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SPECIAL APPLICATION OF THE COMPUTER PROGRAM XRDPLT

--Accessing a User-Generated Data Base

By

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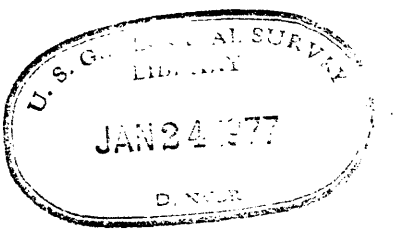

Open File Report 77-53
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Introduction

The program XRDPLT (VanTrump and Hauff, 1976a), operating on the mineral X-ray diffraction data base -- XRDFIL (VanTrump and Hauff, 1976b), is capable of retrieving and/or plotting data from any of the reference entries in this file. These plots are simulated X-ray diffractograms or powder film patterns expressed in degrees two-theta (Figure 1). In certain instances, however, it would be convenient for a user to create a specialized data file from the main data base, XRDFIL, or from his own data sources.

Two methods have been designed to build these special-purpose data files. The first method (Figure 2) enables a user to build a file of X-ray powder diffraction data from his own sources using the program, BLDMIN. The second method, shown in Figure 4, uses an option in the program XRDLST, which accesses the main data base, XRDFIL, and creates the smaller, specialized data file that the user requests. Because the format of these data files or small data bases is standardized, XRDPLT can operate directly on them as it would on XRDFIL.

Before these methods for building specialized files are outlined in detail, a brief discussion of the main program, XRDPLT, is required.

The programs and procedures discussed in this report have been designed for the DEC System-10 computer. It is suggested that the reader consult the references cited on the program XRDPLT and the data file, XRDFIL, for more specific details. As much versatility as possible has been built into this system so that it is adaptable for other computers. The control language commands listed in this report are for the DEC-10. Since this manual is written for users of the DEC System, a detailed attempt to explain the DEC control language commands has not been made. A DEC users manual may be consulted for explanation of these commands; for the most part, they have been kept to a minimum in this report.

The Program XRDPLT

The Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program -- XRDPLT -- is used to retrieve and/or plot mineral X-ray powder diffraction data. The program operates on a file (XRDFIL) of mineral powder diffraction data that contains two-theta or 'd' values, intensities, chemical formula, mineral name, identification number, and mineral-group code. XRDPLT prompts the user in a conversational format to provide the required input information from a time-sharing terminal.

The program offers two major options: retrieval only, retrieval and plot. The first operation retrieves from the file by identification number, by the mineral-group code (a classification by chemistry or structure), or by searches on the formula components; it lists the mineral names, formulas, and groups which meet the retrieval criteria. For example it enables the user to search for minerals by major groups, that is, micas, feldspars, amphiboles, oxides, phosphates, carbonates; by elemental composition, that is, Fe, Cu, Al, Zn, Si; or by a combination of these, that is, all copper-bearing arsenates.

The second option retrieves as described above, but also plots the retrieved two-theta and intensity values as diagrammatic X-ray powder patterns on mylar sheets or overlays, simular to Figure 1. These plots can be made using scale combinations compatible with chart recorded diffractograms and 114.59-mm powder camera films. The overlays are then used to separate or sieve out unrelated minerals until knowns are matched and identified.

All the options contained in the program, detailed operating instructions, and examples are given in the operating manual for the program (Hauff and VanTrump, 1976).

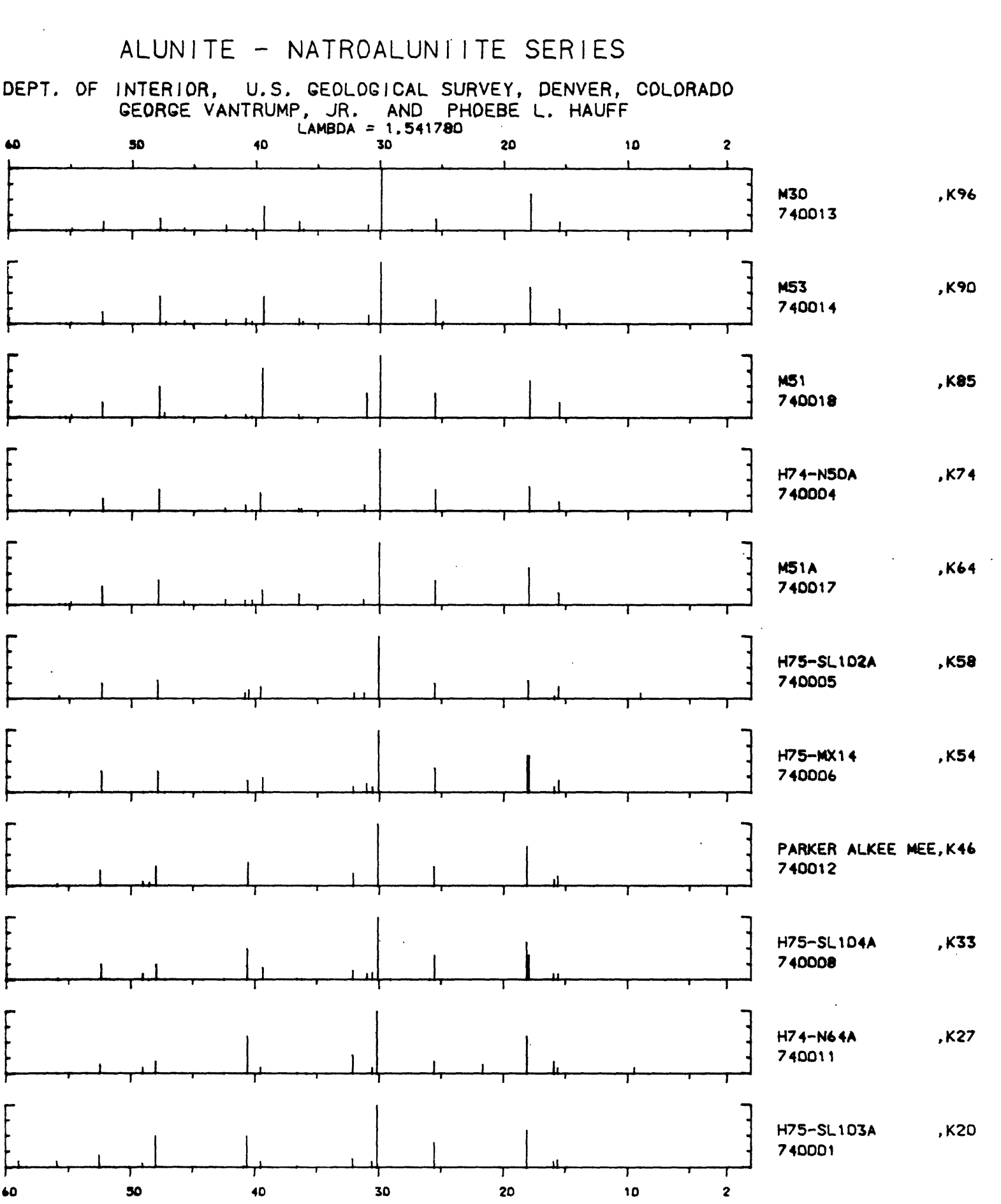

Figure 1. Example of a Sieve Created by the Program XRDPLT

Building A Special-Purpose Data File

Method with User Source Data File.--Figure 2 is a step-by-step flow chart of the procedure to be followed when creating a plot from a user-generated data base. An applied example of this method is found in Cunningham and others (1976).

Data Entry To Create A New File.--The coding sheet for data entry shown in Figure 3 has been standardized to the main data base (XRDFIL). This was done because XRDFIL is accessed by programs other than XRDPLT. These forms are available through the mineralogy laboratory in Denver. Detailed instructions for completing this form start on page 9.

Use one sheet per mineral. The sequence lines 001 and the 400 series must contain data, as these refer to the mineral name, formula, and X-ray data. Obviously the program XRDPLT will not function satisfactorily if these data are not provided.

After the sheets have been completed, each mineral must be assigned a unique identification number (IDNO), because the XRDPLT program retrieves on this number. Conventionally this number would be assigned by the mineralogy laboratory personnel if there is any possibility of the data being included in the master data base, XRDFIL. However, when the data are special-purpose and restricted to a private file, the user may assign his own IDNO as long as the six-digit format is retained.

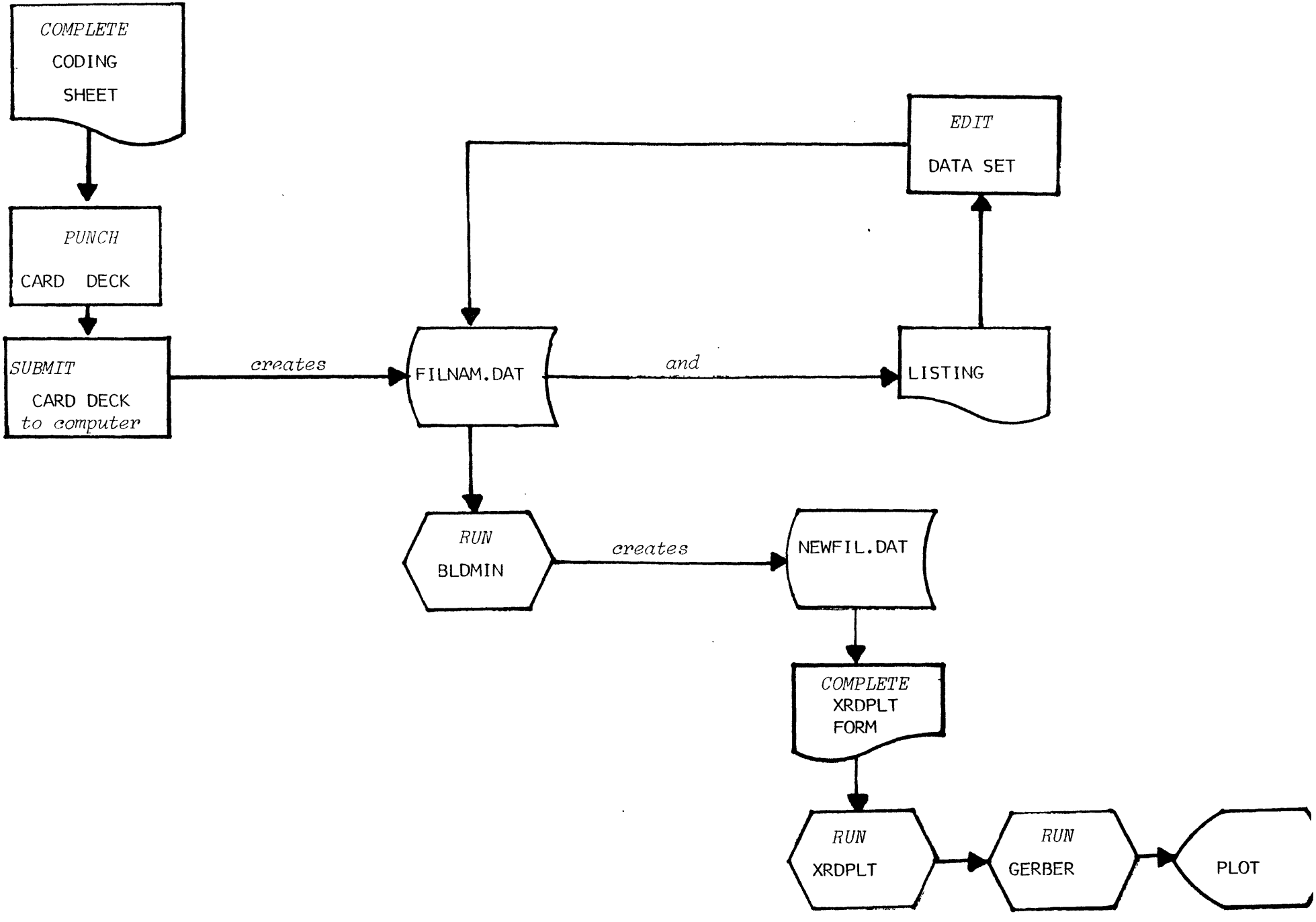

FIGURE 2. -- Flow chart showing how to create sieves from user initiated input

MINERAL X-RAY DATA FILE CODING SHEET

U.S. Geological Survey mineralogy laboratory, Denver, Colorado

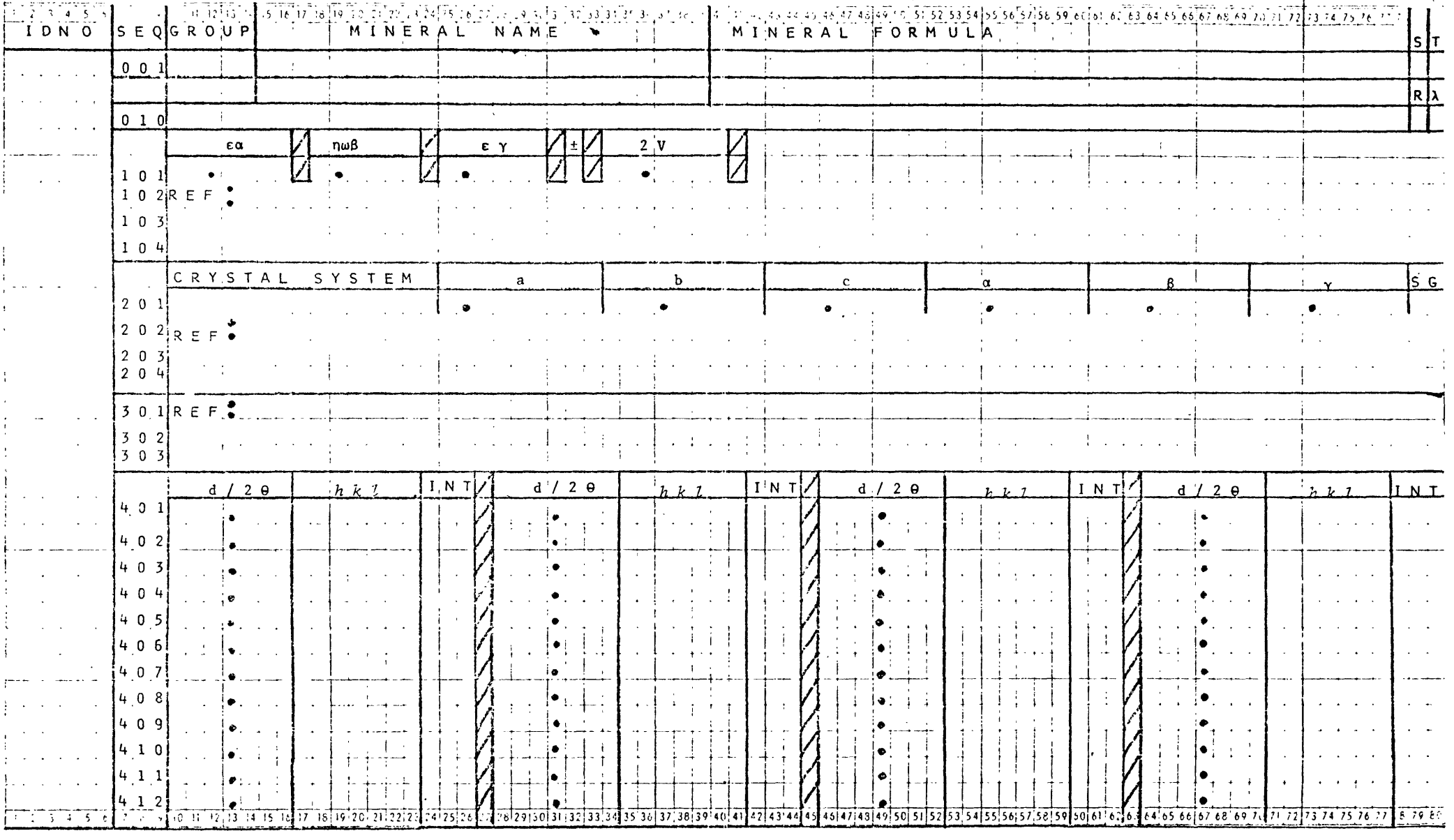

Figure 3 Data Coding Sheet

MINERAL X-RAY DATA-FILE CODING SHEET -- Instructions for Completing

The coding sheet is set up for direct keypunching. When filling in data, put only one character per square. The main data base is capable of holding many other types of data not used by the program XRDPLT. VanTrump and Hauff (1976b) discusses in detail all the various types of data accommodated by the data base. This report will explain only those data fields utilized by the program XRDPLT.

IDENTIFICATION

CARD 001	LABEL	COLUMN
	IDNO	1-6
		Fill in with six-digit number. This may be the Powder Diffraction File number (PDF). If non-JCPDS data, then a user-generated number is used.
	SEQ NO.	7-9
		The three-digit number - 001 - unique to this card must be punched into this field. This number identifies the card to the program building the data file.
	GROUP	10-14
		Use this field only if data is to go into XRDFIL. Codes are found in VanTrump and Hauff (1976b)
	MINERAL NAME	15-39
		Name of mineral limited to a maximum of 24 characters. Use element abbreviations when possible: for example, magnesium chlorite = chlorite, mg
	MINERAL FORMULA	40-78
		Put blanks between elements. Treat subscripts as characters: MgSo 4 · 7H2O = MG S04· 7H2O

CARD 001	LABEL	COLUMN
	TYPE OF RADIATION	80

A = CU-A1 M = MO-A1
B = CU-A N = MO-A
C = CU-A2 O = MO-A2
D = FE-A1 P = AG-A1
E = FE-A Q = AG-A
F = FE-A2 R = AG-A2
G = CO-A1 S = W-A1
H = CO-A T = W-A
I = CO-A2 U = W-A2
J = NI-A1 V = CR-AI
K = NI-A W = CR-A
L = NI-A2 X = CR-A2

If this column is left blank it is assumed that the data found on the 400-series cards is in 'd' values.

X-RAY DIFFRACTION DATA

CARD 401 +

IDNO	1 - 6
SEQ NO	7 - 9

Each card in the 400 series is capable of containing four sets of 'd' or two-theta intensity pairs. The form is filled out from left to right sequentially, not down. The sequence number must be changed as data is entered on each new line. This must also be done sequentially: 401, 402, 403, 404.

'd'/TWO-THETA	10 - 16 starts field

Enter 'd' OR two-theta values in this field, as indicated on Card 001. Do not mix these two different types of data.

I	24 - 26	These are right justified in their field. (One- and two-digit intensities should occupy the right-hand column(s) of the field.)

Card Deck Setup for DEC 10

After the coding sheets are completed and checked, punch a card deck from them. Use the following commands, one line per card, to enter the data into the computer.

```
$JOB  LIST(000,000)/NAME:YOUR NAME/CORE:20K/TIME: 100
$DECK FILNAM.DAT
  DATA CARDS
$EOD
.PROT FILNAM.DAT<257>
.PRI/FILE:ASCII  FILNAM.DAT          command to print a listing
                                     of file for editing

.DIR
EOF     (END OF FILE CARD)
```

Where (000,000) is the project, programmer number assigned by the computer center.

FILNAM.DAT — FILNAM is any five-character or less name that the user assigns to the data set.

.DAT designates to the computer that this file is a data set as opposed to a program.

This punched deck has two purposes. It first creates a data file in the computer and then lists the contents of the file for editing.

After the command cards have been punched and the deck arranged according to the above format, submit the card deck to the computer. Retrieve the listing of the file and manually edit it for errors. If there are errors, correct them

by re-punching the cards that have mistakes and then re-submit the deck. This will recreate the data file and delete the incorrect file. If the user is knowledgable about the text-edit program for the system, the file may be edited directly in the computer. A listing should still be made to check for accuracy.

The data file is now in the user's private area in the computer and ready for the next operation.

Operating Instructions for the Program BLDMIN

The program BLDMIN reads as input the pre-formatted, card-image data file built by the steps described in the previous section. It creates an output file in binary that has the same structure as the main data base, XRDFIL. User-entered responses are underlined.

An example of this program is as follows:

```
.RUN BLDMIN(200,200)
ENTER INPUT CARD FILE NAME:  SKIP
ENTER NAME OF OUTPUT DATA FILE TO BE BUILT: SKIPI
    18 MINERALS ARE CONTAINED IN OUTPUT FILE.
NORMAL TERMINATION
END OF EXECUTION
CPU TIME: X.XX ELAPSED TIME:  XX.XX
EXIT
(X.XX XX XX)
```

Where:	SKIP	in this example is the name of the input data file made using a card deck.
	SKIP1	is the name of the output data file structured so that XRDPLT can operate on it. The data remains unchanged; only the manner in which it is stored in the computer differs. Listing this file with the "PRINT" command is not possible as it is now expressed in binary.

Although the data set is put into the computer using a punched card deck, the programs are run through the terminal. They are time-sharing programs.

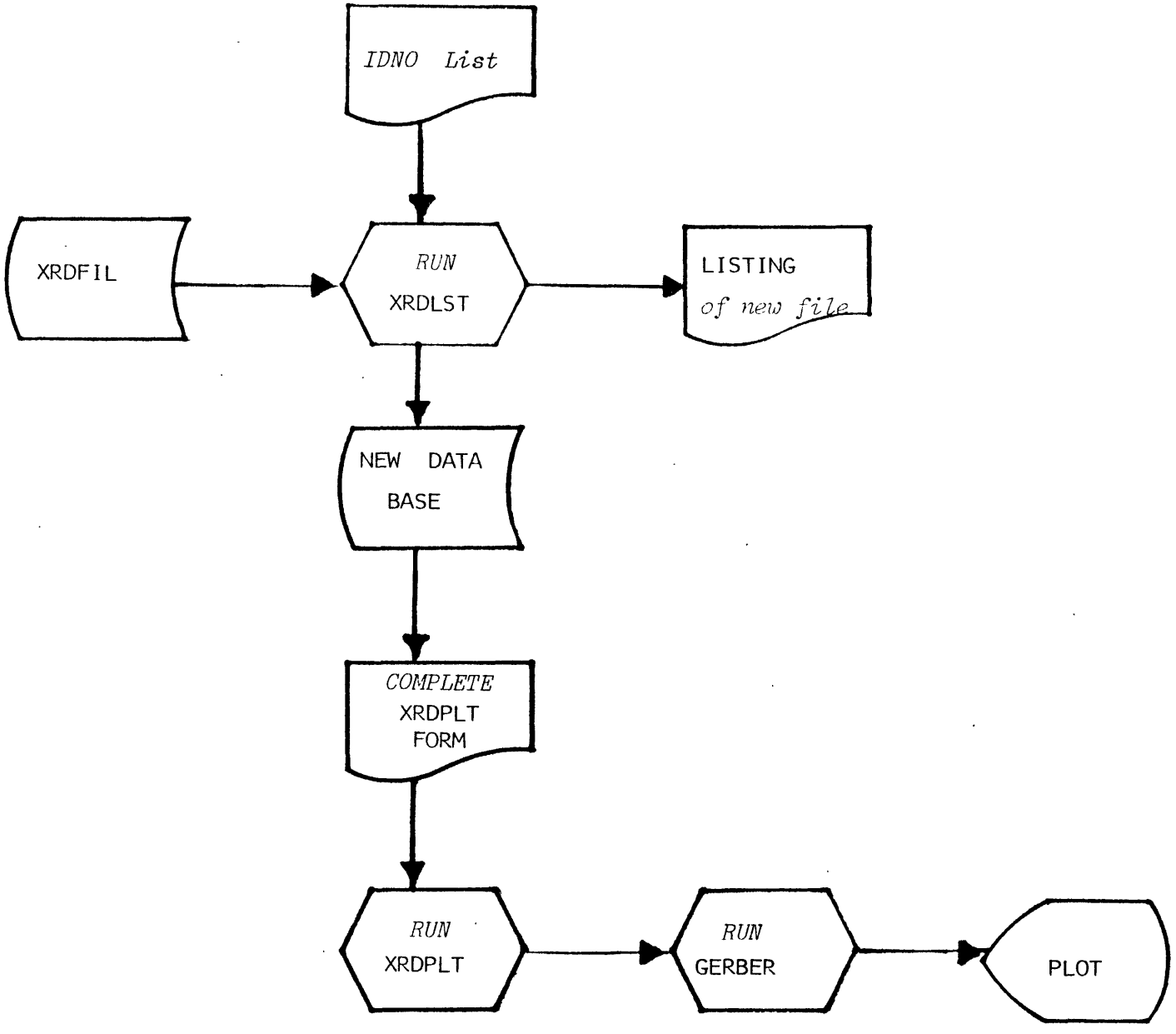

FIGURE 4.--Flow chart showing how to create sieves from Main Data Base, XRDFIL.

Method Using the Program XRDLST

XRDLST is the program used to build a special-purpose data file from the main data base, XRDFIL. It was written for a dual purpose: to look at the contents of a data file and also to build subfiles of the main data base. After a subfile is created, it can be repeatedly accessed for review with XRDLST.

Figure 4 is a step-by-step flow chart of the procedure to follow when creating a subfile from the main data base XRDFIL. Access through XRDLST to any file is by the six-digit IDNO or PDF (Powder Diffraction File) Number. If a subfile is to be built from the main data base, use the indices found in VanTrump and Hauff (1976b) to compile a list of the desired numbers. These identification numbers are used as a common access method by all programs using XRDFIL.

The format of XRDLST follows, with an explanation of the interactive questions:

RUN XRDLST (200,200)	Instruction to excute the program.
ENTER BASE FILE NAME:	This defaults following a carriage return to the main data base, XRDFIL. Any other data file that has the proper format may be entered here and accessed by XRDLST.
DO YOU WANT TO BUILD AN OUTPUT FILE?	If the answer is 'yes', the next question is:
ENTER NEW BASE FILE NAME:	And an output file with the '.DAT' extension is automatically built with the user supplied filename: i.e. SKIP1.

ENTER IDNO'S TO BE SELECTED FROM INPUT FILE:

Enter one IDNO per line. Terminate the input list with an additional carriage return.

DO YOU WANT TO LIST DATA FOR ID'S SELECTED:

If the answer is 'YES,' an output table with the following format is listed on the terminal:

```
ID = 740001    CODE =                NO = 23
NAME = H75-SL103A          K20
FORM =

  NO 2THETA INT   NO 2THETA INT   NO 2THETA INT   NO 2THETA INT   NO 2THETA INT

   1 64.65    3    6 55.93   10   11 40.9    3    16 30.56   10   21 15.9    10
   2 62.59   15    7 52.53   20   12 40.63  50    17 30.13  100   22 15.58   13
   3 61.8    10    8 50.13    2   13 39.51  10    18 26.66  100   23  8.91    2
   4 58.97   10    9 49.05    7   14 36.61   3    19 25.33   40
   5 58.33    2   10 48.00   50   15 32.13  14    20 18.08   60
```

It is not necessary to list the contents of the file created. XRDLST has other uses, however; listing files is one of them.

If the user does not wish the contents of the file being built to be listed, a negative response is given to the last question. The computer then indicates the number of entries in the newly created file and exits the program.

```
 18 MINERALS ARE CONTAINED IN OUTPUT FILE.

 NORMAL TERMINATION

END OF EXECUTION
```

Now that the file has been built and stored in the user's area through the program XRDLST, the processes for creating the plot are the same as those described in the preceding section. XRDLST creates a binary data file as output in the same format as the file created by BLDMIN. XRDPLT can therefore operate directly on any file created by XRDLST.

The user may now return to page 19 and run XRDPLT.

OPERATING INSTRUCTIONS FOR THE PROGRAM XRDPLT - To create a Plot

After the new file has been successfully created and stored in the computer, the next step is preparation for the running of the program XRDPLT. The following interchange between the computer and the user is solely for DEC users. It assumes a basic familiarity with the 1070 system. For the non-DEC user, this is merely the method used to determine availability of tape drives, to mount a plot tape, and to assure that the "mount" command was registered with the command request queue.

.RES

This command requests that the computer check what input devices are available for use. To plot, there must be a plot-tape mounted. Therefore a 7-track tape drive (MTA100 or MTA101) must be free. If one of these devices appears in the resources list, then issue the following command:

.MOUNT MTA:PLOT/REELID:PLOTAP/VID:7-TRK/WE

This is the command to mount the 7-track plot tape.

The computer responds with:

```
REQUEST QUEUED
WAITING...2↑C'S TO EXIT
```

A check may be made of the mount queue to see if the command was entered and its status:

.MO/C

As can be seen the command was entered:

```
1. M JOB18 TTY34 200,00 1 MOUNT MTA PLOT/REELID:PLOTAP/V:7-TRK/WE
1 COMMAND IN QUEUE
```

After the tape has been mounted, the operator sends a message giving the plot-tape number.

```
;;OPR; - YOUR PLOT TAPE IS PLTXXX
```

The "Plot Request Form", shown in Figure 5, should have been completed before starting the program. This form was designed to facilitate the running of the program XRDPLT, as an aid in setting up a plot. The form should be self-explanatory.

R E Q U E S T F O R X R D P L O T S

U.S. GEOLOGICAL SURVEY
mineralogy laboratory
Denver, Colorado

Before requesting a special plot, check the listing of currently available plots

FILL OUT A SEPARATE SHEET FOR EACH PLOT REQUESTED.

REQUESTOR_____BRANCH_____EXT_____ACCOUNT NO._____

MINERALS TO BE PLOTTED: *List minerals to be plotted in REVERSE ORDER from how they are to appear on the plot. Alphabetical, PDF No., and Group Indexes are available in the mineralogy laboratory.*

PDF NO.	MINERAL NAME	PDF NO.	MINERAL NAME

PLOT TAPE NO. _____X = _____ Y = _____PAPER TYPE_____

PLOT PARAMETERS:

ANGSTROM SCALE_____INTENSITY SCALE (UNITS/INCH)_____

DEGREE SCALE (PER INCH) _____2-THETA MAX _____

TITLE _____

Figure 5. Request for XRDPLT plot form.

The program XRDPLT can now be put into execution with the following command;

```
. RUN XRDPLT (200,200)
```

The program then prompts with the following questions. The answers given are those used to create Figure 1.

```
                                                        default answers

ENTER BASE FILE TO BE SEARCHED          :SKIP1

INTENSITY SCALE (UNITS PER INCH)        :200            100

DEGREE SCALE (DEGREES PER INCH)         :9.5            4

MAX 2-THETA VALUE TO BE PLOTTED         :60             70

      BASIC CHARACTER SIZE              : .08           (SUPPLIED BY PROGRAM)

ANGSTROM SCALE (YES OR NO)              :NO             YES

GROUP HEADING (UP TO 50 CHARS)          :ALUNITE - NATROALUNITE SERIES

RETRIEVAL BY (IDNO, GROUP, OR FORM):IDNO                IDNO

ENTER ONE, SIX DIGIT ID NO. PER LINE
ENTER "CARRIAGE RETURN" AS THE LAST ID NO.
740001
740010
740011
740008
740012
740016
740007
740006
740005
740017
740004
740018
740003
740014
740015
740013
740002
740009

18 IDNO'S WERE ENTERED.
```

After all the input IDNO's have been entered, the program starts the retrieval processes. As it finds each entry given in the input list, it prints the IDNO of that entry and the mineral name. If an entry is not found, the message "(MINERAL NOT FOUND)" is printed. The output list finishes with the dimensions of the plot. The option to cycle the program is also offered.

```
ID NO     GROUP       MINERAL NAME                LINES OVER 70.0
          CODE                                    DEGREES (LINES NOT
                                                  PLOTTED)

740001              H75-SL103A          ,K20
740010              PARKER 18           ,21
740011              H74-N64A            ,K27
740008              H75-SL104A          ,K33
740012              PARKER ALKEE MEE    ,K46
740016              M48                 ,K47
740007              H75-MX13            ,K54
740006              H75-MX14            ,K54
740005              H75-SL102A          ,K58
740017              M51A                ,K64
740004                 (MINERAL NOT FOUND)
740018              M51                 ,K85
740003              H74-N63A            ,K87
740014              M53                 ,K90
740015              M47B                ,K93
740013              M30                 ,K96
740002              H74-N52             ,K96
740009              PARKER 2            ,K96

PLOT DIMENSIONS. X/Y:25.2/20.0

WANT TO PROCESS ANY FURTHER DATA     : NO
NORMAL TERMINATION

END OF EXECUTION
CPU TIME:
EXIT
```

When the retrieval is completed, instructions to the plotter operator are created by running the GERBER program. Plot dimensions are entered in the "X" and "Y" size lines. Many plots may be stacked on a plot tape. It is suggested that a log be kept of the file numbers and the dimensions of the plot in each file so that these may be accurately transmitted to the plotter operator through the GERBER program. After the GERBER program is run, the tape must be re-wound, dismounted, and removed; and the computer operator must be instructed to keep it. An example of these instructions follows:

```
.RUN GERBER(51,45)

GERBER PLOTTER REQUEST (10-FEB-76)

THIS VERSION OF THE PROGRAM ALLOWS AS MANY LINES
FOR SPECIAL INSTRUCTIONS AS YOU WANT.  JUST BE SURE
TO GIVE AN EXTRA RETURN AFTER THE LAST LINE.

WHEN ENTERING THE FILENAME FOR THE REQUEST FORM,
PLEASE USE ONLY THE ALPHABETIC CHARACTERS A-Z.
THE EXTENSION WILL BE PROVIDED BY THE PROGRAM.

ENTER THE FILENAME FOR REQUEST (          )
                                  SKIP

NAME: (              )
       CUNNINGHAM
ORGANIZATION (          )
                 G9
ACCOUNT NO:  (              )
               XXXX-XXXXX
USER NO:  (     )
TAPE NO: (          )
          PLTXXX
PROGRAM NO:  (     )
             XRDPLT
NUMBER OF PLOTS  (     )
                   1
```

```
INITIAL PEN POSITION FROM THE LOWER LEFT CORNER OF THE PLOT IN
INCHES.
X = 1
Y = 1
PEN POINT:(TYPE X IN THE CORRECT BLANK)
00-X FINE (  ): 0-FINE (  ): 1-MED(   ): 2-COARSE (    )
           X
PHONE NO. (           )
            3504
PAPER TYPE:  (    )
                MYLAR
PAPER (    )/PLOT (  ) SIZE: (PLACE X IN ONE)
                    X

FOR PLOT     1  ENTER
FILE NUMBER = 1
X SIZE = 25
Y SIZE + 20

IF YOU DO NOT WANT THE PLOT LEFT IN BLDG 53,
PLEASE INDICATE WHERE IT SHOULD GO, ETC.

ENTER ANY SPECIAL INSTRUCTION (EXTRA CARRIAGE RETURN WHEN THROUGH)

STOP

END OF EXECUTION

EXIT

.REW MTA:
(X.XX  X X)

.DIS MTA:/REM

(MTA100:PLOTAP WRITE(C/H/S) = 45666/0/0)
MTA100 DISMOUNTED

.SEND OPR: PLEASE KEEP PLTXXX/INSTRUCTIONS IN 51,45/THANKS
```

The plot tape is now given to the plotter operator with the instructions from the GERBER program.

References

Cunningham, C. G., Jr., Hall, R. B., Hauff, Phoebe L., and VanTrump, George, Jr., 1976, Alunite-natroalunite identification using field tests and a computer plotted overlay for X-ray diffraction charts: U.S. Geological Survey Open-File Report 76-402, 9p.

Hauff, Phoebe L., and VanTrump, George Jr., 1976, Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program-Laboratory Manual: U. S. Geological Survey Open-File Report 76-407, 55p.

VanTrump, George, Jr., and Hauff, Phoebe L., 1976a, Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program--Program Listing: U. S. Geological Survey Open-File Report 76-404, 24p.

----1976b, The Mineral X-Ray Diffraction File: U. S. Geological Survey Open-File Report 76-406, 144p.