UNITED STATES DEPARTMENT OF THE INTERIOR

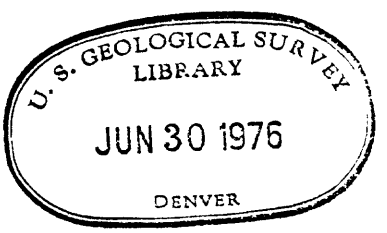
GEOLOGICAL SURVEY

# Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program

## Program Listing

By

George Van Trump and Phoebe L. Hauff
U.S. Geological Survey

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This report is preliminary and has not been edited or reviewed for conformity with U.S. Geological Survey standards and nomenclature.

Contents

## Program Description

The Mineral X-Ray Diffraction Data Retrieval/Plot Computer Program, XRDPLT, is used to retrieve mineral X-ray diffraction data and to create a plot tape of the retrieved information. The use of this information facilitates the identification of minerals. The program operates on The Mineral X-Ray Diffraction Data file (Hauff and Van Trump, 1975) 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 except for the Gerber plot subroutines (Evenden, 1974). The program operates in timesharing mode on a DEC System 10 computer prompting the user from a remote terminal to respond 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 either by identification number, by the mineral group code which is a classification by chemistry or structure, or by searches on the formula components. For example it enables the user to search for minerals by major group; i.e., feldspars, micas, amphiboles, oxides, phosphates, carbonates; or by elemental composition; i.e., Fe, Cu, Al, Zn; or a combination of both; i.e., all copper-bearing arsenates.

The second option retrieves as the first, but also plots the retrieved 2-theta and intensity values as diagramatic X-ray powder patterns on mylar sheets or overlays. These plots can be made using scale combinations compatible with chart recorder diffractograms and 115.59 mm powder camera films. The overlays are then used as standards to separate or sieve out incompatible minerals until unknowns are matched and identified.

Detailed instructions on the operation of the program, its options, and examples of the output are contained in the Laboratory Manual (Hauff and Van Trump, 1975) to the program.

Further information and copies of the general plots can be obtained from the Mineralogy Laboratory, Experimental Geochemistry and Mineralogy Branch, Denver Federal Center.

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C      * * * * *  XRD POWDER DATA RETRIEVAL & PLOT PROGRAM   * * * * * *
C                          U S GEOLOGICAL SURVEY
C                    GEOLOGIC DIVISION, DENVER, COLORADO
C                      WRITTEN BY GEORGE VAN TRUMP, JR.
C                            ON JUNE 20, 1975
C     ------------------------------------------------------------------
C        THIS PROGRAM IS USED TO RETRIEVE MINERAL DATA FROM A MINERAL
C     X-RAY DIFFRACTION DATA FILE AND TO CREATE A GERBER 622 PLOT TAPE
C     OF THE RETRIEVED INFORMATION, THEREBY FACILITATING THE IDENTIFICA-
C     TION OF MINERALS.
C        THE PROGRAM IS MACHINE INDEPENDENT EXCEPT FOR THE PLOTTER
C     CALLS, FILE HANDLING TECHNIQUES, AND THE PROMPTING FORMATS FOR THE
C     INPUT DATA.
C        SUBROUTINES PLTSET, ENDPLT, SCALE, CHAR, XAXIS, AND LINE ARE
C     ROUTINES FOR THE USGS GERBER 622 PLOTTER.  THESE ROUTINES WERE
C     WRITTEN BY GERALD I. EVENDEN, GEOLOGIC DIVISION, DENVER, COLORADO.
C        FOR THE OPERATING INSTRUCTIONS OF THE PROGRAM, SEE THE LAB
C     MANUAL FOR THE PROGRAM.
C     ------------------------------------------------------------------
C
C
1       INTEGER ID(50),IDNUM,IDCNT,IDPRE,FIRST,BAD,FMNUM
2       DIMENSION NID2(2),NEW(150),FORM(8),MINER(5),X(2),Z(2),ILABEL(10),
2      1 XGP(2),YGP(2),XGP2(2),XIN(22),IXIN(22),IXIN1(3),IXIN2(2),IXIN3(6)
2      2 ,GHDG(10),GPREQ(5,10),BUFF(50),DEGSET(5),TENSET(5),CHASET(5)
2      3 ,FORREQ(80)
3       COMMON XSCL,YSCL,NO,XP(4),YP(4),DXP(2),DYP(2)
4       COMMON /INIT/ ICODE,MCODE,NOPTS,IDCNT,FIRST,BAD
5       DATA IDSK/10/,DEGSET/2.0,2.0,4.0,4.0,25.4/,TENSET/100.0,200.0,
5      1 100.0,200.0,0.0/,CHASET/0.10,0.06,0.08,0.06,0.05/
6       DATA ILABEL/' 70',' 60',' 50',' 40',' 30',' 20',' 10','  0','  2',
6      1 ' '/
7       DATA IXIN/'100','50','  ','  ',' ','30','25','20',' ',' ',' ',
7      1 '  ','15','  ','  ','12','11','10','   ',' 9 ','   ',' 8 '/
8       DATA IXIN1/'7.0','6.0','5.0'/,IXIN2/'4.0','3.0'/
9       DATA IXIN3/'2.0','1.9','1.8','1.7','1.6','1.5'/
10      DATA XIN/100.,50.,45.,40.,35.,30.,25.,20.,19.,18.,17.,16.,15.,
10     1 14.,13.,12.,11.,10.,9.5,9.0,8.5,8.0/
11      CALL ILL
C
C ... OPEN MASTER INPUT MINERAL FILE AND INITALIZE VALUES.
C
12      OPEN (UNIT=IDSK,FILE='MINERL',DIRECTORY='200,257')
13      CALL PLTSET (0,XBD,YBD,1)
14  100 CALL INITPR (XBD,YBD)
C     ------------------------------------------------------------------
C ... READ NEW DATA FOR PROCESSING A NEW RETRIEVAL.
C     ------------------------------------------------------------------
15      TYPE 110
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```
16      110 FORMAT (//' WANT TO PLOT DATA?  (YES OR NO)    : ',$)
17          ACCEPT 1000,ANS
18          IPT=0
19          IF (ANS.EQ.'N') IPT=1
20          IF (IPT.NE.0) GO TO 290
21          TYPE 120
22      120 FORMAT (/' INTENSITY SCALE(UNITS PER INCH)    : ',$)
23          ACCEPT 130,XSCL,SIZE
24      130 FORMAT (2F)
25          IF (XSCL.LE.0.0) XSCL=100.0
26      140 TYPE 150
27      150 FORMAT (/' DEGREE SCALE (DEGREES PER INCH)    : ',$)
28      160 ACCEPT 130,YSCL
29          IF (YSCL.LE.0.0) YSCL=4.0
30          TYPE 170
31      170 FORMAT (/' MAX 2-THETA VALUE TO BE PLOTTED    : ',$)
32          ACCEPT 130,DYP(2)
33          IF (DYP(2).LE.0.0) DYP(2)=70.0
34          YP(1)=DYP(2)/YSCL
35          IF (SIZE.GT.0.0) GO TO 200
36          DO 190 I=1,5
37          IF (ABS(YSCL-DEGSET(I)).GT.0.1) GO TO 190
38          IF (I.EQ.5) GO TO 180
39          IF (ABS(XSCL-TENSET(I)).GT.0.1) GO TO 190
40      180 SIZE=CHASET(I)
41          GO TO 200
42      190 CONTINUE
43          SIZE=0.08
44      200 YP(3)=AMAX1(2.0,0.4+25*SIZE)
45          YP(4)=YP(1)+YP(3)+0.1
46          IF (YP(4).LE.YBD) GO TO 220
47          TYPE 210,YP(4),YBD
48      210 FORMAT (/' ERROR *** Y-PAPER SIZE(',F4.1,') GREATER THAN MAX PLOTT
48         1ER SIZE(',F4.1,')'/' TRY RE-ENTERING VALUES AGAIN.')
49          GO TO 140
50      220 SIZBOR=0.80*SIZE
51          TYPE 230,SIZE
52      230 FORMAT (/8X,' BASIC PLOT CHARACTER SIZE : ',F4.2)
53          SIZSUB=1.80*SIZE
54          SIZTIT=2.50*SIZE
55          IF (YSCL.LE.10.0) GO TO 240
56          MCODE=0
57          GO TO 260
58      240 TYPE 250
59      250 FORMAT (/' ANGSTROM SCALE(YES OR NO)          : ',$)
60          ACCEPT 1000,MCODE2
61          IF (MCODE2.EQ.'N') MCODE=0
62      260 TYPE 270
63      270 FORMAT (/' GROUP HEADING(UP TO 50 CHARS)      : ',$)
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64          ACCEPT 280,GHDG
65      280 FORMAT (10A5)
66      290 TYPE 300
67      300 FORMAT (/' RETRIEVAL BY(IDNO, GROUP, OR FORM): ',$)
68          ACCEPT 280,ANS
69          KIND=0
70          IF (ANS.EQ.'GROUP') KIND=1
71          IF (ANS.EQ.'FORM') KIND=2
72          GO TO (310,390,460),KIND+1
    C
    C ... READ ID NUMBERS REQUIRED FOR PLOTTING.
    C
73      310 TYPE 320
74      320 FORMAT (/' ENTER ONE, SIX DIGIT ID NO. PER LINE.'/
74         1 ' ENTER "CARRIAGE RETURN" AS THE LAST ID NO.')
75          I=0
76      330 I=I+1
77          IF (I.LE.50) GO TO 350
78          TYPE 340
79      340 FORMAT (' WARNING *** MORE THAN 50 ID NO ENTERED.'/
79         1' THESE 50 WILL BE PROCESSED.')
80          GO TO 370
81      350 ACCEPT 360,ID(I)
82      360 FORMAT (I)
83          IF (ID(I).NE.0) GO TO 330
84      370 IDNUM=I-1
85          TYPE 380,IDNUM
86      380 FORMAT (1X,I2,' ID NO''S WERE ENTERED.')
87          GO TO 520
    C
    C       ENTER GROUP NAMES REQUIRED FOR PLOTTING.
    C
88      390 TYPE 400
89      400 FORMAT (/' ENTER ONE, FIVE CHAR GROUP NAME PER LINE.'/
89         1 ' ENTER "CARRIAGE RETURN" AS LAST NAME.')
90          I=0
91      410 I=I+1
92          IF (I.LE.10) GO TO 430
93          TYPE 420
94      420 FORMAT (' WARNING *** MORE THAN 10 GROUP NAMES ENTERED.'/
94         1 ' THESE 10 WILL BE PROCESSED.')
95          GO TO 450
96      430 ACCEPT 440,(GPREQ(J,I),J=1,5)
97      440 FORMAT (5A1)
98          IF (GPREQ(1,I).NE.' ') GO TO 410
99      450 IDNUM=I-1
100         GO TO 520
    C
    C ... ENTER FORMULA COMPONENTS REQUIRED FOR PLOTTING.
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```
      C
  101    460 TYPE 470
  102    470 FORMAT (/' ENTER FORMULA COMPONENTS REQUIRED ON ONE LINE.'/
  102       1 4X,'SEPARATE BY COMMAS FOR "AND" LOGIC.'/13X,'BY SLASHES FOR "OR"
  102       2 LOGIC.')
  103    480 ACCEPT 930,FORREQ
  104        CALL CONFOR (FORREQ,FMNUM,IERR,ITYPE)
  105        IF (IERR.EQ.0) GO TO 510
  106        IF (IERR.EQ.1) TYPE 490
  107    490 FORMAT (/' ERROR *** THE FIRST CHAR OF ONE OF THE COMPONENTS IS NO
  107       1N-ALPHABETIC.'/' TRY RE-ENTERING FORMULA COMPONENTS AGAIN.')
  108        IF (IERR.EQ.2) TYPE 500
  109    500 FORMAT (/' ERROR *** NEGATIVE LOGIC CANNOT BE USED IN AN "EXCLUSIV
  109       1E SEARCH".'/11X,'RE-ENTER FORMULA COMPONENTS WITHOUT NEGATIVE LOGI
  109       2C.')
  110        GO TO 480
  111    510 IDNUM=1
  112    520 REWIND IDSK
  113        IHD=0
  114        IFD=0
  115        ICT=0
      C      ------------------------------------------------------------
      C ... BEGIN RETRIEVING REQUIRED MINERALS FROM GROUP NAMES OR ID NUMBERS.
      C      ------------------------------------------------------------
  116    530 IF (IDCNT.GT.IDNUM) GO TO 890
  117        IF (IHD.NE.0) GO TO 590
  118        IF (KIND.EQ.0) IHD=1
  119        IF (KIND.EQ.1) TYPE 540,(GPREQ(J,IDCNT),J=1,5)
  120    540 FORMAT (//' GROUP REQUIRED: ',5A1)
  121        IF (KIND.EQ.2) TYPE 550,(FORREQ(J),J=1,FMNUM)
  122    550 FORMAT (//' FORMULA COMP REQD: ',80A1)
  123        IF (KIND.EQ.2.AND.ITYPE.EQ.1) TYPE 560
  124    560 FORMAT (/' EXCLUSIVE RETRIEVAL')
  125        IF (IPT.EQ.0) TYPE 570,DYP(2)
  126    570 FORMAT (/' ID NO   GROUP    MINERAL NAME',13X,'LINES OVER',F6.1,
  126       1 ' DEGREES'/9X,'CODE',T46,'(LINES NOT PLOTTED)')
  127        IF (IPT.NE.0) TYPE 580
  128    580 FORMAT(/' ID NO  GROUP  MINERAL',T42,'CHEMICAL FORMULA'/8X'CODE')
  129    590 IF (KIND.NE.1.AND.KIND.NE.2) TYPE 600,ID(IDCNT)
  130    600 FORMAT (1X,I6)
  131    610 READ (IDSK,END=640) GP,NK,NID,MINER,FORM,NO2
  132        READ (IDSK) (NEW(I),I=1,NO2)
  133        IF (KIND.EQ.1.OR.KIND.EQ.2) GO TO 680
  134        IF (FIRST.NE.0) GO TO 620
  135        FIRST=1
  136        IDPRE=NID
  137        IF (NID.EQ.ID(IDCNT)) GO TO 670
  138        GO TO 610
  139    620 IF (NID.EQ.ID(IDCNT)) GO TO 670
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      IF (NID.NE.IDPRE) GO TO 610
      TYPE 630
630   FORMAT ('+',17X,'(MINERAL NOT FOUND)')
      IDCNT=IDCNT+1
      BAD=BAD+1
      GO TO 530
640   REWIND IDSK
      IF (KIND.EQ.0) GO TO 610
      IF (IFD.NE.0) GO TO 660
      TYPE 650
650   FORMAT (/' NO MINERALS FOUND')
660   IFD=0
      IDCNT=IDCNT+1
      GO TO 530
670   IDCNT=IDCNT+1
      IDPRE=NID
      GO TO 730
680   IF (KIND.EQ.1) CALL COMPAR (GP,GPREQ(1,IDCNT),IGD)
      IF (KIND.EQ.2) CALL CPRFOR (FORM,IGD)
      IF (IGD.NE.1) GO TO 610
      IFD=1
      ICT=ICT+1
      IF (IPT.EQ.0) GO TO 720
      DECODE (39,930,FORM) BUFF
      DO 690 I=39,1,-1
      N=I
690   IF (BUFF(I).NE.' ') GO TO 700
700   TYPE 710,NID,GP,MINER,(BUFF(I),I=1,N)
710   FORMAT (1X,I6,1X,A5,1X,5A5,1X,39A1)
      GO TO 880
720   TYPE 600,NID
730   TYPE 740,GP,MINER
740   FORMAT ('+',8X,A5,2X,5A5)
C
C ... PLOT RETRIEVED MINERALS.
C
      IF (IPT.EQ.1) GO TO 880
C
C ... START THE FIRST PLOT TWO INCHES OUT AND EACH ADDITIONAL PLOT WILL
C     START ON THE RIGHT BOUNDARY OF THE PREVIOUS PLOT.
C
      XP(3)=XP(3)+XP(1)+.25
      XP(1)=DXP(2)/XSCL
      IENCOD=1
      IF (MCODE.NE.1) GO TO 820
      IF (NO.GT.0) GO TO 820
C
C ... DRAW ANGSTROM SCALE AT BOTTOM OF PLOT.
C
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```
179         TEMP=XP(3)
180         XP(3)=XP(3)-(1.+SIZBOR)
181         CALL SCALE(DXP,DYP,XP,YP,NOPTS,ICODE)
182         IF (ICODE.NE.0) GO TO 1010
183         NOPTS=3
184         X4=XP(3)-1.8*SIZBOR
185         XP(3)=TEMP
186         XGP(1)=SIZBOR*XSCL
187         YGP(1)=0
188         XGP(2)=XGP(1)
189         YGP(2)=DYP(2)
190         X3=0
191         X5=.5*SIZBOR*XSCL
192         X6=.75*SIZBOR*XSCL
      C
      C ... DRAW THE Y AXIS FOR ANGSTROM UNITS.
      C
193     750 CALL LINE(XGP,YGP,2,ICON,IPN)
      C
      C ... DRAW ANGSTROM ANOTATION ALONG Y AXIS.
      C
194         DO 760 I=1,22
195         D=(1.54051*1.00082)/(2.*XIN(I))
196         THET=ASIN(D)
197         THET=2.*THET*57.2958
198         XGP(2)=X3
199         IF (IXIN(I).EQ.' ') XGP(2)=X5
200         YGP(1)=THET
201         YGP(2)=THET
202         CALL LINE(XGP,YGP,2,ICON,IPN)
203         YPLC=(THET/YSCL+SIZBOR)+YP(3)
204     760 CALL CHAR(X4,YPLC,IXIN(I),3,3,SIZBOR,-1.5708,0,0)
205         DO 780 I=1,3
206         YIN=8.0-I
207         D=(1.5405*1.00082)/(2.*YIN)
208         XGP(2)=X3
209         THET=ASIN(D)
210         THET=2.*THET*57.2958
211         YGP(1)=THET
212         YGP(2)=THET
213         CALL LINE(XGP,YGP,2,ICON,IPN)
214         YPLC=(THET/YSCL+SIZBOR)+YP(3)
215         CALL CHAR(X4,YPLC,IXIN1(I),3,3,SIZBOR,-1.5708,0,0)
216         DO 770 K=1,9
217         YIN=8.0-I-K*0.1
218         D=(1.54051*1.00082)/(2.*YIN)
219         THET=ASIN(D)
220         THET=2.*THET*57.2958
221         YGP(1)=THET
```

```
      YGP(2)=THET
      XGP(2)=X5
      CALL LINE(XGP,YGP,2,ICON,IPN)
  770 CONTINUE
  780 CONTINUE
      DO 800 I=1,2
      YIN=5-I
      DO 790 K=1,10
      YIN=5-I-(K-1)*0.1
      D=(1.54051*1.00082)/(2.*YIN)
      THET=ASIN(D)
      THET=2.*THET*57.2958
      XGP(2)=X5
      XGP2(1)=XGP(1)
      XGP2(2)=X3
      YGP(1)=THET
      YGP(2)=THET
      IF (K.NE.1) CALL LINE(XGP,YGP,2,ICON,IPN)
      IF (K.EQ.1) CALL LINE(XGP2,YGP,2,ICON,IPN)
      YPLC=(THET/YSCL+SIZBOR)+YP(3)
      IF (K.EQ.1) CALL CHAR(X4,YPLC,IXIN2(I),3,3,SIZBOR,-1.5708,0,0)
      YIN=YIN-0.05
      D=(1.54051*1.00082)/(2.*YIN)
      THET=ASIN(D)
      THET=2.*THET*57.2958
      XGP(2)=X6
      YGP(1)=THET
      YGP(2)=THET
      CALL LINE(XGP,YGP,2,ICON,IPN)
  790 CONTINUE
  800 CONTINUE
      DO 810 K=1,6
      YIN=2.0-(K-1)*.1
      D=(1.54051*1.00082)/(2.*YIN)
      THET=ASIN(D)
      THET=2.*THET*57.2958
      XGP(2)=X3
      YGP(1)=THET
      YGP(2)=THET
      CALL LINE(XGP,YGP,2,ICON,IPN)
      YPLC=(THET/YSCL+SIZBOR)+YP(3)
      CALL CHAR(X4,YPLC,IXIN3(K),3.3,SIZBOR,-1.5708,0,0)
      YIN=YIN-0.05
      D=(1.54051*1.00082)/(2.*YIN)
      THET=ASIN(D)
       THET=2.*THET*57.2958
      XGP(2)=X5
      YGP(2)=THET
      YGP(1)=THET
```

```
271         CALL LINE(XGP,YGP,2,ICON,IPN)
272     810 CONTINUE
273         IF (IENCOD.LE.0) GO TO 920
274     820 CONTINUE
275         CALL SCALE(DXP,DYP,XP,YP,NOPTS,ICODE)
276         IF (ICODE.NE.0) GO TO 1010
277         NOPTS=3
278         XGP(1)=0
279         YGP(1)=0
280         XGP(2)=DXP(2)
281         YGP(2)=0
282         ICON=0
283         IPN=0
      C
      C ... DRAW THE X BOUNDARY.
      C
284         CALL LINE(XGP,YGP,2,ICON,IPN)
      C
      C ... PUT THE TICK MARKS ON THE X BOUNDARY.
      C
285         CALL XAXIS(DXP,DYP,XP,25.,4,0.06,-1,0)
286         YGP(1)=DYP(2)
287         YGP(2)=DYP(2)
288         CALL LINE (XGP,YGP,2,ICON,IPN)
289         XPLC=XP(3)+XP(1)*0.6
290         YPLC=YP(3)-0.25
291         CALL CHAR(XPLC,YPLC,MINER,25,3,SIZE,-1.5708,0,0)
292         XPLC=XPLC-2*SIZE
      C
      C ... PLOT THE MINERAL NAME.
      C
293         ENCODE (6,830,NID2) NID
294     830 FORMAT (I6)
295         CALL CHAR (XPLC,YPLC,NID2,10,3,SIZE,-1.5708,0,0)
      C
      C ... ANNOTATE THE Y AXIS.
      C
296         TEMP=XP(3)
297         XP(3)=XP(3)-SIZBOR
298         CALL SCALE(DXP,DYP,XP,YP,NOPTS,ICODE)
299         IF (ICODE.NE.0) GO TO 1010
300         CALL ANOTAT (SIZBOR)
301         XP(3)=TEMP
302         CALL SCALE(DXP,DYP,XP,YP,NOPTS,ICODE)
303         IF (ICODE.NE.0) GO TO 1010
      C
      C ... DRAW THE Y AXIS.
      C
304         XGP(1)=0
```

```
      YGP(1) =0
      XGP(2)=0
      YGP(2)=DYP(2)
      ICON=0
      IPN=0
      CALL LINE(XGP,YGP,2,ICON,IPN)
C
C ... PLOT THE INTENSITY LINE.
C
      IOFF=0
      DO 850 I=1,NO2
      IX=NEW(I)/1000
      RINT=NEW(I)-(IX*1000)
      AX=IX/1000.
      Z(1)=2.0*ASIN(1.54051/(2.0*AX))*57.29577
      Z(2)=Z(1)
      X(1)=0.0
      X(2)=RINT
      IF (Z(1).LE.DYP(2)) GO TO 840
      IOFF=IOFF+1
      GO TO 850
  840 CALL LINE (X,Z,2,ICON,IPN)
  850 CONTINUE
      IF (IOFF.NE.0) TYPE 860,IOFF
  860 FORMAT ('+',48X,I3)
      NO=1
C
C ... CHECK TO SEE IF X-PLOT SIZE WILL EXCEED MAX X-SIZE OF PLOTTER.
C
      XSIZE=XP(1)+XP(3)+0.25+2*(XP(1)+MCODE+8*SIZTIT)
      IF (XSIZE.LE.XBD) GO TO 880
      TYPE 870
  870 FORMAT (/' WARNING *** X-PAPER SIZE WILL BE EXCEEDED AFTER PLOTTIN
     1G NEXT MINERAL.'/11X,'THEREFORE PLOTTING OF ANY FURTHER MINERALS W
     2ILL BE TERMINATED.')
      GO TO 900
  880 IF (KIND.EQ.0) GO TO 530
      IF (KIND.NE.0) GO TO 610
  890 CONTINUE
C
C ... RETRIEVAL COMPLETED.
C
  900 IF (IPT.NE.0) GO TO 980
      NUM=IDCNT-BAD-1
      IF (KIND.NE.0) NUM=ICT
      IF (NUM.LT.1) GO TO 980
      XPS=NUM*100.0/XSCL+0.1*NUM+6.5
      TYPE 910,XPS,YP(4)
  910 FORMAT (//' PLOT DIMENSIONS. X/Y:',F4.1,'/',F4.1//)
```

```
      XP(3)=XP(3)+XP(1)
      CALL SCALE (DXP,DYP,XP,YP,NOPTS,ICODE)
      IF (ICODE.NE.0) GO TO 1010
      XGP(1)=DXP(1)
      XGP(2)=DXP(1)
      YGP(1)=0
      YGP(2)=DYP(2)
      CALL LINE (XGP,YGP,2,ICON,IPN)
      NO=999
      CALL ANOTAT (SIZBOR)
      IF (MCODE.NE.1) GO TO 920
C
C ... DRAW ANGSTROM SCALE AT TOP OF PLOT.
C
      XP(3)=XP(3)+1
      X6=.25*SIZBOR*XSCL
      X5=.5*SIZBOR*XSCL
      X3=SIZBOR*XSCL
      X4=XP(3)+2.8*SIZBOR
      IENCOD=-1
      XGP(1)=0
      XGP(2)=0
      YGP(1)=0
      YGP(2)=DYP(2)
      CALL SCALE (DXP,DYP,XP,YP,NOPTS,ICODE)
      IF (ICODE.NE.0) GO TO 1010
      GO TO 750
  920 CONTINUE
C
C ... DRAW TITLING AT TOP OF PLOT.
C
      DECODE (50,930,GHDG) BUFF
  930 FORMAT (80A1)
      DO 940 I=50,1,-1
      N=I
  940 IF (BUFF(I).NE.' ') GO TO 950
  950 CONTINUE
      YPLC=YP(3)+0.5*YP(1)
      IF (N*SIZTIT.LE.YP(1).AND.60*SIZSUB.LE.YP(1)) GO TO 960
      SIZE=AMIN1(YP(1)/N/2.5,YP(1)/60/1.8)
      SIZSUB=1.8*SIZE
      SIZTIT=2.5*SIZE
  960 SIZT=SIZSUB
      XPLC=XP(3)+4.8*SIZT
      CALL CHAR (XPLC,YPLC,'GEORGE VAN TRUMP,JR.  AND  PHOEBE L. HAUFF',
     1 42,3,SIZT,-1.5708,-SIZT*42/2.0,0.0)
      XPLC=XP(3)+6.5*SIZT
      CALL CHAR (XPLC,YPLC,'DEPT. OF INTERIOR,  U.S. GEOLOGICAL SURVEY,
     1 DENVER, COLORADO',61,3,SIZT,-1.5708,-SIZT*61/2.0,0.0)
```

```
      IF (N.LE.1.AND.GHDG(1).EQ.' ') GO TO 970
      SIZT=SIZTIT
      XPLC=XP(3)+7.0*SIZT
      CALL CHAR (XPLC,YPLC,GHDG,N,3,SIZT,-1.5708,-SIZT*N/2.0,0.0)
  970 CALL ENDPLT(0)
C     ------------------------------------------------------------
C ... RETRIEVAL & PLOT FINISHED.  RECYCLE FOR NEW INPUT DATA, IF ANY.
C     ------------------------------------------------------------
  980 TYPE 990
  990 FORMAT (//' WANT TO PROCESS ANY FURTHER DATA  ? ',$)
      ACCEPT 1000,ANS
 1000 FORMAT (A1)
      IF (ANS.EQ.'Y') GO TO 100
C
C ... NORMAL TERMINATION OF PROGRAM.
C
      STOP 'NORMAL TERMINATION'
C
C ... ABNORMAL TERMINATION OF PROGRAM.  SCALING ERROR.
C
 1010 TYPE 1020
 1020 FORMAT (///' ERROR *** SCALING ROUTINE')
      TYPE 1030,(I,DXP(I),DYP(I),I=1,2),(I,XP(I),YP(I),I=1,4)
 1030 FORMAT (/' SCALING SUBROUTINE PARMS:'/(1X,I2,2F10.4))
      CALL ENDPLT (0)
      STOP 'ABNORMAL TERMINATION'
      END
```

```
1           SUBROUTINE COMPAR (GP,GPREQ,IGD)
      C
      C        THIS ROUTINE IS USED TO COMPARE REQUIRED GROUP NAMES WITH FILE
      C     GROUP NAMES.
      C
2           DIMENSION GPREQ(5),GPNAM(5)
3           IGD=1
4           DECODE (5,100,GP) GPNAM
5       100 FORMAT (5A1)
6           DO 110 I=1,5
7           IF (GPREQ(I).EQ.'?') GO TO 110
8           IF (GPREQ(I).EQ.GPNAM(I)) GO TO 110
9           IGD=0
10          RETURN
11      110 CONTINUE
12          RETURN
13          END
```

```
1           SUBROUTINE INITPR (XBD,YBD)
      C
      C        THIS ROUTINE IS USED TO INITALIZED VALUES AT THE BEGINNING OF
      C     EACH RETRIEVAL.
      C
2           INTEGER FIRST,BAD,IDCNT
3           COMMON XSCL,YSCL,NO,XP(4),YP(4),DXP(2),DYP(2)
4           COMMON /INIT/ ICODE,MCODE,NOPTS,IDCNT,FIRST,BAD
5           ICODE=0
6           MCODE=1
7           NO=0
8           NOPTS=4
9           IDCNT=1
10          FIRST=0
11          BAD=0
12          DXP(1)=0.0
13          DXP(2)=100.0
14          DYP(1)=0.0
15          DYP(2)=70.0
16          XP(1)=0.0
17          XP(2)=1.0
18          XP(3)=2.0
19          XP(4)=XBD
20          YP(1)=0.0
21          YP(2)=1.0
22          YP(3)=2.0
23          YP(4)=YBD
24          RETURN
25          END
```

```
1           SUBROUTINE ANOTAT (SIZBOR)
      C
      C        THIS ROUTINE IS USED TO ANNOTATE THE HORIZONTAL AXIS WITH THE
      C     2-THETA VALUES.
      C
2           DIMENSION XGP(2),YGP(2),NUM(18)
3           COMMON XSCL,YSCL,NO,XP(4),YP(4),DXP(2),DYP(2)
4           DATA NUM/'10','20','30','40','50','60','70','80','90','100','110',
4          1 '120','130','140','150','160','170','180'/,TWO/'2'/
5           ICON=0
6           IPN=0
7           A1=0
8           A2=0.5*SIZBOR*XSCL
9           A3=SIZBOR*XSCL
10          IF(NO.EQ.999) A3=0
11          IF(NO.EQ.999) A1=SIZBOR*XSCL
12          XGP(2)=A3
13          YGP(1)=2.0
14          YGP(2)=2.0
15          XGP(1)=A1
16          CALL LINE(XGP,YGP,2,ICON,IPN)
17          IF (NO.GT.0 .AND. NO.NE.999) GO TO 100
18          X=XP(3)-2*SIZBOR
19          IF (NO.EQ.999) X=XP(3)+3*SIZBOR
20          Y=YGP(1)/YSCL+YP(3)
21          CALL CHAR(X,Y,TWO,1,3,SIZBOR,-1.5708,0,0)
22      100 YGP(1)=0
23          YGP(2)=0
24          N=(DYP(2)+0.001)/10.0
25          DO 110 I=1,N
26          YGP(1)=5+YGP(1)
27          YGP(2)=YGP(2)+5
28          XGP(1)=A2
29          CALL LINE (XGP,YGP,2,ICON,IPN)
30          YGP(1)=A1
31          XGP(2)=A3
32          YGP(1)=YGP(1)+5
33          YGP(2)=YGP(2)+5
34          CALL LINE(XGP,YGP,2,ICON,IPN)
35          IF (NO.GT.0 .AND. NO.NE.999) GO TO 110
36          X=XP(3)-2*SIZBOR
37          IF (NO.EQ.999) X=XP(3)+3*SIZBOR
38          Y=YGP(1)/YSCL+YP(3)
39          NN=2
40          IF (I.GT.9) NN=3
41          CALL CHAR(X,Y,NUM(I),NN,3,SIZBOR,-1.5708,0,0)
42      110 CONTINUE
43          RETURN
44          END
```

```
1           SUBROUTINE CONFOR (FORREQ,NCHAR,IERR,ITYPE)
      C
      C        THIS ROUTINE IS USED TO COMPARE FORMULA COMPONENTS REQUIRED TO
      C     THE COMPONENTS OF THE FORMULA IN THE FILE.
      C
2           LOGICAL GOOD,KD(50),COND(50),A(50)
3           DIMENSION FORREQ(80),NO(50,2),NS(50,2),FORM(8),FORSEP(39)
4           COMMON /NAME/ CHARS(42)
      C     ------------------------------------------------------------
      C ... WORK ON REQUIRED COMPONENTS OF FORMULA.
      C     ------------------------------------------------------------
      C
      C ... DETERMINE NO. OF CHARS IN STRING.
      C
5           DO 100 I=80,1,-1
6           IF (FORREQ(I).EQ.' ') GO TO 100
7           NCHAR=I
8           IF (FORREQ(I).NE.'.'.AND.FORREQ(I).NE.'/') GO TO 110
9           FORREQ(I)=' '
10          NCHAR=NCHAR-1
11          GO TO 110
12        100 CONTINUE
13          NCHAR=0
14          RETURN
      C
      C ... COMPRESS OUT BLANKS AND CLOSE UP STRING.
      C
15        110 I=1
16          ITYPE=0
17        120 IF (I.GT.NCHAR) GO TO 170
18          IF (FORREQ(I).EQ.' ') GO TO 150
19          IF (I.NE.1) GO TO 130
20          IF (FORREQ(1).EQ.'.') GO TO 150
21          IF (FORREQ(1).EQ.'/') GO TO 150
22          IF (FORREQ(1).EQ.'+') GO TO 140
23        130 I=I+1
24          GO TO 120
25        140 ITYPE=1
26        150 DO 160 J=I+1,NCHAR
27        160 FORREQ(J-1)=FORREQ(J)
28          FORREQ(NCHAR)=' '
29          NCHAR=NCHAR-1
30          GO TO 120
      C
      C ... SEPARATE STRING INTO GROUPS.
      C
31        170 DO 180 I=1,50
32        180 KD(I)=.TRUE.
33          I=1
```

```
      IERR=0
      IGP=1
      NO(1,1)=1
      IF (FORREQ(1).NE.'-') GO TO 190
      IF (ITYPE.EQ.1) IERR=2
      KD(I)=.FALSE.
      NO(1,1)=2
      GO TO 200
  190 IF (INDEX(FORREQ(1)).NE.-1) IERR=1
  200 DO 220 J=1,NCHAR
      IF (FORREQ(J).NE.',',.AND.FORREQ(J).NE.'/') GO TO 220
      IF (ITYPE.EQ.1.AND.FORREQ(J).EQ.',')IGP=IGP+1
      NO(I,2)=J-1
      IF (J.EQ.NCHAR) GO TO 220
      I=I+1
      NO(I,1)=J+1
      IF (FORREQ(J+1).NE.'-') GO TO 210
      IF (ITYPE.EQ.1) IERR=2
      KD(I)=.FALSE.
      NO(I,1)=J+2
      GO TO 220
  210 IF (INDEX(FORREQ(J+1)).NE.-1) IERR=1
  220 CONTINUE
      NO(I,2)=NCHAR
      NGP1=I
      RETURN
C     ------------------------------------------------------------
C ... WORK ON FORMULA NAME.
C     ------------------------------------------------------------
      ENTRY CPRFOR(FORM,IGD)
C
C ... DETERMINE NO. OF CHARS IN STRING.
C
      IGD=1
      IF (NCHAR.EQ.0) RETURN
      DECODE (39,230,FORM) FORSEP
  230 FORMAT (80A1)
      DO 250 I=39,1,-1
      IF (FORSEP(I).EQ.' ') GO TO 250
      NC=I
      IF (FORSEP(I).NE.'.') GO TO 240
      FORSEP(I)=' '
      NC=NC-1
  240 IF (FORSEP(1).EQ.'.') FORSEP(1)=' '
      GO TO 260
  250 CONTINUE
      IGD=0
      RETURN
C
```

```
      C ... BLANK OUT OF FORMULA ALL PARENTHESIS, MINUS, COMMA, & PERIOD CHARS
      C
 76     260 DO 330 I=1,NC
 77         DO 270 J=37,42
 78         N1=J-36
 79     270 IF (FORSEP(I).EQ.CHARS(J)) GO TO 280
 80         GO TO 330
      C                  . ,BLK, ( , ) , - , ,
 81     280 GO TO (320,330,290,300,310,310),N1
 82     290 FORSEP(I)=' '
 83         IF (I-1.LT.1) GO TO 330
 84         IF (INDEX(FORSEP(I-1)).EQ.1) FORSEP(I-1)=' '
 85         GO TO 330
 86     300 FORSEP(I)=' '
 87         IF (I+1.GT.NC) GO TO 330
 88         IF (INDEX(FORSEP(I+1)).EQ.1) FORSEP(I+1)=' '
 89         GO TO 330
 90     310 FORSEP(I)=' '
 91         GO TO 330
 92     320 IF (I-1.LT.1.OR.I+1.GT.NC) GO TO 330
 93         IF (FORSEP(I-1).NE.' ') GO TO 330
 94         IF (FORSEP(I+1).NE.' ') GO TO 330
 95         FORSEP(I)=' '
 96     330 CONTINUE
      C
      C ... SEPARATE STRING INTO GROUPS.
      C
 97         I=1
 98         J=0
 99     340 J=J+1
100         IF (J.GT.NC) GO TO 380
101         IF (INDEX(FORSEP(J)).EQ.-1) GO TO 350
102         GO TO 340
103     350 NS(I,1)=J
104     360 J=J+1
105         IF (J.LE.NC) GO TO 370
106         NS(I,2)=NC
107         NGP2=I
108         GO TO 380
109     370 IF (FORSEP(J).NE.' ') GO TO 360
110         NS(I,2)=J-1
111         NGP2=I
112         I=I+1
113         GO TO 340
      C
      C ... COMPARE REQ'D COMPONENTS WITH FORMULA.
      C
114     380 IF (ITYPE.EQ.1) GO TO 490
      C
```

```
      C ... INCLUSIVE RETRIEVAL.
      C
  115       DO 390 I=1,NGP1
  116   390 COND(I)=.FALSE.
  117       DO 430 K=1,NGP2
  118       IS2=NS(K,1)-1
  119       IT2=NS(K,2)-NS(K,1)+1
  120       DO 420 I=1,NGP1
  121       IS1=NO(I,1)-1
  122       IT1=NO(I,2)-NO(I,1)+1
  123       NGP=MINO(IT1,IT2)
  124       DO 410 M=1,NGP
  125       IF (FORREQ(IS1+M).EQ.FORSEP(IS2+M)) GO TO 410
  126       IF (M.EQ.1) GO TO 420
  127       IF (FORREQ(IS1+M).NE.'?') GO TO 420
  128       IF (IS2+M.GT.NS(K,2)) GO TO 420
  129       DO 400 N=IS2+M,NS(K,2)
  130       IF (INDEX(FORSEP(N)).LT.0) GO TO 420
  131   400 CONTINUE
  132       COND(I)=.TRUE.
  133       GO TO 420
  134   410 CONTINUE
  135       IF (IT1.EQ.IT2) COND(I)=.TRUE.
  136   420 CONTINUE
  137   430 CONTINUE
  138       DO 440 I=1,NGP1
  139   440 COND(I)=COND(I).EQV.KD(I)
  140       IF (NGP1.GT.1) GO TO 450
  141       IF (COND(1)) RETURN
  142       IGD=0
  143       RETURN
  144   450 K=0
  145       DO 470 I=1,NGP1
  146       IF (I.EQ.1) GO TO 460
  147       IF (FORREQ(NO(I-1,2)+1).NE.'/') GO TO 460
  148       A(K)=COND(I).OR.A(K)
  149       GO TO 470
  150   460 K=K+1
  151       A(K)=COND(I)
  152   470 CONTINUE
  153       IGD=0
  154       DO 480 I=1,K
  155   480 IF (.NOT.A(I)) RETURN
  156       IGD=1
  157       RETURN
      C
      C ... EXCLUSIVE RETRIEVAL.
      C
  158   490 IF (NGP2.GE.IGP) GO TO 500
```

```
      IGD=0
      RETURN
  500 DO 540 K=1,NGP2
      IS2=NS(K,1)-1
      IT2=NS(K,2)-NS(K,1)+1
      DO 530 I=1,NGP1
      IS1=NO(I,1)-1
      IT1=NO(I,2)-NO(I,1)+1
      NGP=MIN0(IT1,IT2)
      DO 520 M=1,NGP
      IF (FORREQ(IS1+M).EQ.FORSEP(IS2+M)) GO TO 520
      IF (M.EQ.1) GO TO 530
      IF (FORREQ(IS1+M).NE.'?') GO TO 530
      IF (IS2+M.GT.NS(K,2)) GO TO 530
      DO 510 N=IS2+M,NS(K,2)
      IF (INDEX(FORSEP(N)).LT.0) GO TO 530
  510 CONTINUE
      GO TO 540
  520 CONTINUE
      IF (IT1-IT2) 530,540,530
  530 CONTINUE
      IGD=0
      RETURN
  540 CONTINUE
      RETURN
      END
```

```
1           FUNCTION INDEX (A)
      C
      C     INDEX = -2  SPECIAL CHARS
      C           = -1  A THRU Z
      C           =  0  BLANK
      C           =  1  INTEGERS & DECIMAL POINT
      C
2           COMMON /NAME/ CHARS(42)
3           DATA CHARS/'A','B','C','D','E','F','G','H','I','J','K','L','M',
3          1           'N','O','P','R','Q','S','T','U','V','W','X','Y','Z',
3          2           '0','1','2','3','4','5','6','7','8','9','.',' ','(',
3          3           ')','-','+','/'
4           DO 100 I=1,38
5           IF (A.NE.CHARS(I)) GO TO 100
6           NO=I
7           GO TO 110
8       100 CONTINUE
9           INDEX=-2
10          RETURN
11      110 IF (NO.GE.1.AND.NO.LE.26) INDEX=-1
12          IF (NO.EQ.38) INDEX=0
13          IF (NO.GE.27.AND.NO.LE.37) INDEX=1
14          RETURN
15          END
```

## References

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