UNITED STATES DEPARTMENT OF THE INTERIOR

GEOLOGICAL SURVEY

Laboratory Manual

Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program

By

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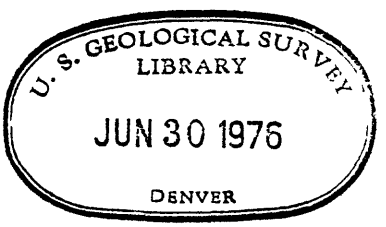

Open File Report 76-407
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Contents

Abstract

The Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program--XRDPLT (VanTrump and Hauff, 1976a) is used to retrieve and plot mineral X-ray diffraction data. The program operates on a file of mineral powder diffraction data (VanTrump and Hauff, 1976b) which contains two-theta or "d" values, and intensities, chemical formula, mineral name, identification number, and mineral group code. XRDPLT is a machine-independent Fortran program which operates in time-sharing mode on a DEC System 10 computer and the Gerber plotter (Evenden, 1974). The program prompts the user to respond from a time-sharing terminal in a conversational format with the required input information.

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

The second option retrieves as the first, but also plots the retrieved 2-theta and intensity values as diagrammatic X-ray powder patterns on mylar sheets or overlays. These plots can be made using scale combinations compatible with chart recorder diffractograms and 114.59 mm powder camera films. The overlays are then used to separate or sieve out unrelated minerals until unknowns are matched and identified.

Introduction

This is a technical manual written to assist the potential user in the exact operation and function of the Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program (XRDPLT). This manual and the program were developed to facilitate the identification of minerals using X-ray diffraction data.

The program performs two main functions. It enables the user to retrieve information from the "Mineral X-Ray Diffraction Data File" (see Appendix A) (VanTrump and Hauff, 1976b). It is also capable of plotting this information as diagramatic X-ray diffraction traces. When these data are plotted on transparent mylar, the overlays or sieves become standards with which other X-ray traces may be compared and from which minerals may be identified.

Description of the program

XRDPLT is a Fortran program (VanTrump and Hauff, 1976a) written to operate on the DEC System 10 computer, located in the U.S. Geological Survey facility at the Denver Federal Center. The program is machine independent, except for the plotter routines (Evenden, 1974), and can be adapted to other time-sharing computers.

The program "questions" the user from a time-sharing terminal for the required information to create a plot tape which is then plotted by a Gerber plotter on transparent mylar sheets. The user picks up the completed plot at the computer center. The advantage of this is that the instructions for both retrieval and plotting are transmitted through the terminal at one time.

The plot option.--The program is designed to plot simulated X-ray diffraction traces from X-ray powder diffraction data stored in a file on a disk of the computer. The completed plots are titled and contain 2-theta and angstrom scales at top and bottom. To the right (at the start) of each plot is the mineral name and ID or PDF number. A choice of scales is offered, for both vertical (intensity) and horizontal (2-theta) axes. The horizontal size of the plots is further controlled by the maximum 2-theta value given the program. The 2-theta range is 0°-180°. Title and heading sizes are automatically assigned when the standard scale factors are given as input. These standards are discussed in the "options" section of this manual.

Output may be in the form of a single plot of one mineral, or a sheet with multiple plots. The number of minerals accommodated on one sheet is a function of the vertical scale chosen and the size limitations of the plotter. Appendix D illustrates various scales that may be selected.

The U.S. Geological Survey's mineralogy laboratory in Denver, Colorado has produced a series of mylar overlays containing the more common mineral groups; i.e. feldspars, amphiboles, garnets, pyroxenes, carbonates, borates, etc. Appendix C lists these groups. At present, these overlays may only be used within the U.S. Geological Survey, since the Joint Committee on Powder Diffraction Standards considers some of its source data as proprietary information available only through them. Many of the minerals on these sieves are from the JCPDS data file.

Figure 1.--Near here

Figure 1.--An example of a plot scaled to exact powder film size (114.59 mm) The vertical scale = 1/2 inch, the horizontal scale is 25.4° 2-theta per inch. Page 4 contains a detailed description of the plot contents.

S I L I C A M I N E R A L S

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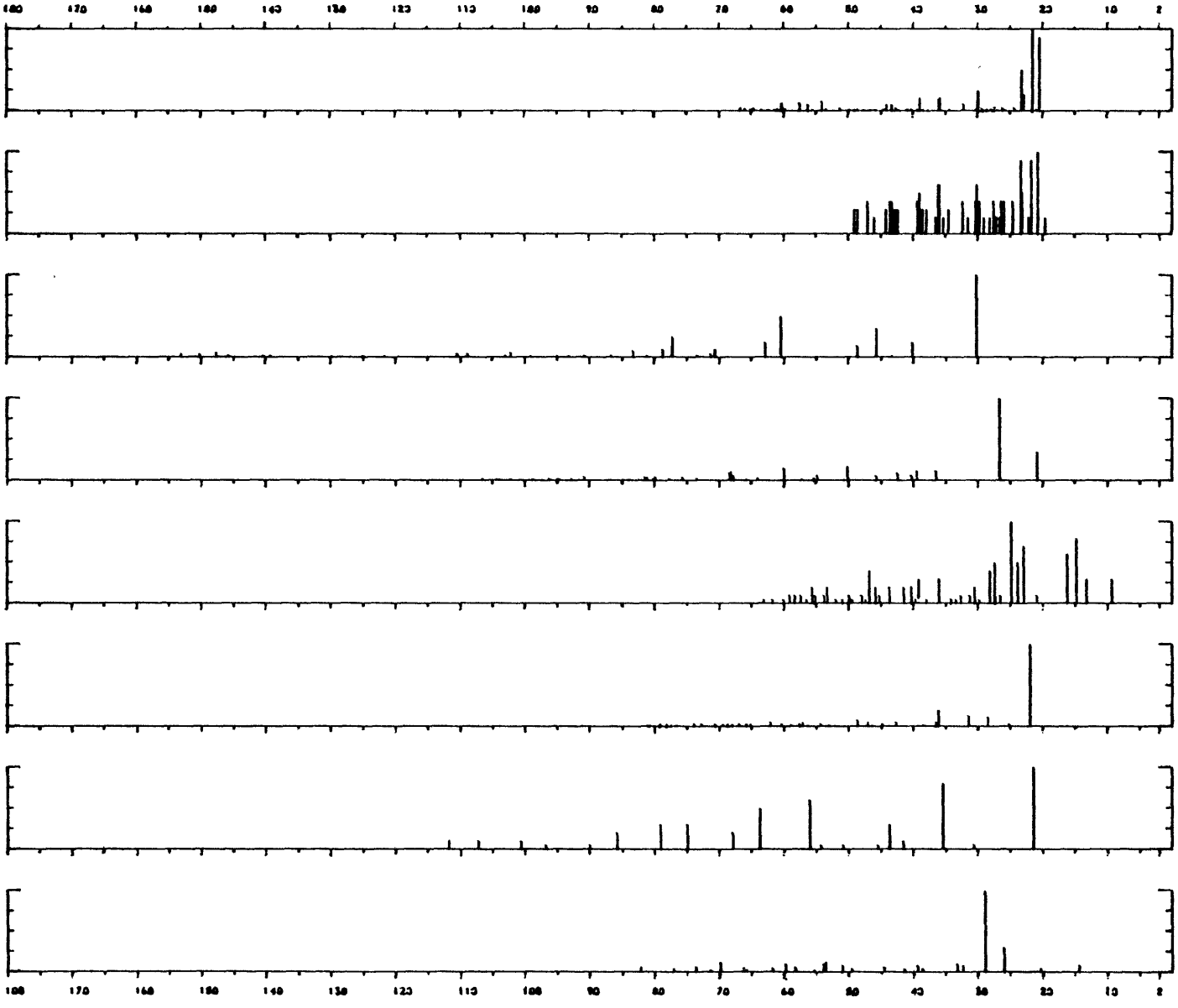


These overlays are an invaluable tool for mineral identification. Since standards of the same size as the chart recorder diffractogram or the powder camera films can be produced, direct comparison of the unknown to the standard may be made. This eliminates interpolation, hand plotting, X-ray machine and operator errors. The relationships of the reflections are graphically displayed. The user is not restricted to precise numerical values, but may shuffle the overlays matching the peaks themselves.

Another possible use of the program is the generation of unique mineral suite sieves required by a specific project. Examples of these might be: igneous and sedimentary zeolites, playa minerals, lithium-bearing minerals, saline minerals, minerals from a specific geographic location (Montezuma, Colorado Mining District), or those from a geologic formation (Pierre shale minerals). Whatever combination the user requires can be retrieved and plotted if the data are in the file.

The ability to create overlays the exact size of a powder camera film is most helpful. The sharp lines on the mylar plot are accurate indicators of even the faintest reflections on the film.

Retrieve option.--The XRDPLT program also has the ability to operate as a retrieval system. Actually this is its primary function as it must search and retrieve from the "Mineral X-Ray Diffraction Data File" before the data can be plotted. When the user wishes to retrieve without plotting, this retrieval is a relatively simple operation. An example of the terminal printout of a retrieval is included with the directions for running the program in the next section.

Three different approaches to retrieval are possible. Retrieval may be made by mineral groups such as oxides, phosphates, sulfides, silicates, amphiboles, feldspars. Retrieval may also be based on the individual formula components; i.e., a user may request all lithium (Li)-bearing minerals, all carbonates with copper (Cu), all arsenates with bismuth (Bi) and silver (Ag). Finally, retrieval can be made by the identification number, a six-digit number unique to each mineral entered into the data file (which can be a PDF#).

The group retrieval process was developed before it was possible to base a search on the actual formula components. Although parts of this five-character code are now archaic, enough of it is useful to retain it in the program. Appendix B includes the key to the groups. When retrieving with the GROUP option, the user enters the codes for the groups desired.

Examples of this are as follows:

SIG	retrieves garnets
SIFP	retrieves plagioclase feldspars
PHMM	retrieves members of the monazite group

Retrieval by group does not necessarily result in an ordered sequence useful to the requestor. If sequence is important for a plot, it is suggested that retrieval without plotting be done first to determine the desired IDNO's, and that a plot search then be done with the IDNO's arranged in the correct sequence.

The second method of retrieval is perhaps the most versatile. Using this option, retrieval is based directly on the formulas. The data file is so structured that the formula components are isolated and can be individually retrieved. Exceptions were made for the following radicals:

SO_4 CO_3 OH H_2O PO_4 NH_4

This was done because these combinations are consistent.

The uniqueness of this method lies in the retrieval combinations. The following are possible:

element only	Cu
element with subscripts	Cu?
("?" indicates numerical subscripts)	
element only OR element-subscripts	Cu/Cu?
("/" indicates "OR" operator)	
Combinations of the above	Cu/Cu?,As/As?
("," indicates "AND" operator)	

Negative retrievals can also be made. The logic is expressed as:

NOT element AND NOT element-subscript	-Cu,-Cu?
("-" designates "NOT" operator)	

It is essential that the comma rather than the slash be used for negative operations. Using the "/" would result in the following interpretation "NOT Cu OR NOT Cu-Subscript." This gives the program a choice which can result in one OR the other expression (Cu or Cu?) being retrieved when the user actually wants neither expression.

The five radicals listed above can be substituted for the elements, in which case there is no need for the "?" (subscript). Any other radicals must be retrieved on their individual components; i.e., SiO_2 would be Si, O_2 = silica AND oxygen 2.

Formula-component searches can further be divided into two types of retrievals: "inclusive" and "exclusive." An inclusive retrieval lists minerals with the specified components, but may include additional components. An exclusive retrieval, which is preceeded by a "+", i.e.; +Cu/Cu?,As/As?, finds those minerals containing only the specified components.

Examples of these various options are given in the next section, which contains instructions on running the program.

The option of retrieval without plotting is an exceptionally powerful tool, especially if the user knows the potential mineral group (amphibole, feldspar, pyroxene) or any of the chemistry of his sample. This option provides the user with a quick list of chemical compositions and mineral group members with which unknowns may be compared.

Instructions for running

X-Ray Data Plot/Retrieve Program

This is an interactive program. The computer prompts the user for the correct input information. Following are simulated listings, as they appear on the terminal with responses for computer and user indicated. The two main options of the program are given: Plot only; retrieve only.

The section on "OPTIONS" lists the various choices available for each question from the computer.

When using the "PLOT" option of the program, it is necessary not only to run the "XRDPLT" program but also "GERBER," which creates instructions to the plotter operator about the tape to be plotted. When stacking more than one plot on the plot tape, a "PLOT TAPE LOG" form is available for convenience in recording the data required by the program, "GERBER." A form is available from the U.S. Geological Survey computer center which may be utilized in lieu of the plotter instruction program. However, from the terminal it is more efficient to make use of the "GERBER" program. Forms are provided by the mineralogy lab to request plots or searches. It is recommended that these forms be completed prior to a plot or search run whether the user is running the programs himself or asking that the laboratory personnel process his request.

Each instruction in the following listings is necessary for a successful and accurate plot to result.

Instructions for Running Program

I. Plot.--If output is to be a plot:
(Underscored commands are user entered.)

The actual commands to the computer do change, sometimes frequently. Before running these programs or if problems are encountered while running check with the computer center or the mineralogy laboratory to update the "job control language."

To exercise the "default option" given hit "carriage return" (<CR>) (see p. 20).

```
.MOUNT MTA:PLOT/REELID:PLOTAP/VID:7-TRK/WE
REQUEST QUEUED
WAITING...2  C'S TO EXIT
PLTO MOUNTED, MTAO USED
[0.XX XXX]

;;OPR: - YOUR PLOT TAPE IS PLTXXX

.RUN XRDPLT[200,200]
```

			Default Answers
WANT TO PLOT DATA? (YES OR NO)	: YES	<CR>	YES
INTENSITY SCALE(UNITS PER INCH)	:	<CR>	100
DEGREE SCALE (DEGREES PER INCH)	:	<CR>	4°
MAX 2-THETA VALUE TO BE PLOTTED	:	<CR>	70°
BASIC PLOT CHARACTER SIZE	: .08		
ANGSTROM SCALE(YES OR NO)	:	<CR>	YES
GROUP HEADING(UP TO 50 CHARS)	: EXAMPLE	<CR>	
RETRIEVAL BY (IDNO,GROUP, OR FORM)	:	<CR>	IDNO

```
ENTER ONE, SIX DIGIT ID NO. PER LINE.
ENTER "CARRIAGE RETURN" AS THE LAST ID NO.
90429
90333
130581
230957
240454
21251
130568
150261                                  <CR>
                                        <CR>

8 IDNO'S WERE ENTERED.
```

```
  IDNO        GROUP      MINERAL                    LINES OVER 70.0 DEGREES
              CODE                                    (LINES NOT PLOTTED)
 90429        ARC        ALGODONITE                          10
 90333        ARC        DOMEYKITE-ALPHA                     26
130581        ARC        KOUTEKITE                            4
230957        ARCA       KUTINAITE                            3
140454        ARC        DOMEYKITE-BETA                      18
 21251        ARC        DOMEYKITE                            8
130568        ARCA       NOVAKITE                             9
150261        ARC        PACITE


PLOT DIMENSIONS. X/Y:16.4/20.0


<<GBR622 X/Y:60.0/20.0-IN CH I/O:181 LN I/O:2074/2074
<<  DEV:MTAO BLKS:41


WANT TO PROCESS ANY FURTHER DATA: NO
NORMAL TERMINATION

END OF EXECUTION
CPU TIME: 00.00 ELAPSED TIME: 0.00.00
EXIT
[XX.XX  XXX X]

.RUN GERBER[51,45]

ENTER THE FILE NAME FOR INSTRUCTIONS(       )
                                      EXAMPL
NAME:(                          )
      JOHN SMITH
ORGANIZATION:(      )
             G9
ACCOUNT NO.:(           )
            123456789
USER NO.:(     )
         987
TAPE NO.:(          )
          PLTXXX
PROGRAM NO.:(       )
             XRDPLT
NUMBER OF PLOTS (    )
                1
INITIAL PEN POSITION FROM THE LOWER LEFT CORNER OF THE PLOT IN IN.
X=1.0
Y=1.0
PEN POINT:(TYPE X IN THE CORRECT BLANK)
00-EXTRA FINE( );0-FINE( ); 1-MED( ); 2-COARSE( )
              X
```

```
PHONE NO.: (            )
            1234/6789
PAPER TYPE: (           )
             MYLAR
PAPER( )/PLOT( ) SIZE:(PLACE X IN ONE)
              X


FOR PLOT  1 ENTER
FILE NUMBER = 1
XSIZE = 16.4
Y SIZE = 20.0
DO YOU WANT THE PLOT TAPE RETURNED? NO
SPECIAL INSTRUCTIONS
NONE
STOP

END OF EXECUTION
CPU TIME: 0.00  ELAPSED TIME: 0.00.00
EXIT
[X/XX  XX X]

.REW MTA:
[X.XX X X]

.DISM MTA:/REM
MTA0DVR135 READ (W/H/S)= 24284/0/0 WRITE (W/H/S)= 25095/0/0
MTA0 DISMOUNTED
[X.XX  XX X]

.SEND OPR: PLEASE SAVE TP PLTXXX, PLOT WITH INST IN [51,45] THANKS
```

The format of this computer center system program, GERBER, may also change. However, the requested information should remain the same.

II. Inclusive retrieval by Group.--If output is retrieval only (no plotter output):

```
.RUN XRDPLT[200,200]


WANT TO PLOT DATA? (YES OR NO)      : NO

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

ENTER ONE, FIVE CHAR GROUP NAME PER LINE.
ENTER "CARRIAGE RETURN" AS LAST NAME.
*ARC??

IDNO       GROUP     MINERAL                 CHEMICAL FORMULA
           CODE
GROUP     REQUIRED:  ARC??
 90429     ARC       ALGODONITE              CU6 AS
 90333     ARC       DOMEYKITE-ALPHA         CU3 AS
130581     ARC       KOUTEKITE               CU2 AS
230957     ARCA      KUTINAITE               CU2 .07 AG.84 AS
140454     ARC       DOMEYKITE-BETA          CU3 AS
 21251     ARC       DOMEYKITE               CU3 AS
130568     ARCA      NOVAKITE                ( CU, AG )4 AS3
150261     ARC       PAXITE                  CU2 AS3


WANT TO PROCESS ANY FURTHER DATA: NO
NORMAL TERMINATION

END OF EXECUTION
CPU TIME: XX.XX ELAPSED TIME: X:X.XX
EXIT
[XX.XX  XXXX X]

.
```

When the retrieval only option is used the chemical formula is printed out in place of "Lines over 70° not plotted."

* The group asked for was arsenates; element was copper (See Appendix B for Group Code key).

III. Inclusive retrieval by Formula Components.--A formula component is defined as a single element, as elements with subscripts, and as the special CO_3, SO_4, H_2O, OH, PO_4, and NH_4. Any other radicals or molecules are retrieved by their individual components; i.e. to find minerals containing various silica radicals, Si_2O_8, Si_8O_{22}, Si_3O_{18}, the search string would be; Si?,O?.

If the previously explained logical operations are not used exactly as defined, this may result in an error message. However, it is possible to insert logic that has the correct syntax, relative to the computer, but which would result in invalid mineral retrievals.

INCLUSIVE

This example retrieves all barium-bearing sulfates.

```
.SET TTY WIDTH 80
.RUN XRDPLT[200,200]
WANT TO PLOT DATA? (YES OR NO)        :NO
RETRIEVAL BY(IDNO, GROUP, OR FORM)    : FORM
ENTER FORMULA COMPONENTS REQUIRED ON ONE LINE.
   SEPARATE BY COMMAS FOR "AND" LOGIC.
            BY SLASHES FOR "OR" LOGIC.
BA/BA?,SO4

FORMULA COMP REQD;  BA/BA?,SO4
```

IDNO	GROUP CODE	MINERAL	CHEMICAL FORMULA
50448	SF**	BARITE	BA SO4
150071	SFX Z	INNELITE	BA- TI- MN- SI- O- OH . NA- SO4
191419	SF**$E	WEILERITE	BA AL3 (AS 04) (SO4) (OH)6
191418	SF**XO	WENKITE	BA CA AL SI O SO4 OH
191421	SCX Z	YOSHIMURAITE	BA MN TI FE O SI O PO4 SO4 (OH)

WANT TO PROCESS ANY FURTHER DATA : NO

INCLUSIVE - with radicals and negatives

This is an example of retrieval using radicals and negative operators. Specific zeolites were sought, those containing sodium, calcium, aluminum and water with subscripted silica radicals, but not unsubscripted silica (i.e. SiO_2).

.SET TTY WIDTH 80

.RUN XRDPLT[200,200]

WANT TO PLOT DATA : NO

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

ENTER FORMULA COMPONENTS REQUIRED ON ONE LINE.
SEPARATE BY COMMAS FOR "AND" LOGIC.
BY SLASHES FOR "OR" LOGIC.

NA/NA?,CI/CA?,AL/AL?,H2O,-SI,SI?

FORMULA COMP REQD; NA/NA?,CA/CA?,AL/AL?,H2O,-SI,SI?

IDNO	GROUP CODE	MINERAL	CHEMICAL FORMULA
120275	SIZ	ERIONITE	K NA CA AL4 SI14 036 . 14 H2O
160148	SIZ	GARRONITE	NA CA2.5 AL6 SI13 032 . 13 . 5 H2O
100473	SIZ	GONNARDITE	CA NA2 SI6 AL4 020 . 7 H2O
110173	SIZ	MESOLITE	NA2 CA2 AL6 SI9 030 . 8 H20
60239	SIZ	MORDENITE	(CA NA2 K2) AL2 SI10 024 . 7 H20
181203	SIZ	STILBITE,NA	NA CA2 AL5 SI13 036 . 14 H2O

WANT TO PROCESS ANY FURTHER DATA : NO

INCLUSIVE

This retrieval became too specific. It has the same search components as the above example. However, eliminating "Si" from the formula components makes the search too narrow, resulting in no components which satisfy the criteria.

```
.SET TTY WIDTH 80
.RUN XRDPLT[200,200]

WANT TO PLOT DATA                    :    NO
RETRIEVAL BY(IDNO, GROUP OR FORM)    :    FORM

ENTER FORMULA COMPONENTS REQUIRED ON ONE LINE.
   SEPARATE BY COMMAS FOR "AND" LOGIC.
            BY SLASHES FOR "OR" LOGIC.

NA/NA?,CA/CA?,-SI,-SI?,AL/AL?,H2O

FORMULA COMP REQD: NA/NA?,CA/CA?,-SI,SI?,AL/AL?,H2O

IDNO   GROUP   MINERAL                          CHEMICAL FORMULA
       CODE

NO MINERALS FOUND

WANT TO PROCESS ANY FURTHER DATA    :    NO
```

IV. Exclusive Retrieval.--The exclusive search, which is initiated by a "+" in front of the search string, retrieves minerals containing only or exclusively the specified components. In this first example the program is told to retrieve only arsenides containing copper. Note also that the "GROUP CODE" for all minerals retrieved is the same.

```
.SET TTY WIDTH 80
.RUN XRDPLT[200,200]

WANT TO PLOT DATA?  (YES OR NO)          :  NO
RETRIEVAL BY  (IDNO, GROUP, OR FORM)     :  FORM

ENTER FORMULA COMPONENTS REQUIRED ON ONE LINE.

     SEPARATE BY COMMAS FOR "AND" LOGIC.
              BY SLASHES FOR "OR" LOGIC.

+CU/CU?,AS/AS?

FORMULA COMP REQD:  CU/CU?,AS/AS?

EXCLUSIVE RETRIEVAL

IDNO     GROUP    MINERAL                    CHEMICAL FORMULA
         CODE

 90429   ARC      ALGODONITE                 CU6 AS
 90333   ARC      DOMEYKITE-ALPHA            CU3 AS
130581   ARC      KOUTEKITE                  CU2 AS
```

```
140454  ARC     DOMEYKITE-BETA                  CU3,AS
 21251  ARC     DOMEYKITE                       CU3 AS
150261  ARC     PAXITE                          CU2 AS3
```

```
WANT TO PROCESS ANY FURTHER DATA    : NO
```

EXCLUSIVE

This example illustrates an exclusive retrieval on a radical where the program was requested to search only for aluminum hydroxide minerals.

```
.SET TTY WIDTH 80

.RUN XRDPLT[200,200]

WANT TO PLOT DATA                   : NO

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

ENTER FORMULA COMPONENTS REQUIRED ON ONE LINE.
   SEPARATE BY COMMAS FOR "AND" LOGIC.
            BY SLASHES FOR "OR" LOGIC.

+AL/AL?,OH

FORMULA COMP REQD:  AL/AL?,OH

EXCLUSIVE RETRIEVAL

IDNO    GROUP   MINERAL                         CHEMICAL FORMULA
        CODE

200011  HX$     BAYERITE                        AL (OH)3
 70324  HX$     HYDRAGILLITE                    AL (OH)3
120460  HX$     GIBBSITE                        AL (OH)3
180031  HX$     NORDSTRANDITE                   AL (OH)3
```

```
WANT TO PROCESS ANY FURTHER DATA      : NO
NORMAL TERMINATION

END OF EXECUTION
CPU TIME:  0:00.00                ELAPSED TIME:  00:00.00
EXIT
 :00:00    000 0
```

Please note that using negative logic with the exclusive option is redundant.

V. Suggestion for a More Efficient Search based on Formula Components

The computer does not search each formula simultaneously for all components given in a search string, but evaluates each separately, searching the entire formula every time. Therefore, on a formula component retrieval, to make the most efficient use of the computer, set up the search string with the component least likely to be found listed first. For example, this method could be used to retrieve beryllium-aluminum silicates. There are numerous aluminum and silica bearing minerals in the file, but few which also contain beryllium. Construct the search string with the beryllium listed first:

BE/BE?,AL/AL?,SI/SI?

When the computer searches a formula and does not find "BE", it will cease to evaluate that formula and go on to the next formula immediately. It will not look for the other constituents until it finds a formula which contains "BE". Using this method therefore cuts computer search time considerably.

Options--Plot and Retrieval Routines

The XRDPLT program has built into it default answers to the various questions asked by the computer. When the carriage return (<CR>) is entered rather than an answer given these defaults are automatically used by the computer. The questions and the defaults are:

RUN XRDPLT[200,200]		DEFAULT
WANT TO PLOT DATA? (YES OR NO)	:	YES
INTENSITY SCALE (UNITS PER INCH)	:	100
DEGREE SCALE (DEGREES PER INCH)	:	4°
MAX 2-THETA VALUE TO BE PLOTTED	:	70°
BASIC PLOT CHARACTER SIZE	: .08	
ANGSTROM SCALE (YES OR NO)	:	YES
GROUP HEADING (UP TO 50 CHARS)	:	_____
RETRIEVAL BY (IDNO,GROUP,OR FORM):		IDNO

ENTER ONE, SIX DIGIT ID NO. PER LINE.
ENTER "CARRIAGE RETURN" AS THE LAST ID NO.

0 IDNO'S WERE ENTERED.

WANT TO PROCESS ANY FURTHER DATA : NO
NORMAL TERMINATION

END OF EXECUTION

Values other than these defaults must be manually entered. This section explains the various questions asked by the computer and gives the choices available to the user when responding to these questions.

1. Intensity Scale (units per inch).--The intensity or vertical scale is a representation of the relative intensities of the reflections. These values are scaled from 0-100 units. This vertical scale can be set up for any value within the paper size of the plotter (60 inches). Following is a list of the more convenient sizes:

Inches	Units per inch
.25	400
.50	200
.67	150
.75	133.33
.80	125
1.00	100
1.25	80
1.33	75
1.50	66.67
2.00	50
4.00	25

The formula for computing the units is:

$$\frac{100}{y \text{ (inches)}} = X \text{ (units)}$$

The program default is 100 units.

2. Degree scale (degrees per inch).--The degree scale lies along the horizontal axis. It is an expression of the 2-theta value in degrees per inch. This scale must also be set up within the limits of the paper, which is 50 inches. The common settings are:

2°/inch	which yields a plot ≈ 40 inches
4°/inch	which yields a plot ≈ 20 inches
25.4°/inch	which yields a plot equal in size to a powder film
1°/ inch	no more than 45° 2-theta can be plotted

The default in the program is 4°/inch.

3. MAX 2-theta value.--All plots start at 0° 2-theta. The default for this option is 70° 2-theta. It is suggested that this value be used except in two cases. The first exception would be when plotting a simulation of a powder film. The maximum 2-theta value must then be 180° to achieve the correct length to the plot. The other exception would be a plot where the 2-theta scale = 1° per inch. Here paper size limits Max 2-theta to 45°.

The program is flexible and accepts any number between 0-180°. However, 70° was chosen as an optimum size for the standard plots.

If the user enters a Max 2-theta which when coupled with the value given for the degree scale exceeds the available paper size, an error message is printed out:

```
ERROR **** Y-PAPER SIZE(93.0) GREATER THAN MAX PLOTTER SIZE(50.0)
TRY RE-ENTERING VALUES AGAIN.
```

4. Character size.--Following is a list of automatic title and heading character size defaults. When these degree-unit combinations are entered the program automatically computes and assigns these values.

Degrees per inch	Units per inch	Character size default
25.4°	any	.05
2°	100=1"	.10
2°	200=1/2"	.06
4°	100=1"	.08
4°	200=1/2"	.06

In addition a further default is built into the program. If a combination of scales other than those listed above is chosen, the program automatically uses .08 as its character size.

The character size can be entered to override the defaults. This is done by adding the value of the character size to the intensity scale line and separating it from the intensity value by a comma.

EXAMPLE:

Intensity scale (units per inch): 100,.05

Examples of the various character sizes are kept on file in the Denver mineralogy lab. Some are included in Appendix D of this manual.

5. Angstrom Scale.--The angstrom scale appears at the top and bottom of each plot when chosen.

If the degrees per inch value is 11° per inch or greater, the angstrom scale will not be plotted. It is not possible to neatly show all the numbers when a plot becomes this small. If 11° or greater is entered as the degree scale, then the program does not ask the angstrom scale question.

The default for this option is "yes"--it prints the angstrom scale.

6. Group heading.--The group heading is the title which appears centered across the top of the specific plot. It is limited to a maximum of 50 characters. It also always includes the lines:

Dept. of Interior, U.S. Geological Survey, Denver, Colorado

George VanTrump Jr. and Phoebe L. Hauff Lambda = 1.5405

7. Retrieval by IDNO or GROUP.--When the user chooses to plot or retrieve by IDNO, these 6-digit identification numbers may be entered in any sequence desired. The program is capable of cycling the data file for these numbers and retrieving in order submitted. However, because of the physical setup of the plotter it is necessary to give the computer the numbers in reverse order from that in which they are to appear on the actual plot.

Terminal input

140654

110695

160331

150026

Plots as:

150026

160331

110695

140654

A maximum of 50 IDNO's may be entered per search. If more data are retrieved than the plotter is capable of plotting, the program computes plot sizes for as much of the data as space allows and prints out the following error message:

WARNING ::::: X-PAPER SIZE WILL BE EXCEEDED AFTER PLOTTING NEXT MINERAL.
THEREFORE PLOTTING OF ANY FURTHER MINERALS WILL BE TERMINATED.

Group.--When plotting or retrieving with the "GROUP" option, the order is not as easily determined. The computer chooses the minerals of the groups as they are arranged in the file. This is not necessarily an ordered sequence useful to the requestor.

If a plot is the ultimate objective and the user requires a specific sequence on the plot, then it is suggested that the file first be searched by "GROUP" option (with "NO PLOT" option). The "NO PLOT" option does not require that the "Mount Plot Tape" command be given, and "NO" is used as the answer to the first question "WANT TO PLOT DATA." The IDNO's retrieved by this search can be put in the desired order, and then the "PLOT" option can be taken, submitting the IDNO's in the desired sequence.

When the "GROUP RETRIEVE/NO PLOT" option is taken the minerals print out with their formulas in addition to the IDNO. A maximum of 10 group names may be entered per search. If more than 10 are entered, the following error message appears:

```
WARNING ***** MORE THAN 10 GROUP NAMES ENTERED.
THESE 10 WILL BE PROCESSED.
```

APPENDIX A

MINERAL X-RAY DIFFRACTION DATA FILE

Mineral X-Ray Diffraction Data File

The Mineral X-Ray Diffraction Data File (XRDFIL) (Van Trump and Hauff, 1976b) is a computer file containing selected X-ray diffraction information. It is a subfile of MINBAS, the master data base which is a more detailed file of varied and comprehensive mineral data. XRDFIL and MINBAS have been installed on the DEC System 10 computer in Denver, Colorado. The programs which operate on XRDFIL are time sharing oriented.

Contents of file.--XRDFIL contains considerable information relating to published and unpublished mineral X-ray diffraction data. It was created to provide standards of comparison for various methods of mineral X-ray identification. The file has the ability to accommodate the following information for each entry: mineral name, chemical formula, two-theta and "d" values, intensities, crystal system, hkl designations, mineral group, and bibliographic references.

Organization of the file.--Since each program which operates on the file requires different combinations of the data contained within the file, XRDFIL can be manipulated to accommodate the varying formats of these programs.

Indexes have also been created to make XRDFIL more understandable and efficient for the user to access. These indexes contain five columns of information. The first column is a five-character alphanumeric code which designates mineral groups and further defines cation and anion relationships within these groups. The X-Ray Diffraction Mineral Retrieval/ Plot Computer Program uses this code to search and retrieve from the file. The mineral groups are based on those found in Dana-Frondel (7th ed.) and Deer, Howie, and Zussman (1962). The second column is an internal numbering system for the program. In the third column is a unique six digit identification number which may also be used to search the file. The mineral name is found in the fourth column and its formula in the fifth.

Example:

Mineral Group		I D Number	Mineral Name	Mineral formula
ASK U	1	160386	ABERNATHYITE	K U 02 AS 04 . 3 H2 O
SCR#	146	210173	ABUKUMALITE	CA2 Y3 SI3 012 (OH)
SCR#	147	210174	ABUKUMALITE	CA2 Y3 SI3 012 (OH)
SPA	2	140072	ACANTHITE	AG2 S
SIXC	3	181222	ACMITE	NA FE SI2 06

Four indexes are provided. Their acronyms are: MINALP, GRPALP, GRPSRT, and IDNOST. MINALP is a strict alphabetical listing of all the minerals in the file. In GRPALP, the file has been sorted by the mineral group code into the respective mineral groups. Each group has then been sorted alphabetically within itself. GRDSRT is also sorted by mineral groups and then further sorted within each group by anion or element distribution. IDNOST is an index sorted by the unique six digit identification number assigned to each entry in the file. Since many of these numbers are the same as the "PDF" numbers assigned by the Joint Committee on Powder Diffraction Standards, it was felt that an ascending numerical sort of these numbers would be useful to have when accessing the XRDFIL.

APPENDIX B

KEY TO GROUP CODES

This appendix contains the key to the group codes by which minerals may be retrieved from the "Mineral X-Ray Diffraction Data File." The following pages are alphabetical lists of mineral groups and the codes which retrieve them from the file.

These codes, as originally set up, allowed the user, with some restrictions, to search on chemical composition. However, improvements in the program allow now for direct search based on the individual formula components, and have made parts of this group code outdated. Therefore, only the more useful parts of the old code are listed in this appendix.

Listing by Mineral Group

Mineral Group	Search Code	Mineral Group	Search Code
Alkali feldspars	SIFA	Clinoamphiboles	SIA
Aluminum silicates	SC$$	Clinopyroxenes	SIXC
Alunite group	SFAA	Clintonite-mica	SIPMC
Amphiboles-clino	SIA	Elements	EL
Amphiboles-ortho	SIO	Epidote	SCEE
Antimonates	AA	Feldspars-alkali	SIFA
Antimonides	AI	Feldspars-barium	SIFB
Apatite group	PHAA	Feldspars-plagioclase	SIFP
Arsenates	AS	Feldspathoids	SIS
Arsenides	AR	Friedelite group	SICP
Autunite group	PHUU	Garnets	SIG
Barium feldspars	SIFB	Halides	HD
Beryllium silicates	SCBB	Humite group	SICH
Biotites	SIPMB	Hydroxides	HX
Borates	BR	Illites	SIPCI
Carbonates	CR	Kandites	SIPCK
Chlorites	SIPR	Lepidolite-mica	SIPML
Chromates	CM	Margarite-mica	SIPMG
Clays-illite	SIPCI	Melilite group	SICM
Clays-kandites	SIPCK	Mica	SIPM
Clays-mixed layer	SIPCL	Biotite	SIPMB
Clays-palygorskite	SIPCP	Clintonite	SIPMC
Clays-smectites	SIPCS	Lepidolite	SIPML

Mineral Group	Search Code	Mineral Group	Search Code
Mica (cont.)		Pyroxenoids	SID
Margarite	SIPMG	Scapolite group	SICS
Muscovite	SIPMM	Selenates	SO
Phengite	SIPMH	Selenides	SE
Phlogopite	SIPMP	Septachlorites	SIPS
Misc. phyllosilicates	SIYM	Serpentines	SIPP
Mixed-layer clays	SIPCL	Silica	SA
Molybdates	MO	Silicates by chemistry	SC
Monazite group	PHMM	Silicates with subgroups	SI
Muscovite-mica	SIPMM	Smectites	SIPCS
Niobates/tantalates	NT	Spinel group	SL
Nitrates	NA	Sulfates	SF
Olivine group	SICO	Sulfides	SP
Orthoamphiboles	SIO	Sulfosalts	SS
Orthopyroxenes	SIXO	Tellurates	TO
Oxides	OX	Tellurides	TE
Palygorskite-clay	SIPCP	Titanates	TI
Phengite-mica	SIPMH	Titano silicates	SCTT
Phlogopite-mica	SIPMP	Tourmaline group	SICT
Phosphates	PH	Tungstates	TU
Phillosilicates	SIP	Turquoise group	PHTT
Plagioclase feldspars	SIFP	Uranates	UR
Pyroxenes-clino	SIXC	Vanadates	VD
Pyroxenes-ortho	SIXO	Vermiculites	SIPCU
Pyroxenoids	SID	Zeolites	SIZ
Pyroxenes-clino	SIXC		
Pyroxenes-ortho	SIXO		

Listing by Mineral Group Code

Search Code	Mineral Group	Search Code	Mineral Group
AA	Antimonates	SE	Selenides
AI	Antimonides	SF	Sulfates
AR	Arsenides	SFAA	Alunite group
AS	Arsenates	SI	Silicates with subgroups
BR	Borates	SIA	Clinoamphiboles
CM	Chromates	SICP	Friedelite group
CR	Carbonates	SICH	Humite group
EL	Elements	SICM	Melilite group
HD	Halides	SICO	Olivine group
HX	Hydroxides	SICS	Scapolite group
MO	Molybdates	SICT	Tourmaline group
NA	Nitrates	SID	Pyroxenoids
NT	Niobates/tantalates	SIFA	Alkali feldspars
OX	Oxides	SIFB	Barium feldspars
PH	Phosphates	SIFP	Plagioclase feldspars
PHAA	Apatite group	SIG	Garnets
PHMM	Monazite group	SIO	Orthoamphiboles
PHTT	Turquoise group	SIPCI	Clays-illite
PHUU	Autunite group	SIPCK	Clays-kandites
SA	Silica	SIPCL	Clays-mixed layer
SC	Silicates by chemistry	SIPCP	Clays-palygorskite
SC$$	Aluminum silicates	SIPCS	Smectites
SCBB	Beryllium silicates	SIPCV	Vermiculites
SCEE	Epidote	SIPM	Mica
SCTT	Titano silicates	SIPMB	Biotite

Search Code	Mineral Group
SIPMC	Clintonite
SIPMG	Margarite
SIPMH	Phengite
SIPML	Lepidolite
SIPMM	Muscovite
SIPMP	Phlogopite
SIPP	Serpentines
SIPR	Chlorites
SIPS	Septachlorites
SIS	Feldspathoids
SIXC	Clinopyroxenes
SIXO	Orthopyroxenes
SIYM	Misc. phyllosilicates
SIZ	Zeolites
SL	Spinel group
SO	Selenates
SP	Sulfides
SS	Sulfosalts
TE	Tellurides
TI	Titanates
TO	Tellurates
TU	Tungstates
UR	Uranates
VD	Vanadates

APPENDIX C

STANDARD SIEVES AVAILABLE

Standard mineral sieves available

from the file

The mineralogy laboratory of the U.S. Geological Survey has set up a file of sieves or overlays of the most commonly used minerals. Copies are kept in the Denver laboratory. They have been generated by XRDPLT program (VanTrump and Hauff, 1976a). The following list includes those available as of September 1975. It is anticipated that the file of these sieves will be enlarged and revised as the data base itself undergoes changes. However, these sieves contain some information considered proprietary by the Joint Committee on Powder Diffraction Standards (JCPDS) and subsequently are presently available for use only by members of the U.S. Geological Survey. A magnetic tape containing their version of this data is available from the JCPDS, Swarthmore, Pa.

Amphiboles

Aluminum silicates

Alunite group

Antimony minerals

Apatite group

Arsenate minerals

Arsenide minerals

Autunite group

Beryllium silicates

Borate minerals

Carbonate minerals

Chlorite minerals

Chromate minerals

Clay minerals

kaolinites/illites/vermiculite/

mixed layer/palygorskite

Clay minerals

smectites

Columbite/tantalate minerals

Elements - simple

Elements - compound

Epidote group

Feldspars - all

Feldspars - alkali/barium

Feldspars - plagioclase

Feldspathoids

Garnet group

Halide minerals

Heavy mineral concentrates

Hydroxide minerals

Manganese oxide minerals

Manganese-bearing oxide minerals

Metamorphic accessory minerals

Mica minerals

Molybdenum minerals

Niobate/tantalate minerals

Nitrate minerals

Olivine group minerals

Oxide minerals - simple

Pyroxene group minerals

Pyroxenoid minerals

Rare earth phosphates

Rare earth silicates

Schultz mineral sieve

Selenium minerals

Serpentine minerals

Silica minerals

Spinel group

Sulfate minerals

Sulfide minerals

Sulfosalt minerals

Tellurium minerals

Titanium-bearing oxides

Titano silicate minerals

Tungstate minerals

Uranium minerals

Zeolite minerals

APPENDIX D

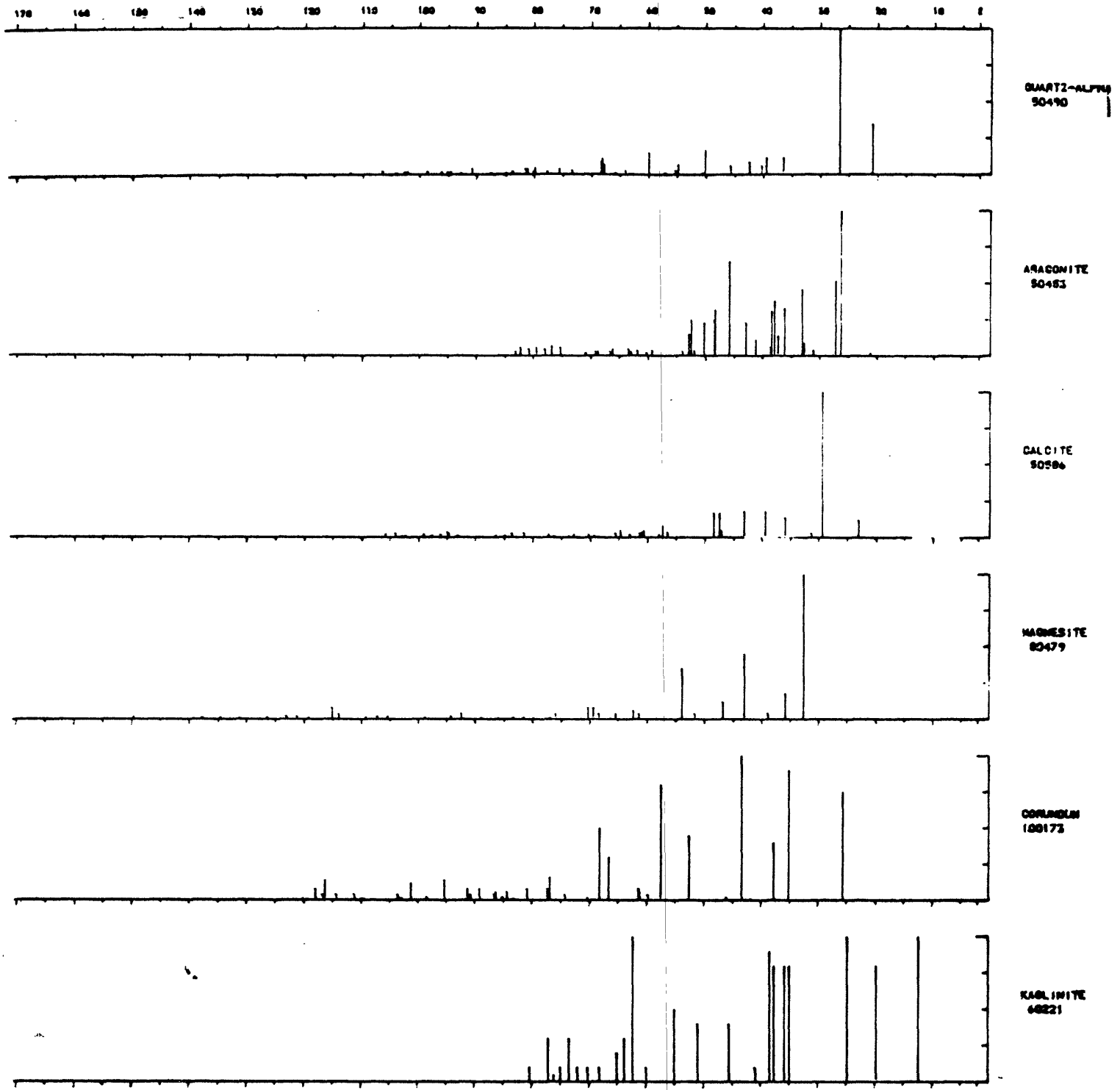
EXAMPLES OF

TITLE AND HEADING SIZES

VERTICAL AND HORIZONTAL SCALES

POWDER FILM SIEVE - NICHOLS SANDIA

DEPT. OF INTERIOR, U.S. GEOLOGICAL SURVEY, DENVER, COLORADO
GEORGE VAN TRUMP, JR. AND PHOEBE L. HAUFF

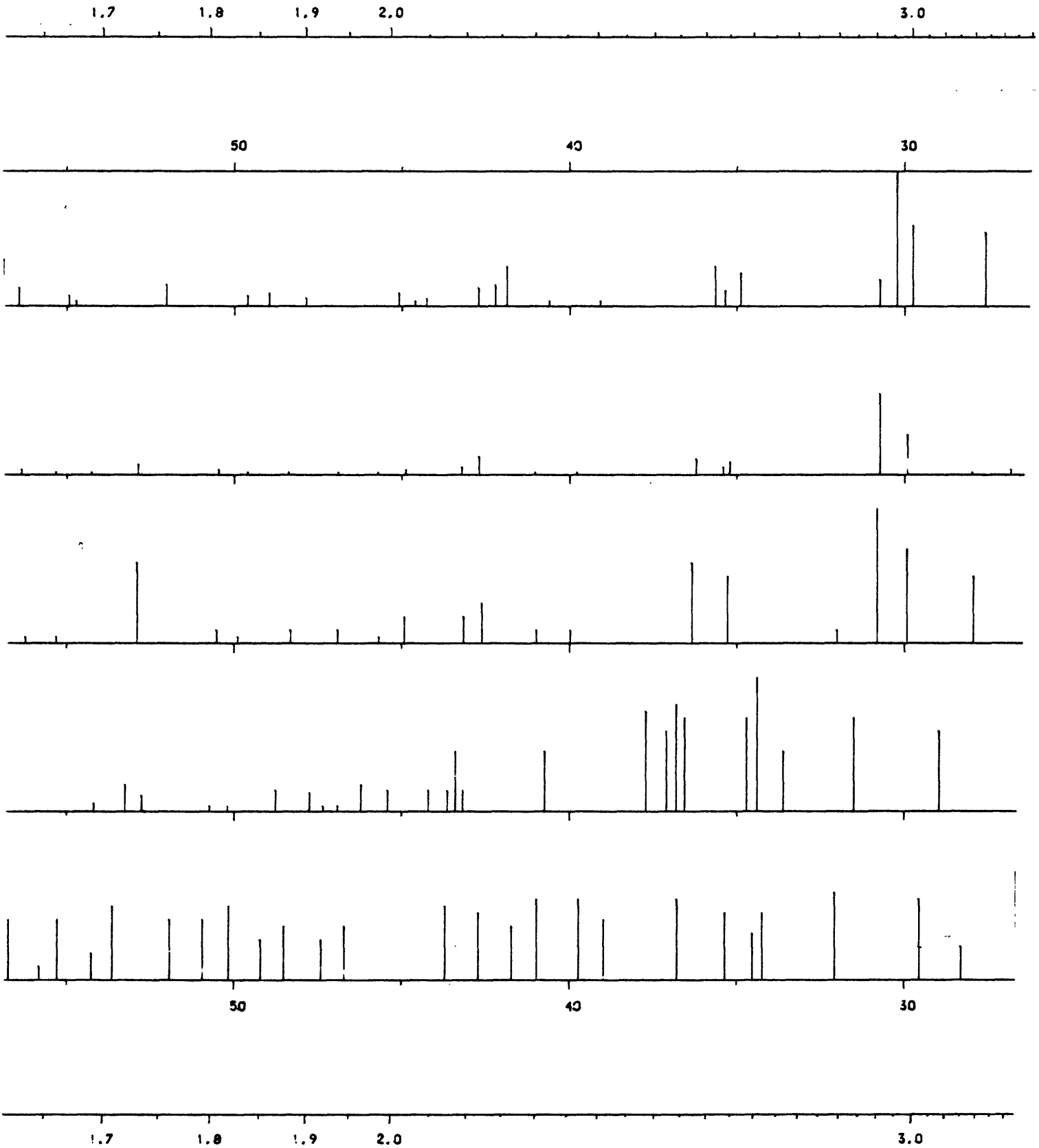


Vertical scale = 1 inch, horizontal scale = 25.4° 2-θ per inch

Character size = .06

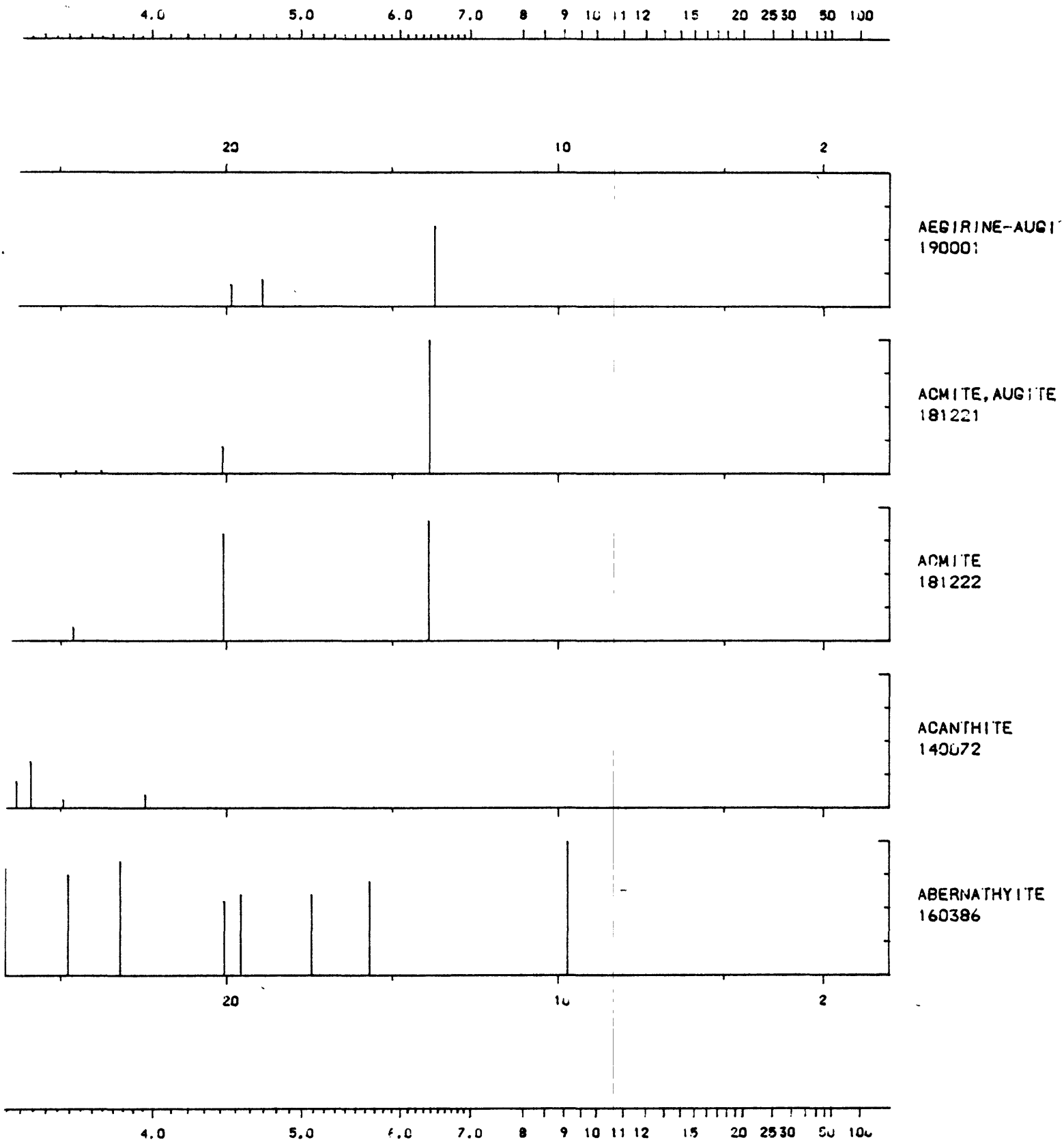
TEST / 4 / 100 / .08

DEPT. OF INTERIOR, U.S. GEOLOGICAL SURVEY, DE
GEORGE VAN TRUMP, JR. AND PHOEBE L.

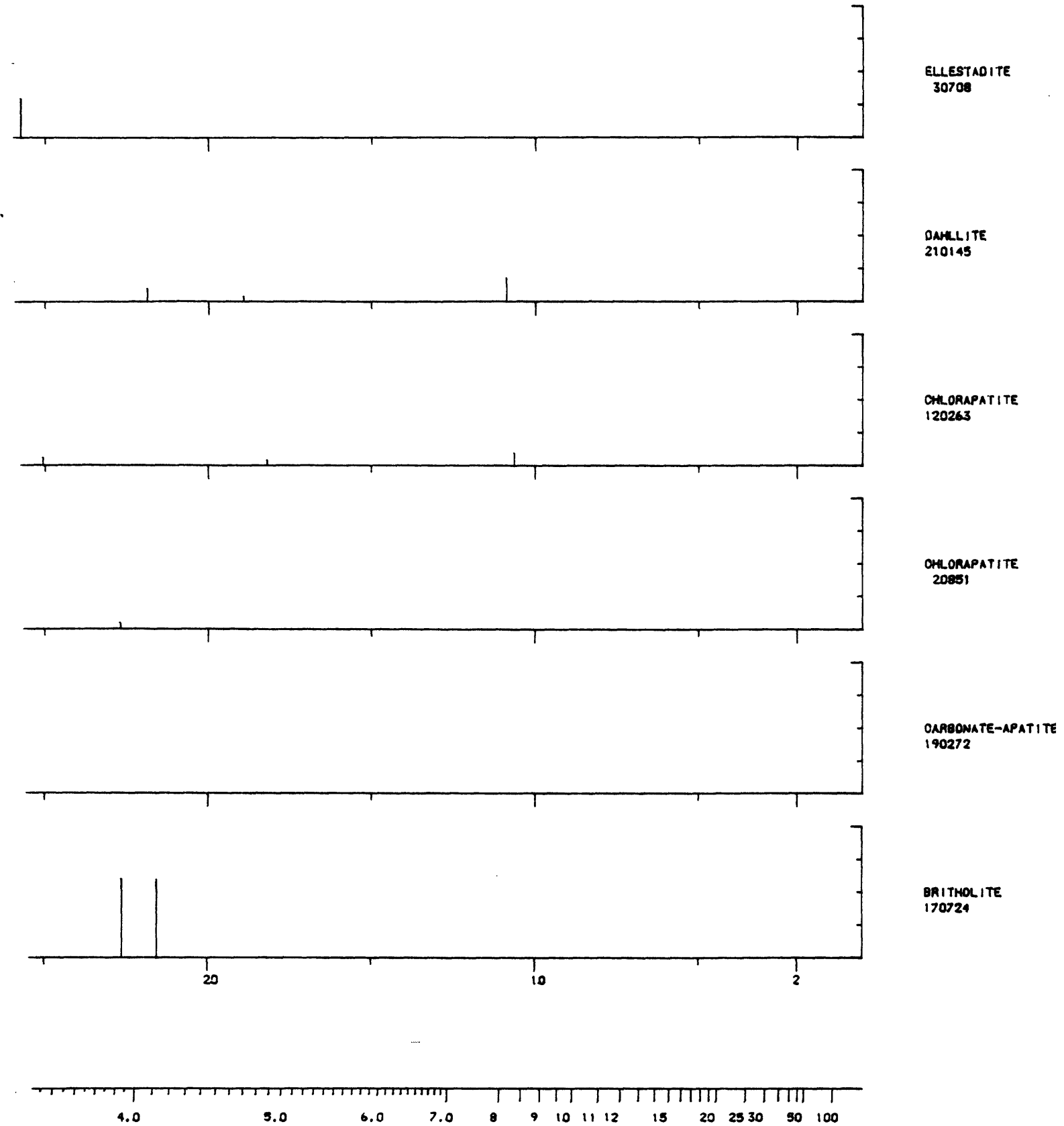


Vertical Scale = 1 inch, Horizontal scale = 4° 2-θ per inch
Character size = .08

ENVER, COLORADO
HAUFF

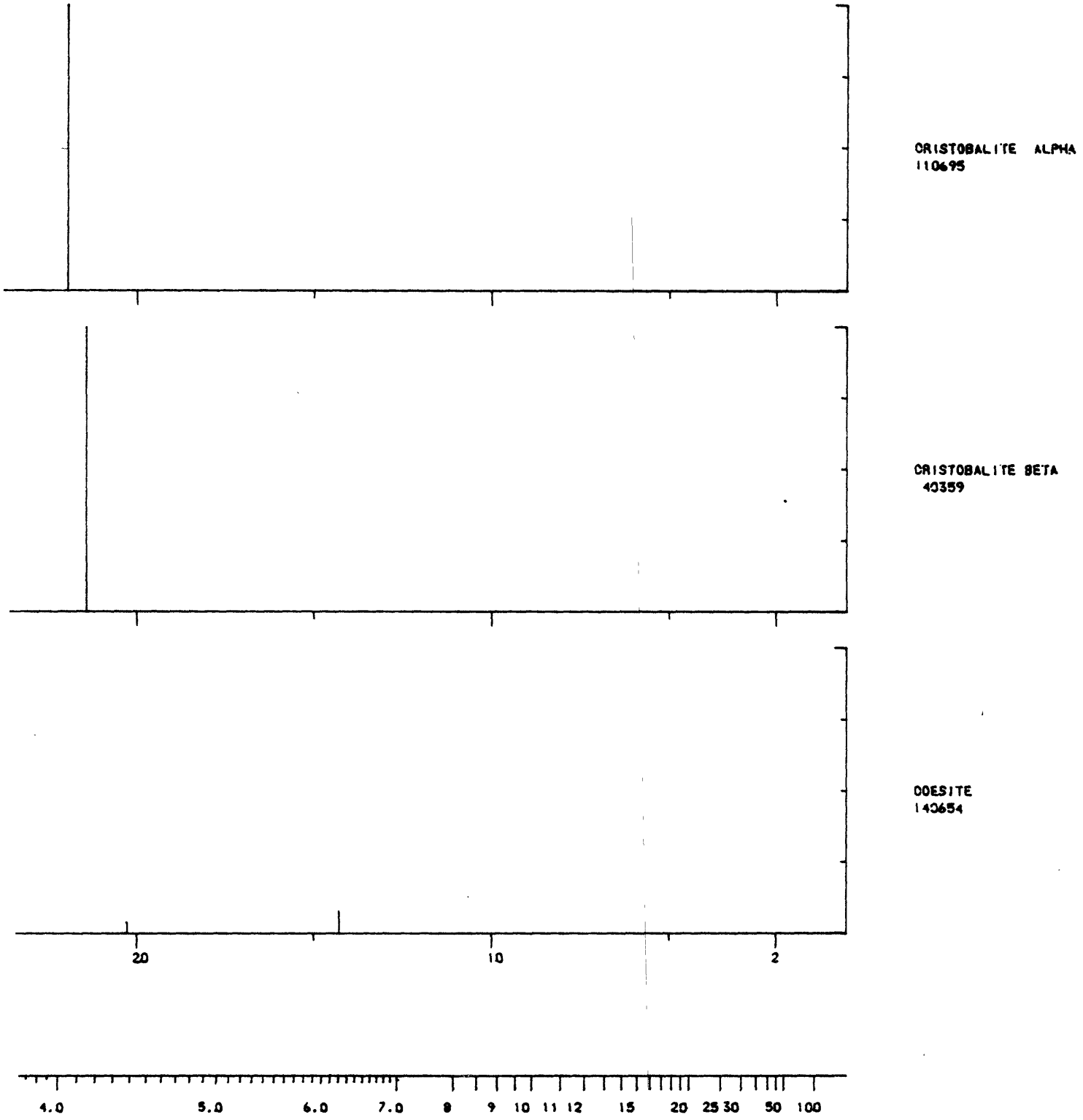


Vertical Scale = 1 inch, horizontal scale = 4° 2-θ per inch
Character size = .08



Vertical scale = 1 inch, horizontal scale - 4° 2-θ per inch

Character size = .06

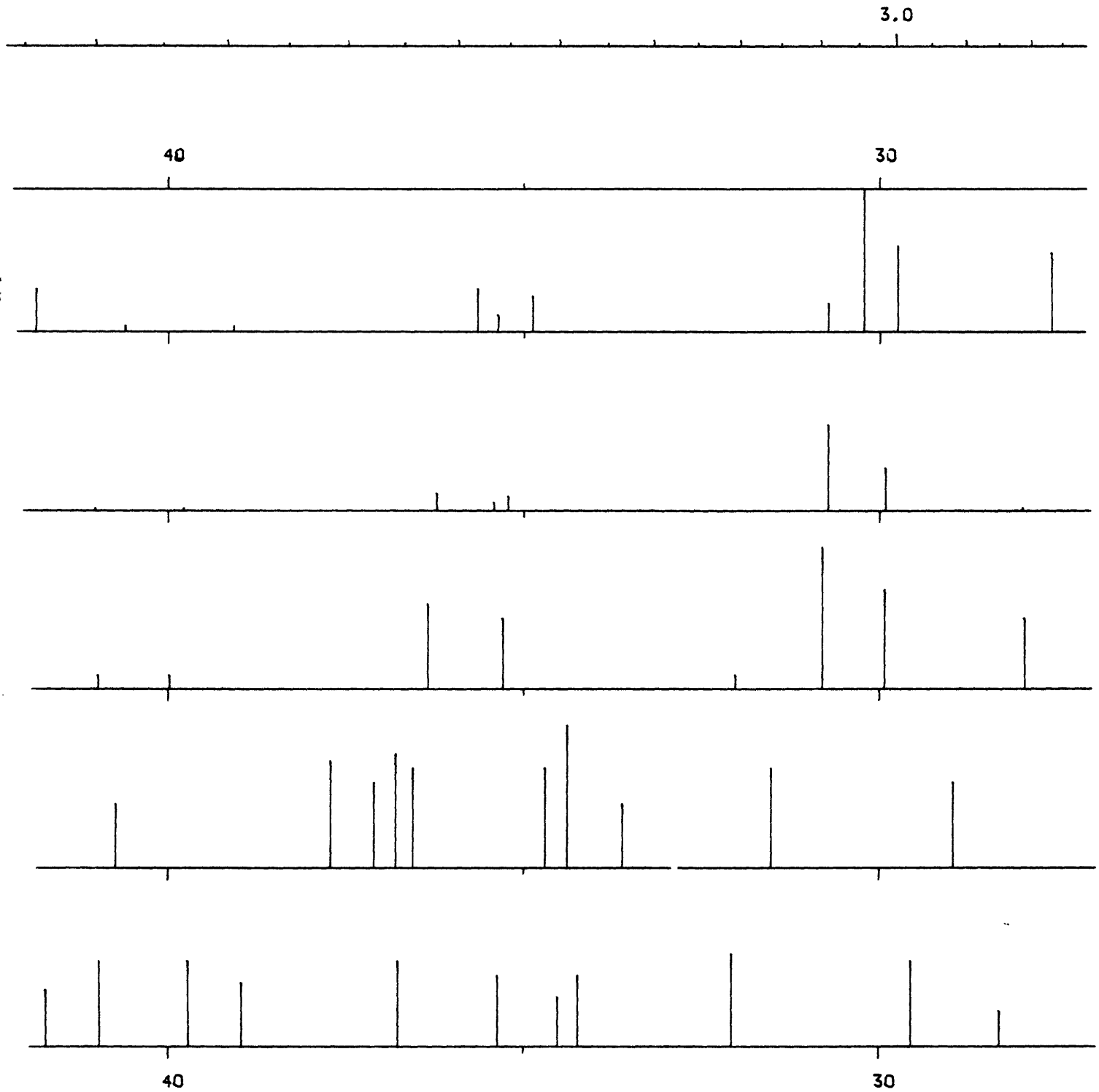


Vertical scale = 2 inches, horizontal scale = 4° 2-θ per inch

Character size = .06

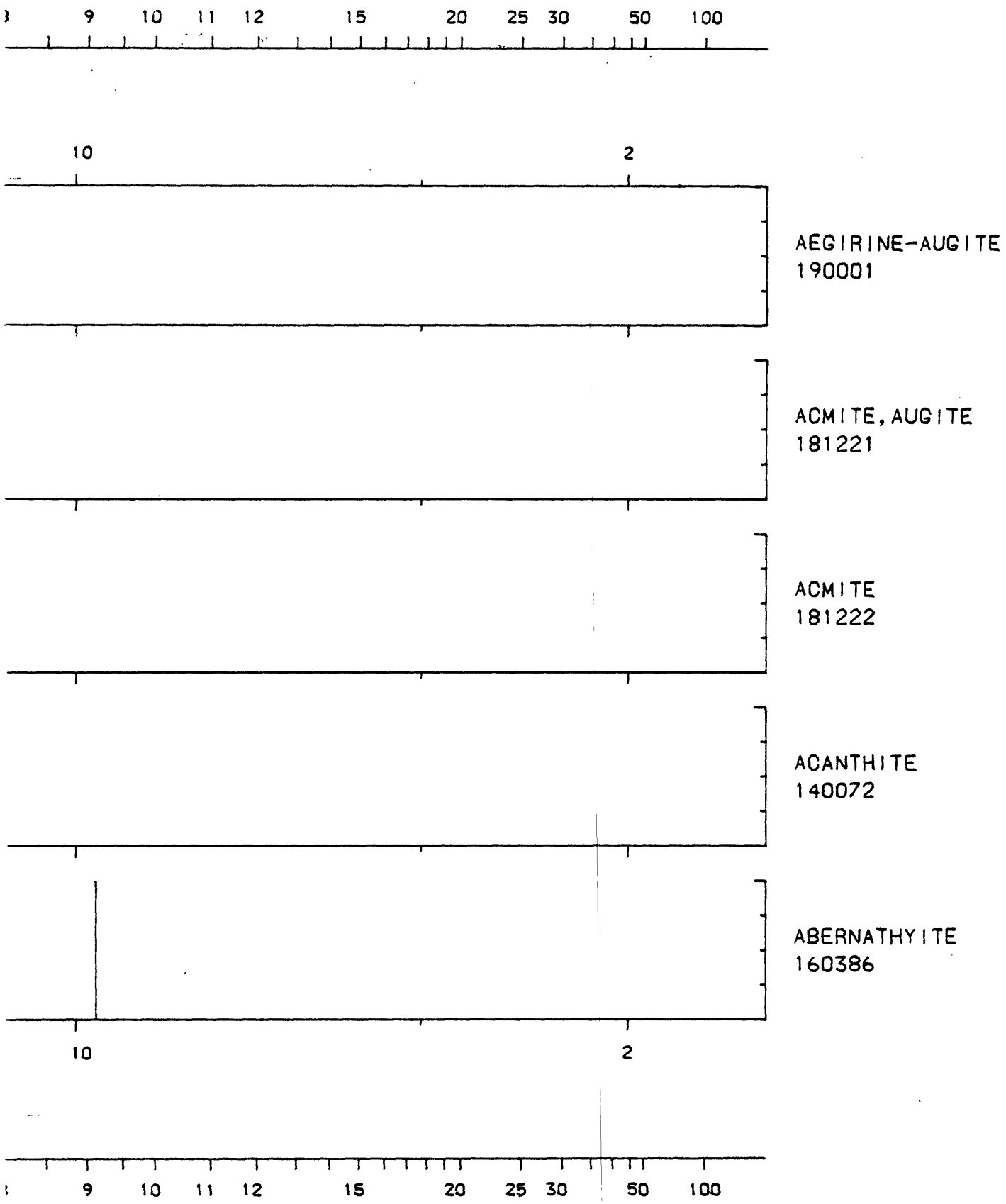
TEST / 2 / 100 / .10

NTERIOR, U.S. GEOLOGICAL SURVEY, DENVER,
EORGE VAN TRUMP, JR. AND PHOEBE L. HAUFF



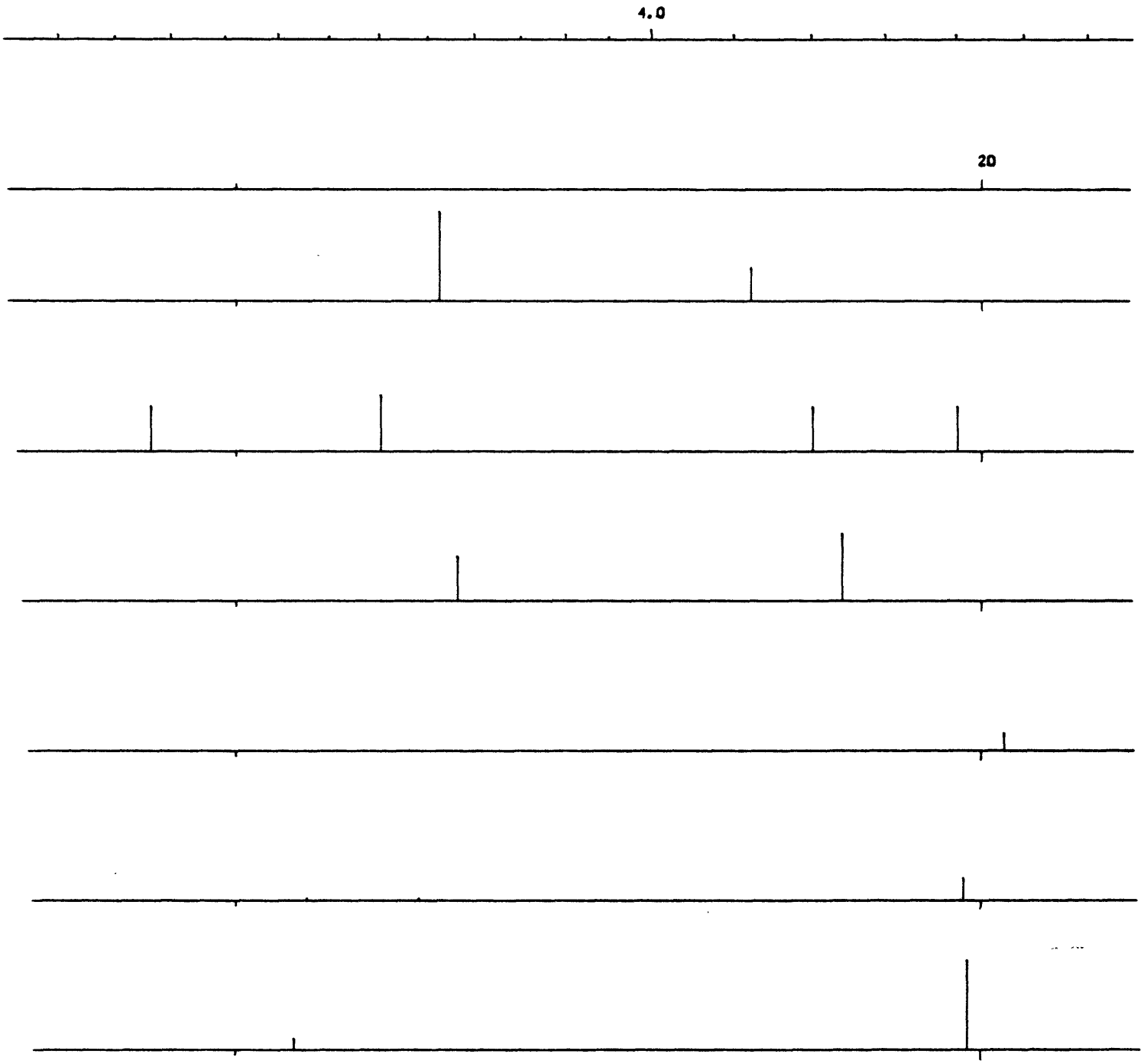
Vertical scale = 1 inch, horizontal scale = 2° 2-θ per inch

Character size = .10



Vertical scale = 1 inch
Horizontal scale = 2° 2θ per inch
Character size = .10

'T. OF INTERIOR, U.S. GEOLOGICAL SURVEY, DENVER, COL(
GEORGE VAN TRUMP, JR. AND PHOEBE L. HAUFF



Vertical scale = .75 inch, horizontal scale = 1° 2-θ per inch

Character size - .08

APPENDIX E

FORMS

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 please check the standard plots currently available from the Denver Mineralogy Lab. Fill out a separate request sheet for each plot.

Requestor name _____ Branch _____ Ext _____

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 Lab.

PDF No.	MINERAL NAME

SEARCH OPTION
Consult Group code index (10 max)

SEARCH ON:

_____ _____
_____ _____
_____ _____
_____ _____
_____ _____

Plot _____ No Plot _____

Listing _____

_____

Plot tape No. _____

X _____ Y _____

Paper type _____

PLOT PARAMETERS:

Angstrom scale _____ Intensity scale (Units/inch) _____

Degree scale (per inch) _____ 2 θ Max _____

Title _____

P L O T T A P E L O G

DATE _____ PLOT TAPE NO. _____ /

FILE #	TITLE	2Ø	INT	X	Y
1.					
2.					
3.					
4.					
5.					
6.					
7.					
8.					
9.					
1Ø					
11.					
12.					
13.					
14.					
15.					
16.					
17.					
18.					
19.					
2Ø.					

References

Deer, W. A., Howie, R. A., and Zussman, J., 1962, Rock-forming minerals: John Wiley and Sons, Inc., 270 p.

Evenden, G. I., 1975, A general purpose contouring system: U.S. Geological Survey, Open file report 75-317, 104 p.

Palache, Charles, Berman, Harry, and Frondel, Clifford, 1951, The system of mineralogy of James Dwight Dana and Edward Salisbury Dana, Yale University 1837-1892: John Wiley and Sons, Inc., 7th Edition.

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, 24 p.

_____1976b, The Mineral X-Ray Diffraction Data File--Description and Indices: U.S. Geological Survey, Open file report 76-406, 144 p.