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AN INTEGRATED SERIES OF CRYSTALLOGRAPHIC
COMPUTER PROGRAMS

III. COMPARISON OF EQUIVALENT REFLECTIONS

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**AN INTEGRATED SERIES OF CRYSTALLOGRAPHIC
COMPUTER PROGRAMS**

III. COMPARISON OF EQUIVALENT REFLECTIONS

by

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Abstract

The procedures employed and the computer program used to compare and average the experimental intensities obtained for crystallographic equivalent reflections are described. The program performs this comparison for data in any of the 230 space groups. Output is a magnetic tape containing an asymmetric unit of data. This tape may be further used in a Fourier Series Analysis (report IV of the series) or a General Least-Squares Refinement (report V of the series) of the crystal structure.

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Introduction to the Series of Reports

The program described in this report is one of an integrated series of crystallographic computer programs. This series encompasses the entire subject of single-crystal structure analysis and includes programs for such items as:

- (1) crystal orientation for the collection of intensity data
- (2) processing of collected data to allow correction for Lorentz-polarization, absorption, background, and crystal-shape effects
- (3) comparison of processed data over equivalent reflections to ascertain the general validity of the data and to obtain a set of relative F^2 (F has the conventional structure factor meaning.)
- (4) a Fourier series analysis coupled with a plotting routine for obtaining Patterson vector maps and electron density maps of the Fourier and difference Fourier types
- (5) a least-squares procedure for determining the positions and thermal motions (isotropic and/or anisotropic) of the atoms in a single crystal
- (6) various subroutines (two per space group) for the least-squares procedure
- (7) miscellaneous procedures employed during and after a structure analysis, e.g., calculation of interatomic distances and angles, of the

orientation relationship of thermal ellipsoid axes to the crystallographic axes of the crystal, and of the polyhedral coordination of atoms; and the ordering of calculated and observed structure factors to prepare tables for publication.

Since each of the above items involves many repetitious procedures and calculations, it has been the authors' philosophy to employ computer techniques wherever possible and as early in the process of a structure determination as it is feasible to do so. Following this philosophy greatly reduces manual labor, minimizes clerical errors, and allows the maximum information to be obtained from the data.

Introduction to the Present Report

For the determination of a crystal structure, the minimum amount of three-dimensional data normally required is a reliable set of intensity measurements made on an asymmetric portion of the crystal. Utilizing an Eulerian cradle fitted with a eucentric goniometer for the collection of single-crystal intensity data, we find it convenient, in this Laboratory, to usually measure more than the minimum required asymmetric unit.

The purpose of the program described in this report is to compare and average the relative values of F^2 for crystallographic equivalent reflections in order to prepare an asymmetric unit of data for our Fourier series program or our general least-squares program. Normal input to the program is the output from our DATAPREP* program.

This report lists the FORTRAN II and FAP program used to perform

* DAPREP in LA-3043.

the comparison and averaging procedures. A brief description of the logic used in the program is as follows. (1) After some control data and basic unit cell information are read (if needed), the experimental data is read from tape to the memory of the computer. A total of 4,000 measured intensities may be processed by this program with a maximum of 48 measurements being made on any one set of equivalent reflections. (2) The experimental data is then sorted and rearranged in order of increasing $\sin^2\theta$. (3) On the basis of space group number, a selection is made of control numbers required by SMTRY, a subroutine used to generate equivalent reflections. (4) The entire list of sorted experimental data is then searched, in blocks of $\sin^2\theta$, for a match between an experimental hkl and a generated hkl . (5) When a match is found, the experimental intensity is temporarily stored. (6) When all possible matches for equivalent hkl 's in the list have been found, the average of the intensities is formed, the individual contributions to an internal reliability index are formed, and a test is made to insure that positive values of h , k , and l (only if permitted by the general symmetry requirements, however), are utilized in the preparation of the output. (7) The positive hkl 's and averaged intensities are written on the output tape, and items (4), (5), and (6) are repeated for the other experimental hkl 's in the list.

The input/output sequence is either a Patterson tape or a LES-7 tape. There is no provision to input a Patterson tape and output a LES-7 tape, or vice versa.

The operating deck consists of a general program, *COMPAR*, and several subroutines. These are described and listed in a later section.

CØMPAR reads control data from cards in the Monitor Deck and experimental data from either a Patterson tape or a LES-7 tape. Data that are to be compared but have not been processed by our DATAPREP program may be transcribed from cards (punched in the appropriate format) to tape, and input made from this tape. In this procedure it is assumed that the data has been uniformly scaled. In addition to the preparation of an asymmetric data set on the output tape from CØMPAR, the results of this program are written on tape for off-line printing.

The program is normally run through the Monitor system. In addition to the Monitor system tapes, the program requires the use of two tape units, one for the input tape and one for the output tape. A test is made to insure that these tape unit numbers are equal to any number from 2 to 9, but are not equal to each other. The following is a description of the complete Monitor Deck:

- * I.D. (Monitor Identification Card)

- * XEQ (Monitor Card)

- Main Program Binary Cards for CØMPAR

- Subroutine Binary Cards for SMTRY

- Subroutine Binary Cards for SØRT

- Subroutine Binary Cards for UNLØAD

- * DATA (Monitor Card)

- Control Cards, etc.

- END OF JOB (Monitor Card)

Mathematical Equations

The following equations are used by CØMPAR for determining the various items of interest from a set of unscaled relative F^2 values. Such a set may have been prepared from our data processing program (LA-3043) as either a Patterson tape or a general least-squares LES-7 tape. For the preparation of a compared Patterson vector map input tape, the average value of F^2 for a reflection hkl is taken as the gross average of the F^2 values for the hkl equivalent reflections, i.e.,

$$(F^2)_{\text{AVG}} = \frac{\sum_{i=1}^N F_i^2}{N}$$

where N = the number of equivalent reflections.

A weighting scheme is not required for Patterson vector maps, and the $\text{AVGW} = 0.0$ and $W = 0.0$ columns in the printed output from CØMPAR may be interpreted as unit weights if desired.

For the preparation of a compared LES-7 least-squares input tape, the average value of F^2 for a reflection hkl is, again, taken as the gross average of the F^2 values for the hkl equivalent reflection, i.e.,

$$(F^2)_{\text{AVG}} = \frac{\sum_{i=1}^N F_i^2}{N}$$

where N = the number of equivalent reflections.

However, for a compared LES-7 data tape, a weight is required. This weight may be used by the least-squares refinement program. DATAPREP

(LA-3043) gives for each value of F_i^2 a preliminary weight based on counting statistics after a method suggested by Evans.*

In deriving the proper weight to be applied to the average value of F (where $F_{\text{AVG}} = \sqrt{(F^2)_{\text{AVG}}}$) but to be associated with the average value of F^2 written on the LES-7 tape prepared by the COMPARE program, we start with the definition of the variance of the average value of F^2 , i.e.,

$$\sigma_{(F^2)_{\text{AVG}}}^2 = \frac{\sum_{i=1}^N \sigma_{F_i^2}^2}{N} \quad (1)$$

where F_i^2 = an individual unscaled F^2 of a set of equivalent reflections, and

N = the number of equivalent reflections over which the average is taken.

The standard deviation of an individual F_i^2 is related to the standard deviation of an individual F_i by

$$\sigma_{F_i^2} = 2F_i \sigma_{F_i} \quad (2)$$

Squaring (2) and substituting in (1) we obtain

$$\sigma_{(F^2)_{\text{AVG}}}^2 = \frac{4 \sum_{i=1}^N F_i^2 \sigma_{F_i}^2}{N} \quad (3)$$

* Evans, H. T. (1961). Acta Cryst. 14, 689.

From the general form of (2) we can also see that

$$\sigma_{F_{AVG}} = \frac{1}{2F_{AVG}} \cdot \sigma_{(F^2)_{AVG}} \quad (4)$$

Squaring, we obtain

$$\sigma_{F_{AVG}}^2 = \frac{1}{4(F_{AVG})^2} \cdot \sigma_{(F^2)_{AVG}}^2 \quad (5)$$

Substituting (3) into (5) we obtain

$$\sigma_{F_{AVG}}^2 = \frac{1}{4(F_{AVG})^2} \cdot \frac{\sum_{i=1}^N F_i^2 \sigma_{F_i}^2}{N} \quad (6)$$

The square root of (6) is

$$\sigma_{F_{AVG}} = \frac{1}{F_{AVG}} \left(\frac{\sum_{i=1}^N F_i^2 \sigma_{F_i}^2}{N} \right)^{\frac{1}{2}} \quad (7)$$

The weight we wish to apply is given by

$$w = \left(\frac{1}{\sigma_{F_{AVG}}} \right)^{\frac{1}{2}} = \left[\frac{F_{AVG} \cdot N^{\frac{1}{2}}}{\left(\sum_{i=1}^N F_i^2 \cdot \sigma_{F_i}^2 \right)^{\frac{1}{2}}} \right]^{\frac{1}{2}} \quad (8)$$

The weight written on the LES-7 tape prepared by DATAPREP is

$$w_{DATAPREP} = \frac{1}{(\sigma_{F_i})^{\frac{1}{2}}} \quad (9)$$

Transposing

$$(\sigma_{F_i})^{\frac{1}{2}} = \frac{1}{w_{\text{DATAPREP}}} \quad (10)$$

Squaring

$$\sigma_{F_i}^2 = \frac{1}{w_{\text{DATAPREP}}^2} \quad (11)$$

Squaring again

$$\sigma_{F_i}^4 = \frac{1}{w_{\text{DATAPREP}}^4} \quad (12)$$

Substituting (12) into (8) we have

$$w_{\text{COMPAR}} = \left[\frac{F_{\text{AVG}} \cdot N^{\frac{1}{2}}}{\left(\sum_{i=1}^N F_i^2 / w_{\text{DATAPREP}}^4 \right)^{\frac{1}{2}}} \right]^{\frac{1}{2}} \quad (13)$$

As a measure of the internal consistency of the data being processed by COMPAR we form a residual, R, based on the structure factors squared, F_i^2 :

$$R_{F^2} = \frac{\sum |F_i^2 - (F^2)_{\text{AVG}}|}{\sum (F^2)_{\text{AVG}}}$$

where the summations occur over all the sets of equivalent reflections

and $(F^2)_{\text{AVG}}$ is the average for a given set.

An alternative residual, based on the structure factors is given by

$$R_F = \frac{\sum |F_i - F_{\text{AVG}}|}{\sum F_{\text{AVG}}}$$

where $F_{\text{AVG}} = \sqrt{(F^2)_{\text{AVG}}}$

For example, if the reflections 111 , $1\bar{1}1$, $\bar{1}11$, and $\bar{1}\bar{1}1$ in the orthorhombic system had measured values of F_i^2 equal to 36, 31, 29, and 25, respectively, then for R_{F2} :

$F_i^2 = 36$	$ F_i^2 - (F^2)_{\text{AVG}} = 5.75$
31	0.75
29	1.25
<u>25</u>	<u>5.25</u>
121	13.00
$(F^2)_{\text{AVG}} = 30.25$	$R_{F2} = 0.1074$

Using the same data, then for R_F :

$F_i = 6.00$	$ F_i - F_{\text{AVG}} = 0.50$
5.57	0.07
5.38	0.12
5.00	<u>0.50</u>
	1.19
$F_{\text{AVG}} = \sqrt{30.25} = 5.50$	$R_F = 0.0541$

In the formation of the residual, R, single reflections (i.e., intensities measured only once) are excluded. Also, unobserved reflections (characterized by a minus sign on F^2 on LES-7 tapes) are not included in the determination of R.

Glossary of Program Terms

A	Unit cell <u>a</u> axis
B	Unit cell <u>b</u> axis
C	Unit cell <u>c</u> axis
CA	Unit cell α angle or cosine α
CB	Unit cell β angle or cosine β
CC	Unit cell γ angle or cosine γ
CØUNT (I)	I = 1 to 4, a Boolean number designation for a control character number used by the subroutine SMTRY
IC	Number of equivalent reflections generated by SMTRY
IH (3,48)	Integer values of h,k,l used by SMTRY and CØMPAR to generate equivalent crystallographic indices
JMAX	Twice the number of equivalent reflections generated by SMTRY; includes those related by a center of symmetry
LIST (4001)	An internal indexing variable
N1	The number of CØUNT (I) associated with a given Laue symmetry class

SA	$(1.0 - \cos^2 \alpha)^{\frac{1}{2}}$, i.e., $\sin \alpha$
SB	$(1.0 - \cos^2 \beta)^{\frac{1}{2}}$, i.e., $\sin \beta$
SC	$(1.0 - \cos^2 \gamma)^{\frac{1}{2}}$, i.e., $\sin \gamma$
TEMP (4001)	Temporary storage for items being sorted; subsequently used as temporary storage for items being averaged
L1, L2, L3, and S	Variables not used at the present time
AIK(3)	Floating point form of IK; used in preparation of binary LES-7 output tape
F (4001)	Experimental F^2 (structure factor squared) on either Patterson or LES-7 input tape
HKL (4001)	The combination of experimental values h,k, and ℓ into a single number. See statement lll of the FORTRAN listing for a specific definition
IK(3)	The decombination of the maximum value of HKL into the quantities h,k, ℓ that are used in both a test for the positive values permitted by symmetry and in the output
I ϕ H, I ϕ K, I ϕ L	Indexed quantities of h,k, ℓ for the same reflection
NAME	Problem identification
NAMPAT	Patterson tape identification
PHKL	A combination of generated values of h,k, ℓ into a single number
SQ	$\sin^2 \theta / \lambda^2$
TEMP1	Temporary storage for relative weights

W	Relative weight assigned to F_{hkl}^2
ASTAR	$1/2(A*SC*SINBSR)$
AVGF	Average value of experimental F^2
AVG	Number of F^2 being averaged
AVGW	Average weight associated with AVGF
BAC ϕ SC	$BSTAR*ASTAR*C\phi SCSR*2.0$
BCC ϕ SA	$BSTAR*CSTAR*C\phi SASR*2.0$
BSTAR	$1/2(B*SC*SINASR)$
CAC ϕ SB	$CSTAR*ASTAR*C\phi SBSR*2.0$
C ϕ SASR	$(CB*CC-CA)/(SB*SC)$
C ϕ SBSR	$(CA*CC-CB)/(SA*SC)$
C ϕ SCSR	$(CA*CB-CC)/(SA*SB)$
CSTAR	$1/2(C*SA*SINBSR)$
H1,H2,H3	Experimental values of h,k,l
HKLMAX	Maximum value of HKL
ID	Temporary storage for IK(1) while testing for permissible positivity of h
IE	Temporary storage for IK(2) while testing for permissible positivity of k
IMAX	Maximum value of experimental F^2 to be examined (Equal to 1 less than the total number of F^2 , i.e., F_{000} is the last item read in but is not examined)
IP	Page number; fixed point
I	General indexing variable

J	General indexing variable
K	General indexing variable
J1	Designator for Patterson or LES-7 input-output
J2	Space group number
J3	Tape number of input
J4	Tape number of output
J5	Data field number of Patterson input
J6	Origin choice for rhombohedral space group
J7	A number such that, if the percentage discrepancy between an individual F_i^2 and the average F^2 exceeds J7 per cent, a comment to this effect is written in the output
LINE	Line count per output page
L	General indexing variable; total number of equivalent reflections found per set
M	Scale factor number
N	General indexing variable; total number of $-F^2$ found per set
Z	Total number of $+F^2$ found per set of equivalent reflections, i.e., $Z = L - N$
PAT1,PAT2,PAT3	First, second, and third data fields on a Patterson tape
R1	Storage for sum of the residuals between F_i^2 and F_{AVG}^2
R2	Storage for sum of F_i^2
R	$R1/R2$

R4	Storage for sum of the residuals between F_i and F_{AVG}
R5	Storage for sum of F_i
R3	$R4/R5$
RFFAVG	F_i^2/F_{AVG}^2
SINASR	$(1.0 - C\phi SASR^2)^{\frac{1}{2}}$
SINBSR	$(1.0 - C\phi SBSR^2)^{\frac{1}{2}}$
SQ000	$\sin^2 \theta / \lambda^2$ for $h = 0, k = 0, l = 0$, i.e., $= 0.0$
SUM	Storage for sum of $-F_i^2$
SUM1	Storage for partial sum of modified weight associated with $-F_i^2$
SUM2	Storage for sum of F_i^2
SUM3	Storage for partial sum of modified weight associated with F_i^2
X	Upper percentage limit of J7
Y	Lower percentage limit of J7

Data Cards and/or Tape Description

Data cards for C ϕ MPAR consist of three cards for processing a Patterson tape and two cards for processing a LES-7 tape. Data tapes are either the Patterson type or the LES-7 type and are fully described in LA-3043.

DATA CARDS: (for Patterson and LES-7)

Card 1: 72 Hollerith characters for problem identification

Card 2: In format 7I5, the information J1, J2, J3, J4, J5, J6, and J7

J1 < 7 for Patterson input/output tape

≥ 7 for LES-7 input/output tape

J2 = space group number (1 to 230)

J3 = tape number of input (2 to 9); if J3 is negative, unload
tape J3

J4 = tape number of output (2 to 9); if J4 is negative, unload
tape J4

J5 = data field number of Patterson input; may equal 1, 2, or 3

J6 = origin choice for rhombohedral space group; may equal 1 or 2,
signifying rhombohedral or hexagonal axes

J7 = A number such that if an individual F^2 disagrees with the
average F^2 by more than J7 per cent, a comment to this effect
is written. If J7 is not punched, it is set equal to 25 per
cent.

Card 3: (for Patterson input only) In format 6F10.5, the unit cell
parameters a, b, c and three angles or three cosines.

Output Description

The output from CØMPAR consists of the magnetic tape prepared with
the averaged values of F^2 plus an off-line printout. The off-line print-
out lists on each page the following information: problem identification
and page number; then, in columns, the positive values of h, k, and l with
h always positive and k and l positive if permitted (that is, if consis-

tent with the symmetry requirements of an asymmetric unit of data); the average value of F^2 ; the average weight; then the h, k, l values of the experimental equivalent reflections; the values of F^2 measured for these reflections; the weight computed by DATAPREP for these reflections; the ratio F_i^2/F_{AVG}^2 ; and, if needed, the information that F_i^2 disagrees with F_{AVG}^2 by J7 per cent.

The last page of the off-line output contains F^2 for the reflection 000, the R factor based on F and F^2 , the sum of residuals, the sum of F , and the sum of F^2 used in forming the R factors.

Illustrative Example: Input

As an illustrative example of the use of this program, we consider the preparation of a compared LES-7 tape for the material $\text{CuCN} \cdot \text{NH}_3$.^{*} We assume that an input tape is available from the DATAPREP program and we wish to mount this tape on unit 7 and have it unloaded when the program has processed the data. The output tape will come from unit 8 and also be unloaded. The compound $\text{CuCN} \cdot \text{NH}_3$ is monoclinic, space group No. 14, $P2_1/c$ with $a = 5.814$, $b = 7.977$, $c = 8.193$ Å, $\beta = 125.8^\circ$, and four formula units in the unit cell. The two data cards needed for this example are shown in Fig. 1.

^{*} Cromer, D. T., Larson, A. C., Roof, R. B., Jr., The Crystal Structure of $\text{CuCN} \cdot \text{NH}_3$, Acta Cryst. (in press).

Fig. 1 Data cards for the illustrative example.

Illustrative Example: Output

Figure 2 gives an example of a typical page of output from COMPAR. The column headings are self-explanatory. Negative values of $\text{AVG } F(\text{SQD})$ represent unobserved reflections and in general are not used in a least-squares refinement of the structure. The ratio $F(\text{SQD})/\text{AVG } F(\text{SQD})$ in these cases is relatively meaningless and is not listed. For single positive reflections this ratio is, of course, equal to 1.00. Negative $F(\text{SQD})$ and single reflections are not included in the formation of an R index.

Figure 3 shows the last page of output for the illustrative example.

H	K	L	AVG F(SQD)	AVG W	H	K	L	F(SQD)	W	F(SQD)/AVG F(SQD)
4	6	=4	158.799	1.41086	-4	-6	4	165.414	1.41433	1.04165
					-4	6	4	152.185	1.40713	0.95835
1	8	0	-10.673	0.72317	1	8	0	-10.673	0.72317	
					1	-8	0	-10.673	0.72317	
0	4	6	-11.177	0.77846	0	4	6	-10.777	0.71965	
					0	-4	6	-11.577	0.86489	
1	8	=2	64.635	1.22594	-1	8	2	60.177	1.16018	0.93102
					-1	-8	2	69.094	1.30237	1.06898
5	3	=7	-13.173	0.32722	-5	3	7	-15.554	0.28810	
					-5	-3	7	-10.793	0.71913	
5	4	=6	-13.739	0.56537	-5	-4	6	-13.739	0.56537	
					-5	4	6	-13.739	0.56537	
4	6	=2	-11.077	0.79834	4	6	-2	-9.032	0.86182	
					4	-6	-2	-13.123	0.76574	
5	0	=8	101.122	1.40116	-5	0	8	101.122	1.40116	1.00000
6	1	=5	26.988	0.93955	-6	-1	5	29.237	1.23335	1.08333
					-6	1	5	24.739	0.81299	0.91667
1	0	6	65.330	1.28467	1	0	6	65.330	1.28467	1.00000
6	0	=4	29.321	1.23157	6	0	-4	29.321	1.23157	1.00000
3	7	=1	29.322	1.11388	3	-7	-1	38.344	1.18141	1.30769
					3	7	-1	20.300	1.02471	0.69231
3	3	3	-12.404	0.31612	3	3	3	-9.080	0.49624	
					3	-3	3	-15.728	0.28650	
3	7	=4	-9.098	0.49575	-3	7	4	-9.098	0.49575	
					-3	-7	4	-9.098	0.49575	
6	0	=6	92.745	1.33302	-6	0	6	92.745	1.33303	1.00000
2	4	4	-10.822	0.55146	2	4	4	-9.116	0.49528	
					2	-4	4	-12.529	0.62417	

F DISAGREES WITH FAVG BY MORE THAN 25 PERCENT
F DISAGREES WITH FAVG BY MORE THAN 25 PERCENT

Fig. 2. Typical page of output from COMPAR.

LES-7 FROM COMPARE PROGRAM FOR COPPER CYANIDE AMMONIA

PAGE 37

H K L AVG F(SQD) AVG W H K L F(SQD) W F(SQD)/AVG F(SQD)
0 0 0 43264.000

THE R FACTOR BASED ON F IS 0.0248

THE SUM OF THE RESIDUALS IS 151.83555

THE SUM OF THE STRUCTURE FACTORS IS 6130.17834

THE R FACTOR BASED ON F SQUARED IS 0.0384

THE SUM OF THE RESIDUALS IS 3205.02768

THE SUM OF THE STRUCTURE FACTORS SQUARED IS 83397.28906

068967 1670 LINES OUTPUT THIS JOB.

Fig. 3. Last page of output for the illustrative example.

Fortran II Listing of Program

On the following pages the Fortran II listing of the C/MPAR program is given. The subroutine SMTRY is written in FAP. SMTRY generates equivalent reflections for the 11 Laue symmetry classes.

In the "Fourier Series Analysis" report of this series (LA-3198), SMTRY is expanded to SMTRY1 which generates not only equivalent reflections but also the proper phase relationship for these reflections for each of the 230 space groups. The subroutines UNLOAD and SORT used by C/MPAR have been listed in the first report of this series, "I. Crystal Orientation," LA-2974.

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CCOMPARE PROGRAM TO AVERAGE EQUIVALENT REFLECTIONS
C   CARD 1 IS PROBLEM IDENTIFICATION
C   CARD 2 IS CONTROL CARD IN 15 FIELDS. READS J1 TO J7.
C   J1=7 OR GREATER FOR LES-7 INPUT/OUTPUT TAPE
C   J1=LESS THAN 7 FOR PATTERSON INPUT/OUTPUT TAPE
C   J2=SPACE GROUP NUMBER
C   J3=TAPE NUMBER OF INPUT, IF NEGATIVE UNLOAD TAPE J3
C   J4=TAPE NUMBER OF OUTPUT, IF NEGATIVE UNLOAD TAPE J4
C   J5=DATA FIELD NUMBER OF PATTERSON INPUT, = 1,2, OR 3
C   J6=ORIGIN CHUICE FOR RHOMBOHEDRAL SPACE GROUPS, =1 OR 2
C   J7 IF AN INDIVIDUAL F DISAGREES WITH THE AVERAGE F BY MORE
C   THAN J7 PERCENT, A COMMENT TO THIS EFFECT IS WRITTEN
C   IF J7 IS NOT PUNCHED, IT IS SET EQUAL TO 25 PERCENT
C   CARD 3 GIVES CELL PARAMETERS IN 6F10.5 FIELDS.
C   A,B,C AND THREE ANGLES OR THREE COSINES.
C   DIMENSION NAME(12),NAMPAT(12),F(4001),W(4001),SQ(4001),
C   IHKL(4001),LIST(4001),TEMP(4001),SI(4001),COUNT(4),AIK(13),
C   ZIH(3,48),TEMP1(48),PHKL(48),IK(3),IOH(50),IOK(50),IOL(50)
C   EQUIVALENCE (LIST(1),SI(1),N1(7),IC(6),COUNT(5),IH(15))
C   COMMON A,B,C,CA,CB,CC,SA,SB,SC,L1,L2,L3,TEMP,JMAX,S
1   FORMAT (12A6)
2   FORMAT (14I5)
3   FORMAT (6F10.5)
4   FORMAT (3I5,F10.4,F10.2,F10.0)
5   FORMAT(7BH0 'H K L' AVG F(SQD) 'AVG W' 'H K L' 'F(SQD)'
C   'W' 'F(SQD)/AVG F(SQD)')
6   FORMAT(1H0,3I3,F11.3,F10.5)
7   FORMAT (1H1,12A6,10X,4HPAGE,13)
8   FORMAT (32X,3I3,F11.3,2F10.5)
9   FORMAT (32H0J6 HAS BEEN PUNCHED INCORRECTLY)
10  FORMAT (27H0THE R FACTOR BASED ON F IS,F7.4)
11  FORMAT (35H0THE R FACTOR BASED UN F SQUARED IS,F7.4)
12  FORMAT (32H0J7 HAS BEEN PUNCHED INCORRECTLY)
13  FORMAT (32X,3I3,F11.3,F10.5)
14  FORMAT (32X,3I3,F11.3,2F10.5,37H 'F DISAGREES WITH FAVG BY MORE T
C   IHAN, 13,8H PERCENT)
15  FORMAT (3F5.0,3F10.5)
16  FORMAT(28H0THE SUM OF THE RESIDUALS IS,F15.5)
17  FORMAT(136H0THE SUM OF THE STRUCTURE FACTORS IS,F15.5)
18  FORMAT(44H0THE SUM OF THE STRUCTURE FACTORS SQUARED IS,F15.5)
19  FORMAT (56H0INPUT/OUTPUT TAPE NUMBERS HAVE BEEN PUNCHED INCORRECTL
C   Y)
100 READ INPUT TAPE 10,1,NAME
    READ INPUT TAPE 10,2,J1,J2,J3,J4,J5,J6,J7
    IF (XABSF(J3)-2)70,75,75
    WRITE OUTPUT TAPE 9,19
    CALL EXIT
    75 IF (XABSF(J3)-9)80,80,70
    80 IF (XABSF(J4)-2)70,85,85
    85 IF (XABSF(J4)-9)86,86,70
    86 IF (XABSF(J3)-XABSF(J4))87,70,87
    87 IF(J7)90,91,92
    90 WRITE OUTPUT TAPE 9,12
    CALL EXIT
    91 J7 = 25
    92 X = 1.0 + (FLOATF(J7)/100.0)
    Y = 1.0 - (FLOATF(J7)/100.0)
    REMIND J3
    99 IF (J1-7) 101,102,102
101 J1=2
    READ INPUT TAPE 10,3,A,B,C,CA,CB,CC
    IF (CA-1.0) 1041,1041,1040

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1040 CA=COSE(CA/57.29578)
1041 IF (CB-1.0) 1043,1043,1042
1042 CB=COSE(CB/57.29578)
1043 IF (CC-1.0) 105,105,1044
1044 CC=COSE(CC/57.29578)
105 SA=SQRTE(1.0-CA**2)
SB=SQRTE(1.0-CB**2)
SC=SQRTE(1.0-CC**2)
COSASR=(CB*CC-CA)/(SB*SC)
COSBSR=(CA*CC-CB)/(SA*SC)
COSCSR=(CA*CB-CC)/(SA*SB)
SINASR=SQRTE(1.0-COSASR**2)
SINBSR=SQRTE(1.0-COSBSR**2)
SINCSR=SQRTE(1.0-COSCSR**2)
ASTAR=0.5/(A*SC*SINBSR)
BSTAR=0.5/(B*SC*SINASR)
CSTAR=0.5/(C*SA*SINBSR)
BCCOSA=HSTAR*ASTAR*COSASR*2.0
CACOSB=CSTAR*ASTAR*COSBSR*2.0
BACOSC=BSTAR*ASTAR*COSCSR*2.0
GO TO 103
102 J1=1
103 REWIND J4
I=1
GO TO (107,106),J1
106 READ INPUT TAPE J3,1,NAMPAT
107 GO TO (110,120),J1
110 READ TAPE J3,H1,H2,H3,F(1),W(1),M,SQ(1)
LIST(I)=I
GO TO 124
120 READ INPUT TAPE J3,15,H1,H2,H3,PAT1,PAT2,PAT3
LIST(I)=I
SQ(I)=(H1*ASTAR)**2 + (H2*USTAR)**2 + (H3*CSTAR)**2 +
H1*H2*BACOSC + H1*H3*CACOSB + H2*H3*BCCOSA
GO TO (121,122,123),J5
121 F(I)=PAT1
GO TO 124
122 F(I)=PAT2
GO TO 124
123 F(I)=PAT3
124 IF (SQ(I)) 111,112,111
111 HKL(I)=H3 + 256.0 + 512.0*((H2+256.0) + 512.0*(H1+256.0))
I=I+1
GO TO 107
112 IMAX=I-1
CALL SORT (IMAX,SQ(1),LIST(1))
DO 113 J=1,IMAX
L=LIST(J)
113 TEMP(J)=F(L)
DO 114 J=1,IMAX
F(J)=TEMP(J)
DO 115 J=1,IMAX
L=LIST(J)
115 TEMP(J)=HKL(L)
DO 116 J=1,IMAX
HKL(J)=TEMP(J)
GO TO (140,143),J1
140 DO 141 J=1,IMAX
L=LIST(J)
141 TEMP(J)=W(L)
DO 142 J=1,IMAX
W(J)=TEMP(J)
142 W(J)=TEMP(J)
143 IF (J3)150,155,155

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150 CALL UNLOAD (J3)
GO TO 1000
155 REWIND J3
1000 IF (J2-2) 1001,1001,1002
1001 N1=0
GO TO 2000
1002 IF (J2-15) 1003,1003,1004
1003 N1=1
8 COUNT(1)=001000
GO TO 2000
1004 IF (J2-74) 1005,1005,1006
1005 N1=2
8 COUNT(1)=100000
8 COUNT(2)=001000
GO TO 2000
1006 IF (J2-88) 1007,1007,1008
1007 N1=2
8 COUNT(1)=302000
8 COUNT(2)=101000
GO TO 2000
1008 IF (J2-142) 1009,1009,1010
1009 N1=3
8 COUNT(1)=202000
8 COUNT(2)=100010
8 COUNT(3)=001010
GO TO 2000
1010 IF (J2-145) 1011,1011,1012
1011 N1=1
8 COUNT(1)=2000000
GO TO 2000
1012 IF (J2-146) 1013,1013,1014
1013 IF (J6-1) 1313,1113,1213
1113 N1=1
8 COUNT(1)=1000000
GO TO 2000
1213 IF (J6-2) 1011,1011,1313
1313 WRITE OUTPUT TAPE 9,9
CALL EXIT
1014 IF (J2-148) 1011,1013,1015
1015 IF (J2-167) 1016,1016,1017
1016 K=J2-148
GO TO (162,164,162,164,162,164,166,164,162,164,162,166,166,162,
1162,164,164,166,166),K
162 N1=2
8 COUNT(1)=202000
8 COUNT(2)=2000000
GO TO 2000
164 N1=2
8 COUNT(1)=303000
8 COUNT(2)=2000000
GO TO 2000
166 IF (J6-1) 1313,1661,1662
1661 N1=2
8 COUNT(1)=202000
8 COUNT(2)=1000000
GO TO 2000
1662 IF (J6-2) 164,164,1313
1017 IF (J2-176) 1117,1117,1023
1117 N1=2
8 COUNT(1)=101000
8 COUNT(2)=2000000
GO TO 2000

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1023 IF (J2-194) 1118,1118,1024
1118 N1=3
      COUNT(1)=202010
      COUNT(2)=101000
      COUNT(3)=2000000
      GO TO 2000
1024 IF (J2-206) 1119,1119,1025
1119 N1=3
      COUNT(1)=101000
      COUNT(2)=001010
      COUNT(3)=1000000
      GO TO 2000
1025 IF (J2-230) 1120,1120,1313
1120 N1=4
      COUNT(1)=202000
      COUNT(2)=100010
      COUNT(3)=001010
      COUNT(4)=1000000
2000 M=1
      IP=1
      IC = 1
      LINE = 65
      R1 = 0.0
      R2 = 0.0
      R4 = 0.0
      R5 = 0.0
      GO TO (1999,1998),J1
1998 WRITE OUTPUT TAPE J4,1,NAMPAT
1999 DO 3000 I=1,IMAX
      IF (HKL(I))2001,3000,2001
2001 IH(1,1)=XF(XF(HKL(I))/262144.0)-256
      IH(2,1)=XF(XF(HKL(I))/512.0)-512*(IH(1,1)+256)-256
      IH(3,1)=XF(XF(HKL(I))-512*(IH(2,1)+256+512*(IH(1,1)+256)))-256
2002 CALL SMTRY
      DO 2006 J=1,IC
      K=J+IC
      DO 2004 L=1,3
      IF (IH(L,J))2003,2005,2003
2005 IH(L,K)=IH(L,J)
      GO TO 2004
2003 IH(L,K)=-IH(L,J)
2004 CONTINUE
2006 CONTINUE
      HKLMAX=0.0
      JMAX=2*IC
      DO 2009 J=1,JMAX
      TEMP(J)=0.0
      H1=IH(1,J)
      H2=IH(2,J)
      H3=IH(3,J)
      PHKL(J)=H3 + 256.0 + 512.0*((H2 + 256.0) + 512.0*(H1 + 256.0))
      HKLMAX=MAX(HKLMAX,PHKL(J))
2009 CONTINUE
      L = 0
      N = 0
      SUM=0.0
      SUM1=0.0
      SUM2 = 0.0
      SUM3 = 0.0
      DO 2014 K=1,IMAX
      IF (SQ(K)-(SQ(1)+0.0001)) 2011,2011,2015
2011 DO 2013 J=1,JMAX

```

```

      IF (PHKL(J)-HKL(K)) 2013,2012,2013
2012 L = L+1
      IOH(L) = IH(1,J)
      IOK(L) = IH(2,J)
      IOL(L) = IH(3,J)
      IF (F(K)) 2100,2100,2110
2100 TEMP(L) = F(K)
      TEMP1(L) = W(K)
      N = N+1
      SUM = SUM+TEMP(L)
      SUM1 = SUM1+TEMP(L)/(TEMP1(L))**.4
      HKL(K) = 0.0
      GO TO 2014
2110 TEMP(L) = F(K)
      TEMP1(L) = W(K)
      SUM2 = SUM2+TEMP(L)
      SUM3 = SUM3+TEMP(L)/(TEMP1(L))**.4
      HKL(K) = 0.0
      GO TO 2014
2013 CONTINUE
2014 CONTINUE
2015 IF (SUM2 + SUM) 2500,2500,2501
2500 AVG = N
      AVGF = SUM/AVG
      AVGW = SQRTF(SQRTF(SUM/SUM1))
      GO TO 2540
2501 Z = L-N
      AVG = Z
      AVGF = SUM2/AVG
      AVGW = SQRTF(SQRTF(SUM2/SUM3))
      IF (Z-1.0) 2530,2540,2530
2530 DO 2532 J=1,L
      IF (TEMP(J)) 2532,2532,2531
2531 R1 = R1 + ABSF(TEMP(J)-AVGF)
      R2 = R2 + AVGF
2532 CONTINUE
2540 IK(1)=XFIXF(HKLMAX/262144.0) - 256
      IK(2)=XFIXF(HKLMAX/512.0) - 512*(IK(1) + 256) - 256
      IK(3)=XFIXF(HKLMAX)-512*(IK(2)+256+512*(IK(1)+256))-256
      IF (J2-74) 5600,5600,5542
5542 IF (J2-88) 5543,5543,5550
5543 IF (IK(2)) 5544,5600,5600
5544 ID=IK(1)
      IE=IK(2)
      IK(1) = -IE
      IK(2) = ID
      GO TO 5600
5550 IF (J2-142) 5600,5600,5555
5555 IF (J2-167) 5556,5556,5575
5556 IF (J6-1) 6556,5600,6556
6556 K=J2-148
6557 IF (K-2) 5557,7578,6558
6558 IF (K-4) 5557,7578,6559
6559 IF (K-6) 5557,7578,6560
6560 IF (K-8) 5557,7578,6561
6561 IF (K-10) 5557,7578,6562
6562 IF (K-16) 5557,7578,6563
6563 IF (K-17) 5557,7578,5557
7578 IF (IK(3)) 5562,8578,8578
8578 IF (IK(2)) 7579,5600,5600
7579 IK(1)=IK(1)+IK(2)
      IK(2)=-IK(2)

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```

GO TO 5600
5557 IF (IK(2)) 5558,5572,5572
5558 IF (IK(3)) 5562,5578,5562
5562 IK(3) = -IK(3)
GO TO 5578
5572 IF (IK(3)) 5562,5600,5600
5575 IF (J2-168) 5550,5577,5577
5577 IF (J2-194) 5576,5576,5600
5576 IF (IK(2)) 5578,5600,5600
5578 ID = IK(1)
IE = IK(2)
IF (IE) 5579,5580,5580
5579 IK(1) = -IE
GO TO 5581
5580 IK(1) = IE
5581 IK(2) = ID+IE
5600 LINE = LINE+ L + 2
IF (LINE-60) 2560,2560,2550
2550 WRITE OUTPUT TAPE 9,7,NAME,IP
IP = IP+1
WRITE OUTPUT TAPE 9,5
LINE = L+2
2560 WRITE OUTPUT TAPE 9,6,(IK(L),L=1,3),AVGF,AVGM
2590 DO 2600 J=1,L
IF (TEMP(J)) 2591,2591,2592
2591 WRITE OUTPUT TAPE 9,13,IOH(J),IOK(J),IOL(J),TEMP(J),TEMP1(J)
GO TO 2600
2592 IF (AVGF) 2591,2591,2570
2570 RFFAVG = TEMP(J)/AVGF
IF (RFFAVG-X) 2593,2593,2594
2593 IF (RFFAVG-Y) 2594,2594,2595
2594 WRITE OUTPUT TAPE 9,14,IOH(J),IOK(J),IOL(J),TEMP(J),TEMP1(J),RFFAV
1G,J7
GO TO 2600
2595 WRITE OUTPUT TAPE 9,8,IOH(J),IOK(J),IOL(J),TEMP(J),TEMP1(J),RFFAVG
2600 CONTINUE
2700 GO TO (2701,2702),J1
2701 AIK(1)=IK(1)
AIK(2)=IK(2)
AIK(3)=IK(3)
WRITE TAPE J4,(AIK(L),L=1,3),AVGF,AVGM,M,SQ(1)
GO TO 2740
2702 WRITE OUTPUT TAPE J4,4,(IK(L),L=1,3),AVGF,AVGF,AVGF
2740 IF (L-N) 3000,3000,2745
2745 IF (Z-1.0) 2750,3000,2750
2750 DO 2760 J = 1,L
IF (TEMP(J)) 2760,2760,2755
2755 TEMP(J) = SQRTF(TEMP(J))
2760 CONTINUE
AVGF = SQRTF(AVGF)
DO 2770 J = 1,L
IF (TEMP(J)) 2770,2770,2765
2765 R4 = R4+ABSF(TEMP(J)-AVGF)
R5 = R5+AVGF
2770 CONTINUE
3000 CONTINUE
IK(1)=0
IK(2)=0
IK(3)=0
AVGF=F(IMAX+1)
R = -R1/R2
R3 = R4/R5

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```

WRITE OUTPUT TAPE 9,7,NAME,IP
WRITE OUTPUT TAPE 9,5
WRITE OUTPUT TAPE 9,6,(IK(L),L=1,3),AVGF
WRITE OUTPUT TAPE 9,10,R3
WRITE OUTPUT TAPE 9,16,R4
WRITE OUTPUT TAPE 9,17,R5
WRITE OUTPUT TAPE 9,11,R
WRITE OUTPUT TAPE 9,16,R1
WRITE OUTPUT TAPE 9,18,R2
GO TO (4000,4001),J1
4000 AVGW=0
M=M+1
SQ000=0
WRITE TAPE J4,(IK(L),L=1,3),AVGF,AVGW,M,SQ000
GO TO 4004
4001 WRITE OUTPUT TAPE J4,4,(IK(L),L=1,3),AVGF,AVGF,AVGF
4004 END FILE J4
IF (J4) 4002,4003,4003
4002 CALL UNLOAD (J4)
GO TO 100
4003 REWIND J4
GO TO 100
END

```

```

*SMTRY      PROGRAM TO GENERATE EQUIVALENT REFLECTIONS FOR COMPARE
COUNT      200
ENTRY       SMTRY
REM         CONTROL NUMBERS AND THEIR FUNCTION
REM
REM         10      L = -L
REM         1000    K = -K
REM         2000    K = H
REM         3000    K = -H
REM         4000    K = H+K
REM         5000    K = -H-K
REM         6000    K = H
REM         7000    K = -H
REM         100000   H = -H
REM         200000   H = K
REM         300000   H = -K
REM         400000   H = H+K
REM         500000   H = -H-K
REM         600000   H = K
REM         700000   H = -K
REM         1000000  CUBIC TRIPLE
REM         2000000  HEXAGONAL TRIPLE
REM
SMTRY      CLA      N1
TZE      RET
SXA      RET-1,4
SXA      RET-2,2
SXA      RET-3,1
LXD      THREE,2
PDX      ,4
CLA      K-2
ARS      9
ADD      K-1
ARS      9
ADD      K
E1      STO      A-2
LXD      ZERO,1
LDI      NCOUNT+1,4
SXA      E4,4
PXD      ,2
SUB      THREE
STO      E3
E2      LFT      1
TRA      C1          CUBIC TRIPLE
LFT      2
TRA      H1          HEX TRIPLE
ALPHA    CLA      K,1
RFT      400000      H+K
ADD      K-1,1
RFT      200000      K
CLA      K-1,1
RFT      100000      -H
CHS
STO      K,2
CLA      K-1,1
RFT      4000      H+K
ADD      K,1
RFT      2000      H
CLA      K,1
RFT      1000      -K
CHS
STO      K-1,2

```

```

CLA      K-2,1
RFT      10
CHS
STO      K-2,2
TSX      DUP,4
TXI      **1,2,3
TXI      **1,1,3
E3      TXL      E2,1
E4      AXT      ,4
TIX      E1+1,4,1
PXD      ,2
LRS      17
DVP      THREE
STO      1C
AXT      ,1
AXT      ,2
AXT      ,4
RET      TRA      1,4
REM
DUP      SXA      E11,4
SXA      E12,4
LXD      ZERO,4
PXD      ,2
SUB      THREE
STD      E5
CLA      K-2,2
ARS      9
ADD      K-1,2
ARS      9
ADD      K,2
STO      A-2,2
E6      GAS      A-2,4
TRA      **2
TRA      E3-1
CHS
CAS      A-2,4
TRA      **2
TRA      E3-1
E7      TXI      **1,4,3
E5      TXL      E6,4
E11     AXT      ,4
TRA      1,4
E12     AXT      ,4
TRA      2,4
REM
C1      CLA      K,1
STO      K-1,2
CLA      K-1,1
STO      K-2,2
CLA      K-2,1
STO      K,2
TSX      DUP,4
TXI      **1,2,3
CLA      K,1
STO      K-2,2
CLA      K-1,1
STO      K,2
CLA      K-2,1
STO      K-1,2
TRA      E3-3
REM
REM      CUBIC TRIPLE.      HKL TO LHK AND-KLH
REM      HEXAGONAL TRIPLE,      HKL TO KIL AND IHL

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```

      REM
H1    CLS      K,1
      SUB      K-1,1
      STO      K-1,2
      STO      K-3,2
      CLA      K-1,1
      STO      K,2
      CLA      K,1
      STO      K-4,2
      CLA      K-2,1
      STO      K-2,2
      STO      K-5,2
      TSX      UUP,4
      TXI      *+1,2,3
      TRA      E3-3
ZERO  DEC      0
THREE DEC      3B17
K      COMMON  72
A      COMMON  72
N1     COMMON  1
IC     COMMON  1
NCUNT  COMMON  4
      END

```