

27  
2-2-77  
25-10-77  
IS-4169

USERS GUIDE TO FINGER, THUMB, AND  
TRIPLE AXIS REAL TIME EXPERIMENT  
CONTROL PROGRAMS

**MASTER**

Thomas G. Pinter and Elaine M. Notis



AMES LABORATORY, USERDA  
IOWA STATE UNIVERSITY  
AMES, IOWA

Date Transmitted: April 1977

PREPARED FOR THE U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION  
UNDER CONTRACT W-7405-eng-82

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

## **DISCLAIMER**

**This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.**

## **DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

USERS GUIDE TO FINGER, THUMB, AND TRIPLE AXIS  
REAL TIME EXPERIMENT CONTROL PROGRAMS

Thomas G. Pinter and Elaine M. Notis

Ames Laboratory, ERDA

Iowa State University

Ames, Iowa 50011

NOTICE  
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Date Transmitted: April 1977

PREPARED FOR THE U. S. ENERGY RESEARCH AND  
DEVELOPMENT ADMINISTRATION UNDER CONTRACT NO. W-7405-eng-82

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

*[Handwritten signature]*

—NOTICE—

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Available from: National Technical Information Service  
U. S. Department of Commerce  
P.O. Box 1553  
Springfield, VA 22161

Price: Microfiche	\$3.00
Printed	\$4.50

## TABLE OF CONTENTS

	PAGE
ABSTRACT	iv
I. USER-SYSTEM INTERACTIONS	1
II. EXPERIMENT START UP	4
III. TRIPLE AXIS SPECTROMETER	9
A. GENSCAN	9
B. DBLRCK	12
C. QESCAN	16
1. SEMI-PERMANENT DATA	17
2. SCAN DATA	19
IV. FINGER AND THUMB SPECTROMETERS	22
A. GENSCAN	22
B. DBLROCK	23
C. Q(E)SCAN	24
1. SEMI-PERMANENT DATA	25
2. SCAN DATA	27
V. UTILITIES	27
A. DISKREAD	27
B. DUMPSPD	28
C. TAPESTART	28
D. TESTQ(E)	29
E. UPDATE	30
VI. PLOTTER	33
VII. ACKNOWLEDGEMENTS	37
VIII. APPENDICES	38
A. TRIPLE AXIS INPUT SUMMARY	38
B. FINGER AND THUMB INPUT SUMMARY	40
C. PLOTTER SUMMARY	42
D. LOADING DATA SETS FROM OBJECT CARDS	43
E. DATA SET AND FILE ORGANIZATION	46

## ABSTRACT

This manual provides the user with instructions for using the real time control system for the neutron scattering spectrometers: finger, thumb, and triple axis. The input requirements of the various programs are described in detail. Logging on procedures, program loading, and data set organization are also discussed.

Distribution List

Chicago Patent Office	1
USERDA-TIC	27
Ames Laboratory Library	5
Thomas G. Pinter	10
Elaine M. Notis	9
	—
Total	52



## I. User-System Interactions

Communication with the PDP-15 system is by teletypewriter. Turning the teletype to LINE activates it for this communication to the PDP-15. For those teletypes with a black box, switching the toggle switch from AUTO to ON also activates the teletype. After all input has been entered, the switch should be toggled back to AUTO, so that it is activated only during printing. To initiate a session, a CONTROL A (SOM) is struck. The CONTROL (CNTL) key is to the left of the keyboard and is used to generate non-printable ASCII characters for communication to the PDP-15. The commonly used characters are shown in Figure 1. After typing (SOM) the computer responds with REQ, INQ OR ZAP?. This is how the user gains access to the procedures he/she desires to execute. The responses to this statement will be discussed separately. See Figure 2 for examples of these uses.

CONTROL A (SOM)	Activates log-on routines in PDP-15 system.
CONTROL D (EOT)	Signals end of transmission, all user entered lines must end with EOT.
CONTROL U (ERROR)	Erases the input from the last question mark.
CONTROL F	Erases the last character of the present input line. Repeating N times erases N characters.
CONTROL X	Terminates the output message.

Figure 1. Teletypewriter control characters.

REQ Response: To initiate a set of user procedures, the response to REQ, INQ OR ZAP? is REQ. At this point the teletype will type the statement: LIBRARY NAME(S)?. Here the response is the library in which the procedures are stored. Libraries may be concatenated together by separating each library name with a period, e.g., TRIAX.FINGER. The library named UNIVERSAL is automatically concatenated to the libraries entered and does not need to be explicitly entered by the user unless it is to be the only library accessed. The libraries are searched in the order given in the input list. In the example above TRIAX would first be searched for the requested procedure, followed by a search of FINGER if it was not found, and finally by a search of UNIVERSAL.

After the request for the library name has been satisfied, the teletype will print the query: USER TASK NAME?. The response to this is the main procedure which is to be executed. The teletype then prints a line of start up information. The information includes the time and date, the starting address in core, the user I.D., and the libraries to be searched for programs.

Upon task completion, the system prints the message

TASK START COMPLETED \*-\* CODE = ##### ADDRESS = #####

USER ID = #### \*-\*

Upon normal completion, the completion code will be 000000 or 004000 and END will be printed at end of line. ABEND is printed at the end

of the line for an abnormal end. The nature of an abnormal end can be identified by looking up the completion code in the ALECS language manual.

(SOM)

REQ, INQ OR ZAP? REQ (EOT)

LIBRARY NAME(S)? TRIAX (EOT)

USER TASK NAME? START (EOT)

DATE/TIME TASK START @ 027400.2034 LIB(S): TRIAX

DISPATCH

- a.) Example of initial start up using REQ. Note the core address 27400 followed by the user I.D., 2034.

(SOM)

REQ, INQ OR ZAP? ZAP (EOT)

TYPE IN USER ID? 2034 (EOT)

- b.) Example of ZAP of task START.

INQ Response: If the user desires to communicate with his procedures, he may do this by using the inquiry mode. To do this he/she responds INQ to the REQ, INQ OR ZAP? request. The teletype answers TYPE IN USER I.D.. The number requested is the number the system assigned the program during the original REQ. At this point control is transferred to the ON ATTENTION block of the main procedure. If no ON ATTENTION block is there, then the request is ignored. The ON ATTENTION block may allow user interaction with his procedures when they are being executed.

ZAP Response: The final response is ZAP. This allows the user to terminate any task currently in core. After the user responds ZAP, the teletype responds with TYPE IN USER I.D.? as before. The user responds with the USER I.D. assigned by the system to the task he/she wishes to ZAP. Two remarks must be made:

1.) Usually a task must be zapped at a teletype different than the one from which the task was initiated. 2.) If the task is waiting for input, an (EOT) must be entered on the original teletype before the task will be removed from core.

## II. Experiment Start Up

In this section, the procedure for initiating an experiment will be described. The initial start up procedure is the same for each spectrometer; hence they will be described collectively below.

After a REQ response for a program load, the user responds FINGER, THUMB, or TRIAX depending upon which spectrometer he/she is using. The task which drives each spectrometer is START. Two other initial tasks are available: RESTART, which restarts the experiment at the point at which it was interrupted; and UPDATE, which allows user control of the scan file. RESTART will be described below, while UPDATE will be described in Section V. START is used to input the scans to be executed and requires input of the scans which will be executed. The rest of this section will describe the common input to START.

After calling START, the teletype prints CHANGE TITLE--YES OR NO?.\* If the user desires to change the title, which is stored on disk and printed at the top of each scan, he/she responds YES. The desired title is then entered. This title consists of 56 (finger/thumb) or 69 (triax) alphanumeric characters. A response of NO or (EOT) retains the title currently stored on disk.

For the triax spectrometer alone, the teletype responds FIX ANGLES--YES OR NO. This is to allow certain angles to remain stationary throughout the scans. The control word which marks those angles which are not to be moved is stored on disk. Thus, the user needs only to set this word when he/she desires to change it. To set this control word, the user responds YES; then he/she enters '0' for angles which are to be backlashed and/or scanned, '1' for any angle which is never to be moved. The order of entry is  $\theta_M$ ,  $2\theta_M$ ,  $\psi$ ,  $\phi_1$ ,  $\theta_{A1}$ ,  $2\theta_{A1}$ ,  $\phi_2$ ,  $\theta_{A2}$ ,  $2\theta_{A2}$ . The user enters NO or (EOT) if this control word is not to be changed.

The teletype next responds STARTING FILE?. This request allows the user control of the file upon which to begin storing the count data (Appendix E). Thus, data currently stored on the count data set can be preserved for later use. If user enters 3 say, the first 2 data files are saved. The data for the first scan is then stored in file 3, the rest of the scans following in order. The user may not enter a starting

---

\*All requests requiring a yes or no response will print yes or no as part of the request; otherwise, a numerical response is necessary.

scan number greater than  $n+1$  where  $n$  is the last file currently stored. If he/she does so, the task will abend with a completion code 000013, i.e., the end of the data set was encountered.

Now the teletype responds GENSCAN, DBLRCK, OR QESCAN?. The user enters the type of scan he/she desires to perform. Only the first three characters are necessary, although all will be accepted. The program will now branch to the proper input routine for the desired scan. See Figure 3 for an example of the start procedure.

When entering scan data, the user may accidentally enter an improper character. This causes a conversion error which is trapped by the program. When this happens, the teletype prints REPEAT. The user then enters the line number he/she wishes to repeat, and control is transferred to that line. These lines are identified by the numbers printed on the extreme left of each input line. If no line numbers appear, then control is automatically returned to the beginning of the input.\*

Each separate scan is identified by a scan number. The first scan is always SCAN 1. SCAN I is typed before the  $i^{\text{th}}$  input scan is entered so that the user may readily identify where he/she is. The number of scans which can be entered is limited by the size of the data set (Figure 4). When this number is exceeded, the teletype types FILE FULL. The input program is then exited.

---

\*The user can generate a conversion error if he/she desires to correct an error in the data already entered.

When the last scan has been entered, the teletype prints LAST  
SCAN N where N is the scan number appearing above the last entry.  
 This is followed by the request CHANGE OR ADD?. If the user desires  
 to change any scan on the data set, he enters its corresponding scan

(SOM)

REQ, INQ OR ZAP? REQ (EOT)

LIBRARY NAME(S)? TRIAX (EOT)

USER TASK NAME? START (EOT)

DATE/TIME TASK START @ 027400.2034 LIB(S): TRIAX

DISPATCH

CHANGE TITLE--YES OR NO? YES (EOT)

FIX ANGLES--YES OR NO? YES (EOT) ? 1 (EOT) ? 1 (EOT)  
 ? 0 (EOT) ? 0 (EOT) ? 0 (EOT) ? 0 (EOT) ? 1 (EOT)  
 ? 1 (EOT) ? 1 (EOT)

THIS IS A SAMPLE OF INPUT FOR START. (EOT)

STARTING FILE? 2 (EOT)

GENSCAN, DBLOCK, OR QESCAN? GENSCAN (EOT)

Figure 3. Example showing initiation of procedure START fixing  
 angles  $\theta_M$ ,  $2\theta_M$ ,  $\varphi_2$ ,  $\theta_{A2}$ , and  $2\theta_{A2}$  throughout the scan  
 and storing data starting with file 2.

number, I. The program accepts new input data for this scan only.

The user may add scans to the end of the data set by entering the number  
 N+1. This allows the user to add scans until he/she terminates the  
 input program normally. To start the experiment, the user enters a 0 or  
 (EOT) to the CHANGE OR ADD request.

As each scan is performed, the teletype prints the scan title followed by FILE I. Here *i* is the number of the file on the count data set (Appendix E). If the user wishes to access this spectrum from one of the utilities, he enters the appropriate file number when requested.

The teletype also prints initial scan data. The spectrum is printed with the associated key number for the count file and the non-preset counting interval. The key marks the location of the data point on the count data set. The maximum key value which can be stored is currently 1280.

<u>Program</u>	<u>Directory</u>		
	Thumb	Finger	Triax
stepscan	50	50	17
doublerock	50	50	17
q(e)-scan	25	25	17

Figure 4. Maximum number of scan files on each data set.

If the program is stopped for any reason, the user can continue from the point of interruption by calling program RESTART rather than START. RESTART has no input data, but it reads the scan data set to see where the scan was terminated. The program then restarts the experiment at that point.

Each spectrometer has a button for stopping the scan immediately. For all spectrometers, the scan is immediately stopped if it is in



progress. If programs are computing between scans, it is better to zap the program rather than stop the program with the dump button. For the doublerock experiment, pushing the dump button causes the current scan to terminate. The program then proceeds to the mean calculation. Doublerocks must be zapped to stop the programs.

### III. Triple Axis Spectrometer

This section describes the input required for scans on the triple axis spectrometer (triax). The three possible scan types, GENSCAN, DBLRCK, or QESCAN, will be discussed separately below. All angle related input is in the order: monochromator,  $\theta_M$ ; drum,  $2\theta_M$ ; sample table,  $\Psi$ ; G-arm 1,  $2\theta_{S1}$ ; analyzer crystal 1,  $\theta_{A1}$ ; V-arm 1,  $2\theta_{A1}$ ; G-arm 2,  $2\theta_{S2}$ ; analyzer crystal 2,  $\theta_{A2}$ ; V-arm 2,  $2\theta_{A2}$ .

#### A. GENSCAN

GENSCAN is a set of programs which steps selected angles by a constant stepsize. Upon entry the teletype prints TYPE END TO EXIT. This is the input termination command. The teletype next prints SCAN 1. Next 1--? is printed and the program is ready for input.

The entry on line 1 is the scan type specified by a three character code. The first character is a 2 if  $\theta$ - $2\theta$   $\frac{1}{2}$  angling is to be performed. The increment for the  $\frac{1}{2}$  angling scan must be the  $\theta$  angle. The second character specifies the  $2\theta$  angle when  $\frac{1}{2}$  angling. The first and second characters specify the scan angle when there is

no  $\frac{1}{2}$  angling. The third character specifies the detector(s) and is either 1, 2, or B. The user responds with one of the three character codes from Figure 5.

Next the teletype prints 2--? requesting the stepsize, the number of steps on each side of the center, and the preset value. The preset value is negative for counting against time and positive for counting against monitor. Finally the teletype prints 3--? requesting the center angle of the scan for each angle which moves, and the proper position for each angle which does not move. An input of zero for an angle value uses its current position; however, the angle will be backlash unless its corresponding FIX word bit is 1. If 0 is the desired angle value, the user must enter 360.

Type of Scan Code1/2 Angle1st Character Specifies  $\theta$  -  $2\theta$  Action2nd Character Specifies  $2\theta$ 

3rd Character Specifies Detector

<u>Code</u>	<u>1st Angle</u>	<u>2nd Angle</u>	<u>Detector</u>
2G1	Sample Table ( $\psi$ )	G-Arm 1 ( $\varphi_1$ )	1
2G2	Sample Table ( $\psi$ )	G-Arm 2 ( $\varphi_2$ )	2
2D1	Monochromator ( $\theta_M$ )	Drum ( $2\theta_M$ )	1
2D2	Monochromator ( $\theta_M$ )	Drum ( $2\theta_M$ )	2
2V1	Analyzer Xtal ( $\theta_{A1}$ )	V-Arm 1 ( $2\theta_{A1}$ )	1
2V2	Analyzer Xtal ( $\theta_{A2}$ )	V-Arm 2 ( $2\theta_{A2}$ )	2
2VB	Both $\theta_{A1}$ , $\theta_{A2}$	Both $2\theta_{A1}$ , $2\theta_{A2}$	1,2

No 1/2 Angle

1st and 2nd Characters Specify Scanning Angle

3rd Character Specifies Detector

<u>Code</u>	<u>Angle</u>	<u>Detector</u>
GA1	G-Arm 1 ( $\varphi_1$ )	1
GA2	G-Arm 2 ( $\varphi_2$ )	2
GAB	Both $\varphi_1$ and $\varphi_2$	1,2
ST1	Sample Table ( $\psi$ )	1
ST2	Sample Table ( $\psi$ )	2
MN1	Monochromator ( $\theta_M$ )	1
MN2	Monochromator ( $\theta_M$ )	2
DM1	Drum ( $2\theta_M$ )	1
DM2	Drum ( $2\theta_M$ )	2
AX1	Analyzer Xtal ( $\theta_{A1}$ )	1
AX2	Analyzer Xtal ( $\theta_{A2}$ )	2
AXB	Both $\theta_{A1}$ , $\theta_{A2}$	1,2
VA1	V-Arm 1 ( $2\theta_{A1}$ )	1
VA2	V-Arm 2 ( $2\theta_{A2}$ )	2
VAB	Both $2\theta_{A1}$ , $2\theta_{A2}$	1,2

Figure 5. Scan types for GENSCAN.

The user enters END as the scantype to terminate the input. The program then asks for corrections, and either updates the scan data set or starts the scan (see Figure 6).

```

GENSCAN, DBLRCK, OR QESCAN?  GEN (EOT)

TYPE END TO EXIT

SCAN 1

1--?  MN1 (EOT)

2--?  .02 (EOT) ? 25 (EOT) ? -10 (EOT)

3--?  116 (EOT) ? 41.87 (EOT) ? 0 (EOT) ? 0 (EOT)
? 0 (EOT) ? 0 (EOT) ? 0 (EOT) ? 0 (EOT) ? 0 (EOT)

SCAN 2

1--?  END (EOT)  LAST SCAN 1

CHANGE OR ADD?  (EOT)

```

Figure 6. Example showing genscan to step  $\theta_M$  angle .02 degree steps about 116 degrees with 2 $\theta_M$  41.87 degrees. All other angles remain at current positions. If the user noted an error or wished to add a scan, he/she would have responded 1 or 2 to the CHANGE OR ADD request. The program would then return to the input routine.

## B. DBLRCK

DBLRCK is a set of procedures which performs two step scans consecutively in order to maximize the peak of each scan. This is continued, alternating scans, until the change in the weighted mean of each spectrum is less than a predetermined value for two successive scans.

The teletype prints TYPE END TO EXIT. Next the teletype prints SCAN 1 followed by 1--?. The user then enters the desired 3 character scantype (see Figure 7). The first character is 1 if the doublerock angles are uncoupled, or 2 if the first scan angle is stepped by  $\theta/2$  when the second angle is stepped by  $\theta$ . The second character indicates the first angle of the doublerock: M for monochromator, A for analyzer crystal, or S for sample table. The third character is 1 for counting on detector 1 or 2 for counting on detector 2.

Next the teletype prints 2--?. The user enters the scan multiplier, the counting interval preset value, and the starting scan. The multiplier is a factor which multiplies the stepsize of scan 1 if the scan "looks" too narrow when doing a quickscan. This is determined by comparing the initial scan count and the final scan count to see if they are reasonably close together. The preset value is negative to count against time and positive to count against monitor. If preset is 0, then a preliminary quickscan is performed at every other scan point. The preset is then adjusted so that the maximum of the scan is 2000 counts. Start is 1 if the doublerock is to start with the first scan angle, or 2 if the second angle is the starting scan.

The teletype then responds 3--?. The user enters the stepsize, the convergence criterion, and number of steps on each side of the center angle. These quantities are entered for scan angle 1 and then for scan angle 2 respectively. The convergence criterion is

Type of Scan Code

1st Character Specifies Independent Angles or 1/2 Angling

2nd Character Specifies  $\theta$  of  $\theta - 2\theta$  Pair

3rd Character Specifies Detector

Independent Angles

<u>Code</u>	<u>1st Angle</u>		<u>2nd Angle</u>		<u>Detector</u>
1S1	Sample Table	( $\psi$ )	G-Arm 1	( $\varphi_1$ )	1
1S2	Sample Table	( $\psi$ )	G-Arm 2	( $\varphi_2$ )	2
1M1	Monochromator	( $\theta_M$ )	Drum	( $2\theta_M$ )	1
1M2	Monochromator	( $\theta_M$ )	Drum	( $2\theta_M$ )	2
1A1	Analyzer Crystal	( $\theta_{A1}$ )	V-Arm 1	( $2\theta_{A1}$ )	1
1A2	Analyzer Crystal	( $\theta_{A2}$ )	V-Arm 2	( $2\theta_{A2}$ )	2

Dependent Angles

Scan 1: 1st Angle Moves  $\Delta\theta_1$ , 2nd Angle Does Not Move

Scan 2: 1st Angle Moves  $\Delta\theta_2/2$ , 2nd Angle Moves  $\Delta\theta_2$

<u>Code</u>	<u>1st Angle</u>		<u>2nd Angle</u>		<u>Detector</u>
2S1	Sample Table	( $\psi$ )	G-Arm 1	( $\varphi_1$ )	1
2S2	Sample Table	( $\psi$ )	G-Arm 2	( $\varphi_2$ )	2
2M1	Monochromator	( $\theta_M$ )	Drum	( $2\theta_M$ )	1
2M2	Monochromator	( $\theta_M$ )	Drum	( $2\theta_M$ )	2
2A1	Analyzer Crystal	( $\theta_{A1}$ )	V-Arm 1	( $2\theta_{A1}$ )	1
2A2	Analyzer Crystal	( $\theta_{A2}$ )	V-Arm 2	( $2\theta_{A2}$ )	

Figure 7. Scan types for DOUBLEROCK.

the maximum increment the mean can change from one scan on the same angle to another such that the crystal is considered centered. When both scans satisfy their respective convergence criteria consecutively, the crystal is considered centered.

Finally the teletype prints 4--?. The user then enters the center angle values as described above. Again a 0 entry uses the current angle setting, and 360 is required for a 0 setting (see Figure 8 for a sample input).

Each data file for a doublerock contains two spectra. The spectrum for the first angle of the doublerock is followed by the spectrum for the second angle of the doublerock. As the scans are repeated, the new spectra are stored on top of the old spectra.

After each scan is complete, the program searches for the background on each side of the spectrum. The key numbers marking the background and the key numbers marking the peak are printed. The curve is then corrected for the background by subtracting a straight line from the spectrum. Finally the area is computed by both a Simpson's rule calculation as well as a direct sum of the counts. The weighted mean is then calculated. These values are all printed on the teletype.

```

GENSCAN, DBLROCK, OR QESCAN? DBL (EOT)

TYPE END TO EXIT

SCAN 1

1--? 2S1 (EOT)

2--? 1.0 (EOT) ? 10 (EOT) ? 1 (EOT)

3--? .02 (EOT) ? .03 (EOT) ? 10 (EOT)
? .04 (EOT) ? .01 (EOT) ? 10 (EOT)

4--? 0 (EOT) ? 0 (EOT) ? 207 (EOT) ? 248 (EOT)
? 0 (EOT) ? 0 (EOT) ? 0 (EOT) ? 0 (EOT) ? 0 (EOT)

SCAN 2

1--? END (EOT) LAST SCAN 1

CHANGE OR ADD? (EOT)

```

Figure 8. Example showing the double rocking of the sample table,  $\Psi$ , and G-Arm 1,  $2\theta_{S1}$ ; when  $2\theta_{S1}$  steps by  $\Delta\theta$ ,  $\Psi$  advances by  $\Delta\theta/2$ .

### C. QESCAN

QESCAN is a set of procedures which performs a step scan in momentum ( $q$ ) space, energy ( $\nu$ ) space, or both simultaneously. The procedures compute the proper angles from the desired  $q$  and  $\nu$  values and drive the angles to those positions. Since calibration data are required, both semi-permanent data, i.e., the calibration data which are not necessarily changed with each scan, and scan data are requested.

After entry into QESCAN input, the teletype prints NAMES WRITTEN--YES OR NO?. The user responds YES if he/she desires a



description of each input line of the semi-permanent data and/or the scan data. Otherwise he/she enters NO or (EOT). Next the teletype prints ENTER 0 FOR PSI, 1-7 FOR SPD, 8 FOR SCAN?. The user enters 0 if he/she desires to change the  $\Psi$  calibration angles; 1-7 to start on the respective input line of the semi-permanent data; or 8 if no semi-permanent data are to be entered.

Below is a list of the inputs for lines 1-7 of the semi-permanent data. At the end of each line, the teletype requests the next desired input line.\* The user can respond with the line number desired or an (EOT) for the next line.

#### 1. Semi-permanent data

1. The teletype prints 1--? or 1--CALIBRATION 1?.  
The user responds with H,K,L indices,  $\Psi$ ,  
and  $2\theta_{S1}$  for calibration 1.
2. The teletype prints 2--? or 2--CALIBRATION 2?.  
The user responds with H,K,L indices,  $\Psi$ ,  
and  $2\theta_{S1}$  for calibration 2.
3. The teletype prints 3--? or 3--LATTICE SPACINGS?.  
The user enters the lattice d-spacings for the  
monochromator, analyzer 1, and analyzer 2 crystals  
in order.
4. The teletype prints 4--? or 4--ZERO REFERENCE  
ANGLES?. The user enters the zero reference  
angles in the following order:  $\theta_M$ ,  $2\theta_M$ ,  $\varphi_1$ ,  $\theta_{A1}$ ,  
 $2\theta_{A1}$ ,  $\varphi_2$ ,  $\theta_{A2}$ ,  $2\theta_{A2}$ .

---

\*After line 7, the program automatically enters the input routine for the scan data.

5. The teletype prints 5--? or 5--LOW,HIGH LIMIT ANGLES?.  
The user enters the low/high limit angles in ordered pairs in the following order:  $\theta_M$ ,  $2\theta_M$ ,  $\Psi$ ,  $2\theta_{S1}$ ,  $2\theta_{A1}$ ,  $2\theta_{S2}$ ,  $2\theta_{A2}$ .
6. The teletype prints 6--? or 6--ANGLE SIGNS?.  
The user enters "1" for positive sense of angle, or "0" for negative sense of angle for  $2\theta_M$ ,  $2\theta_{S1}$ ,  $2\theta_{A1}$ ,  $2\theta_{S2}$ ,  $2\theta_{A2}$  in order.
7. The teletype prints 7--? or 7--CALIBRATION WAVELENGTH?.  
The user enters the calibration wavelength. After this input control is automatically shifted to the scan input routine.

In this manner selected lines of the semi-permanent data can be changed without affecting the rest of the semi-permanent data. The user can enter 8 as the line number when he/she wishes to exit from the semi-permanent data routine.

Since angle  $\Psi$  may pass through zero, the low/high limits may be on either side of zero, say, 300 and 100 so that allowable angles are between 300/360 and 0/100.\* To achieve these limits, the high limit should be set to 460 so that it is larger than the low limit. Thus all angles between 300 and 460 will be allowed.

---

\*The limits are limit imposed internally in the software, not physically on the spectrometer. This means that any computed angle outside these limits will be eliminated from the scan. If this occurs, a message will be printed on the teletype giving which angle exceeded its limits along with its calculated value.

Upon entry into the scan input routine, the teletype prints TYPE -1 TO EXIT followed by SCAN 1. Below are the entries for the scan data:

## 2. Scan data

1. The teletype prints 1--? or 1--STEPS,COUNTS,PRESET?. The user enters the number of steps each side of center, the number of counts at each angle setting, and the counting interval. It is best to count at least three times per angle setting for statistical checking as the highest point normally is accepted for only two counts. When performing one count per angle setting, only one detector may be used. The preset value is negative for counting against time and positive for counting against monitor as before.
2. The teletype prints 2--? or 2--DET, FIX E, ENERGY?. The user enters the principal detector, 1 or 2; the energy to be held constant, "0" for the incident energy or "1" for the final energy; and the value of the fixed energy.
3. The teletype prints 3--? or 3--QX1,QY1,QZ1,NU,DQ1,DQ2,DQ3,DNU?. The user enters the components of the principal q-vector of the scan, the phonon energy, the increments of the principal q-vector, and the phonon energy increment.
4. The teletype prints 4--? or 4--QX2,QY2,QZ2?. The user enters the weaker q-vector of the scan. If this vector is "0", then no weaker q-vector enters the angle calculations and only one detector is used.\*

The user enters -1 for the number of steps to terminate the scan input routine (see Figure 9 for sample input). For long counts, it may

---

\*This input may not always be implemented. If not, the teletype will print SCAN 2; and the next scan can be entered.

be desirable to divide the counting interval into several shorter intervals. This allows for statistical checking of each separate interval. If an abnormal number of counts is noted for one of these intervals, say the reactor loses power for awhile, then this point is recounted. These shorter counts are then summed, and the result is written on the data file and printed on the teletype. The teletype experiment output contains the file number at which the spectrum is stored on the count data set. This is followed by the initial scan data and initial angles. As each count completes, the teletype prints the count, background, and non-preset counting interval. For multiple counts this is preceded by the count number. When all counts at a given angle setting have been completed, the teletype prints the data file key, the sum and adjusted sum for each detector being used. Normally the sum and adjusted sum are identical. However, if a count does not statistically check, then the adjusted sum is computed on the average of the accepted counts, and the count is retaken.

GENSCAN, DBLROCK, OR QESCAN? QES (EOT)  
NAMES WRITTEN--YES OR NO? YES (EOT)  
ENTER 0 FOR PSI, 1-7 FOR SPD, 8 FOR SCAN? 2 (EOT)  
2--CALIBRATION 2? 1 (EOT) ? 1 (EOT) ? 1 (EOT)  
 ? 353.92 (EOT) ? 269.98 (EOT) ? 8 (EOT)  
TYPE -1 TO EXIT  
SCAN 1  
1--STEPS,COUNTS,PRESET? 5 (EOT) ? 4 (EOT) ? +1000 (EOT)  
2--DET, FIX E, ENERGY? 1 (EOT) ? 1 (EOT) ? 3.2856 (EOT)  
3--QX1,QY1,QZ1,NU,DQ1,DQ2,DQ3,DNU? 1 (EOT) ? 1 (EOT)  
 ? 1 (EOT) ? 0 (EOT) ? .1 (EOT) ? .1 (EOT) ? .1 (EOT)  
 ? 0 (EOT)  
4--QX2,QY2,QZ2? 0 (EOT) ? 0 (EOT) ? 0 (EOT)  
SCAN 2  
1--? .1 (EOT) REPEAT? 1 (EOT)  
1--? -1 (EOT) LAST SCAN 1  
CHANGE OR ADD? (EOT)

Figure 9. Example of QESCAN input replacing line 2 of the semi-permanent data. The line headings are printed. There are 11 scan points with 4 counts being performed at each angle setting. Note the input error in line 1 of scan 2.

#### IV. Finger and Thumb Spectrometers

The discussion of the input for thumb and finger will be combined in this section since they are almost identical.\* The driving routines are the same as triple axis when procedure START is invoked. However, since the Mitsubishi's have the ability to be driven by paper tape (in fact the computer system emulates this paper tape), a further set of procedures has been installed to allow the user to punch paper tapes for a general scan or a q-space scan (see Section V).

##### A. GENSCAN

Genscan is a set of procedures which performs a simple step scan. Three different scans are possible: the sample table is stepped, code ST; the GA-arm is stepped by angle  $\theta$  and the sample table is stepped by angle  $\theta/2$ , code GA1; finally the GA-arm is stepped by angle  $\theta$  and sample table is not stepped, code GA2. (Finger has an additional scan in which the analyzer crystal is driven, code VA.)

Because the GA1 scan is automatically performed by the Mitsubishi, the sample table does not appear to move during this scan. Thus the sample table must physically be backed up during a GA2 scan in order to remain unmoved. Hence, the sample table appears not to move during a GA1 scan and to move during a GA2 scan.

---

\*Input required for the finger, but not for the thumb, will be enclosed in parentheses.

(SOM)

REQ, INQ OR ZAP? REQ (EOT)

LIBRARY NAME(S)? THUMB (FINGER) (EOT)

USER TASK NAME? START (EOT)

DATE/TIME TASK START @ 027400.2034 LIB(S): THUMB

DISPATCH

CHANGE TITLE--YES OR NO? YES (EOT)

? THIS IS SAMPLE INPUT FOR START (EOT)

STARTING FILE? 3 (EOT)

GENSCAN, DBLROCK, OR Q(E)SCAN? GEN (EOT)

Figure 10. Example showing initiation of procedure START with data files starting at file 3 preserving files 1 and 2.

Upon entry to GENSCAN input program, the teletype prints TYPE END TO EXIT followed by SCAN 1. The user enters one of the above scan codes: ST, GA1, GA2, (VA); the number of steps each side of center; the stepsize; the counting interval; and the center angles for ST, GA, (VA). The teletype responds SCAN 2. The user continues entering scans. After the last scan the user types END for the scan type to exit from the input routine.

#### B. DBLROCK

The only doublerock for thumb or finger involves the sample table and the GA-arm. The sample table is scanned. The weighted

mean is calculated. The sample table is set at its mean and the GA-arm is then scanned in either coupled or uncoupled mode.

Upon entry to DBLOCK, the teletype prints TYPE END TO EXIT followed by SCAN 1. The teletype then prints 1--? requesting the scan code: either GA1 or GA2. The teletype then prints 2--?. The user enters the multiplier factor, the preset value, and the starting scan. The teletype prints 3--?. The user enters the stepsize, the convergence criterion, and the number of steps each side of center for sample table scan followed by the same quantities for the GA-arm scan. After the teletype prints 4--?, the user enters the center angles in order: sample table, GA-arm, (VA-arm). See Section III.B for a complete description of these parameters along with sample inputs for triple axis spectrometer.

### C. Q(E)SCAN

QSCAN or QESCAN are a set of procedures which perform a step scan in momentum,  $q$ , space (QSCAN), energy,  $\nu$ , space, or both (QESCAN). These procedures compute the proper angles from the desired  $q$  and  $\nu$  values using the calibration data. This calibration data or semi-permanent data are stored separately from the scan data. Thus it need not be entered from one run to the next.

Upon invoking QSCAN, the teletype responds with NAMES WRITTEN--YES OR NO?. This allows the user to have the input for each line printed as headings before entry. If these headings are desired, the user responds YES. Any other response suppresses the headings for the semi-permanent data as well as the scan data.



The teletype then types the line ENTER 0 FOR ST, 1-4 FOR SPD, 5 FOR SCAN. The user responds with the line number he wishes to begin the data input. A 0 allows the user to change either/both values of the sample table calibration. Lines 1-4 are semi-permanent data which are described below. Line 5 starts the scan data which are also described below. After each line in the semi-permanent data, the line number of the next entry is requested. Typing (EOT) automatically gets the next line. For example, the user can enter lines 1 and 4 of the semi-permanent data only and then enter the desired scans (see Figure 11).

#### 1. Semi-permanent data

1. The teletype responds 1--? or 1--CALIBRATION 1?. The user enters the calibration indices H,K,L; and the calibration sample table and GA-arm angles. An (EOT) or 2 response gets the next line.
2. The teletype responds 2--? or 2--CALIBRATION 2?. The user then enters the respective data for the second calibration. Again an (EOT) or 3 response gets the next line.
3. The teletype responds 3--? or 3--LOW,HIGH LIMIT ANGLES?. The user enters the limit angles in low/high ordered pairs for the sample table, the GA-arm, (and the VA-arm). A response of (EOT) or 4 requests the next line.
4. The teletype responds 4--? or 4--LAMDA,GA(Z), SIGN(GA)? (or 4--LAMDA,D,GA(Z),VA(Z),SIGN(GA), SIGN(VA)?). The user then enters the calibration wavelength, (the d-spacing of the analyzer crystal), the zero reference GA-arm angle, (the zero reference VA-arm angle), the sign of GA, (the sign of VA). The user enters "1" for positive sign and "0" for negative sign.

NAMES WRITTEN--YES OR NO? YES (EOT)  
ENTER 0 FOR ST, 1-4 FOR SPD, 5 FOR SCAN? 1 (EOT)  
1--CALIBRATION 1? 1 (EOT) ? 0 (EOT) ? 0 (EOT)  
 ? 164.39 (EOT) ? 74.39 (EOT) ? 4 (EOT)  
4--LAMDA,GA(Z),SIGN(GA)? 1.08452 (EOT) ? .38 (EOT)  
 ? 1 (EOT)  
TYPE -1 TO EXIT  
SCAN 1  
1--STEPS,COUNTS,PRESET? 2 (EOT) ? 1 (EOT) ? 2 (EOT)  
2 QX,QY,QZ,DQX,DQY,DQZ? 1 (EOT) ? 0 (EOT)  
 ? 0 (EOT) ? .005 (EOT) ? 0 (EOT) ? 0 (EOT)  
SCAN 2  
1--? -1 LAST SCAN 2  
CHANGE OR ADD? 2 (EOT)  
1--? 2 (EOT) ? 1 (EOT) ? 2 (EOT)  
2--? 0 (EOT) ? 0 (EOT) ? 2 (EOT) ? .005 (EOT)  
 ? 0 (EOT) ? 0 (EOT)  
SCAN 3  
1--? -1 LAST SCAN 2  
CHANGE OR ADD? (EOT)

Figure 11. Example thumb input for Q-SCAN changing lines 1 and 4 of the semi-permanent data. Scan 2 was added as an after thought before the experiment was started.

Upon entry into the scan input routine, the teletype prints  
TYPE -1 TO EXIT followed by SCAN 1. Below are the entries for  
 the scan data:

## 2. Scan data

1. The teletype responds 1--? or 1--STEPS,COUNTS,PRESET?. The user enters the number of steps each side of center, the number of counts at each angle setting, and the preset value. Preset is negative for counting against time and positive for counting against monitor.
2. The teletype prints 2--? or 2--QX,QY,QZ,(NU),DQX,DQY,DQZ,(DNU)?. The user enters the components of the q-vector, (the phonon energy for inelastic scattering), the increments of the q-vector, (the increment of the phonon energy).

After all of the scans have been entered, the user enters -1 for the number of steps to terminate the scan input. The user is then asked for updates before the scans are run. See Section III.C for details of scan input.

## V. Utilities

Several utility programs have been written for the user's convenience. Since these are virtually identical for all three spectrometers, they will all be described in this section. They provide functions such as dumping semi-permanent and count data sets, updating the scan data set, trial calculations for  $q(e)$  scans, and paper tape generation for the Mitsubishis.

### A. DISKREAD

This program dumps the contents of a given data file residing on the count data set. Upon starting this program, the teletype prints DUMP FILE. The user enters the file number corresponding to the hard copy file number he/she desires to dump. The teletype prints the type of scan which generated the data file, and the

initial angles or q-values along with their respective step sizes. Finally the key values and the data are printed. Upon completion of the dump of the file, the teletype prints DUMP FILE? The user can now dump another file or terminate the dump by entering (EOT).

If the file containing the count data is a doublerock scan, then the teletype prints DUMP SCAN 1 OR 2?. If the user desires the first angle scan he/she responds 1, otherwise he/she responds 2. The same file must be dumped a second time to get both scans.

#### B. DUMPSPD

This routine dumps the semi-permanent data stored on data set SCANTEST (see Paragraph D). This allows the user to interrogate the semi-permanent data. The program requires no input. It prints the following table:

- a.) Calibration 1 data
- b.) Calibration 2 data
- c.) Limit angles and zero reference angles
- d.) d-spacings
- e.) Angle signs
- f.) Calibration wavelength.

The order of this print out varies for the different spectrometers.

#### C. TAPESTART

This program generates a paper tape which can be read by the Mitsubishi. This routine can be used whenever hardware problems cause problems in the computer control. The input for this routine is identical to that of program START and will not be discussed here.

## D. TESTQ(E)

This routine allows the user to make a trial calculation for the q-scan angles. Its input is similar to that required by Q(E)SCAN with the exception of the TITLE, FIX ANGLES, and STARTING FILE requests. The user is referred to the Q(E)SCAN sections for discussion of the input.

The program prints the calculated angles for the triple axis spectrometer. It prints the q-vector values (and the phonon energy) as well for the thumb and finger spectrometers.

This routine maintains its own scan data set SCANTEST for use while the respective spectrometer is operating. Thus two versions of the semi-permanent data are stored: one on data set SCANTEST and one on data set SCANIN, the data set used by program START. Whenever the semi-permanent data is changed in program START, both data sets SCANIN and SCANTEST are updated so that these copies are identical. If the semi-permanent data are changed during a TESTQ(E) calculation, these data are restored to the values at the beginning of the run. Thus the semi-permanent data can only be permanently changed from program START.

If the angle calculation routine Q(E)CALC terminates with a completion code of 000033, the scan q-vector or phonon energy is inconsistent with the input data. The 000033 is caused when the routine attempts to calculate the square root of a negative number. This means the data would generate non-physical angles.

## E. UPDATE

This program is used for updating the currently active scan file. The experiment in progress is terminated. Then program UPDATE is called which allows the user to repeat, add, delete, or replace scans on the scan data set. The input is as follows (see Figure 12):

The teletype prints REPEAT SCAN NO?. If the user desires to repeat a GENSCAN or QESCAN which has been completed, he/she enters its number. The program automatically transfers control to the proper scan. The scan must have completed before this option can be used. If no scan is to be repeated, the user responds (EOT).

After an (EOT) to the repeat scan request, the teletype prints ADD TO SCANS--YES OR NO?. If the user desires to add scans to the end of the scan data set, he/she responds YES. The program passes control to the proper input routine to enter the scans. Input proceeds as described in the appropriate subsection above. If the user responds NO or (EOT), the program skips this option.

The teletype prints DELETE SCAN NO? as the next option. If the user desires to delete any scan, he/she enters that number. Any scan can be deleted including one in progress. If a scan is deleted, then the DELETE SCAN NO? request is printed again. This continues until the user enters (EOT) to this request.

The teletype prints REPLACE SCAN NO? as the final option. If the user desires to replace a scan, he/she enters that number. The

program then transfers control to the appropriate input routine. After the replacement scan has been entered, the teletype prints REPLACE SCAN NO?. The user continues replacing scans until he/she is finished. Then the response is (EOT).

After the updating has been completed, the teletype prints CHANGE OR ADD--YES OR NO?. This allows the user to correct any mistakes he/she may have noticed. If the response is YES, the updating options are available again starting with the ADD option. The user starts the scans at the point at which they were interrupted by responding NO (EOT).

```

(SOM)

REQ, INQ OR ZAP?  REQ (EOT)

TYPE IN USER LIBRARY NAME?  THUMB (EOT)

TYPE IN TASK NAME?  UPDATE (EOT)
.
.
.
.
REPEAT SCAN NO?  (EOT)

ADD TO SCANS--YES OR NO?  YES (EOT)

SCAN 5

1--?  5 (EOT) ? 1 (EOT) ? 10 (EOT)

2--?  0 (EOT) ? 0 (EOT) ? 2 (EOT) ? .005 (EOT)
? 0 (EOT) ? 0 (EOT)

SCAN 6

1--?  -1

DELETE SCAN NO?  2 (EOT)

DELETE SCAN NO?  3 (EOT)

DELETE SCAN NO?  (EOT)

REPLACE SCAN NO?  4 (EOT)

SCAN 4

1--?  5 (EOT) ? 1 (EOT) ? 10 (EOT)

2--?  0 (EOT) ? 0 (EOT) ? 2.5 (EOT) ? 0 (EOT)
? 0 (EOT) ? .005 (EOT)

REPLACE SCAN NO?  (EOT)

CHANGE OR ADD--YES OR NO?  NO (EOT)

```

Figure 12. Input to program UPDATE. Initially the scan data set contained 4 scans: scans 2 and 3 were deleted, scan 5 was added, and scan 4 was replaced. Control then returned to the interruption point to continue the scans.



## VI. Plotter

The plotter is a series of programs initiated from the directory containing the data set to be used by these programs. The driving routine for these programs is GRAPH. Calling this program allows the user several options: plotting data from the count data set; calculating the weighted mean and area under the spectrum either automatically or by input of salient peak features. The various options will be described below.

The program initially prints OPTION to request one of the available options: CAL, PLOT, AUTO, AREA, XMAX, CHK, END. When the calibration options CAL and CHK are invoked, the program will ask for the next option immediately. The user should not enter a new option until he/she is finished with the CAL or CHK option.

CAL: This option allows the user to calibrate the plotter for the abscissa(x) and ordinate(y) scales being used. The plotter marks points at the origin and the ordered pair (x,y) at the maximum to allow the user to adjust the x and y gains as he/she desires. Six points are plotted at each point.

PLOT: This is the plot command. When PLOT is specified, the teletype prints FILE. The user then enters the file number he/she desires plotted. The program then prints the initial abscissa value and the scan increment. This is followed by YO,YMAX?. The user enters the minimum and maximum number of counts to appear on the plot. For example, the user might enter 0 and 1000 if the background were in

neighborhood of 10 counts, and the peak in the neighborhood of 900 counts. Invoking the plot option when the plotter is calibrating stops the calibration.

CHK: This option checks the calibration by plotting points at the origin and at the ordered pair (x,y) for the respective maximum values. One point is plotted at each point.

AUTO: This option allows the user to compute the weighted mean and the area under the curve automatically, i.e., the program searches for the peak features and prints them on the teletype. When this option is invoked, the teletype prints FILE, and the user enters the file number to be used as input.

AREA: This option allows the user to compute the weighted mean and the area under user specified parts of the spectrum on a given file. In this case, however, he/she must enter the salient features of the curve: the start and end of the background on each side of the spectrum; and the start and end of the peak. As above the teletype requests the file number. This is followed by the following requests:

START,END LEFT BACKGROUND?. The user enters the key number of the data point at which the left background begins followed by the key number of the data point at which the left background ends.

START,END PEAK?. The user enters the keys for the data points at which the peak begins and ends respectively. If the user enters keys for the peak that are different by a number greater than 7, the programs treat the peak as a plateau. When this occurs, the

average of right and left peak values is calculated and used as the mean. Otherwise, the weighted mean is calculated.

START,END RIGHT BACKGROUND?. The user enters the key numbers for the data points at the beginning of the right background and the end of the right background.

If any feature is not to be included, then the same key number should be entered for each member of an ordered pair. Do not enter zero. The key numbers must be in ascending order (see Figure 13).

a.)  
Spectrum appearing  
on teletype

b.)  
Entries for GRAPH

FILE 1

KEY DATA

33	3	<u>OPTION?</u> AREA (EOT)
34	4 left background	<u>FILE?</u> 1 (EOT)
35	3	<u>START,END LEFT BACKGROUND?</u> 33(EOT) ? 36 (EOT)
36	16	<u>START,END PEAK?</u> 39 (EOT) ? 41 (EOT)
37	152	<u>START,END RIGHT BACKGROUND?</u> 44 (EOT) ? 47 (EOT)
38	348	
39	601	<u>SIMPSON</u> 146. <u>SUM</u> 145. <u>MEAN</u> 30.001
40	692 peak	
41	593	
42	341	
43	173	
44	20	
45	4	
46	5 right background	
47	2	

Figure 13. Example of area calculation using GRAPH.

XMAX: This option scales the abscissa,  $x$ . The minimum  $x$ -value is assumed zero. The user enters the maximum  $x$ -value to appear on the plot. If the number of data points to be plotted is entered, the plot will span the entire abscissa.

END: This option terminates the program.

## VII. Acknowledgements

The authors wish to thank the neutron scattering group, particularly J. Traylor, for their patience and encouragement during the development and implementation of this system.

Special thanks are due to W. Lembke for her expert typing as well as her handling of the details of getting this manual printed.

## VIII. Appendices

## A. Triple Axis Input Summary

Short summary of input data for the three experiments performed on the triple axis spectrometer.

## 1.) GENSCAN

- Line 1: Scan type (see Figure 4 for codes). Enter END to terminate input.
- Line 2: Stepsize; # of steps to one side of center; preset value.
- Line 3: Nine center angles in order  $\theta_M$ ,  $2\theta_M$ ,  $\Psi$ ,  $\phi_1$ ,  $\theta_{A1}$ ,  $2\theta_{A1}$ ,  $\phi_2$ ,  $\theta_{A2}$ ,  $2\theta_{A2}$ . (Zero entry will use current angle value. To set angle to 0 degrees, enter 360.)

## 2.) DOUBLEROCK

- Line 1: Scan type (see Figure 6 for codes). Enter END to terminate input.
- Line 2: Multiplier factor (for quickscan correction if scan too narrow), preset value (0 for quickscan starting scan), 1 to do  $\theta$  scan first, 2 to do  $2\theta$  scan first.
- Line 3: Stepsize angle 1; convergence criterion angle 1; number of steps each side of center for angle 1; stepsize angle 2; convergence criterion angle 2; number of steps for angle 2.
- Line 4: Nine center angles as above. (Zero entry will use current angle value. To set angle to 0 degrees, enter 360.)

## 3.) QESCAN

## Semi-permanent data

- Line 1: Indices for calibration one,  $H_1, K_1, L_1$ ; calibration 1 values for  $\Psi$  and  $\phi$ .
- Line 2: The above values for calibration 2.
- Line 3: The lattice d-spacings in order  $d_M$ ,  $d_{A1}$ ,  $d_{A2}$ .

- Line 4: The zero reference angles in order  $\theta_M$ ,  $2\theta_M$ ,  $\varphi_1$ ,  $\theta_{A1}$ ,  $2\theta_{A1}$ ,  $\varphi_2$ ,  $\theta_{A2}$ ,  $2\theta_{A2}$ .
- Line 5: The low and high limit angles in ordered pairs  $\theta_M$ ,  $2\theta_M$ ,  $\psi$ ,  $\varphi_1$ ,  $2\theta_{A1}$ ,  $\varphi_2$ ,  $2\theta_{A2}$ .
- Line 6: 1 if angle sign is to be positive and -1 if angle sign is to be negative in order  $2\theta_M$ ,  $\varphi_1$ ,  $2\theta_{A1}$ ,  $\varphi_2$ ,  $2\theta_{A2}$ .
- Line 7: The wavelength used during the calibration.

#### Scan data

- Line 1: Number of steps each side of center, number of counts at each scan point, preset. Enter -1 to terminate input.
- Line 2: Principal detector number (1 or 2); 1 if E' fixed, 0 if E<sub>0</sub> fixed; fixed energy value.
- Line 3: Central q, energy values, q and energy increments in order  $Q_{X1}$ ,  $Q_{Y1}$ ,  $Q_{Z1}$ ,  $\nu$ ,  $\Delta Q_{X1}$ ,  $\Delta Q_{Y1}$ ,  $\Delta Q_{Z1}$ ,  $\Delta \nu$ .
- Line 4: Weaker Q value (leave zero if no second scan) in order  $Q_{2X}$ ,  $Q_{2Y}$ ,  $Q_{2Z}$  (may not be included).

#### Sample table data only

- Line 1: Calibration angles  $\psi_1$  and  $\psi_2$ . Input 0 if they are to remain the same.

## B. Finger and Thumb Input Summary

Short summary of input data for three experiments performed on the thumb and finger spectrometers. Input data valid only for the finger spectrometer is in parentheses.

### 1.) GENSCAN

- Line 1: a.) Scan type: ST, GA1 (coupled GA scan), GA2 (uncoupled GA scan). Enter END to terminate input.  
 b.) Number of steps each side of center.  
 c.) The stepsize.  
 d.) The preset value.  
 e.) Center angles for the sample table, GA-arm center angle, (the VA-arm) respectively.

### 2.) DOUBLE ROCK

- Line 1: Scan code: GA1 (coupled GA scan) or GA2 (uncoupled GA scan). Enter END to terminate input.  
 Line 2: Multiplier factor (for quickscan correction if scan too narrow), preset value (0 for quickscan), and 1 for sample table scan first, 2 for GA-arm scan first.  
 Line 3: Stepsize, convergence criterion, and number of steps each side of center for sample table scan. Respective values for GA-arm scan.  
 Line 4: Center angles for the sample table, GA-arm, (VA-arm) respectively.



## 3.) QESCAN

## Semi-permanent data

Line 1: Calibration 1 indices, sample table and GA-arm angles.

Line 2: Calibration 2 indices, sample table and VA-arm angles.

Line 3: Low/high limit angles for sample table and GA-arm.

Line 4: Calibration wavelength, zero reference for GA-arm,  
(analyzer crystal d-spacing), (zero reference for  
VA-arm), sign of GA-arm, (sign of VA-arm).

## Sample table input only

Line 1: Calibration 1 sample table angle, calibration 2 sample  
table angle. Enter zero if they are to remain the same.

## Scan data

Line 1: a.) Number of steps each side of center.  
b.) Number of counts at each angle setting.  
c.) Preset value.

Line 2: a.) Components of q-vector at scan center,  
(value of  $\nu$  at scan center).  
b.) Increments of q-vector, (increment of  $\nu$ ).

## C. Plotter Summary

Short summary of input data for GRAPH.

Line 1: GRAPH option:

AREA-calculate area under spectrum and  
weighted mean with user input of  
salient features  
AUTO-calculate area under spectrum and  
weighted mean with computer search  
for salient features  
CAL-calibrate the plotter  
CHK-check the plotter calibration  
END-exit from the program  
PLOT-plot the spectrum  
XMAX-set the maximum abscissa value.

Line 2.a: The file number of the data file being used.  
(Entered when options PLOT, AUTO, or AREA  
are specified.)

Line 2.b: The maximum value of the abscissa, XMAX.  
(Entered only when option XMAX is specified.)

Line 3.a: The minimum value of the ordinate, YO, and the  
maximum value of the ordinate, YMAX. (Entered  
when option (PLOT) is specified.)

Line 3.b: Starting and ending keys for the left background.  
Starting and ending keys for the peak.  
Starting and ending keys for the right background.  
(Entered only when option AREA is specified.)

#### D. Loading Data Sets From Object Cards

The compiler is resident on the 360. Therefore programs must be compiled on the 360 which produces an object deck for the PDP-15. The object deck is then read onto the 15 disk so that it is available for loading when it is called.

For this purpose the disk is divided into libraries or directories. The neutron scattering directories are FINGER, THUMB, and TRIAX. Routines which are shared such as the plotting routines are stored in directory UNIVERSAL.

Since most of the directories have the same routines, the object cards are identified by a one letter code attached to the end of the name. These codes are F for finger, T for thumb, X for triax, and U for universal. The data set name appears on the first card of the object deck. When entering these data sets, the code letter must not be included as it is not part of the task name (see Figure 14).

The program for loading tasks onto the 15 disk is called DISKORG and is located in directory DISK. If a data set is to be reloaded due to a problem with the disk, the procedure in Figure 14 is to be followed. Refer to Users Manual For DISKORG, The Disk Organization Subsystem For The PDP-15 Computer, IS-4105, by Kent R. Brobst, Leonard C. Moon, and Thomas Ekberg, for complete details for using DISKORG.

The procedure is slightly different for loading code for the 910. This code is stored permanently on the 15 disk and can be loaded across the interface whenever desired. All of the machine code for

the neutron scattering programs is located in data set NS910. Hence, the 910 object code is read into this data set and loaded to the 15. This is due to the fact that the 910 cross-assembler is resident on the 360 similarly to the 15 ALECS compiler. Figure 15 shows an example of reading object code and loading to the 910.

```
(SOM)

REQ, INQ OR ZAP?  REQ (EOT)
LIBRARY NAME(S)?  DISK (EOT)
USER TASK NAME?  DISKORG (EOT)
.
.
.
.
DATE--YMD?  770222 (EOT)
YOUR NAME?  TGP (EOT)

OPCODE?  MDS (EOT)
DIRECTORY?  THUMB (EOT)
DATA SET?  STEPSCAN (EOT)
UPDATE?  YES (EOT)
DATA SET TYPE?  TASK (EOT)
UPDATE?  YES (EOT)
```

Figure 14. Example of reloading task STEPSCAN into directory THUMB. Select the object cards headed STEPSCANT and procede as above.

a.) Read the 910 object code from cards

(SOM)

REQ, INQ OR ZAP? REQ (EOT)

LIBRARY NAME(S)? SDS

USER TASK NAME? CARDREAD (EOT)

.

.

.

.

.

DATA SET NAME? NS910 (EOT)

NORMAL END, NEXT DATA SET NAME? (EOT) to exit

b.) Load the object code from 15 disk to 910

(SOM)

REQ, INQ OR ZAP? REQ (EOT)

LIBRARY NAME(S)? SDS

USER TASK NAME? LOADER (EOT)

.

.

.

.

.

DATA SET NAME? NS910 (EOT)

NORMAL END, NEXT DATA SET NAME? (EOT) to exit

Figure 15. Example of loading 910 object code onto the 15 disk and transferring it to the 910.

### E. Data Set and File Organization

The programs for experiment control require two data sets: one to contain the scan files, and one to contain the count files. Each file on the scan data set can be thought as containing one scan. Similarly, each file on the count data set can be thought as containing one spectrum, except for doublerock files.

Upon input the label SCAN N identifies the  $n^{\text{th}}$  file on the scan data set. This number is referred to when updating or modifying this data set.

Each spectrum printed on the teletype is identified by the label FILE M. This is the file on the count data set containing the spectrum. When dumping disk or plotting this is the identifying file number for the spectrum.

If saving data, the number entered for STARTING FILE is the file where the spectrum will be stored. Files 1 through  $m-1$  are still available to the user. Files greater than  $m$  are no longer accessible as each file contains a pointer to the next file.

For doublerock experiments, each file contains both spectra: scans one and two respectively. These spectra are written over as the scans are repeated so that only the latest spectra are stored on the file. In all other cases, each file contains the spectrum of its respective scan.

Each file also contains an experiment identifier. Thus spectra from different experiments can be saved on the same data set without any problems.