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COMPUTER PROGRAMS FOR X-RAY CRYSTALLOGRAPHY

PART III:

PROGRAMS FOR PRELIMINARY PROCESSING OF DIFFRACTOMETER DATA

IIIA, REFLECTION EDITING

IIIB, DATA PREPARATION

S. R. HALL

MINERAL SCIENCES DIVISION

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IIIA, Reflection Editing; IIIB, Data Preparation

by

S. R. Hall*

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ABSTRACT

These two programs perform the preliminary processing of intensity data collected on the Mines Branch automatic diffractometer and are a prerequisite to the XRAY-67 data reduction routine =DATRDN=. The purpose of the first program (IIIA) is to edit the data on magnetic tape, and the second (IIIB) to scale and correlate the multiple segments of data into a unique set of reflections.

*Research Scientist, Crystal Structure Group, Mineral Sciences Division, Mines Branch, Department of Energy, Mines and Resources, Ottawa, Canada.

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PROGRAMMES D'ORDINATEUR POUR LA RADIOCRISTALLOGRAPHIE

PARTIE III :

PROGRAMMES DE TRAITEMENT PRÉLIMINAIRES DES DONNÉES DE DIFFRACTOMÈTRE

IIIA, Apprêtage des données sur les réflexions
IIIB, Préparation des données

par

S.R. Hall*

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RÉSUMÉ

Ces deux programmes servent à effectuer le traitement préliminaire des données d'intensité recueillies au moyen du diffractomètre automatique de la Direction des mines et sont un prérequis à la routine XRAY-67 de réduction des données =DATRDN=. Le programme IIIA sert à porter les données sur bande magnétique, et le programme IIIB sert à établir la corrélation entre les divers éléments des données et à les uniformiser en vue de produire un seul groupe de données sur les réflexions.

*Chercheur scientifique, Groupe des structures cristallines, Division des sciences minérales, Direction des mines, ministère de l'Énergie, des Mines et des Ressources, Ottawa, Canada.

CONTENTS

INTRODUCTION

The two computer programs described in this report are for use in the preliminary processing of intensity data collected on the Mines Branch automatic diffractometer (Research Report R 214*), in preparation for use with the data reduction program =DATRDN= of the XRAY-67 crystallographic program system (Report 67-58, Computer Science Centre, University of Maryland, 1967).

The first program (IIIA) has the function of writing and editing the magnetic tape containing the diffractometer data information. Any errors in the diffractometer measurements or sorting order in equivalent data sets, etc., may be eliminated by manipulation of this routine.

The second program (IIIB) is designed to extract and scale the reflection intensities from the diffractometer measurements and then correlate equivalent segments of reflections into one unique set.

SPECIFICATIONS

These programs have been written in standard FORTRAN IV code excluding logical-IF, complex arithmetic and double precision instructions.

Program IIIB requires a minimum working core memory of 35K words of 24, 32 or 36 bit size and at least two magnetic tape drives. This is the dimensioned limit required to process 10,000 unique reflections, and could be increased or reduced according to requirements.

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*In preparation.

PROGRAM IIIA - DATA EDITING ROUTINE

DESCRIPTION

This program has three basic modes of operation:

1) Read diffractometer data cards, list and write as magnetic tape file
2) Edit and list existing magnetic tape file
3) List existing magnetic tape file

In mode 1), each of the data cards, prepared from the diffractometer paper tape, is stored on magnetic tape as a single card image. Usually these images are listed on the lineprinter with their associated serial number for reference in subsequent editing of the tape.

In operation mode 2), existing magnetic tape files, which may have been prepared in mode 1) or by the diffractometer control routine, are edited using the CHANGE, INSERT or DELETE option cards. All card images are referenced according to the serial numbers on the input magnetic tape, not according to the new serial numbers on the output tape.

Edit cards must reference the card image serial numbers sequentially. For example, editing of image number 1157 must precede any reference to image number 2351, etc.

In operation mode 3), the entire contents of the input magnetic tape are listed. This is usually to examine a diffractometer-generated tape and identify the image serial numbers for editing purposes.

The reflection data stream, whether it be in the form of cards or be card images on magnetic tape, must fulfil the following structure considerations:

(a) As described in the diffractometer control routine, the reflection data are divided into segments of reciprocal space, the boundaries of which are usually defined by the reciprocal cell axes. Within a set of data,

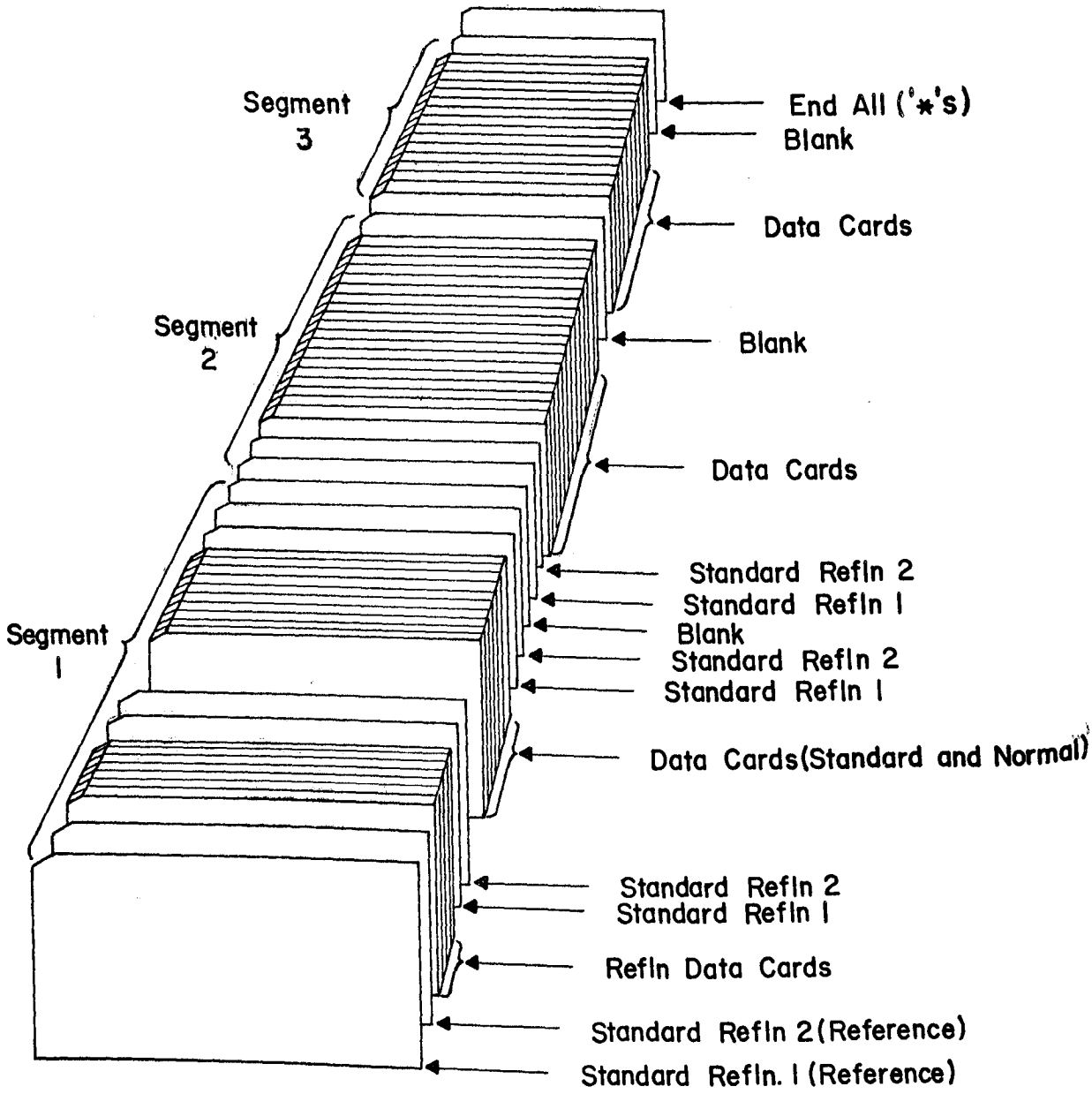
the segments may be either non-equivalent (such as $hk\ell$, and $\bar{h}k\ell$ reflections in a triclinic cell) or equivalent (such as $hk\ell$, $\bar{h}\bar{k}\ell$, $\bar{h}k\ell$ and $\bar{h}k\bar{\ell}$ reflections in an orthorhombic cell; or multiple sets of $hk\ell$ reflections in any cell). Any number of equivalent or non-equivalent segments may be present in the data set, and in any order, provided the total number does not exceed 12. The Data Preparation program stores each non-equivalent segment of reflections in separate areas of core memory and "overlays" these with the equivalent segments in order to provide <u>averaged intensities</u>. It is therefore important that, although the indices of a given reflection in equivalent segments may be numerically different (e.g., 1, 3, 5; 3, 1, 5; 5, 3, 1 in a cubic cell), the symmetry-equivalence order and the number of the reflections be the same. The interval and number of standard reflection groups in equivalent segments need not be identical.

(b) Standard reflection cards (or images) used in the overall scaling of the intensities must not exceed four (4) in number and must be grouped in sequential order. A group of standards must start and end each segment of reflection data, and must appear at intervals, of 0 to 100 reflections, throughout the data. The interval may be zero (i.e., two groups follow consecutively) to allow for a break in continuity of data collection within a given segment. In this case the first group of standards would refer to reflections collected before the stoppage and the second group of standards would be associated with the reflections collected following the restart.

(c) The order of data segments, equivalent or non-equivalent, is immaterial, but a blank spacer "card" must follow the last group of standards in the segment.

(d) A "card" containing all *'s must be placed after the blank spacer of the last segment of data; this is the end-all indicator.

The program source code is listed in APPENDIX 3.



A TYPICAL DECK PROFILE OF DIFFRACTOMETER DATA COMPOSED OF THREE SEGMENTS AND TWO STANDARDS

Figure 1

INPUT FORMATS

Cards

The input cards, which are described in detail below, are as follows:

1. DATA EDIT lead card
2. CHANGE single reflection card
3. DELETE reflections card
4. INSERT reflections card
5. NOMORE editing card

} For optional use with operation mode 2).

1. DATA EDIT lead card

FORMAT (10X, 2I10)

Cols.	Specified punching or function of the field
1-10	DATA EDIT
11-20	Operation mode 1)/ 2)/ 3) to (read data cards and write tape)/ (edit existing tape)/(list existing tape)
21-30	N -- list every Nth card image on the line printer (Blank = 1)
31-80	Blank

2. CHANGE single reflection card (replacement card follows immediately)

FORMAT (A6, 4X, I10)

Cols.	Specified punching or function of the field
1-6	CHANGE
7-10	Blank
11-20	Serial no. of single card image to be replaced for image of card immediately following
21-80	Blank

3. DELETE reflections card

FORMAT (A6, 4X, 2I10)

Cols.	Specified punching or function of the field
1-6	DELETE

7-10	Blank
11-20	Serial no. of first card image to be deleted
21-30	Serial no. of last card image to be deleted; along with all card images between
31-80	Blank

4. INSERT reflection card (cards to be inserted follow immediately)

FORMAT (A6, 14, I10)

Cols.	Specified punching or function of the field
1-6	INSERT
7-10	Number of card images to be inserted
11-20	Serial no. of card image preceding the position of insertion
21-80	Blank

5. NOMORE editing card (must follow last editing card)

FORMAT (A6)

Cols.	Specified punching or function of the field
1-6	NOMORE
7-80	Blank

Data Cards

The data cards required for operation mode 1) must be arranged in the order outlined in the description above. A typical set of data cards, immediately following the DATA EDIT card, has been shown in Figure 1.

The format of the reflection data cards is as follows:

Reflection data card

FORMAT (I1, 3I4, 5F8.3, I2, I5, I7, I5, 8X).

Cols.	Specified punching or function of the field
1	Standard reflection number (1-4). Blank if non-standard reflection.
2-5	Index h
6-9	Index k
10-13	Index ℓ

14-21	Diffractometer setting - 2θ (degrees)
22-29	Diffractometer setting - ϕ
30-37	Diffractometer setting - χ
38-45	2θ(min) of scan range (degrees)
46-53	2θ(max) of scan range
54-55	Attenuator used. (Blank, 1, 2--5)
56-60	Background count at 2θ (min)
61-67	Peak count during scan from 2θ (min) to 2θ(max)
68-72	Background count at 2θ (max)

Magnetic Tape

For operation modes 2) and 3) (see input card 1), the input magnetic tape will be entered from tape drive B*. This tape will contain formatted card images, as output by the diffractometer control routine or by this program in a previous run.

OUTPUT FORMATS

Lineprinter

According to the print option N (see input card 1), every Nth card image will be listed, with the associated image serial number. In operation mode 2), these serial numbers will be the updated values, and images edited by CHANGE or INSERT options will also be printed with their new serial numbers.

---

*See Appendix 2.

Magnetic Tape

For operation modes 1) and 2) (see input card 1), a magnetic tape will output on tape drive A. This tape will be in formatted card images identical in structure to the input card check in mode 1), or the input magnetic tape in mode 2).

PROGRAM IIIB - DATA PREPARATION ROUTINE

DESCRIPTION

The purpose of this program is to scale and correlate intensity data collected on the Mines Branch automatic diffractometer and output it in a form which is acceptable to the data reduction program =DATRDN= of the XRAY-67 system.

The source of the input data stream is either from cards or from magnetic tape. The tape may have been generated directly from the diffractometer control routine or from the editing program IIIA described earlier. The structure and format of the data stream have been discussed in detail in the preceding program IIIA.

The first group of standard reflections entered in the data stream is used as the reference standard reflections. All subsequent standard reflection groups are scaled according to these reflections, in order that the complete data set be on a common scale.

The scaling process in this program is based on four factors:

1) the overall intensity scale, used to bring all the intensities as close as possible to their absolute values;
2) the attenuator scale, initiated by the indicator on each reflection card;
3) the time-of-peak-scan to time-of-background scale (TP/TB) necessary to calculate the net count intensity;

4) the standard reflection(s) scale, interpolated from the relative scale of the group of standards preceding and following each reflection.

This program, in addition to calculating the least squares weight (i.e. the reciprocal variance $1/\sigma^2(F_o)$) of each reflection, determines whether a reflection may be considered to have an intensity that is significant to within a specified limit (commonly referred to as the observed or unobserved criteria). The least squares weight (LSWT) is calculated using an expression derived by Dr. E.J. Gabe in the Institute of Cancer Research program series (No. 16), namely:

$$\text{LSWT} = \frac{1}{\sigma^2(F_o)} = \frac{1}{F_o^2}\left[\frac{4}{\frac{\sigma^2(K)}{K^2} + \frac{\sigma^2(A)}{A^2} + \frac{\sigma^2(LP^{-1})}{(LP^{-1})^2} + \frac{\sigma^2(I)}{I^2}}\right] \quad \ldots(1)$$

In this expression, $\frac{\sigma^2(K)}{K^2} = \frac{\Delta^2(K)}{2K^2}$, ...(2)

where K and $\Delta(K)$ are average scale and scale difference derived from two consecutive groups of standard reflections;

$$\frac{\sigma^2(A)}{A^2} = \frac{n^2\sigma^2(A_1)}{A_1^2}, \quad \ldots(3)$$

where A_n is the scale factor of the nth (n = 0 to 5) attenuator;

$$\frac{\sigma^2(LP^{-1})}{(LP^{-1})^2} = \left\{\frac{4\cos 2\theta \sin^2\theta}{\sin 2\theta} \cdot \left[\frac{1}{\sin 2\theta} + LP^{-1}\right]\frac{\sigma(\sin\theta)}{\sin\theta}\right\}^2, \quad \ldots(4)$$

where the reciprocal of the Lorentz polarization factor

$$LP^{-1} = \frac{2\sin\theta\cos\theta\,(1+K')}{(1+K'\cos^2 2\theta)}; \quad \ldots(5)$$

and

$$\frac{\sigma^2(I)}{I^2} = \frac{I_p + t^2 I_b}{(I_p - tI_b)^2}, \quad \ldots(6)$$

where I is the net intensity, I_p the peak count, I_b the total background count, and t the ratio of time-to-peak-scan to total-time-of-background-count.

The net intensity I is considered insignificant, and therefore unobserved, at a level specified by S (see input card 5), if

$$I < S.\sigma(I), \qquad \ldots(7)$$

that is,

$$I < S.\,(I_p + t^2 I_b)^{1/2} \qquad \ldots(8)$$

or rather,

$$S^2 \geq \frac{(I_p - tI_b)^2}{I_p + t^2 I_b} \qquad \ldots(9)$$

The value of S, at various significance levels, is listed below:

Significance Level	σ (I) Factor S
1%	2.58
2%	2.33
5%	1.96
10%	1.65
20%	1.28
30%	1.04
40%	0.84
50%	0.68

Unless specified otherwise, the value of 1.65 (significance level of 10%) will be used in the program. In addition, any reflection with $tI_b > I_p$ (i.e., I is negative) is considered unobserved. Intensities which are considered unobserved by these criteria are set at the value:

$$I(\text{unobs}) = C.S.\sigma(I) \qquad \ldots(10)$$

$$= C.S.(I_p + t^2 I_b)^{1/2} \qquad \ldots(11)$$

The constant C enables the most probable value of I to be estimated for the unobserved reflection. Unless specified as an input parameter on card 5, the value of C will be taken as 0.5.

Of course, if the reflection is significant, the value of the net intensity will be

$$I(obs) = I_p - tI_b. \qquad \ldots(12)$$

When all the segments of data have been scaled and correlated, the resulting set of unique, averaged reflections is sorted according to the specified order of the index magnitudes $/h/$, $/k/$ and $/\ell/$. All reflections with the same $/h, k, \ell/$ will then be adjacent in core, and the order of the data output on tape will be optimized for subsequent calculations. The sort order is specified as an input parameter on card 3.

The format of the output magnetic tape is discussed in the OUTPUT FORMATS section below. The restrictions placed on the input parameters of the =DATRDN= program by using this tape are discussed in APPENDIX 1.

In the Lorentz-polarization factor (see equation (5) above), the polarization constant K' is 1.0 when there is no crystal monochromator, and K'< 1.0 for the perpendicular arrangement of the Mines Branch Picker diffractometer. In the latter case, the value of the K' should lie somewhere between $\langle 1/\cos^2 2\theta_m \rangle$ for the completely mozaic crystal and $\langle 1/\cos 2\theta_m \rangle$ for the perfect crystal, where $2\theta_m$ is Bragg angle of diffraction at the monochromator.

The program source code is listed in APPENDIX 4.

INPUT FORMATS

Cards

The input cards, which are described below, must be entered in the following order:

1. TITLE card.
2. CELL CONSTANTS card.

3. CONTROL card.
4. SCALES card.
5. COUNT TIMES card.
*6. ABSORPTION parameters card.
*7. EXTINCTION parameters card.
8. DATA LEAD card.
9. Reflection data stream (optional).

*These cards are not entered in this version of the program.

1. TITLE card

FORMAT (8X, 18A4)

Cols.	Specified punching or function of the field
1-8	TITLE
9-80	Any alphanumeric information to be used as printout heading

2. CELL CONSTANTS card

FORMAT (10X, 7F10.5)

Cols.	Specified punching or function of the field
1-10	CELL CONS
11-20	Cell dimension a (Å)
21-30	Cell dimension b
31-40	Cell dimension c
41-50	Cell angle α (degrees)
51-60	Cell angle β
61-70	Cell angle γ
71-80	Wavelength λ (weighted mean of α_1 and α_2) (Å)

3. CONTROL card

FORMAT (10X, 14I5)

Cols.	Specified punching or function of the field
1-10	CONTROL
11-15	Input tape option; (0)/(1) reflection data stream entered on (cards)/(tape drive A)
16-20	Output tape option; (0)/(1) (do not)/(do) output processed data on tape drive C.

21-25	Print option -I; (0)/(1) (do not)/(do) list each input reflection during processing
26-30	Print option -II; (0)/(1) (do not)/(do) list summary of correlated reflections <u>before</u> sort
31-35	Print option -III; (0)/(1) (do not)/(do) is summary of correlated reflections <u>after</u> sort
36-40	Absorption option; (0)/(1) (do not)/(do) calculate extinction corrections (<u>must = 0</u> in this version)
41-45	Extinction option; (0)/(1) (do not)/(do) calculate extinction corrections (<u>must = 0</u> in this version)
46-50	Slowest sort index } for { h put 1
51-55	Medium sort index } for { k put 2
56-60	Fastest sort index } for { ℓ put 3
61-80	Blank

4. <u>SCALES card</u>

FORMAT (10X, 7F10.3)

Cols.	Specified punching or function of the field
1-10	SCALES
11-20	Overall intensity scale factor
21-30	A_1 scale factor of attenuator 1 (assume $A_0 = 1.0$)
31-40	A_2 scale factor of attenuator 2
41-50	A_3 scale factor of attenuator 3
51-60	A_4 scale factor of attenuator 4
61-70	A_5 scale factor of attenuator 5
71-80	$\sigma(A_1)$, standard dev. of attenuator 1 scale factor

5. <u>COUNT TIMES card</u>

FORMAT (10X, 7F10.3)

Cols.	Specified punching or function of the field
1-10	COUNT TIME
11-20	Time of one degree 2θ-scan (seconds)
21-30	Time of 2θ(min) background count (seconds)
31-40	Time of 2θ(max) background count (seconds)
41-50	Value of $\sigma(\sin\theta)/\sin\theta$ used in L.S. weight calculation
51-60	Polarization factor K' (Blank = 1.0)

61-70 Significance factor S used in unobserved refln. test (Blank = 1.65)

71-80 Scale constant C used to calculate I (unobs) (Blank = 0.5)

6. ABSORPTION parameters card

(not used in this version)

7. EXTINCTION parameters card

(not used in this version)

8. DATA LEAD card

FORMAT (10X, 14I5)

Cols.	Specified punching or function of the field	
1-10	DATA LEAD	
11-15	Number of standard reflections per group (max of 4)	
16-20	Number of segments of data (max of 12)	
21-25	Type code of segment 1	Segment 1 is type 1; succeeding non-equivalent segments are types 2, 3, etc. Equivalent segments are given the same type code.
26-30	Type code of segment 2	
31-35	Type code of segment 3	
:	: : : : :	
:	: : : : :	
76-80	Type code of segment 12	

9. Reflection data stream (optional on control card 3, col. 15)

The format and structure of these cards has been described in the Tape Edit program (IIIA).

Magnetic Tape

The input magnetic tape, if specified on control card 3 (col. 15), will be mounted on tape drive A (discussed in Appendix 2). It will contain the reflection data in the form of card images which have been output from either the diffractometer control routine or the Tape Edit program (IIIA).

OUTPUT FORMATS

Lineprinter

The lineprinter output is in several parts which are specified options on the input control card 3.

(i) An overall summary of the input parameters. This is self-explanatory.

(ii) If specified, (i) is followed by the listing of the parameters of each reflection in the input data stream and the standard reflection scale factors.

The notation used in this listing is as follows:

N	=	serial number of the reflection as stored in core. (N.B.: equivalent reflections will have the same number.)
H, K, L	=	Miller indices as entered
AT	=	Attenuator no. (0 to 5)
B1C	=	Background count at 2θ (min)
PKC	=	Peak scan count
B2C	=	Background count at 2θ (max)
TP/TB	=	Ratio of time-of-peak-scan to time-of-background-count
I(NET)	=	PKC - (B1C + B2C)*(TP/TB)
TSCL	=	Total scale product of overall intensity scale, attenuator scale and the interpolated standard reflection scale
ABS	=	Absorption scale factor (=1. in this version)
EXT	=	Extinction scale factor (=1. in this version)
S2/L2	=	$\sin^2\theta / \lambda^2$
1/LP	=	Lp^{-1} factor
LSWT	=	Least squares weight (see equation (1) above)
F(REL)	=	structure factor:
	=	$[\text{TSCL}*1/\text{LP}*\text{I(NET)}]^{1/2}$ for observed reflections
	=	$[\text{TSCL}*1/\text{LP}*(\text{equ. 11})]^{1/2}$ for unobserved reflections

DELTA = For equivalent reflections, the difference between F(REL) and the average structure factor.

(iii) If specified, (ii) is followed by the complete set of unique reflections in order of processing, four reflections per line. The notation used is as follows:

N = Serial number of the reflection as stored in core

H, K, L = Miller indices as stored in core

I(REL) = Average relative intensity

LSWT = Average least squares weight. If any one of the equivalent reflections was considered unobserved (i.e. indicated in (ii) by * or □), this value will be marked as negative. The actual value of the L.S. weight is, however, always positive.

(iv) Following the index sort of reflections, a brief summary of the overall status of the data, and the max-min values of I, $\sin^2\theta/\lambda^2$ and L.S. weight, is listed.

(v) If specified, (iv) is followed by an identical core dump to (iii), except that the reflections have now been sorted into a specified order in preparation for output.

Magnetic Tape

The output magnetic tape, if specified on control card 3, is mounted on tape drive C (discussed in Appendix 2) and will contain the following information in card image format:

1. FORMAT specifying card image

FORMAT (20A4)

Cols.	Specified contents or function of the field
1-22	FORMAT (4I5, 2F20.6, 20X)
23-80	Blank

2. REFIN card image

FORMAT (2A4, 8X, I5, 10X, 6A4, 25X)

Cols.	Specified contents or function of the field
1-8	REFIN
9-16	Blank

17-21	M, the total number of unique reflections in the data set
22-31	Blank
32-55	IH IK IL ID FR FW
56-80	Blank

3 to 2+M. Reflection data images

FORMAT (4I5, 2F20.6, 20X)

Cols.	Specified contents or function of the field
1-5	Index h
6-10	Index k
11-15	Index ℓ
16-20	Status code (obs. =1, unobs. =2)
21-40	Relative intensity
41-60	(Least squares weight)$^{1/2}$ $=w^{1/2}=1/\sigma(F_o)$
61-80	Blank

3+M. FILES card image*

FORMAT (20A4)

Cols.	Specified contents or function of the field
1-7	FILES
8-42	01 03 13 14 02 03 15 08 09 20 21 22
43-80	Blank

-- END OF FILE MARK

*The function of the FILES card is described in the XRAY-67 programming system manual.

APPENDIX 1

Restrictions on =DATRDN= Input Cards

When the output tape of the Data Preparation program (IIIB) is used as input to the Data Reduction program =DATRDN=, the sequence of input cards, and certain parameters on these cards, must be fixed. The order of the =DATRDN= input cards, following either the SYMTRY or DISPER cards, must be:

:	:
:	:
n+1	CONDIT
n+2	ABSORB (optional)
n+3	SCALE
n+4	FILES
n+5	END

These cards contain the following restrictions:

CONDIT

-- as normally specified except,

Cols.

43 =2 (4-circle diffractometer Lp^{-1} correction)

46 =1 (take the square root of the intensity)

SCALE

-- as normally specified except,

Cols.

20 =1 (one scale group only)

32 =3 (value of $w^{1/2}$ stored directly from the input tape)

FILES

-- as normally specified except,

Cols.

8-9 =15 (card reader interchanged for tape drive C)

APPENDIX 2

Magnetic Tape Scheduling for Programs IIIA, IIIB and =DATRDN=

The programs IIIA and IIIB described in this writeup, and the program =DATRDN= in the XRAY-67 system, can be used with only two tape drives. However, it is more convenient for sequential operation if four tape drives are available. This writeup describes the tape operations, assuming three tape drives for data input-output (designated A, B, C) with a fourth drive (D) being used as the system tape. In these programs (see source code listings in Appendices 3 and 4), the tape drives A, B and C have been allocated the device numbers 13, 14 and 15, which are appropriate for the particular computer installation in use at the Mines Branch. The cardreader and lineprinter have the device numbers 01 and 03.

The device numbers for the various input-output units appear also on the FILES card image output by program IIIB, and the FILES card entered by program =DATRDN= (see Appendix 1). These device numbers must be in accord with the particular installation being used.

The usage of tape drives in these programs has been arranged to facilitate sequential execution, as well as avoiding the data from IIIB being overwritten by subsequent XRAY-67 outputs. The tape scheduling can be summarized as follows:

	Tape drives (Nos.)			
	A (13)	B (14)	C (15)	D (16)
1. IIIA (TAPE EDIT)	O/P	I/P		System
2. IIIB (DATA PREP.)	I/P		O/P	System
3. =DATRDN=		O/P	I/P*	System
4. =LOADAT=(e.g.)	O/P	I/P		System

*Data are entered from drive C only when 15 appears in place of the cardreader device no. on the =DATRDN= input FILES card (see Appendix 1).

APPENDIX 3 - Source Listing of Program IIIA

```
C       PROGRAM IIIA  --  CRYSTAL STRUCTURE GROUP, MINES BRANCH, E.M.R.
C       MAGNETIC TAPE STORE AND DUMP PROGRAM.
C
        DIMENSION AD(20),BD(20)
        DATA CODE /4H    /,NN,NP /2*0/,NI/0/
        DATA ICR /1/,LPT/3/,IIT/14/,IOT/13/
C
C       READ TAPDUM CARD
        READ(ICR,100) MODE,NPNT
  100   FORMAT(10X,2I10)
        IF(MODE-2) 200,400,600
C       ***************************************************************
C       READ DATA CARDS AND WRITE NEW TAPE
  200   READ(ICR,210) AD
  210   FORMAT(20A4)
C
        NN=NN+1
        NP=NP-1
        IF(NP) 230,230,350
  230   NP=NPNT
        WRITE(LPT,300) NN,AD
  300   FORMAT(I10,10(',.'),20A4,10(',.'))
C
  350   WRITE(IOT,210) AD
        IF(AD(20)-CODE) 700,200,700
C       ***************************************************************
C       EDIT EXISTING MAGNETIC TAPE
  400   READ(ICR,410) AL,N,N1,N2
  410   FORMAT(A6,I4,2I10)
C
C       IDENTIFY CARD
        IF(N) 415,415,425
  415   IF(N1) 435,435,420
  420   IF(N2) 440,440,430
C
C       =INSERT= CARD
  425   N1=N1+1
        GO TO 440
C
C       =DELETE= CARD
  430   N=-1
        GO TO 440
C
C       =NOMORE= CARD
  435   N1=1000000
        GO TO 440
C
C       READ TAPE IMAGE
  440   READ(IIT,210) AD
        NI=NI+1
        IF(N1-NI) 999,445,480
C
C       MATCH - BRANCH TO FUNCTION
  445   N1=0
```

```
      IF(N) 470,450,460
C
C     CHANGE SINGLE REFLECTION
  450 READ(ICR,210) BD
      WRITE(IOT,210) BD
      NN=NN+1
      NP=NP-1
      WRITE(LPT,455) NN,BD,AL
  455 FORMAT(I10,10('*'),20A4,10('*'),A6)
      GO TO 400
C
C     INSERT 'N' REFLECTIONS
  460 DO 465 I=1,N
      READ(ICR,210) BD
      WRITE(IOT,210) BD
      NN=NN+1
      NP=NP-1
      WRITE(LPT,455) NN,BD,AL
  465 CONTINUE
      GO TO 480
C
C     DELETE REFLECTIONS N1 TO N2 INCLUSIVE
  470 IF(N2-NI)999,515,475
  475 READ(IIT,210) AD
      NI=NI+1
      GO TO 470
C
  480 NP=NP-1
      NN=NN+1
      IF(NP) 490,490,510
  490 NP=NPNT
  500 WRITE(LPT,300) NN,AD
C
  510 WRITE(IOT,210) AD
C
  515 IF(AD(20)-CODE) 650,520,650
  520 IF(N1) 400,400,440
C
C     ***************************************************************
      PRINT ONLY CURRENT TAPE
  600 NN=NN+1
      READ(IIT,210) AD
      WRITE(LPT,300) NN,AD
C     GO TO 600
C
      ERROR - SERIAL NUMBERS OUT OF ORDER
  999 WRITE(LPT,990) NI
  990 FORMAT('0CARD SERIAL NO. OUT OF ORDER -- DETECTED AT I/P TAPE IMAG
     1E NO.',I8)
  650 REWIND IIT
  700 ENDFILE IOT
C     REWIND IOT

      END
```

APPENDIX 4 - Source Listing of Program IIIB

```
C      PROGRAM IIIB  --  CRYSTAL STRUCTURE GROUP, MINES BRANCH, E.M.R.
C-----DATA PREPARATION PROGRAM (PREREQUESITE OF =DATRDN=)
C      TO REDUCE INTENSITIES COLLECTED ON THE MINES BRANCH
C      PICKER AUTOMATIC DIFFRACTOMETER.
C
C-----ARRAY DEFINITION.
       INTEGER  CDR,LPT,TAPIN,TAPOT
       INTEGER   X(10000),ISS(8),ISF(8)
       INTEGER  IH(3,100),IA(100),ISEG(12),R
       REAL TITLE(18),Y(10000),Z(10000),STD1(4),STD2(4),HHH(3)
       REAL  Q(3,3),AS(6),SET(3),B1(100),PK(100),B2(100),T(100)
       REAL FMT1(6),AR(8)
       DATA SMAX,FMAX,WMAX/3*0./,SMIN,FMIN,WMIN/3*10000./
       DATA ISUMUN,ISUMOB /2*0/,AR/8*0./
       DATA FMT1 /6H(I1,3I,6H4,5F8.,6H3,I2,I,6H5,I7,I,6H5,8X) ,6H
       DATA X /10000*0/, Y,Z /20000*0./, ISS,ISF /16*0/
       DATA NL/0/,NP/0/,IRF/0/,AB/1./,EX/1./,SCL2/1./,AS(1)/1./
       DATA HHH /1HH,1HK,1HL/
C**** DEVICE ALLOCATION
       DATA CDR/1/,LPT/3/,TAPIN/13/,TAPOT/15/
C
C-----ENTER PARAMETER CARDS
C
C-----(1).TITLE CARD.
       READ(CDR, 10) TITLE
   10 FORMAT(8X,18A4)
C
C-----(2).CELL CONSTANTS CARD.
       READ(CDR,20) A,B,C,ALP,BET,GAM,WL
   20 FORMAT(10X,7F10.5)
C
C      PREPARE  S2/L2 MATRIX Q(I,J).
       RAD= 3.14159265/180.
       COSA=COS(ALP*RAD)
       COSB=COS(BET*RAD)
       COSG=COS(GAM*RAD)
       SINA=SIN(ALP*RAD)
       SINB=SIN(BET*RAD)
       SING=SIN(GAM*RAD)
       V=A*B*C*SQRT(1.-COSA*COSA-COSB*COSB-COSG*COSG+2.*COSA*COSB*COSG)
       VS=.5/V
       AX=B*C*SINA*VS
       BX=A*C*SINB*VS
       CX=B*A*SING*VS
       Q(1,1)=AX*AX
       Q(1,2)=AX*BX*(COSA*COSB-COSG)/(SINB*SINA)
       Q(1,3)=AX*CX*(COSA*COSG-COSB)/(SINA*SING)
       Q(2,1)=Q(1,2)
       Q(2,2)=BX*BX
       Q(2,3)=BX*CX*(COSB*COSG-COSA)/(SINB*SING)
       Q(3,1)=Q(1,3)
       Q(3,2)=Q(2,3)
       Q(3,3)=CX*CX
       AX=2.*AX
```

```
      BX=2.*BX
      CX=2.*CX
C
C-----(3).  PROGRAM CONTROL CARD.
      READ(CDR,30) IIT,IOT,IOLS,IOL1,IOL2,JA,JE,J1,J2,J3
   30 FORMAT(10X,14I5)
C
C-----(4).SCALES CARD.
      READ(CDR,40) GS,(AS(I),I=2,6),SS
   40 FORMAT(10X,7F10.3)
C
C-----(5).COUNT TIMES CARD.
      READ(CDR,40) TS,TB1,TB2,CLP,POLK,SIGFAC,SIGCON
      IF(POLK) 41,41,42
   41 POLK=1.
   42 IF(SIGFAC) 43,43,44
   43 SIGFAC=1.65
   44 IF(SIGCON) 45,45,46
   45 SIGCON=0.5
C
C-----(6)*  ABSORPTION PARMETER CARDS.
   46 IF(JA) 50,90,50
   50 CONTINUE
C
C-----(7)*  EXTINCTION PARAMETER CARDS.
   90 IF(JE)  100,150,100
  100 CONTINUE
C
C-----(8).DATA LEAD CARD.
  150 READ(CDR,30) NSS,NSG,ISEG
C
C
      PRINT SUMMARY OF PARAMETERS BEFORE PROCEEDING
C
      WRITE(LPT,160) TITLE,A,B,C,ALP,BET,GAM,V,AX,BX,CX,WL
  160 FORMAT( 1H1//  10X,'DATA PREPARATION OF ... ',18A4
     $/  10X,19('-')
     $////  10X,'CELL CONSTANTS'  /  10X,14('-')
     $//  14X,'A =',F09.4,7X,'B =',F09.4,8X,'C =',F09.4,'  ANGSTROMS'
     $//10X'ALPHA =',F8.3,5X'BETA =',F8.3,5X'GAMMA =',F8.3,'   DEGREES'
     $//  10X,'VOLUME=',F09.3,'  CUBIC ANGSTROMS'
     $////  10X,'RECIPROCAL CELL CONSTANTS'  /  10X,25('-')
     $//   13X,'A* =',F09.6,6X,'B* =',F9.6,7X'C* =',F9.6,'  1/ANGSTROMS'
     $//// 10X,'WAVELENGTH =',F8.5,'  ANGSTROMS'  /  10X,10('-')     )
C
C
      WRITE(LPT,200)   GS,(I,AS(I+1),I=1,5)
  200 FORMAT(1H0//  10X,'SCALE FACTORS'  /  10X,13('-')
     $//  10X,'OVERALL INTENSITY SCALE =',F08.4
     $//  10X,'SCALE FOR ',5('ATTENUATOR  ',I1,' =',F08.4 //20X )    )
C
C
      WRITE(LPT,220) TS,TB1,TB2,SS,CLP,SIGFAC,SIGFAC,SIGCON,SIGFAC
  220 FORMAT(1H1/// 10X,'COUNT TIMES'  /  10X,11('-')
     $//  10X,'TWO THETA SCAN COUNT TIME  =',F8.3,'  SECONDS PER DEGREE'
     $//  10X,'PRE -BACKGROUND COUNT TIME =',F8.3,'  SECONDS'
     $//  10X,'POST-BACKGROUND COUNT TIME =',F8.3,'  SECONDS'      /1H1
     $////  10X,'STANDARD DEVIATIONS'  /  10X,19('-')
     $//  10X,'SIGMA(ATTENUATOR 1) =',F8.4,
```

```
     $//   10X,'SIGMA( SINE THETA )' / 10X,19('-'), ' =',F8.4
     $/    14X,'SINE THETA'
     $/// 10X,'REFLECTIONS WITH [INET**2/(IPK+IBG*T*T)] < ('F4.2,')**2
     $ARE CONSIDERED UNOBSERVED (*)'
     $/// 10X,'REFLECTIONS WITH INET NEGATIVE AND'
     $//  27X'[INET**2/(IPK+IBG*T*T)] > (',F4.2,')**2 ARE CONSIDERED UNO
     $BSERVED (#)'
     $/// 10X,'FOR UNOBSERVED REFLECTIONS I(REL) IS PUT EQUAL TO --  ',
     $   F4.2,'*',F4.2,'*SQRT(IPK+IBG*T*T)*SCALING FACTORS'            )
C
C
      WRITE(LPT,230)
  230 FORMAT(1H0/// 10X,'PROGRAM KEYED TO *'  /  10X,16('-')   )
C
C
      IF(IIT) 235,235,245
C
  235 WRITE(LPT,240)
  240 FORMAT(1H0  15X,'*ENTER INTENSITY DATA ON CARDS (ONE/REFLECTION)')
      GO TO 255
C
  245 WRITE(LPT,250)
  250 FORMAT(1H0  15X,'*ENTER INTENSITY DATA ON MAGNETIC TAPE'   )
C
C
  255 WRITE(LPT,260) NSS,NSG,(I,ISEG(I),I=1,NSG)
  260 FORMAT(1H0  15X,'*PROCESS DATA IN BLOCKS BOUNDED BY 'I1,' STANDARD
     $ REFLECTION(S)'/ 37X,'THERE ARE 'I1,' SEPARATE SEGMENTS OF DATA--'
     $/( 77X,'SEGMENT ',I1,' IS OF TYPE ',I1  )  )
C
      IF(IOLS) 263,263,261
  261 WRITE(LPT,262)
  262 FORMAT(1H0 15X'*PRINT REFLECTIONS DURING PROCESSING'   )
C
  263 IF(JA) 270,270,265
C
  265 WRITE(LPT,267)
  267 FORMAT(1H0  15X,'*APPLY ABSORPTION CORRECTIONS'   )
C
  270 IF(JE) 280,280,275
  275 WRITE(LPT,277)
  277 FORMAT(1H0  15X,'*APPLY EXTINCTION CORRECTIONS'   )
C
C
  280 IF(IOL1) 295,295,290
  290 WRITE(LPT,292)
  292 FORMAT( 1H0 15X,'*PRINT SUMMARY OF I(REL) DATA IN ORDER OF INPUT')
C
C
  295 WRITE(LPT,300) HHH(J1),HHH(J3)
  300 FORMAT(1H0 15X,'*SORT I(REL) DATA WITH ',A1,' SLOW, ',A1,' FAST VA
     $RYING'   )
C
      IF(IOL2) 310,310,305
C
  305 WRITE(LPT,307)
  307 FORMAT(1H0  15X,'*PRINT SUMMARY OF I(REL) DATA IN SORTED ORDER' )
C
```

```
  310 IF(IOT) 320,320,315
C
  315 WRITE(LPT,317)
  317 FORMAT(1H0  15X,'*OUTPUT I(REL) DATA ON MAGNETIC TAPE'  )
  320 CONTINUE
C
C-----SET UP ARRAYS AND CONSTANTS.
      WL=WL*WL
      TS=TS/(TB1+TB2)
      SS=SS*SS/(AS(2)*AS(2))
      SIGF=SIGFAC*SIGCON
      SIGFAC=1./(SIGFAC*SIGFAC)
C
      IDEV=CDR
      IF(IIT) 340,350,340
  340 REWIND TAPIN
      IDEV=TAPIN
  350 IF(IOT) 360,370,360
  360 REWIND TAPOT
  370 I1=0
C
C
C-----START OF SEGMENT LOOP.
      DO 3000 I1=1,NSG
C
C-----INITIALIZE COUNTERS, ETC..
      R=ISEG(I1)
      IF(ISF(R)) 400,400,425
  400 J=1
      DO 420 K=1,8
      IF(ISF(J)-ISF(K)) 410,420,420
  410 J=K
  420 CONTINUE
      ISS(R)=ISF(J)
      GO TO 430
  425 AR(R)=AR(R)+1.
      ARW=AR(R)
      RRW=1./(ARW+1.)
  430 IS=ISS(R)
      DF=0.
C
C-----ENTER REFLECTION DATA ON CARDS OR TAPE.
  440 IB=0
  450 IB=IB+1
C
  460 READ(IDEV,FMT1) K,(IH(I,IB),I=1,3),SET,SB1,SB2,IA(IB),L,M,N
      IF(SB1) 650,2900,650
C
C
      CALCULATE TIME RATIO 2THETA/BACKGROUND SCANS
  650 T(IB)=TS*(SB2-SB1)
      B1(IB)=L
      PK(IB)=M
      B2(IB)=N
C
C-----IS REFLECTION STANDARD OR NORMAL.
      IF(K)1000,700,1000
C
C-----PROCESS NORMAL REFLECTIONS.
```

```
  700 IF(JA) 750,800,750
C
C-----BRANCH TO ABSORPTION CORRECTION SUBROUTINE.
  750 CONTINUE
  800 IF(JE) 850,900,850
C
C-----BRANCH TO EXTINCTION CORRECTION SUBROUTINE.
  850 CONTINUE
C
C-----BRANCH TO NEXT REFLECTION.
  900 CONTINUE
      GO TO 450
C
C-----PROCESS STANDARD REFLECTION.
 1000 STD2(K)=PK(IB)-T(IB)*(B1(IB)+B2(IB))
      IF(NSS-K) 1020,1020,450
 1020 IF(IB-K) 1024,1024,1030
 1024 IF(IRF) 1030,1025,1030
C
C-----STORE REFERENCE COUNT OF FIRST STANDARDS.
 1025 DO 1026 I=1,NSS
 1026 STD1(I)=STD2(I)
C
C-----CALCULATE INDIVIDUAL STD. SCALES.
 1030 IB=IB-NSS
      J=IB
      A=0.
      DO 1100  I=1,NSS
      B=STD1(I)/STD2(I)
      J=J+1
C     BRANCH ON PRINT FLAG
      IF(IOLS) 1080,1080,1035
 1035 L=B1(J)
      M=PK(J)
      N=B2(J)
      NL=NL-2
      IF(NL) 1040,1040,1060
C-----NEW PAGE-PRINT TITLE, HEADINGS.
 1040 NL=50
      NP=NP+1
      WRITE(LPT,1050) TITLE,I1,R,NP
 1050 FORMAT('1',4X,18A4,9X,'SEGMENT NO.',I3,'  TYPE',I3,15X,'PAGE',I4//
     1'      N      H    K    L     AT     B1C      PKC      B2C    TP/TB    I(NET
     2)    TSCL      ABS      EXT    S2/L2     1/LP      LSWT     F(REL)    DELT
     3A'/)
      IF(IRF) 1060,1052,1060
 1052 WRITE(LPT,1054)
 1054 FORMAT('0',11X,'**** REFERENCE STANDARD REFLECTION(S) ****')
C
 1060 WRITE(LPT,1070)   (IH(K,J),K=1,3),L,M,N,STD2(I),B
 1070 FORMAT('0',11X,'STANDARD REFLECTION' ,3I4,'   WITH COUNTS',3I6,'
     1 WHICH GIVES I(NET) =',F8.0,'   AND SCALE OF',F8.5)
 1080 A=A+B
 1100 CONTINUE
      IF(IRF) 1106,1102,1106
 1102 IRF=1
C     CHECK PRINT FLAG
      IF(IOLS) 440,440,1103
```

```
 1103 WRITE(LPT,1104)
 1104 FORMAT('0',11X,'-----------------------------------------------------'//)
      NL=NL-6
      GO TO 440
C-----CALCULATE AVERAGE SCALE
 1106 CONTINUE
      SCL1=SCL2
      SCL2=A/NSS
C-----CALCULATE SCALE INCREMENT.
 1110 DS=SCL2-SCL1
      DD=0.5*DS*DS
      DS=DS/(IB+1)
C     BRANCH ON PRINT FLAG
      IF(IOLS) 1130,1130,1115
 1115 WRITE(LPT,1120) SCL2,SCL1,IB,DS
 1120 FORMAT('0',11X,'AVERAGE SCALE ='F10.5,'  PREVIOUS SCALE =',F10.5,
     1'  NO. OF REFLNS. =',I3,'  SCALE INCR. =',F08.5/)
      NL=NL-3
 1130 IF(IB) 1140,450,1140
C
C
C-----REDUCE ONE BLOCK OF INTENSITY DATA.
C
 1140 DO 2500 N=1,IB
C
C-----CALCULATE SIN**2(THETA)/LAMBDA**2.
      S=0.
      DO 1160 I=1,3
      B=0.
      DO 1150 J=1,3
 1150 B=B+IH(J,N)*Q(I,J)
 1160 S=S+IH(I,N)*B
C
C-----CALCULATE LORENTZ-POLARIZATION FACTOR.
      SMAX=AMAX1(SMAX,S)
      SMIN=AMIN1(SMIN,S)
      A=S*WL
      B=SQRT(A)
      C=SQRT(1.-A)
      D=1.-2.*A
      RLP=2.*B*C*(1.+POLK)/(1.+POLK*D*D)
C
C-----CALCULATE TOTAL SCALE.
      SCL1=SCL1+DS
      M=IA(N)
      TK=SCL1*AS(M+1)*GS
C
C-----CALCULATE OBSERVED S.F.
      G=T(N)*(B1(N)+B2(N))
      CN=PK(N)-G
      TEN=ABS(TK*AB*EX*CN)
      FOB=SQRT(RLP*TEN)
C
C-----CALCULATE SFLS WEIGHT.
C     ATTENUATOR SCALES CONTRIBUTION.
C     SIG=M*M*SS
      STANDARD REFLECTION SCALE CONTRIBUTION.
      SIG=SIG+DD/(SCL1*SCL1)
```

```
C       LORENTZ-POLARIZATION CORRRECTION CONTRIBUTION
        E=0.5/(B*C)
        E=4.*A*D*E*(E+RLP)*CLP
        SIG=SIG+E*E
C       COUNTING STATISTICS CONTRIBUTION.
        D=(PK(N)+T(N)*G)/(CN*CN)
        SIG=SIG+D
C
C-----TOTAL WEIGHT.
        WT=4./(FOB*FOB*SIG)
C
C-----TEST FOR 0.01 SIGNIFICANCE LEVEL--- * INDICATES TEST FAILED.
        IF(SIGFAC-D) 1800,1800,1900
 1800   FS=1H*
        SWT=-WT
        GO TO 1915
 1900   IF(CN) 1910,1910,1920
C-----NEGATIVE NET COUNT- MARK WITH # (12-8-7)
 1910   FS=1H#
        SWT=-WT
 1915   TEN=ABS(TK*AB*EX*SIGF*SQRT(PK(N)+G*T(N)))
        FOB=SQRT(RLP*TEN)
        GO TO 2000
 1920   FS=1H
        SWT= WT
C
C-----STORE REFLECTION IN PERMANENT ARRAY.
 2000   IS=IS+1
        IF(X(IS)) 2180,2100,2180
C-----NEW REFLECTION.
C       PACK INDICES WORD IN SORTING ORDER (SLOW,MEDIUM,FAST).
 2100   I=1
        IF(IH(J3,N)) 2110,2120,2120
 2110   I=I+1
 2120   IF(IH(J2,N)) 2130,2140,2140
 2130   I=I+2
 2140   IF(IH(J1,N)) 2150,2160,2160
 2150   I=I+4
 2160   X(IS) = I +IABS(IH(J1,N))*100000
       1          +IABS(IH(J2,N))*1000
       2          +IABS(IH(J3,N))*10
        Y(IS)=TEN
        Z(IS)=SWT
        GO TO 2200
C
C       EQUVALENT REFLECTION TO BE AVERAGED.
 2180   DF=SQRT(RLP*Y(IS))-FOB
        Y(IS)=(Y(IS)*ARW+TEN)*RRW
        D     =4./(1./ABS(Z(IS))+1./WT)
        IF(Z(IS)) 2184,2184,2182
 2182   IF(SWT) 2184,2184,2186
 2184   D=-D
 2186   Z(IS)=D
C
C-----PRINT DATA SUMMARY- ONE REFLECTION PER LINE.
C
 2200   IF(IOLS) 2500,2500,2205
 2205   NL=NL-1
```

```
      IF(NL) 2210,2210,2250
C-----NEW PAGE -PRINT TITLE,HEADINGS.
 2210 NL=50
      NP=NP+1
      WRITE(LPT,1050) TITLE,I1,R,NP
C-----PRINT REFLECTION DATA.
 2250 M=CN+.5
      L=B1(N)
      K=B2(N)
      J=PK(N)
      WRITE(LPT,2260) IS,(IH(I,N),I=1,3),IA(N),L,J,K,T(N),M,TK,AB,EX,S,
     1RLP,WT,FOB,FS,DF
 2260 FORMAT(2I6,2I4,I6,I7,I9,I7,F8.3,I9,3F8.4,F8.5,F8.4,F9.4,F9.3,A1,
     1 F7.3)
C
C-----END OF BLOCK LOOP.
 2500 CONTINUE
      GO TO 440
C
 2900 NL=0
      ISF(R)=IS
C
C-----END OF SEGMENT LOOP.
 3000 CONTINUE
C
      IF(IOL1) 3100,3500,3100
C
C---- PRINT PERMANENT ARRAY OF HKL,IREL,LSWT
 3100 J=1
      DO 3120 K=1,8
      IF(ISF(J)-ISF(K)) 3110,3120,3120
 3110 J=K
 3120 CONTINUE
      IS=ISF(J)
C     SET COUNTER FOR BLOCK PRINTOUT.
 3130 I=1
      J=50
      K=IS-1
 3135 IF(K-200) 3140,3140,3150
 3140 J=(K/4)+1
 3150 L=I+J-1
      NP=NP+1
      WRITE(LPT,3170) TITLE,NP
 3170 FORMAT('1',06X,18A4,43X,'PAGE ',I3//
     1 4('        N   H  K  L   I(REL)  LSWT')/)
C-----PRINTOUT REFLECTIONS 4 COLS./PAGE.
      DO 3400 I1=I,L
      M=0
      DO 3300 I2=1,4
      N=M+I1
      IA(I2)=N
C-----UNPACK INDICES WORD X(N).
      CALL HKL(X(N),IH(J1,I2),IH(J2,I2),IH(J3,I2))
 3230 ISS(I2)=Y(N)
      B2(I2)=Z(N)
 3300 M=M+J
C
      NN=4
```

```
      IF(X(N)) 3320,3310,3320
 3310 NN=3
 3320 CONTINUE
C
C-----PRINT OUT LINE OF FOUR (4) REFLECTIONS.
      WRITE(LPT,3350) (IA(M),(IH(N,M),N=1,3),ISS(M),B2(M),M=1,NN)
 3350 FORMAT(4(I8,I4,2I3,I8,F7.3))
 3400 CONTINUE
      I=I+200
      K=K-200
      IF(K) 3450,3450,3135
 3450 IF(II) 3500,3500,4000
C
C-----SORT ROUTINE.
C
 3500 II=1
      DO 3600 I=1,IS
      K=I
      L=I+1
      IF(L-IS) 3520,3520,3580
 3520 DO 3560  J=L,IS
      IF(X(K)-X(J)) 3560,3560,3540
 3540 K=J
 3560 CONTINUE
 3580 J=X(I)
      X(I)=X(K)
      X(K)=J
      A=Y(I)
      FMAX=AMAX1(FMAX,Y(K))
      FMIN=AMIN1(FMIN,Y(K))
      Y(I)=Y(K)
      Y(K)=A
      A=Z(I)
      IF(Z(K)) 3585,3590,3590
 3585 ISUMUN=ISUMUN+1
      B=-Z(K)
      GO TO 3595
 3590 ISUMOB=ISUMOB+1
      B=Z(K)
 3595 WMAX=AMAX1(WMAX,B)
      WMIN=AMIN1(WMIN,B)
      Z(I)=Z(K)
      Z(K)=A
 3600 CONTINUE
      WRITE(LPT,3650) HHH(J1),HHH(J3)
 3650 FORMAT('1',///,09X,'REFLECTIONS HAVE BEEN SORTED INTO ',A1,' SLOW'
     1 ',A1,' FAST VARYING.')
      WRITE(LPT,3800) IS,ISUMOB,ISUMUN,FMAX,FMIN,SMAX,SMIN,WMAX,WMIN
 3800 FORMAT(1H0///  9X,'THERE ARE',I5,' UNIQUE REFLECTIONS OF WHICH --'
     $// 18X,I5,' ARE CONSIDERED OBSERVED'
     $// 18X,I5,' ARE CONSIDERED UNOBSERVED (LSWT MARKED -VE)'
     $////  9X,'MAXIMUM  RELATIVE  INTENSITY          =',F10.1
     $//   9X,'MINIMUM  RELATIVE  INTENSITY          =',F10.1
     $////  9X,'MAXIMUM (SINE THETA/ LAMBDA)**2       =',F10.5
     $//   9X,'MINIMUM (SINE THETA/ LAMBDA)**2       =',F10.5
     $////  9X,'MAXIMUM LEAST SQUARES WEIGHT          =',F10.4
     $//   9X,'MINIMUM LEAST SQUARES WEIGHT          =',F10.4  )
      IF(IOL2) 3100,4000,3100
```

```
 4000 IF(IOT) 4010,4200,4010
C
C-----OUTPUT =FORMAT= AND =REFIN= CARD IMAGES ON MAG. TAPE.
C
 4010 WRITE(TAPOT,4020)
 4020 FORMAT('FORMAT(4I5,2F20.6,20X)',58X)
      WRITE(TAPOT,4030) IS
 4030 FORMAT('REFIN',10X,16,9X,' IH IK IL ID FR FW    ',28X)
C
C-----OUTPUT PERMANENT ARRAYS AS CARD IMAGES ON MAG. TAPE.
C
 4050 DO 4100 I=1,IS
      CALL HKL(X(I),IA(J1),IA(J2),IA(J3))
      J=1
      A=Y(I)
      B=Z(I)
      IF(B) 4060,4080,4080
 4060 B=-B
      J=2
 4080 B=SQRT(B)
      WRITE(TAPOT,4090) IA(1),IA(2),IA(3),J,A,B
 4090 FORMAT(4I5,2F20.6,20X)
 4100 CONTINUE
C
C-----RESET DEVICE NUMBERS WITH =FILES= CARD IMAGE.
C
      WRITE(TAPOT,4150)
 4150 FORMAT('FILES  01 03 13 14 02 03 15 08 09 20 21 22',38X)
      END FILE TAPOT
      REWIND TAPOT
C
 4200 IF(IIT) 4250,4300,4250
 4250 REWIND TAPIN
 4300 CALL EXIT
C
C
C
C
      *****SUBROUTINE TO UNPACK INDICES WORD.
      SUBROUTINE HKL(I,J,K,L)
C
      INTEGER   IH(8),IK(8),IL(8),W
      DATA IH /+1,+1,+1,+1,-1,-1,-1,-1/
      DATA IK /+1,+1,-1,-1,+1,+1,-1,-1/
      DATA IL /+1,-1,+1,-1,+1,-1,+1,-1/
C
      W=MOD(I,10)
C
      J=ISIGN(I,IH(W))/100000
      K=MOD(ISIGN(I,IK(W)),100000)/1000
      L=MOD(ISIGN(I,IL(W)),1000)/10
C
   60 RETURN
      END
```

CANADA. MINES BRANCH

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