
2.63804	3.12498	4.57962	.00362	.28802	0.00000	125						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	126						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	127						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	130						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	131						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	134						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	135						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	142						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	145						
3.12577	5.09455	5.10075	-.47586	-.01905	-.01944	148						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	153						
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	154						
3.12291	5.05265	5.05265	.50000	0.00000	0.00000	158						
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	159						
3.12291	5.05265	5.05265	.50000	-0.00000	-0.00000	160						
2.92332	3.43682	4.61583	.13242	.31666	.41816	162						
3.12630	5.05457	5.07154	.49809	.01108	0.00000	172						
5.36752	5.37598	5.38520	-.32511	-.33720	-.33543	175						
3.41976	5.17683	5.19557	-.42681	-.21970	-.21349	180						
2.80697	3.56740	4.75057	-.26729	-.16909	-.34195	202						
2.80516	3.56211	4.75032	-.26997	-.16827	-.33988	207						

Fig. 2. (Continued)

2.80697	3.56740	4.75057	-.26729	-.16909	-.34195	202
3.41976	5.17683	5.19557	-.42681	-.21970	-.21349	180
5.36752	5.37598	5.38520	-.32511	-.33720	-.33543	175
3.12630	5.05457	5.07154	.49809	.01108	0.00000	172
2.92332	3.43682	4.61583	.13242	.31666	.41816	162
3.12577	5.09455	5.10075	-.47586	-.01905	-.01944	148
2.63804	3.12498	4.57962	.00362	.28802	0.00000	124
3.12635	5.05459	5.07061	.49814	.01070	.00030	122
2.52643	3.12285	4.37669	-0.00000	-0.00000	-0.00000	104
2.63897	3.12190	4.57343	0.00000	.28851	0.00000	102
3.51783	5.19774	5.28950	-.39914	-.15466	-.18422	85
5.36372	5.36376	5.38968	-.33316	-.32789	-.33358	58
5.37490	5.37600	5.40504	-.32100	-.32210	-.32467	54
5.05677	5.08498	26.78331	-.04523	-.01337	-.49660	23
3.12291	5.05265	5.05265	-.50000	-0.00000	-0.00000	10
16000						
15644						
15063						
14075						
12878						
11983						
11322						
10753						
10788						
10364						
9747						
9372						
8803						
7818						
7294						
6270						
5669						
4690						
4098						
3651						
3114						
2593						
2085						
1563						
1545						
1024						
0521						
27	0	00150	161000	10	1	100
						75
						15
POWDER PATTERN FOR PU-ZR COMPOUND K						
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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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</					

POWDER PATTERN FOR PU-ZR

COMPOUND K

27 0 .00150 1.61000 10 1 100 75 15

1 .0521
 2 .1024
 3 .1545
 4 .1563
 5 .2085
 6 .2593
 7 .3114
 8 .3651
 9 .4098
 10 .4690
 11 .5669
 12 .6270
 13 .7294
 14 .7818
 15 .8803
 16 .9372
 17 .9747
 18 1.0364
 19 1.0788
 20 1.0953
 21 1.1322
 22 1.1983
 23 1.2878
 24 1.4075
 25 1.5063
 26 1.5644
 27 1.6000

1 27

7 27

TCCL = 2

LINES NOT INDEXED FOR 1

LINES NOT INDEXED FOR 7

A	B	C	COS ALPHA	COS BETA	COS GAMMA	CELL NO.
3.12375	5.05364	5.05364	-.50000	-0.00000	-0.00000	1
2.52706	3.12336	4.37629	-0.00000	-0.00000	-0.00000	7

Fig. 4. Information obtained for Example #1, Output #2.

valid a representation as the hexagonal cell on the basis of a powder pattern.

ILLUSTRATIVE EXAMPLE #2: INPUT #1

Indexing of the compound θ (Pu_4Zr) is given as the second example of the use of INDX. Table II is a listing of the Q values obtained from the published³ d spacings. Probable 2nd, 3rd, 4th, and 5th order

Table II

Q values for Pu_4Zr , compound θ of Pu-Zr phase diagram. hkl indexing for an orthorhombic unit cell $a=5.43$, $b=14.84$, $c=10.86$, space group #64, Cmca.

No.	Q	hkl	No.	Q	hkl
1	0.0176	020	24	0.2713	204
2	0.0332	002	25	0.3239	026,082
3	0.0463	111	26	0.3436	116,312,244
4	0.0514	022	27	0.4221	333
5	0.0724	112,040	28	0.4277	351
6	0.0829	131	29	0.4357	264,281,192
7	0.1138	113	30	0.4529	156,352,117
8	0.1357	004,200	31	0.4608	202
9	0.1484	043	32	0.4871	047
10	0.1506	133	33	0.5447	400
11	0.1532	024,220	34	0.5952	086
12	0.1556	151	35	0.6057	373,266
13	0.1625	221,060	36	0.6142	195,316,048
14	0.1692	202	37	0.6250	441
15	0.1736	114	38	0.6622	0121
16	0.1805	152	39	0.6807	391
17	0.1973	062	40	0.6954	228
18	0.2100	134	41	0.7072	460,196,392
19	0.2169	241	42	0.7241	356,119,317
20	0.2298	025,223	43	0.9709	551
21	0.2393	063	44	1.0020	2125
22	0.2498	115	45	1.0309	447,4102
23	0.2652	171			

reflections appear in this list, and on that basis Q_1 and Q_2 may be revised to 0.0180 and 0.0340. The values on Control Card 2 were selected as:

M = 26
N = 5 (and 10)
C = 0.0020
QMAX = 0.3500
Z = 10
M1 = 1
Z3 = 90
Z4 = 60
I2 = 0

ILLUSTRATIVE EXAMPLE #2: OUTPUT #1

Figures 5 and 6 are listings of the outputs obtained when $N = 5$ and 10, respectively. There is a tremendous increase in the number of trial cells generated as N increases.*

*The time taken on a CDC 6600 computer to generate and test 8282 cells is ~ 196 sec, which corresponds to a processing rate of about ~ 40 cells/sec.

Also note that no small cell of high symmetry that will index 90% or more of the listed Q values is found. Sixteen reduced cells are found that will index 26 of 26 lines, but their Niggli matrices reveal that they must remain triclinic since they cannot be transformed to cells of higher symmetry. Three other reduced triclinic cells that are found will transform to reasonably simple monoclinic cells, but they will index only 24 of 26 lines.

ILLUSTRATIVE EXAMPLE #2: INPUT #2

Since no promising unit cell was found in the examination of some 8000 cells, the assumption is made that some of the Q values listed in Table II are 2nd order. A search for higher orders is now necessary. To eliminate the possibility of just mere coincidence matching, at least two higher orders must be found to reinforce the assumption that a particular Q value represents a 2nd order. Table III is a listing of the agreement between the calculated and observed Q values when all Q's are assumed to be second order. There are five implied first-order lines, 0.0045, 0.0085, 0.0130, 0.383, and 0.0425. The last line is included in the list in spite of its having only one higher order, because we observe that if

$$\begin{aligned}a^* &= 0.0045 \\b^* &= 0.0085 \\c^* &= 0.0383,\end{aligned}$$

and if

$$\begin{aligned}100 + 010 &= 110 = 0.0130 \\010 + 001 &= 011 = 0.0468,\end{aligned}$$

then

$$100 + 001 = 101 = 0.0428,$$

and the implied Q at 0.0425 is needed to define a cell of at least orthorhombic symmetry. The five implied first-order lines are added to the observed Q's, and the values on Control Card 2 are selected as:

M = 29
N = 5
C = 0.0020
QMAX = 0.2800
Z = 10
M1 = 1
Z3 = 100
Z4 = 75
I2 = 0

POWDER PATTERN FOR PII-7R THETA COMPOUND

26	5	.00200	.35000	10	1	90	60	0
1		.0180						
2		.0340						
3		.0463						
4		.0514						
5		.0724						
6		.0829						
7		.1138						
8		.1357						
9		.1484						
10		.1506						
11		.1532						
12		.1556						
13		.1625						
14		.1692						
15		.1736						
16		.1805						
17		.1973						
18		.2100						
19		.2169						
20		.2298						
21		.2393						
22		.2498						
23		.2652						
24		.2713						
25		.3239						
26		.3436						
ESPO = 30								
NICO = 313								
PCEL = 459								
6	25							
		1	2	5	13	4	9	2
7	25							
		1	2	5	13	4	9	2
201	24							
		3	4	4	11	4	7	6
204	24							
		3	4	5	20	1	11	6
TCCL = 9								
A	B	C	COS ALPHA	COS BETA	COS GAMMA	CELL NO.		
6.10367	9.69760	11.15744	.14601	.17151	.29806	6		
6.10367	9.69760	11.15744	.14601	.17151	.29806	7		
5.52905	8.13638	12.91781	-.18982	-.16087	-.08169	8		
5.52905	8.13638	12.91781	-.18982	-.16087	-.08169	9		
6.30932	8.22680	10.78675	.30195	.25918	.37592	32		
6.22813	8.18881	9.97587	.26852	.21641	.35649	33		
5.49876	6.05802	7.92750	.16284	.33943	.44719	132		
5.13105	5.84972	7.60083	.07429	.23540	.36630	201		
5.38791	7.26187	7.57332	-.09119	-.13031	-.04446	204		

Fig. 5. Information obtained for Example #2, Output #1, N=5.

POWDER PATTERN FOR PU-ZR THETA COMPOUND

26 10 .00200 .35000 10 1 90 60 0

1	.0180
2	.0340
3	.0463
4	.0514
5	.0724
6	.0829
7	.1138
8	.1357
9	.1484
10	.1506
11	.1532
12	.1556
13	.1625
14	.1692
15	.1736
16	.1805
17	.1973
18	.2100
19	.2169
20	.2298
21	.2393
22	.2498
23	.2652
24	.2713
25	.3239
26	.3436

ESPO = 158
 NICO = 4635
 PCEL = 8282

6	25									
		1	2	5	13	4	9	2	4	4
7	25									
		1	2	5	13	4	9	2	4	4
8	26									
		1	2	5	16	2	8	3	4	4
9	26									
		1	2	5	16	2	8	3	4	4
14	26									
		1	2	6	13	5	14	2	4	4
15	26									
		1	2	6	13	5	14	2	4	4
16	25									
		1	2	6	10	6	14	2	4	4

Fig. 6. Information obtained for Example #2, Output #1, N=10.

4639 24

4 5 6 12 11 17 5 20 1 1

4640 24

4 5 6 12 12 17 5 20 1 1

4932 24

4 5 6 12 12 22 1 15 5 1

TCEL = 86

A	B	C	COS ALPHA	COS BETA	COS GAMMA	CELL NO.
6.10347	9.69740	11.15744	.14601	.17151	.29806	4
6.10347	9.69740	11.15744	.14601	.17151	.29806	7
5.52905	8.13638	12.91781	-.18982	-.16087	-.08169	8
5.52905	8.13638	12.91781	-.18982	-.16087	-.08169	9
7.37011	7.66351	11.28223	.20721	.24191	.15889	14
7.37011	7.66351	11.28223	.20721	.24191	.15889	15
7.19780	7.24738	7.52533	-.10933	-.10385	-.12718	16
7.19780	7.24738	7.52533	-.10933	-.10385	-.12718	17
5.42841	5.71429	7.70109	.08101	.26253	.31506	28
5.42841	5.71429	7.70109	.08101	.26253	.31506	29
9.05063	9.23383	9.23629	.47943	.29611	.47247	33
9.05063	9.23383	9.23629	.47943	.29611	.47247	34
5.42811	8.11517	8.86555	-.40301	-0.00000	-0.00000	35
5.42811	8.11517	8.86555	-.40301	-0.00000	-0.00000	36
9.05468	9.09232	9.22022	.29655	.46332	.46231	37
5.42872	7.49217	7.79639	-.30250	-0.00000	-0.00000	70
5.42872	7.49217	7.79639	-.30250	-0.00000	-0.00000	71
5.30628	5.66114	7.61754	.06250	.22116	.28901	72
5.30628	5.66114	7.61754	.06250	.22116	.28901	73
5.44794	7.43035	10.56133	-0.00000	-.07617	-0.00000	153
5.44794	7.43035	10.56133	-0.00000	-.07617	-0.00000	154
4.91596	8.03613	14.26052	-.21007	-.06966	-.28393	178
5.01001	7.28766	7.83833	-.03480	-.29019	-.22404	180
9.09435	10.77987	23.22713	-.21262	-.55416	-.03547	181
6.56061	8.12964	8.97182	-.39032	-.15577	-.04229	182
7.28770	8.15094	9.18478	-.38881	-.26802	-.00169	183
7.15749	7.87219	11.83890	.27200	.12128	.11811	1951
5.14890	7.45799	7.73271	-.03204	-.17446	-.31234	1957
7.60582	9.01785	12.59934	.13577	.25542	.11857	1958
5.15066	7.43744	7.94656	-.00053	-.27739	-.29834	1965
8.12301	8.73854	10.48684	.58311	.34794	.27325	1993
4.50584	6.93331	7.64494	-.10943	-.19254	-.11194	2029
5.47378	5.73102	7.09487	.04036	.07117	.11411	2052
5.47378	5.73102	7.09487	.04036	.07117	.11411	2053
5.43211	6.08221	8.09794	.13571	.28052	.45403	2189
5.49876	6.05802	7.92750	.16284	.33943	.44719	2500
5.20311	6.01682	22.37234	.04181	.09669	.43238	2553
5.13105	5.84972	7.60083	-.07429	.23540	.36630	2857
5.38791	7.26187	7.57332	-.09119	-.13031	-.04446	2860
7.47248	7.93221	8.30122	.38378	.23959	.00956	2872
5.04200	7.29416	7.77195	-.05800	-.28898	-.21177	2877
5.24323	7.98655	8.73597	.38438	.21653	.17819	3036
5.22848	7.86890	8.31956	.34048	.25223	.19893	3037
5.44017	5.95200	7.74217	.10454	.32724	.43058	3354
5.82420	7.91711	8.51924	.25380	.16331	.24983	4639
6.22568	7.93886	9.62263	.27083	.29962	.26861	4640
5.18881	7.51951	7.97939	.28441	.27703	.13019	4932

Fig. 6. (Continued)

Table III

Agreement between calculated and observed Q values
when all Q's of compound 8 are assumed to be second order.

Q No.	1		2		4		11		14	
ORDER	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.
1	0.0045	-	0.0085	-	0.0130	-	0.0383	-	0.0425	-
2	0.0180	0.0176	0.0340	0.0332	0.0520	0.0514	0.1532	0.1532	0.1700	0.1692
3	0.0405	-	0.0765	-	0.1170	-	0.3447	0.3436	0.3829	-
4	0.0720	0.0724	0.1360	0.1357	0.2080	0.2100	0.6128	0.6142	0.6800	0.6807
5	0.1125	0.1138	0.2125	0.2100	0.3250	0.3239				
6	0.1620	0.1625	0.3060	-						
7	0.2205	-	0.4165	-						
8	0.2880	-	0.5440	0.5447						
9	0.3645	-								
10	0.4500	0.4529								
11	0.5445	0.5447								

ILLUSTRATIVE EXAMPLE #2: OUTPUT #2

Figure 7 is a listing of the output obtained from the pass through the program as described in the preceding section. Since Z3 was set at 100%, all 91 cells listed will index 29 of 29 Q values. Several interesting reduced cells are found; for example, No. 1 is a large rhombohedral cell and No. 5 is end-centered orthorhombic. The orthorhombic cell given by Marples³ (a=10.39, b=10.44, c=11.18) was not found. The tetragonal cell proposed by Berndt⁴ (1967) (a=10.89, c=14.89) was found as cell Nos. 66 and 67 as well as other tetragonal cells, cell Nos. 28, 29, 133 and 134. However, the smallest cell of highest symmetry appears to be orthorhombic, cell Nos. 92, 93, 198, and 199.

ILLUSTRATIVE EXAMPLE #2: INPUT #3

To help select the best cell of the 63 different cells discovered, all 63 are sent through the program in several passes utilizing successively smaller values of C. As C is made smaller, certain cells will be rejected as being unable to index 100% of the Q values. The 63 cells are now tested against the 45 Q values listed in Table II, and the values selected for Control Card 2 are:

M = 45
N = 0
C = 0.00200 (0.00175, 0.00150, 0.00125, etc.)
QMAX = 1.04
Z = 10
M1 = 1
Z3 = 90
Z4 = 60
L2 = 63 (If desired, this may be

reduced after each pass by re-introducing only those cells that have passed a C test.)

ILLUSTRATIVE EXAMPLE #2: OUTPUT #3

Figure 8 is a listing of the output obtained when C = 0.0015. Below this value the small orthorhombic cell is not retained. The comment in Fig. 8 that "MG EXCEEDS 2000. REDUCE QMAX OR C." indicates that cell No. 2 (or 39) in the list is so large that more than 2000 hkl's that will match the observed Q values are generated. Such a unit cell is probably incorrect and should be rejected. However, if this cell is the only one retained, the suggestion should be followed. Figure 8 also indicates that there are two lines, Nos. 29 and 41, not indexed by cell No. 22. Other cells also do not index all the lines, as indicated in the figure.

An examination of the hkl indices generated by the small orthorhombic cell (No. 52, Fig. 8) and space group Pmmm reveals that Q values having reflections with $h + l = 2n$ are all that are needed to match the Q values of Table II. The $h + l = \text{odd}$ extinct reflections indicate a space group of Bmmm. Transference to the standard setting of Cmmm reveals further extinctions, namely, $h0l$, l odd, and hko , h odd, indication that the space group is No. 64, Cmca. This is identical with the cell found by Zachariasen.⁵ Table II lists the hkl indexing for compound 8 with a=5.42898, b=14.83869, c=10.86392, space group No. 64, Cmca.

SUGGESTIONS FOR USING INDX

Since low-angle reflections are used to define unit cells for further testing, they should be mea-

POWDER PATTERN FOR PU-ZR THETA COMPOUND

29 5 .00200 .28000 10 1 100 75 0

1 .0045
2 .0085
3 .0130
4 .0180
5 .0340
6 .0383
7 .0425
8 .0463
9 .0514
10 .0724
11 .0829
12 .1138
13 .1357
14 .1484
15 .1506
16 .1532
17 .1556
18 .1625
19 .1692
20 .1736
21 .1805
22 .1973
23 .2100
24 .2169
25 .2298
26 .2393
27 .2498
28 .2652
29 .2713

ESPO = 30

NICO = 234

PCEL = 386

1	29										
		1	1	1	3	1	3	1	3	1	1
2	29										
		1	1	1	3	1	3	1	3	1	2
3	29										
		1	1	1	2	2	3	1	3	1	1
4	29										
		1	1	1	2	2	3	1	3	1	2
5	29										
		1	1	1	2	2	2	2	3	1	1
6	29										
		1	1	1	2	2	2	2	3	1	2
7	29										
		1	1	2	4	2	4	2	3	1	1

Fig. 7. Information obtained for Example #2, Output #2.

8	29	1	1	2	4	2	4	2	3	1	2
9	29	1	1	2	3	3	4	2	3	1	1
10	29	1	1	2	3	3	4	2	3	1	2
11	29	1	1	2	3	3	3	3	3	1	1
12	29	1	1	2	3	3	3	3	3	1	2
15	29	1	1	4	6	2	6	2	3	1	1
26	29	1	1	2	3	3	4	2	2	2	1

295	29	3	3	3	7	2	7	2	8	1	1
297	29	3	3	3	5	4	7	2	8	1	1
317	29	3	3	3	5	4	5	4	7	2	2
TCCL = 91											

A	B	C	COS ALPHA	COS BETA	COS GAMMA	CELL NO.
17.87040	17.87040	17.87040	-.32195	-.32195	-.32195	1
17.37349	17.37349	37.87182	-0.00000	-.22937	-.50000	2
17.64656	17.64656	18.24140	-.30749	-.37956	-.28978	3
17.64656	17.64656	18.24140	-.30749	-.37956	-.28978	4
14.90423	16.89182	16.89182	-.47194	-0.00000	0.00000	5
14.90423	16.89182	16.89182	-.47194	0.00000	0.00000	6
12.18745	17.37922	17.37922	-.37507	-.25289	-.25289	7
16.36883	16.91450	16.91450	-.47385	0.00000	0.00000	8
12.11107	17.29602	17.29603	-.39692	-.22312	-.22312	9
12.11107	17.29602	17.29603	-.39692	-.22312	-.22312	10
10.83218	16.90653	16.90653	-.47317	-0.00000	-0.00000	11
10.83218	16.90653	16.90653	-.47317	0.00000	0.00000	12
17.26274	17.26274	28.40929	-.20683	-.20683	-.40546	15
11.77231	14.84941	15.92289	0.00000	.34483	0.00000	26
11.77231	14.84941	15.92289	0.00000	.34483	0.00000	27
10.83355	14.90370	14.90370	-0.00000	-0.00000	-0.00000	28
10.83355	14.90370	14.90370	-0.00000	-0.00000	-0.00000	29
11.99576	11.99576	16.72406	-.32559	-.26632	-.17478	39
11.99576	11.99576	16.72406	-.32559	-.26632	-.17478	40
10.84276	11.72833	15.79162	.34083	0.00000	0.00000	41
10.84276	11.72833	15.79162	-.34083	-0.00000	-0.00000	42
12.09233	17.55899	17.82449	-.38831	-.24423	-.24723	43

Fig. 7. (Continued)

12.09233	17.55899	17.82449	-.38831	-.24423	-.24723	44
11.61782	11.86083	16.68779	-.30031	-.28549	-.12091	45
11.61782	11.86083	16.68779	-.30031	-.28549	-.12091	46
13.71831	15.95203	16.75585	.20448	.24176	.32992	47
13.33618	15.97638	23.06172	.19762	.04460	.30465	48
12.66437	14.33679	16.09912	-.16506	-.26370	-.36935	49
11.80230	13.33926	16.50280	-.27380	-.33326	-.01816	50
11.82919	11.98450	16.49989	-.26922	-.30288	-.10735	51
11.83165	15.92727	16.68448	-.03193	-.07043	-.35085	58
11.83165	15.92727	16.68448	-.03193	-.07043	-.35085	59
10.86915	10.86915	14.87959	-0.00000	-0.00000	-0.00000	66
10.86915	10.86915	14.87959	-0.00000	-0.00000	-0.00000	67
10.84399	14.69584	14.82987	0.00000	0.00000	.00254	68
10.84399	14.69584	14.82987	0.00000	0.00000	.00254	69
13.65408	18.52710	22.51563	.18138	.03212	.36548	74
13.65408	18.52710	22.51563	.18138	.03212	.36548	75
13.26362	13.86299	15.90505	-.22012	-.20345	-.28165	76
13.26362	13.86299	15.90505	-.22012	-.20345	-.28165	77
11.27112	11.95791	15.89165	.35802	.10060	.27064	78
11.27112	11.95791	15.89165	.35802	.10060	.27064	79
5.57507	10.92244	15.09135	.02078	.17729	.11491	82
5.57507	10.92244	15.09135	.02078	.17729	.11491	83
5.42377	10.87281	14.87353	-0.00000	-0.00000	-0.00000	92
5.42377	10.87281	14.87353	-0.00000	-0.00000	-0.00000	93
12.51082	13.30328	16.32047	.29602	.28159	.07968	102
12.51082	13.30328	16.32047	.29602	.28159	.07968	103
5.71429	13.47607	15.64996	.30561	.09554	.16298	117
5.71429	13.47607	15.64996	.30561	.09554	.16298	118
5.38444	13.36719	15.59119	.29912	0.00000	0.00000	119
5.38444	13.36719	15.59119	-.29912	-0.00000	-0.00000	120
11.70329	11.70329	16.75487	-.27387	-.33198	-.13264	131
11.70329	11.70329	16.75487	-.33198	-.27387	-.13264	132
10.80266	10.80266	31.79234	-0.00000	-0.00000	-0.00000	133
10.80266	10.80266	31.79234	-0.00000	-0.00000	-0.00000	134
10.88224	11.48282	14.36424	.31961	0.00000	0.00000	136
10.88224	11.48282	14.36424	.31961	0.00000	0.00000	137
11.03958	11.91507	17.74691	-.23649	-.14894	-.07496	141
11.03958	11.91507	17.74691	-.23649	-.14894	-.07496	142
10.83640	16.49952	16.49952	-.44422	-.00066	-.00066	170
10.81429	14.73437	14.73437	-.00127	-.00817	-.00817	171
10.84261	16.51496	16.51496	.44542	.00579	.00579	172
10.88536	14.87173	50.62840	.14687	.05673	0.00000	173
11.42362	14.81068	14.86200	.10843	.31603	.04032	174
11.26334	11.78848	15.70710	.35147	.08769	.25717	175
11.30600	11.97756	15.75748	.37566	.09370	.26401	177
10.85365	10.94247	15.72636	.33808	.00020	.00207	178
10.94357	13.91839	15.35085	.25957	.04899	.14418	179
8.67955	11.07252	14.79519	.00635	.01847	.20147	180
8.14240	11.55767	15.20597	.09306	.25132	.34211	181
11.33908	12.41797	15.60815	.32825	.10029	.27627	182
6.03107	11.28869	14.70583	.00458	.01967	.26640	188
6.03107	11.28869	14.70583	.00458	.01967	.26640	189
5.47833	10.94793	14.70173	.00554	.01805	.12335	191
5.79875	10.94668	14.74545	.01480	.03572	.11689	192
5.53568	10.92827	14.97635	.01946	.15786	.11753	193
5.53568	10.92827	14.97635	.01946	.15786	.11753	194
5.42919	10.86348	14.84258	-0.00000	-0.00000	-0.00000	198
5.42919	10.86348	14.84258	-0.00000	-0.00000	-0.00000	199
11.29707	12.05104	15.23724	.39545	.10348	.26168	200
11.13665	11.52980	12.88940	-.21648	-.12674	-.21413	208
11.23498	11.78350	17.57654	.32160	.08217	.26549	209
11.10319	12.48997	18.30543	.18919	.06579	.26588	217
10.83961	10.84453	16.41949	.33023	0.00000	0.00000	227
11.11443	11.62930	14.83674	-.10446	-.17474	-.09333	242
10.36891	15.06431	15.06431	.33100	.19527	.19527	293
14.91916	21.42936	21.86582	.12032	.34115	0.00000	294
9.83622	12.00607	15.38179	-.28208	-.18768	-.33837	295
11.13385	11.53118	14.90626	.32399	.17927	.32194	297
9.63879	11.65188	13.01141	-.12630	-0.00000	-.41362	317

Fig. 7. (Continued)

POWDER PATTERN FOR PU-ZR THETA COMPOUND

45 0 .00150 1.04000 10 1 90 60 63

1	.0180
2	.0340
3	.0463
4	.0514
5	.0724
6	.0829
7	.1138
8	.1357
9	.1484
10	.1506
11	.1532
12	.1556
13	.1625
14	.1692
15	.1736
16	.1806
17	.1973
18	.2100
19	.2169
20	.2298
21	.2393
22	.2498
23	.2652
24	.2713
25	.3239
26	.3436
27	.4221
28	.4277
29	.4357
30	.4529
31	.4608
32	.4871
33	.5447
34	.5952
35	.6057
36	.6142
37	.6250
38	.6622
39	.6807
40	.6954
41	.7072
42	.7241
43	.9709
44	1.0020
45	1.0309

1 45

MG EXCEEDS 2000. REDUCE QMAX OR C.

3 45

4 45

5 45

6 45

7 45

8 45

9 45

10 45

Fig. 8. Information obtained for Example #2, Output #3.

11	44		
12	45		
13	45		
14	45		
15	45		
16	45		
17	45		
18	45		
19	45		
20	45		
21	45		
22	43		
23	45		
24	45		
25	45		
26	45		
27	45		
28	45		
29	45		
30	45		
31	45		
32	44		
33	45		
34	45		
35	45		
36	45		
37	45		
38	45		
MG EXCEEDS 2000. REDUCE QMAX OR C.			
40	45		
41	45		
42	45		
43	45		
44	45		
45	45		
		46	45
		47	45
		48	44
		49	45
		50	45
		51	45
		52	45
		53	45
		54	45
		55	44
		56	45
		57	44
		58	45
		59	45
		60	45
		61	45
		62	45
		63	45
		TCEL = 61	
		LINES NOT INDEXED FOR	1
		LINES NOT INDEXED FOR	3
		LINES NOT INDEXED FOR	4
		LINES NOT INDEXED FOR	5
		LINES NOT INDEXED FOR	6
		LINES NOT INDEXED FOR	7
		LINES NOT INDEXED FOR	8
		LINES NOT INDEXED FOR	9
		LINES NOT INDEXED FOR	10
		LINES NOT INDEXED FOR	11
			6
		LINES NOT INDEXED FOR	12

Fig. 8. (Continued)

LINES NOT INDEXED FOR 13
 LINES NOT INDEXED FOR 14
 LINES NOT INDEXED FOR 15
 LINES NOT INDEXED FOR 16
 LINES NOT INDEXED FOR 17
 LINES NOT INDEXED FOR 18
 LINES NOT INDEXED FOR 19
 LINES NOT INDEXED FOR 20
 LINES NOT INDEXED FOR 21
 LINES NOT INDEXED FOR 22
 29
 41
 LINES NOT INDEXED FOR 23
 LINES NOT INDEXED FOR 24
 LINES NOT INDEXED FOR 25
 LINES NOT INDEXED FOR 26
 LINES NOT INDEXED FOR 27
 LINES NOT INDEXED FOR 28
 LINES NOT INDEXED FOR 29
 LINES NOT INDEXED FOR 30
 LINES NOT INDEXED FOR 31
 LINES NOT INDEXED FOR 32
 22
 LINES NOT INDEXED FOR 33
 LINES NOT INDEXED FOR 34
 LINES NOT INDEXED FOR 35

LINES NOT INDEXED FOR 36
 LINES NOT INDEXED FOR 37
 LINES NOT INDEXED FOR 38
 LINES NOT INDEXED FOR 39
 LINES NOT INDEXED FOR 40
 LINES NOT INDEXED FOR 41
 LINES NOT INDEXED FOR 42
 LINES NOT INDEXED FOR 43
 LINES NOT INDEXED FOR 44
 LINES NOT INDEXED FOR 45
 LINES NOT INDEXED FOR 46
 LINES NOT INDEXED FOR 47
 LINES NOT INDEXED FOR 48
 14
 LINES NOT INDEXED FOR 49
 LINES NOT INDEXED FOR 50
 LINES NOT INDEXED FOR 51
 LINES NOT INDEXED FOR 52
 LINES NOT INDEXED FOR 53
 LINES NOT INDEXED FOR 54
 LINES NOT INDEXED FOR 55
 1
 LINES NOT INDEXED FOR 56
 LINES NOT INDEXED FOR 57
 6
 LINES NOT INDEXED FOR 58
 LINES NOT INDEXED FOR 59

Fig. 8. (Continued)

LINEs NOT INDEXED FOR 60

LINEs NOT INDEXED FOR 62

LINEs NOT INDEXED FOR 61

LINEs NOT INDEXED FOR 63

A	B	C	COS ALPHA	COS BETA	COS GAMMA	CELL NO.
17.88028	17.88028	17.88028	-.32166	-.32166	-.32166	1
17.64486	17.64486	18.24198	-.37936	-.30758	-.28981	3
14.90355	16.88811	16.88811	-.47120	-0.00000	-0.00000	4
12.19891	17.36751	17.36751	-.37429	-.25384	-.25384	5
16.37395	16.90629	16.90629	.47432	0.00000	0.00000	6
12.11225	17.29214	17.29214	-.39646	-.22328	-.22328	7
10.83306	16.90833	16.90833	-.47361	-0.00000	-0.00000	8
17.26481	17.26481	27.49017	-.15980	-.15980	-.40498	9
11.77217	14.84745	15.92282	0.00000	.34485	0.00000	10
10.83897	14.90318	14.90318	-0.00000	-0.00000	-0.00000	11
11.99211	11.99211	16.71635	-.26626	-.32494	-.17590	12
10.84310	11.73908	15.79666	.34010	0.00000	0.00000	13
12.08420	17.56642	17.84011	-.38872	-.24418	-.24751	14
11.61814	11.85239	16.68016	-.30010	-.28521	-.11963	15
13.72103	15.95815	16.75386	.20362	.24209	.32994	16
13.33263	15.97573	23.06604	.19752	.04400	.30449	17
12.65814	14.34175	16.10506	-.16449	-.26338	-.36895	18
11.79287	13.35225	16.49310	-.27369	-.33216	-.01900	19
11.84173	11.98192	16.49818	-.26961	-.30213	-.10883	20
11.83458	15.92288	16.68511	-.03199	-.06862	-.35066	21
10.86783	10.86783	14.87179	-0.00000	-0.00000	-0.00000	22
10.84933	14.68082	14.83981	0.00000	0.00000	.00112	23
13.65175	18.53332	22.51185	.18181	.03202	.36657	24
13.26082	13.86410	15.88892	-.21864	-.20336	-.28198	25
11.26956	11.95597	15.90153	.35905	.10168	.26978	26
5.57534	10.92082	15.08565	.02059	.17806	.11586	27
5.42685	10.87757	14.83337	-0.00000	-0.00000	-0.00000	28
12.51752	13.30655	16.31829	.29495	.28329	.07967	29
5.71686	13.47794	15.64078	.30612	.09479	.16218	30
5.38821	13.37624	15.58576	.29875	0.00000	0.00000	31
11.70028	11.70028	16.74276	-.27334	-.33334	-.13187	32
10.80266	10.80266	31.79234	-0.00000	-0.00000	-0.00000	33
10.88333	11.47391	14.36459	.31797	0.00000	0.00000	34
11.03977	11.90996	17.73695	-.23623	-.14955	-.07427	35
10.83883	16.49322	16.49322	-.44379	-.00040	-.00040	36
10.81735	14.73050	14.73050	-.01212	-.00932	-.00932	37
10.83186	16.51514	16.51514	.44545	.00581	.00581	38
11.43226	14.81270	14.86551	.10884	.31670	.04032	40
11.26449	11.78230	15.70004	.35175	.08791	.25705	41
11.30764	11.98235	15.76739	.37508	.09515	.26414	42
10.85717	10.94590	15.72479	.33893	.00019	.00027	43
10.94602	13.92376	15.34563	.25913	.04861	.14297	44
8.67950	11.07545	14.80117	.00538	.01800	.19998	45
8.13998	11.55747	15.20384	.09324	.25160	.34062	46
11.33734	12.42115	15.61254	.32808	.09868	.27626	47
6.03560	11.29041	14.69541	.00445	.01878	.26678	48
5.47339	10.93875	14.71209	.00545	.01560	.12385	49
5.80278	10.94904	14.72963	.01536	.03578	.11737	50
5.53832	10.92796	14.98738	.01850	.15848	.11728	51
5.42898	10.86392	14.83869	-0.00000	-0.00000	-0.00000	52
11.30673	12.05246	15.23679	.39551	.10387	.26264	53
11.14407	11.52865	12.88762	-.21666	-.12696	-.21500	54
11.23269	11.78152	17.57791	.32130	.08308	.26619	55
11.10819	12.48964	18.30192	.18939	.06678	.26671	56
10.83192	10.83538	16.41961	.32995	0.00000	0.00000	57
11.12581	11.62831	14.83861	-.10386	-.17461	-.09441	58
10.37390	15.05967	15.05967	.33099	.19384	.19384	59
14.92062	21.42387	21.86821	.12021	.34115	0.00000	60
9.83763	12.00526	15.37646	-.28203	-.18767	-.33870	61
11.12725	11.53152	14.91479	.32434	.17901	.32216	62
9.63457	11.65249	13.00760	-.12707	-0.00000	-.41341	63

Fig. 8. (Continued)

sured as accurately as possible. Specifically, they should be corrected for the effects of absorption, or else erroneous results may be obtained.

The list of observed Q values should be examined for higher order reflections that may be used to revise first-order lines as illustrated in Example #1. If first-order lines are not present, their positions may have to be inferred through the stratagem of assuming second- (or higher) order lines as illustrated in Example #2. Other techniques such as searching for common differences (the Hesse-Lipson method) or quick graphical methods for higher symmetries may be helpful.

It may be necessary to employ considerable ingenuity to imply enough first-order lines so that a satisfactory cell can be obtained. The current program allows the experimenter to try a number of possibilities in quite rapid succession.

Limitations on the quantity of data that may be handled by the program are

Q = 100 observed values
ESPQ = 1000 generated values
hkl = 2000 generated triplets
QMAX = 2.00

FORTTRAN IV LISTING OF PROGRAM

The following pages contain the FORTTRAN IV listing of the program described in this report. The

first two lines of the listing define the program name and the various files necessary to run INDX on a Control Data Corporation 6600 computer using a Scope System Version 3.00 compiler. For an IBM 7094 series computer, the first two lines may be either eliminated or handled as comment cards by punching C in column 1. The compiler must be compatible with FORTTRAN IV, and two temporary storage tapes (Tape 7 and Tape 8) must be provided.

ISS (Linear System Solver) and SORT1, two sub-routines used for the solution of a 6 x 7 matrix and the sorting and arranging of a list of numbers from smallest to largest, must also be provided. ISS is labeled IA-FD04 and SORT1 is labeled IA-MA01 in the SHARE library.

REFERENCES

1. L. V. Azaroff and M. J. Buerger, The Powder Method in Crystallography, McGraw-Hill Book Company, Inc., New York, (1958), Chapter 11, pp. 124-159.
2. H. M. Haendler and W. A. Cooney, Acta Cryst. **16**, 1243 (1963).
3. J. P. Marples, J. Less-Common Metals **2**, 331 (1960).
4. A. F. Berndt, J. Less-Common Metals **12**, 82 (1967).
5. W. H. Zachariasen, private communication (1967).


```

PROGRAM INDX(INPUT,TAPE10=INPUT,OUTPUT,TAPE9=OUTPUT,TAPE7,TAPE8,
1PUNCH)
000003   DIMENSION NAME(12),Q(100),D(100),I1(1000),I2(1000),I3(1000),
1I4(1000),LT(100),TH(2000),TK(2000),TL(2000),X(6,6),RMAT(6,7),
2PD(6),TE(2000),TSQ(62),UT(62),VT(62),WT(62),TEMP(124),ISON(900),
3LM(100),NQTAB(20000)
000003   COMMON M,N,C,QMAX,Z,M1,DET,Z3,Z4,I1,I2,I3,I4,
1IA1,IA2,IA3,IA4,IA5,IA6,IA7,IA8,IA9
000003   1 FORMAT(12A6)
000003   2 FORMAT(2I5,2F10.5,F5.0,I5,2F5.0,I5)
000003   3 FORMAT(F10.5)
000003   4 FORMAT(I5,F10.4)
000003   5 FORMAT(1H0,39HEVENLY SPACED PAIRS OF Q=S EXCEEDS 1000)
000003   6 FORMAT(1H0,7HESPO =I7)
000003   7 FORMAT(1H0,7HNICQ =I7)
000003   8 FORMAT(1H0,7HPCEL =I7,/)
000003   9 FORMAT(1H0,7HTCEL =I7)
000003  10 FORMAT(1H0,6X,1HA,9X,1HB,9X,1HC,4X,9HCOS ALPHA,2X,8HCOS BETA,1X,9H
1COS GAMMA,4X,8HCELL NO.,/)
000003  11 FORMAT(6F10.5,I10)
000003  12 FORMAT(10X,I5)
000003  21 FORMAT(1H1,12A6,/)
000003  22 FORMAT(2I5,2F10.5,5I5,/)
000003  32 FORMAT(1H0,2I5)
000003  92 FORMAT(1H0,21HLINES NOT INDEXED FOR,I5,/)
000003  98 FORMAT(1H0,35HMG EXCEEDS 2000. REDUCE QMAX OR C.)
000003  99 FORMAT(1H0,10X,10I5)
000003 100 READ(10,1)NAME
000011   IF(EOF,10)101,102
000014 101 STOP
000016 102 READ(10,2)M,N,C,QMAX,Z,M1,Z3,Z4,L2
000044   WRITE(9,21)NAME
000052   MZ=Z
000054   M2=Z3
000055   M3=Z4
000057   WRITE(9,22)M,N,C,QMAX,MZ,M1,M2,M3,L2
000104   IS1=0
000105   IS12=0
000106   I61=0
000107   ZERO = 0.0
000110   DO 110 I=1,M
000111     READ(10,3)Q(I)
000116 110 WRITE(9,4)I,Q(I)
000131     IM=20000.
000132     IC=C*5000.,.5
000136     DO 103 I=1,IM
000137 103 NQTAB(I)=0
000143     DO 105 I=1,M
000144       NQ=Q(I)*10000.,.5
000150       INQ=NQ-IC
000152       INQ1=NQ+IC
000153       DO 104 J=INQ,INQ1
000155 104 NQTAB(J)=I
000161 105 CONTINUE
000163   IF(L2)119,119,111
000165 111 REWIND 7
000167   DO 112 I=1,L2
000171     READ(10,11)RA,RB,RC,CFAS,CFBS,CFGs,I8
000212     CON=(1.0+2.0*CFAS*CFBS*CFGs-CFAS**2-CFBS**2-CFGs**2)
000225     VOL1=RA*RB*RC*SQRT(CON)
000232 112 WRITE(7)RA,RB,RC,CFAS,CFBS,CFGs,VOL1,I8
000260     I61=1
000261     MF=L2
000262     GO TO 500
000262 113 I61=0
000263     IS12=1
000264     IS1=-1
000265     ME=L2
000267     REWIND 7
000271     REWIND 8
000273     GO TO 411

```

```

000274 119 MA=0
000275 DO 150 I=1,N
000277 DO 141 J=I,N
000300 E=Q(I)+Q(J)
000303 IF(E-Q(M))121,121,150
000306 121 E1=2.0*SQRT(Q(I)*Q(J))
000315 K=1
000316 LO=1
000317 DO 120 L=1,M
000320 LM(K)=L
000322 D(K)=E-Q(L)
000324 IF(D(K).GT.0.0)LO=K
000327 IF((D(K)+E1).LT.0.0)GO TO 122
000332 120 IF(D(K).LE.E1)K=K+1
000341 122 LB=LO+1
000343 K=K-1
000344 DO 140 L=1,LB
000346 LO=MAX0(LO,L)
000351 DO 139 LA=LO,K
000352 E2=D(L)+D(LA)
000355 IF(E2-C)140,130,126
000357 126 IF(E2-C)130,130,139
000362 130 MA=MA+1
000364 I1(MA)=I
000366 I2(MA)=J
000367 I3(MA)=LM(L)
000371 I4(MA)=LM(LA)
000373 IF(MA-1000)139,139,142
000375 139 CONTINUE
000400 140 CONTINUE
000403 141 CONTINUE
000405 150 CONTINUE
000410 GO TO 200
000410 142 WRITE(9,5)
000414 GO TO 100
000415 200 WRITE(9,6)MA
000423 IF(MA)701,701,201
000425 201 REWIND 7
000427 MB=0
000430 II=1
000431 DO 300 J=1,MA
000433 IA1=I1(J)
000435 IA2=I2(J)
000436 IA3=I3(J)
000440 IA4=I4(J)
000441 DO 299 K=J,MA
000442 IF(IA1-I1(K))299,214,299
000444 214 IA5=I2(K)
000446 IA6=I3(K)
000450 IA7=I4(K)
000451 DO 298 L=K,MA
000452 IF(IA2-I1(L))298,220,298
000454 220 IF(IA5-I2(L))298,230,298
000457 230 IA8=I3(L)
000461 IA9=I4(L)
000463 ISON(II)=IA1
000465 ISON(II+1)=IA2
000466 ISON(II+2)=IA5
000470 ISON(II+3)=IA4
000471 ISON(II+4)=IA3
000473 ISON(II+5)=IA7
000474 ISON(II+6)=IA6
000476 ISON(II+7)=IA9
000477 ISON(II+8)=IA8
000501 IF(II-A92)232,231,232
000502 231 WRITE(7)ISON
000507 II=1
000510 GO TO 233
000511 232 II=II+9
000513 233 MB=MB+1
000515 298 CONTINUE

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000520 299 CONTINUE
000523 300 CONTINUE
000525     IF (MOD(MB,100)) 301,302,301
000531 301 WRITE(7) ISON
000536 302 WRITE(9,7) MB
000544     IF (MB) 701,701,303
000546 303 REWIND 7
000550     REWIND 8
000552     ME=0
000553     II=1
000554     DO 400 I=1,MB
000556     IF (II=9) 311,311,312
000560 311 READ(7) ISON
000565 312 IF (II=900) 313,315,315
000570 315 II=1
000571     GO TO 311
000572 313 IA1=ISON(II)
000574     IA2=ISON(II+1)
000576     IA5=ISON(II+2)
000577     IA4=ISON(II+3)
000601     IA3=ISON(II+4)
000602     IA7=ISON(II+5)
000604     IA6=ISON(II+6)
000605     IA9=ISON(II+7)
000607     IA8=ISON(II+8)
000610     II=II+9
000611 340 MC=1
000612     RA=SQRT(Q(IA1))
000615     RB=SQRT(Q(IA2))
000620     RC=SQRT(Q(IA5))
000623     GG=Q(IA4)-Q(IA3)
000626     BB=Q(IA7)-Q(IA6)
000631     AA=Q(IA9)-Q(IA8)
000634     CFAS=0.25*AA/(RB*RC)
000637     CFBS=0.25*BB/(RC*RA)
000642     CFGS=0.25*GG/(RA*RB)
000644 330 IF (ABS(CFAS)-0.99) 331,331,400
000650 331 IF (ABS(CFBS)-0.99) 332,332,400
000654 332 IF (ABS(CFGS)-0.99) 367,367,400
000660 367 WRITE(8) RA,RB,RC,CFAS,CFBS,CFGS,
    1 IA1,IA2,IA5,IA9,IA8,IA7,IA6,IA4,IA3,MC
000723     ME=ME+1
000725 370 IF (MC=2) 382,400,400
000730 382 CFAS=-CFAS
000731     CFBS=-CFBS
000732     CFGS=-CFGS
000733     AS=ACOS(CFAS)
000736     BS=ACOS(CFBS)
000740     GS=ACOS(CFGS)
000742     AS=AS*57.2957795
000743     BS=BS*57.2957795
000744     GS=GS*57.2957795
000745     IF ((AS+BS+GS)-357.0) 381,400,400
000751 381 MC=MC+1
000753     GO TO 330
000753 400 CONTINUE
000756     WRITE(9,8) ME
000763     IF (ME) 701,701,410
000765 410 REWIND 7
000767     REWIND 8
000771 411 MF=0
000772     Z1=FLOAT(M)*Z4/100.0
000775     Z5=FLOAT(M)*Z3/100.0
001000     L11=INT(FLOAT(M)-Z1)
001004     DO 490 I5=1,ME
001006     IF (I5) 445,443,444
001007 444 READ(7) RA,RB,RC,CFAS,CFBS,CFGS,VOL,IA
001032     GO TO 407
001033 443 READ(8) RA,RB,RC,CFAS,CFBS,CFGS,
    1 IA1,IA2,IA5,IA9,IA8,IA7,IA6,IA4,IA3,MC
001076     GO TO 446

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001077 445 READ(8)RA, RB, RC, CFAS, CFBS, CFGS, I8
001120 446 NC=M1
001122 401 CYCLE=Z
001124 407 DO 402 J1=1, M
001126 LT(J1)=0
001127 402 CONTINUE
001131 L1=0
001132 J2=1
001133 L=0
001134 MG=0
001135 TGS=1.0-CFGS**2
001137 IF(TGS)490,480,480
001140 480 SFGS=SQRT(TGS)
001143 TBS=1.0-CFBS**2
001145 IF(TBS)490,481,481
001146 481 SFBS=SQRT(TBS)
001151 CFA=(CFBS*CFGS-CFAS)/(SFBS*SFGS)
001155 IF(ABS(CFA)=.99)412,412,490
001160 412 SFA=SQRT(1.0-CFA**2)
001165 C11=RA
001166 C12=RB*CFGS
001170 C13=RC*CFBS
001172 C14=RB*SFGS
001174 C15=RC*SFBS*CFA
001176 C16=RC*SFA*SFBS
001177 C60=2.0*C11
001201 C61=-2.0*C14
001203 C21=C14**2
001204 C35=C11**2
001205 C62=2.0*C21
001207 C63=2.0*C62
001210 C64=2.0*C35
001211 C65=2.0*C64
001212 XL=0.0
001213 GO TO 404
001213 403 XL=XL+1.0
001215 404 QC=(XL*C16)**2
001217 IF(QC-QMAX)405,420,420
001222 405 IF(QC)415,415,423
001224 423 J3=J2+1
001226 DO 425 J2=.12, M
001227 IF(Q(J2)-QC+C)425,425,426
001233 425 CONTINUE
001236 426 IF(J3.GT.J2)GO TO 415
001242 DO 428 I=J3, J2
001243 IF(LT(I-1))429,429,428
001245 429 L1 = L1+1
001247 428 CONTINUE
001252 IF(L1-L11)415,415,490
001254 415 C40=XL*C13
001256 C41=C60*C40
001260 C42=C40**2
001261 C20=XL*C15
001262 C22=C61*C20
001264 C23=C20**2-QMAX+QC
001267 C24=C22**2
001270 C25=C63*C23
001272 C27=SQRT(C24-C25)
001277 BMIN=(-C22-C27)/C62
001302 BMAX=(-C22+C27)/C62
001303 XKMIN=AINT(BMIN)
001305 XKMAX=AINT(BMAX)
001307 NKROW=XKMAX-XKMIN
001312 IF(NKROW)420,420,406
001313 406 IF(XL)453,453,455
001315 453 XK=0.0
001316 GO TO 456
001317 455 XK=XKMIN
001321 456 QBC=QC+(XK*C14-C20)**2
001325 C30=XK*C12
001327 C31=C60*C30

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001330      C32=C30**2
001331      C36=C31+C41
001333      C45=2.0*C30*C40
001335      C37=C32+C42+C45-QMAX+QBC
001342      C50=C36**2
001344      C51=C65*C37
001346      C52=C50-C51
001350      IF (C52) 457,450,450
001351  450  C53=SQRT(C52)
001354      AMIN=(-C36-C53)/C64
001357      AMAX=(-C36+C53)/C64
001360      XHMIN=AIN(T(AMIN))
001362      XHMAX=AIN(T(AMAX))
001364      NHROW=XHMAX-XHMIN
001367      IF (NHROW) 457,457,458
001370  457  XK=XK+1.0
001372      IF (XK-XKMAX) 456,456,403
001375  458  IF (QBC) 459,459,460
001377  459  XH=1.0
001401      GO TO 461
001401  460  XH=XHMIN
001403  461  GHKL=QBC*(XH*C11+C30+C40)**2
001411      NQHKL=(GHKL+0.00005)*10000.
001414      MD=0
001415      J1=0
001416      I10=NQHKL-IC
001420      I11=NQHKL+IC
001421      IF (I10) 470,470,469
001422  469  IF (NQTAB(I10),NE,0) 471,470
001427  470  IF (NQTAB(I11),NE,0) 472,413
001434  471  J1=NQTAB(I10)
001436      GO TO 473
001437  472  J2=NQTAB(I11)
001441      IF (J2-J1) 475,413,475
001443  475  J1=J2
001445  473  E=Q(J1)-GHKL
001450      MG=MG+1
001451      TE(MG)=E
001453      TH(MG)=XH
001455      TK(MG)=XK
001456      TL(MG)=XL
001460      IF (MG-2000) 408,408,409
001462  409  WRITE(9,98)
001466      GO TO 490
001467  408  IF (LT(J1)) 417,417,414
001471  417  LT(J1)=1
001473  414  MD=MD+1
001475      IF (MD-2) 470,413,413
001477  413  CONTINUE
001477  418  XH=XH+1.0
001501      IF (XH-XHMAX) 461,461,457
001504  420  CONTINUE
001504      IF (I51) 424,424,499
001506  424  DO 422 I=1,M
001510      IF (LT(I)) 422,422,421
001512  421  L=L+1
001514  422  CONTINUE
001517      Z2=FLOAT(L)
001520      IF (Z2-Z1) 490,430,430
001523  430  IF (CYCLE) 440,440,431
001525  431  DO 432 I=1,6
001527      RMAT(I,1)=0.0
001530      DO 432 J=1,6
001532  432  X(I,J)=0.0
001542      XX1=2.0*RA
001544      XX4=2.0*RB
001545      XX7=2.0*RC
001547      XX2=XX4*CFGS
001551      XX3=XX7*CFBS
001553      XX5=XX1*CFGS
001554      XX6=XX7*CFAS

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001556      XX8=XX1*CFBS
001557      XX9=XX4*CFAS
001560      XX10=XX4*RC
001562      XX11=XX7*RA
001564      XX12=XX1*RB
001566      DO 435 I=1,MG
001567          YY1=TH(I)**2
001571          YY2=TK(I)**2
001572          YY3=TL(I)**2
001574          YY4=TH(I)*TK(I)
001576          YY5=TH(I)*TL(I)
001600          YY6=TK(I)*TL(I)
001602          PD(1)=XX1*YY1+XX2*YY4+XX3*YY5
001610          PD(2)=XX4*YY2+XX5*YY4+XX6*YY6
001616          PD(3)=XX7*YY3+XX8*YY5+XX9*YY6
001624          PD(4)=XX10*YY6
001625          PD(5)=XX11*YY5
001627          PD(6)=XX12*YY4
001631          DO 433 J=1,6
001632              RMAT(J,1)=RMAT(J,1)+PD(J)*TE(I)
001636          DO 433 K=1,6
001637      433 X(J,K)=X(J,K)+PD(J)*PD(K)
001652      435 CONTINUE
001654          CALL LSS(6,1,6,X,RMAT,0,DET)
001663          DO 437 J=1,6
001665          IF(ABS(RMAT(J,1)).GT.0.00001)GO TO 436
001672      437 CONTINUE
001673          NC=0
001674          GO TO 441
001675      436 RA=RA+RMAT(1,1)
001677          RB=RB+RMAT(2,1)
001701          RC=RC+RMAT(3,1)
001703          CFAS=CFAS+RMAT(4,1)
001705          CFBS=CFBS+RMAT(5,1)
001707          CFGS=CFGS+RMAT(6,1)
001711          CYCLE=CYCLE-1.0
001713          GO TO 407
001714      440 NC=NC-1
001716      441 IF(Z2-Z5)452,482,482
001721      452 IF(NC)490,490,401
001723      482 CON=(1.0+2.0*CFAS*CFBS*CFGS-CFAS**2-CFBS**2-CFGS**2)
001736          VOL=RA*RB*RC*SQRT(CON)
001743          WRITE(7)RA,RB,RC,CFAS,CFBS,CFGS,VOL,IS
001766          WRITE(9,32)IS,L
001776          IF(IS12)483,483,484
002000      483 WRITE(9,99)IA1,IA2,IA5,IA9,IA8,IA7,IA6,IA4,IA3,MC
002030      484 MF=MF+1
002032      490 CONTINUE
002035          IF(IS1)491,491,485
002036      485 MF=ME
002040          GO TO 500
002040      491 WRITE(9,9)MF
002046          IF(MF)701,701,494
002050      494 REWIND 7
002052          REWIND 8
002054          IF(IS12)500,500,496
002056      496 IS1=1
002057          ME=MF
002061          GO TO 411
002061      499 WRITE(9,92)IS
002067          DO 498 I=1,M
002071          IF(LT(I))497,497,498
002073      497 WRITE(9,12)I
002101      498 CONTINUE
002104          GO TO 490
002104      500 REWIND 8
002106          REWIND 7
002110          DO 600 I=1,MF
002112          READ(7)A1,B1,C1,CFA1,CFB1,CFG1,VOL1,IS
002135          AT=ACOS(CFA1)
002140          BT=ACOS(CFB1)

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002142      GT=ACOS(CFG1)
002144      SFA1=SIN(AT)
002146      SFB1=SIN(BT)
002150      SFG1=SIN(GT)
002152      VOL2=1.0/VOL1
002154      A2=B1*C1*SFA1*VOL2
002157      B2=C1*A1*SFB1*VOL2
002162      C2=A1*B1*SFG1*VOL2
002164      CFA2=(CFB1*CFG1-CFA1)/(SFB1*SFG1)
002170      CFB2=(CFG1*CFA1-CFB1)/(SFG1*SFA1)
002173      CFG2=(CFA1*CFB1-CFG1)/(SFA1*SFB1)
002176      WRITE(8)A2,B2,C2,CFA2,CFB2,CFG2,IS
002217      600 CONTINUE
002222      IF(I61)604,604,113
002223      604 REWIND 8
002225      WRITE(9,10)
002231      DO 700 I7=1,MF
002233      READ(8)A2,B2,C2,CFA2,CFB2,CFG2,IS
002254      L=0
002255      X1=A2**2
002257      X2=B2**2
002260      X3=C2**2
002262      X4=2.0*A2*B2*CFG2
002264      X5=2.0*B2*C2*CFA2
002266      X6=2.0*C2*A2*CFB2
002271      U1=+3.0
002272      V1=+3.0
002273      W1=+3.0
002274      U=U1
002275      DO 612 I=1,5
002277      U=U-1.0
002301      V=V1
002303      DO 611 J=1,5
002304      V=V-1.0
002306      W=W1
002310      DO 610 K=1,5
002311      W=W-1.0
002313      IF(W)601,602,603
002314      601 IF(V)610,610,613
002316      613 IF(U)610,610,607
002320      602 IF(V)614,614,608
002322      614 IF(U)610,610,607
002324      608 IF(U)610,607,607
002326      603 IF(V)609,607,607
002330      609 IF(U)610,607,607
002332      607 L=L+1
002334      TSQ(L)=U**2*X1+V**2*X2+W**2*X3+U*V*X4+V*W*X5+W*U*X6
002351      UT(L)=U
002353      VT(L)=V
002354      WT(L)=W
002356      610 CONTINUE
002360      611 CONTINUE
002362      612 CONTINUE
002364      CALL SORT1(62,3,TSQ(1),TEMP(1),UT(1),VT(1),WT(1))
002374      DO 630 I=1,62
002376      IF(TSQ(I))630,630,631
002400      631 M=I+1
002402      DO 625 L=M,62
002403      D1=UT(I)*VT(L)-VT(I)*UT(L)
002407      D2=VT(I)*WT(L)-WT(I)*VT(L)
002413      D3=UT(I)*WT(L)-WT(I)*UT(L)
002420      IF(D1)634,627,634
002421      627 IF(D2)634,626,634
002422      626 IF(D3)634,625,634
002423      634 K=L+1
002425      DO 629 J=K,62
002426      DIS=UT(I)*(VT(L)*WT(J)-WT(L)*VT(J))
          1=VT(I)*(UT(L)*WT(J)-WT(L)*UT(J))
          2=WT(I)*(UT(L)*VT(J)-VT(L)*UT(J))
002450      IF(DIS)635,629,635
002451      635 RCA=SQRT(TSQ(I))

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002454      RCB=SQRT(TSQ(L))
002457      RCC=SQRT(TSQ(J))
002462      CFRCG=(1.0/(RCA*RCB))*(UT(I)*UT(L)*X1
1*VT(I)*VT(L)*X2*WT(I)*WT(L)*X3
2*0.5*(UT(I)*VT(L)+UT(L)*VT(I))*X4
3*0.5*(VT(I)*WT(L)+VT(L)*WT(I))*X5
4*0.5*(WT(I)*UT(L)+WT(L)*UT(I))*X6)
002516      CFRCB=(1.0/(RCA*RCC))*(UT(I)*UT(J)*X1
1*VT(I)*VT(J)*X2*WT(I)*WT(J)*X3
2*0.5*(UT(I)*VT(J)+UT(J)*VT(I))*X4
3*0.5*(VT(I)*WT(J)+VT(J)*WT(I))*X5
4*0.5*(WT(I)*UT(J)+WT(J)*UT(I))*X6)
002552      CFRCA=(1.0/(RCB*RCC))*(UT(L)*UT(J)*X1
1*VT(L)*VT(J)*X2*WT(L)*WT(J)*X3
2*0.5*(UT(L)*VT(J)+UT(J)*VT(L))*X4
3*0.5*(VT(L)*WT(J)+VT(J)*WT(L))*X5
4*0.5*(WT(L)*UT(J)+WT(J)*UT(L))*X6)
002606      IF(ABS(CFRCG).LT.0.00010)CFRCG=-ZERO
002612      IF(ABS(CFRCB).LT.0.00010)CFRCB=-ZERO
002617      IF(ABS(CFRCA).LT.0.00010)CFRCA=-ZERO
002624      640 IF(CFRCG)644,644,641
002626      641 IF(CFRCB)643,643,642
002630      642 IF(CFRCA)647,647,650
002632      643 IF(CFRCA)649,649,648
002634      644 IF(CFRCB)645,645,646
002636      645 IF(CFRCA)650,650,647
002640      646 IF(CFRCA)648,648,649
002642      647 CFRCB=-CFRCB
002643      CFRCG=-CFRCG
002644      GO TO 650
002645      648 CFRCA=-CFRCA
002646      CFRCG=-CFRCG
002647      GO TO 650
002650      649 CFRCA=-CFRCA
002651      CFRCB=-CFRCB
002652      650 WRITE(9,11)RCA,RCB,RCC,CFRCA,CFRCB,CFRCG,15
002674      PUNCH 11,RCA,RCB,RCC,CFRCA,CFRCB,CFRCG,15
002716      GO TO 700
002717      629 CONTINUE
002721      625 CONTINUE
002723      630 CONTINUE
002725      700 CONTINUE
002730      701 GO TO 100
002731      END

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