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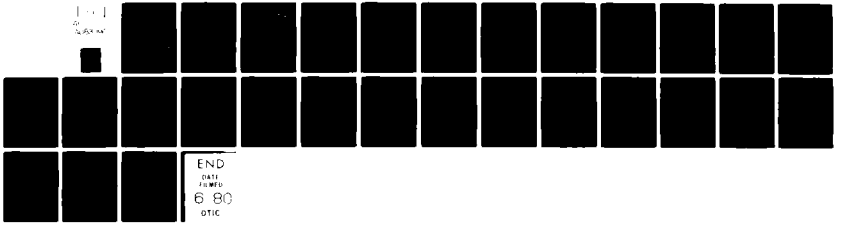
COMPUTERIZED DRAWING OF STEREOGRAPHIC PROJECTIONS.(U)
JAN 80 R E SCHAFRIK
UNCLASSIFIED AFML-TR-79-4137 NL



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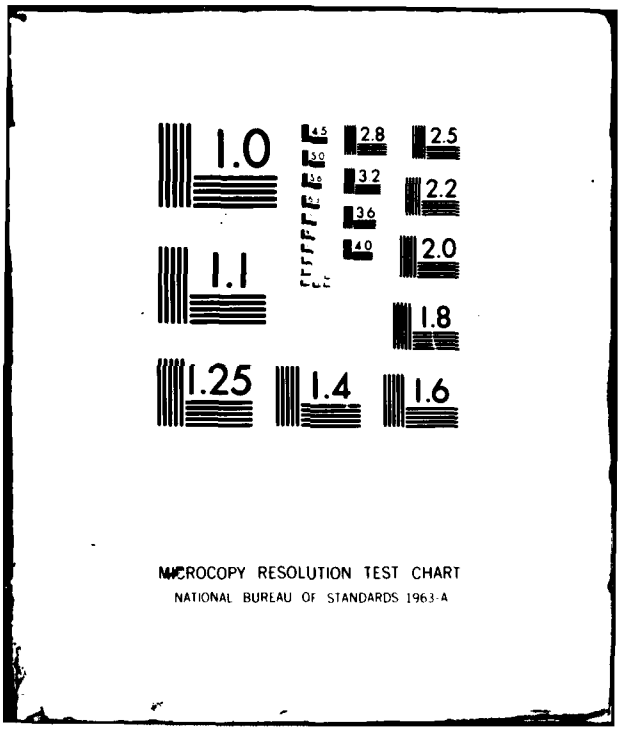
1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963-A

AFML-TR-79-4137

LEVEL II

AD A083990

COMPUTERIZED DRAWING OF STEREOGRAPHIC PROJECTIONS

ROBERT E. SCHAFRIK

PROCESSING AND HIGH TEMPERATURE MATERIALS BRANCH
METALS AND CERAMICS DIVISION

JANUARY 1980

TECHNICAL REPORT AFML-TR-79-4137
Interim Report for period June 1974 — September 1977

Approved for public release; distribution unlimited.

AIR FORCE MATERIALS LABORATORY
AIR FORCE WRIGHT AERONAUTICAL LABORATORIES
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This technical report has been reviewed and is approved for publication.

Robert E Schafrik

ROBERT E. SCHAFRIK, CAPT, USAF
Project Engineer

FOR THE COMMANDER

Henry C. Graham

HENRY C. GRAHAM, CHIEF
Processing and High Temperature Materials Branch
Metals and Ceramics Division

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Computer Program in Materials Science

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A computer program was developed to plot stereographic projections for any crystal system.

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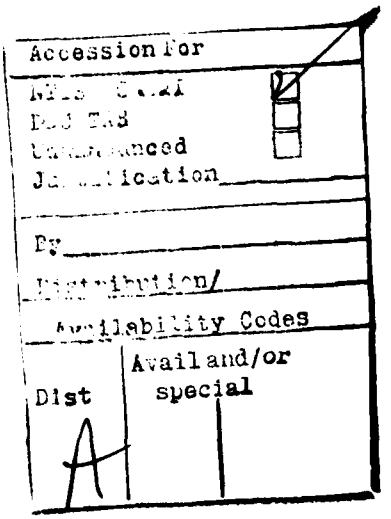
FOREWORD

The preparation of stereographic projections can be time consuming and tedious, especially for non-cubic crystal systems. This study was an attempt to adapt an existing computer program to a CDC 6600/Cyber 76 mainframe computer with Calcomp plotting subroutines. Some modifications to the program plotting capabilities also were made.

The author would like to acknowledge the help of P.J. Moroz, Jr. of the Armco Steel Research Center, Middletown, Ohio in interpreting the functions of the different plotting commands in the original computer program (Reference 1).



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1. INTRODUCTION

Automating the generation of stereographic projections is of great convenience to the materials scientist. A source listing of computer programs which provides the capability to draw stereographic projections for any crystal system is contained in the appendix. This computer program has the following capabilities:

1. Draw stereographic projections of any size up to 5.4 inch radius (13 cm) on the 11 inch on-line plotter or draw stereographic projections up to 14.75 inch radius on the 30 inch off-line plotter.

2. Plot stereographic projections for plane normals, directions, or directions superimposed on plane normal projections. Hexagonal projections use the 4-index notation.

3. Up to nine different plots can be drawn per computer run for a given crystallographic system.

4. The user can adjust the spacing of the plots and the size of the drawn symbols. Also, an enclosing square can be drawn around each projection.

This program is written in FORTRAN EXTENDED code for processing on a CDC 6600/ Cyber 76 computer using Calcomp Plotting Subroutines. The basic reference which was used is given in Reference 1.

2. PROGRAM ARCHITECTURE

A flow chart is contained in Figure 1. Note that subroutines are used extensively throughout the program to perform specialized tasks.

The main program acts as an organizer, reading in the key parameters, and directing the calling of appropriate subroutines. Subroutine PRO1 calculates some geometric quantities from the crystal lattice data and stores them in unlabeled common. Subroutine PRO2 computes some geometric quantities from the plane index value selected to be the center of the projection. Subroutine PRO3 reads in the index value of the center of

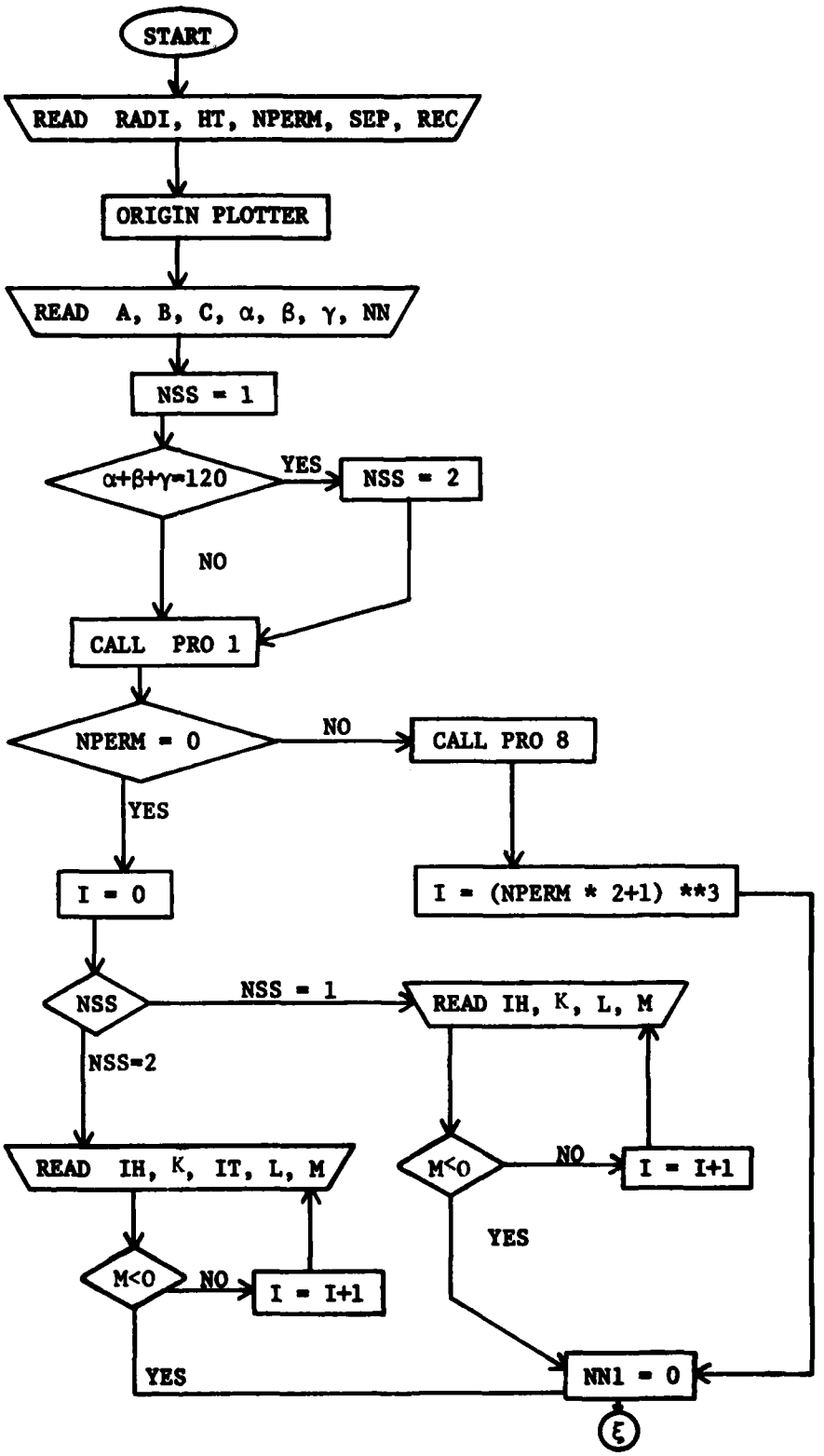

Fig. 1. Flowchart

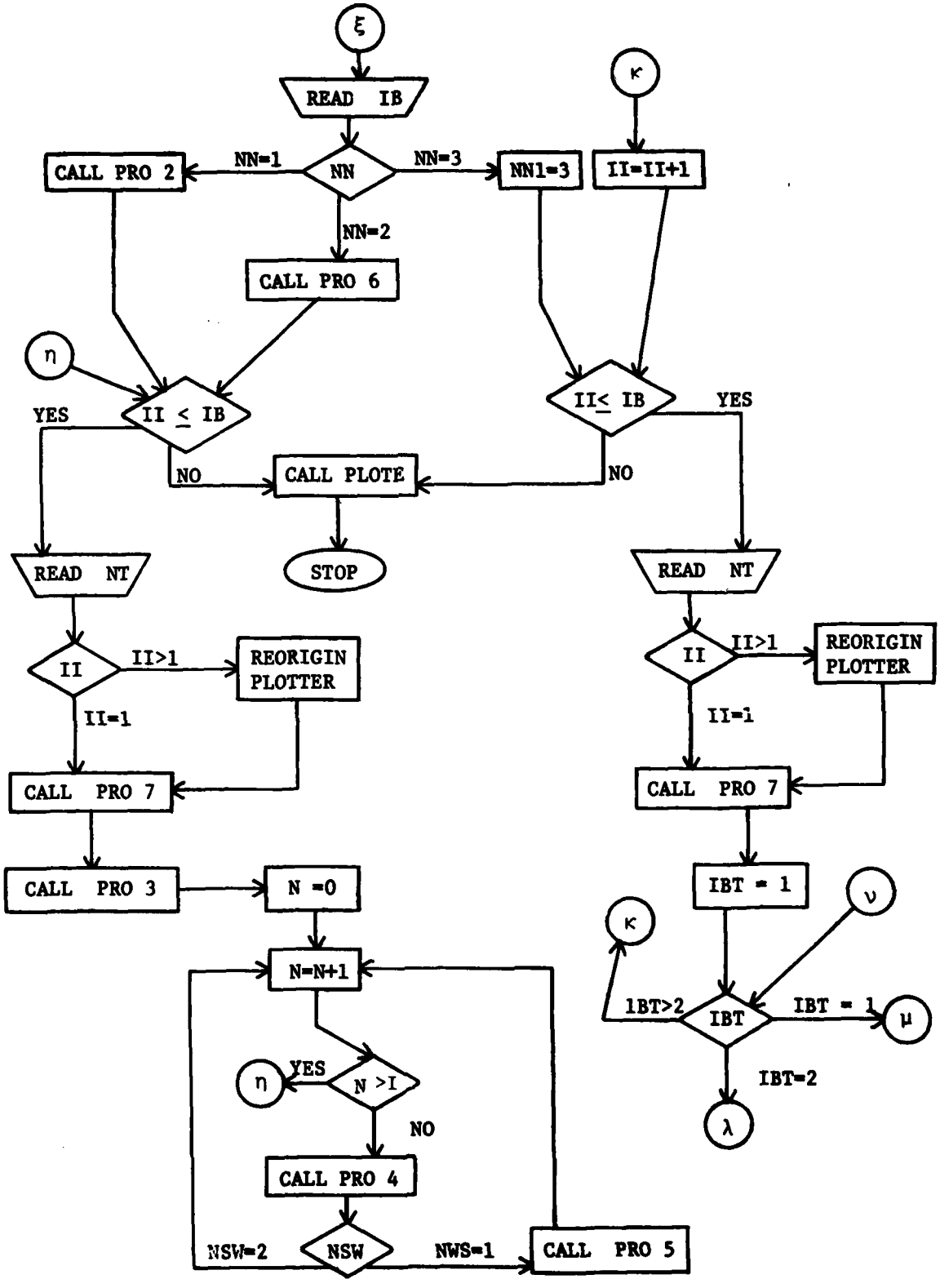

Fig. 1 - Continued

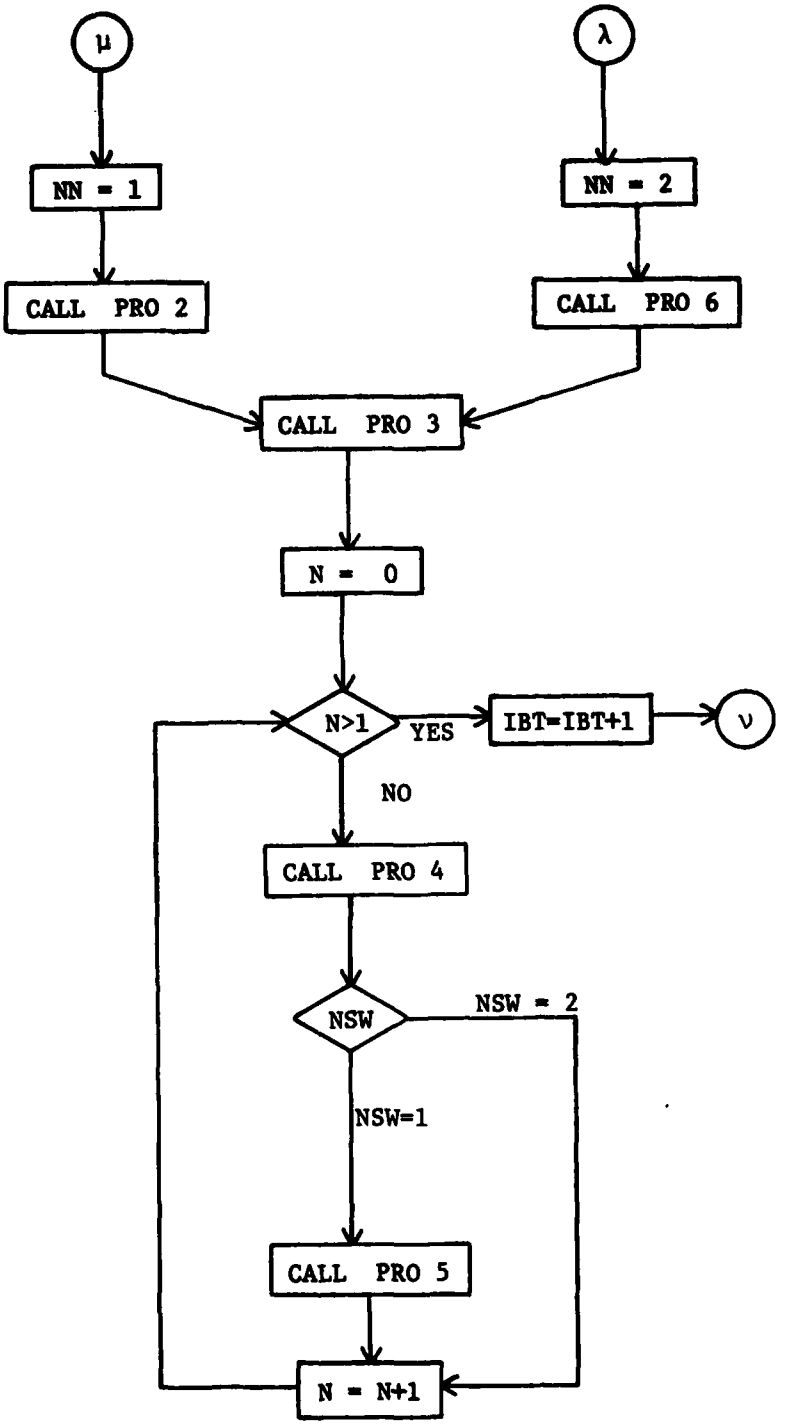

Fig. 1 - Concluded

the projection and calculates various parameters which are placed in Common. Subroutine PR04 calculates the plotting coordinates of the indices (in inches) and determines which indices are within the field of projection. The accuracy is 0.010 radian. The index coordinates are placed in common for use in subroutine PR05. Subroutine PR05 does the actual plotting and labeling of the indices. Subroutine PR06 calculates quantities from the index values of directions and places them in common for use in subroutine PR04. Subroutine PR07 draws the projection circle, the enclosing square, and prints the title. Subroutine PR08 can be used to permute indices for plotting. For example, by reading in a number, N, all possible combinations of indices from NNN to $\bar{N}\bar{N}\bar{N}$ could be generated, thereby simplifying the inputing of data. However, in this version it is inoperative.

3. DATA INPUT DESCRIPTION

The set up for the data deck structure is identical for on-line plotting and off-line plotting.

3.1 On-Line Plotting.

A typical data deck structure is shown in Table 1. The first data card takes care of some "housekeeping" chores. It is this data card which specifies the desired plot radius (in cm), the height of the symbols to be plotted (in inches), the permutation code (must be 0), and the separation distance (in inches) between plots. An unformated read statement is used, so that the parameters must be separated by commas. If the last parameter is a 1, an enclosing square will be drawn.

The second data card which reads in a number to drive the pen to the -Y limit position in order to establish an origin should be at least -11.5.

The third data card provides information about the crystallographic system and the projection option desired. The first three parameters-A,B,C-provide the length of the crystallographic axes. The next three parameters -

TABLE 1. TYPICAL DATA DECK STRUCTURE

```
9.00, .070, 0,  4.0, 1
-12.0
1.00, 1.00, 1.587, 90., 90., 120.,1
-01003-02000
-01003-02001
-01003-02002
-01003-02003
000002-02003
000001-01003
001002-03000
001002-03001
001002-03002
001002-03003
001001-02003
002001-03000
002001-03001
002001-03002
002001-03003
-02000002003
-01000001003
001000-01003
002000-02003
003-01-02000
003-02-01000
002-03001000
001-03002000
-01-02003000
-02-01003000
             -1
1
0 0 0 1  STD PROJ   HEXAGONAL PLANES     C/A=1.587
  0  0  0  1
```

α, β, γ - provide the crystallographic angles. The angles are determined by the usual crystallographic convention(2). The last parameter, NN, specifies the projection type requested: (a) NN=1 specifies a projection of plane normals; (b) NN=2 specifies a projection of directions; and (c) NN=3 specifies a projection of directions superimposed on plane normals. An unformated read statement is used for this data card too.

The next group of data cards provides the indices that are to be plotted. If the hexagonal system is hexagonal ($\alpha+\beta+\gamma$=300 Degrees), the 4 index system must be used. Data is entered under the format specification 3I3 (non hexagonal) or 4I3 (hexagonal). A negative index has the form: -XX. Note that although the capability exists for entering an index value greater than 9, only integers up to 9 will be plotted above the location on the projection. The data set is terminated as follows:

(a) Non-hexagonal system: Place a -1 in card columns 10-11.

(b) Hexagonal system: Place a -1 in card columns 13-14.

The next data card specifies the number of plots to be run.

The final data card set consists of the title for the stereographic projection and the index of the center of the projection. There must be as many of these sets as there are plots to be run. The plotter draws four lines of 20 characters each, so that each line begins with card columns 1, 21, 41, and 61. The index of the center spot must be of the same form as the other indices. Thus, for a hexagonal system, the 4 index notation must be used.

For the cases where plane normals (NN=1) or direction (NN=2) projections are requested, the final data set would have the arrangement:

Title Card
Index of Center of Projection
Title Card
Index of Center of Projection
Etc.

For the case where the plane normals are superimposed on directions (NN=3), the final data set would have the arrangement:

Title Card
Index of Center - Plane Projection
Index of Center - Direction Projection
Etc.

3.2 Off-Line Plotting

The advantages of off-line plotting are: (a) large plots can be run, and (b) the accuracy of plotting is greater than for on-line plotting. The disadvantage is that the turn-around time is much greater (typically, at least one day).

The set up of the data deck is the same as for on line plotting. The second data card which reads in a number to drive the pen to the -Y limit position in order to establish an origin should be at least -19.50.

4. CONTROL CARDS

A detailed description of the control cards used in running a job will not be given since these cards change with changes in the operating systems. However, the following general comments should be helpful:

(a) The library subroutine which draws the projection circle and enclosing square must be accessed, or a similar subroutine added to the computer program.

(b) For off-line plotting, the library subroutine which places the plotting commands on magnetic tape must be accessed.

(c) For off-line plotting,the job card must contain the appropriate parameter to indicate that a magnetic tape is required to man the job. Also, a tape LABEL control card is necessary. The tape library must be notified to load the magnetic tape reel prior to the execution of the job; and after the completion of the job, the tape library must be notified to run the off-line plot.

5. RESULTS

The utility of the stereographic plotting computer program is depicted in Figures 2-4. Figure 2 shows a stereographic projection of plane normals for hexagonal titanium. Figures 3a and 3b show a stereographic projection of plane normals for face centered tetragonal Ni_4W using different unit cells. Figure 4 shows a superimposed projection of directions on plane normals for a tri-clinic crystal. These projections, which can be readily obtained, are extremely useful in x-ray and electron diffraction investigations. For example, they can be used to determine the crystallographic orientation of a portion of a foil in transmission electron microscopy work.

6. CONCLUSIONS

Computer plotting of stereographic projections provides the capability to easily and quickly plot desired projections with good accuracy.

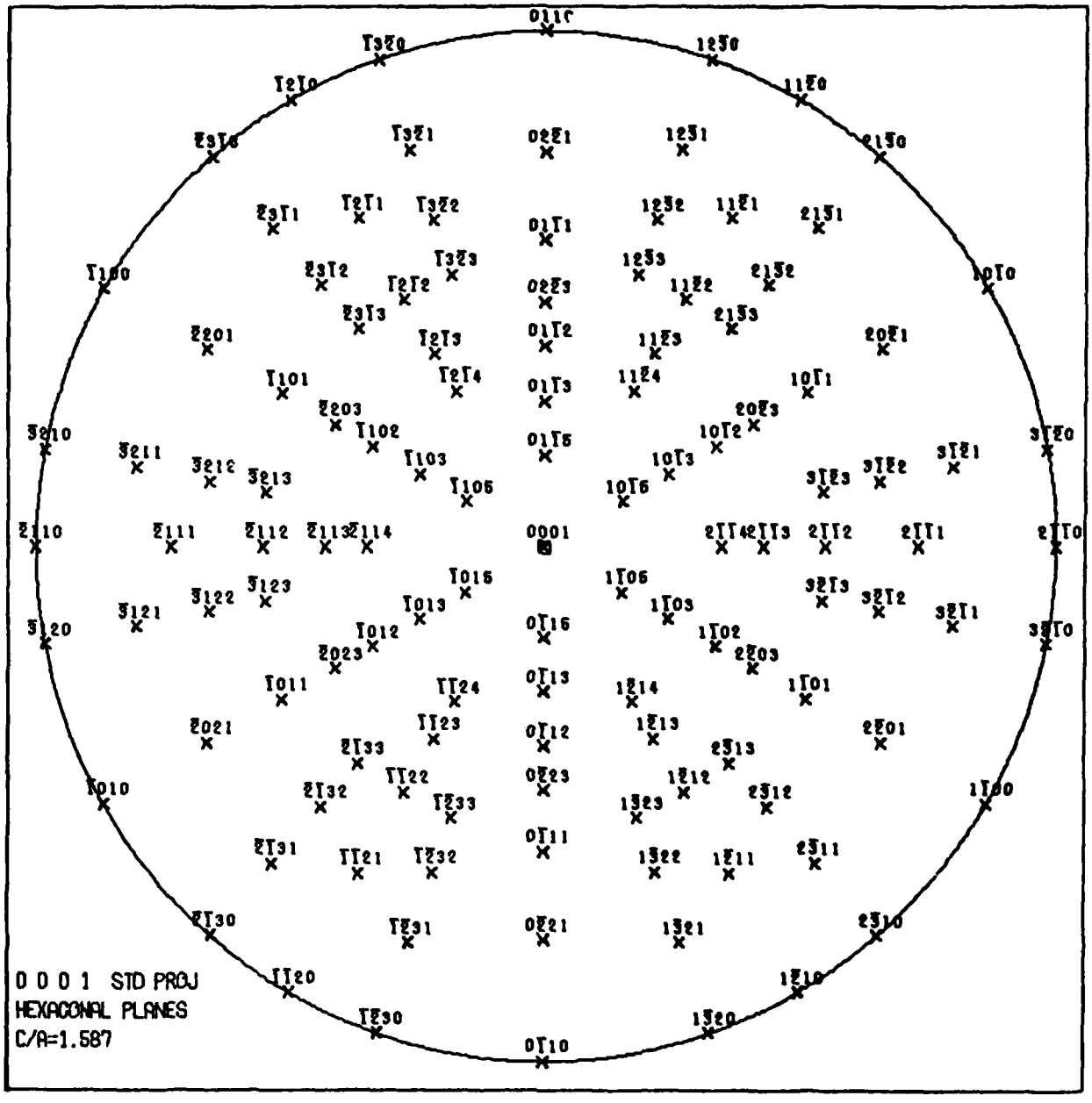

Fig. 2. Stereographic Projection of Plane Normals in an Hexagonal Crystal System for C/A = 1.587.

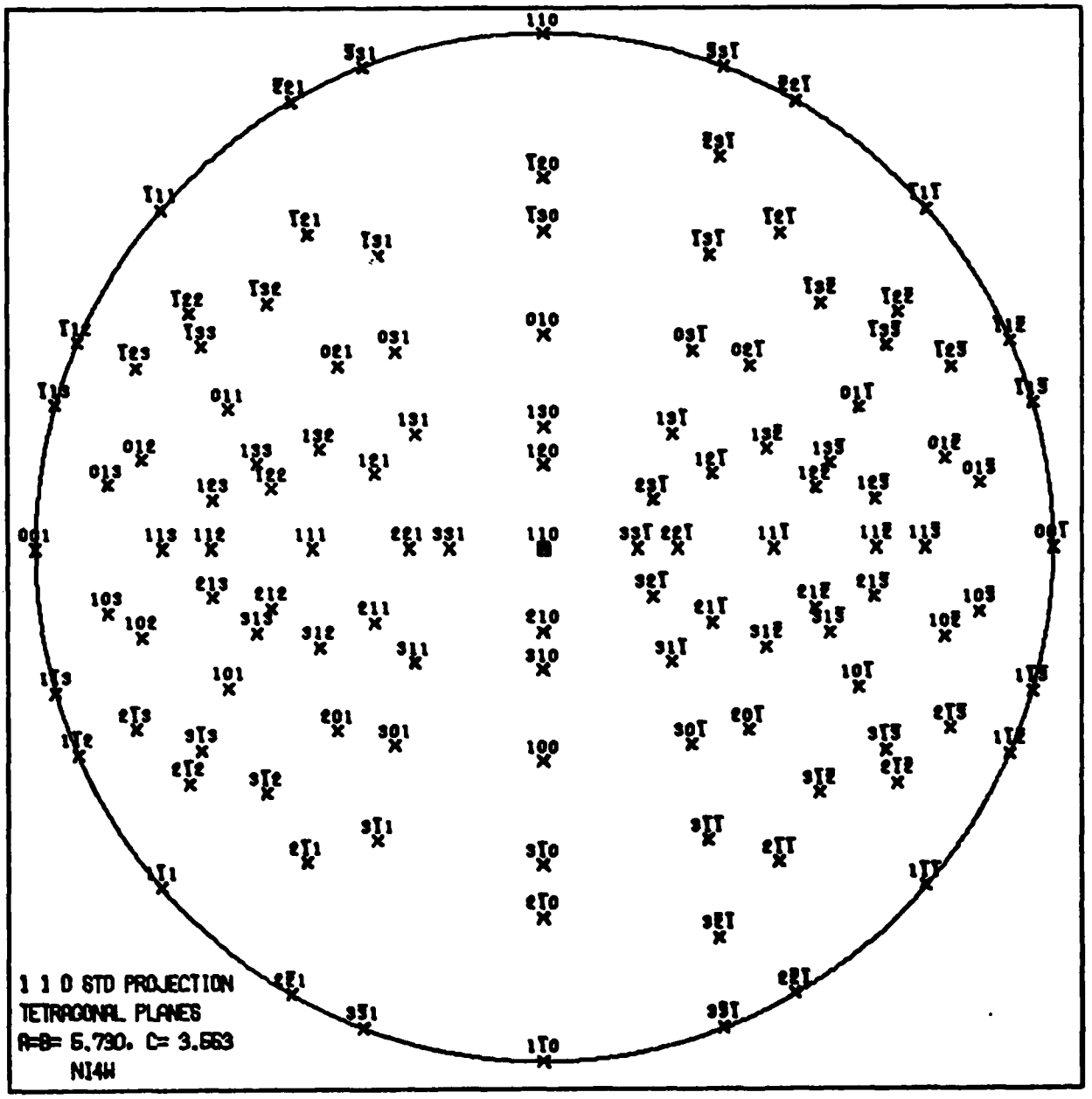

Fig. 3. Stereographic Projection of Plane Normals in a Face Centered Tetragonal Crystal System (a) Projection using a unit cell where A = B = 5.730Å, C = 3.553 Å.

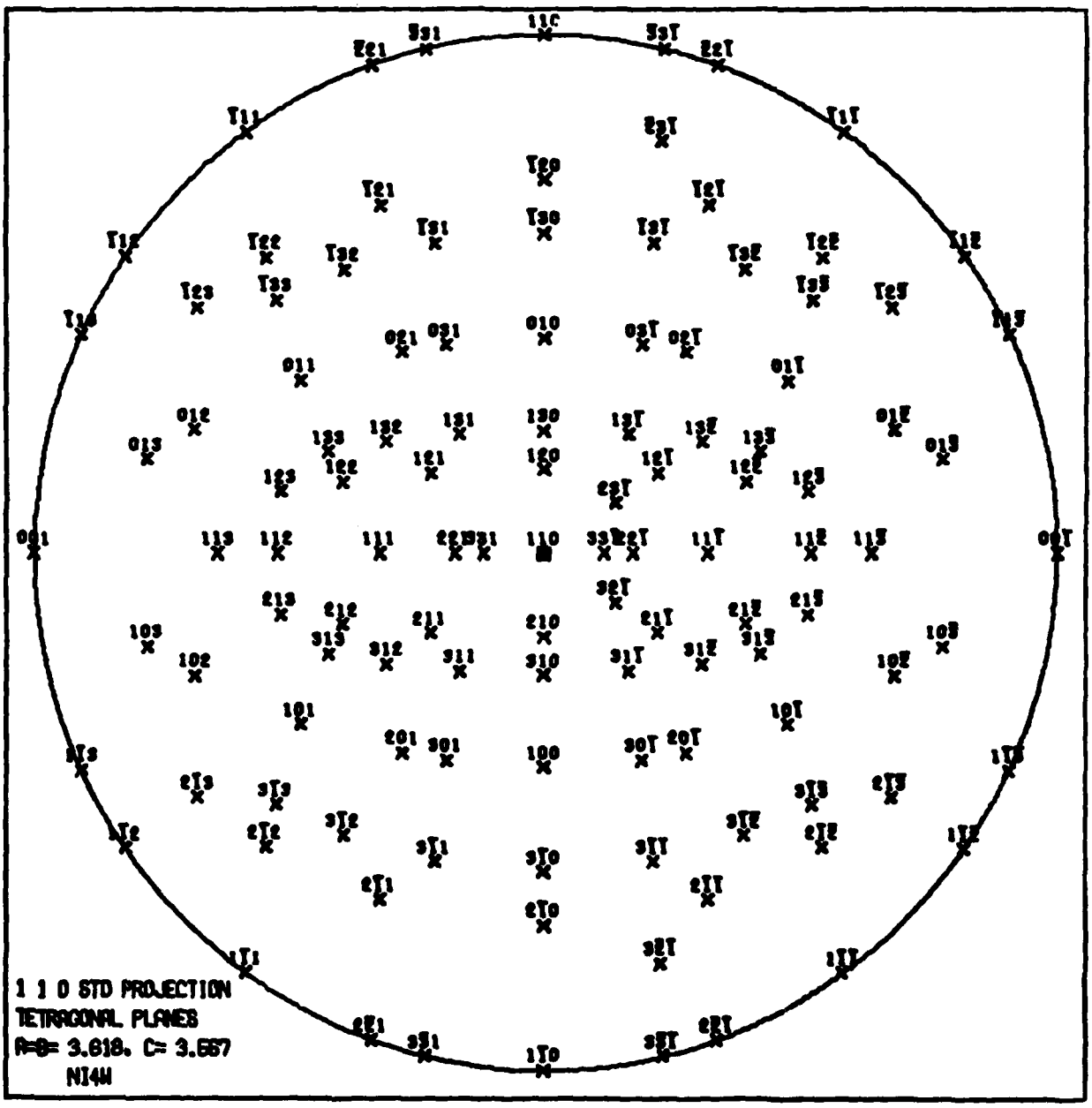

Fig. 3 (b) Projection using a unit cell where A = B = 3.618, C = 3.567.

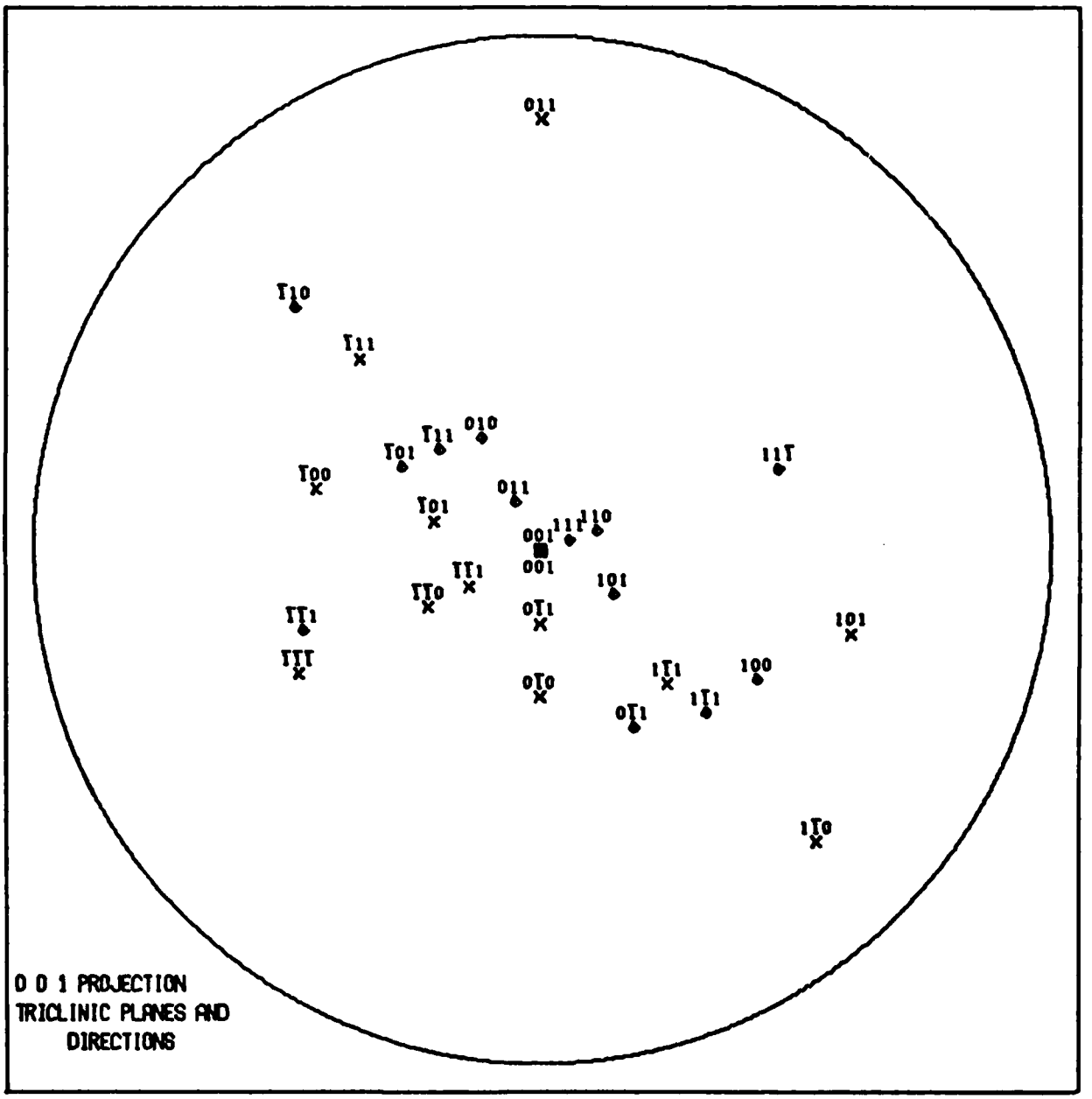

Fig. 4. Stereographic Projection of Plane Normals Superimposed on Directions in a Triclinic Crystal System.

REFERENCES

1. Johari and Thomas, "The Stereographic Projection and its Applications," Techniques of Metal Research, IIA, pp 107-132, Interscience (1969).

2. C. Kittle, Introduction to Solid State Physics, Fifth Edition, p. 15, John Wiley and Sons (1976).

APPENDIX

SOURCE LISTING COMPUTER PROGRAM

```
      PROGRAM STER (INPUT,OUTPUT,PLOT)                                  000001
C                                                                       000002
C     REF  JOHARI AND THOMAS, THE STEREOGRAPHIC PROJECTION AND ITS      000003
C     APPLICATIONS, TECHNIQUES OF METALS RESEARCH,  IIA, INTERSCIENCE,  000004
C     1969, PP 107-132                                                  000005
C                                                                       000006
C     ****************************************************************  000007
C     MODIFIED BY CAPT BOB SCHAFRIK, AFML                               000008
C     ****************************************************************  000009
      DIMENSION NT(4,20)                                                000010
      INTEGER RET                                                       000011
      COMMON /A/ PI                                                     000012
      COMMON N3,ND, P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,      000013
     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SH,   000014
     2SK,SL,E,X2,Y2,Z2,X,Y                                             000015
     3,A,B,C,ALPHA,BETA,GAMMA                                          000016
      COMMON /B/ HT                                                     000017
      COMMON /C/ IH(250),K(250),IT(250),L(250)                          000018
      COMMON /D/ IB,I                                                   000019
      DATA NMAX /250/                                                   000020
      PI=2.*ASIN(1.0)                                                   000021
      PRINT 7                                                           000022
 7    FORMAT (1H1,T2,*OFF-LINE PLOT*/)                                  000023
C  SET-UP FOR ON-LINE PLOT.  NOTE THAT TOTAL PLOT MUST BE  LESS THAN    000024
C     10.5 INCHES                                                       000025
C  READ PLOT RADIUS(CM),HT OF PLOTTED SYMBOLS(IN),NPERM=0, AND         000026
C     SEPERATION DISTANCE BETWEEN PLOTS(IN).                            000027
C  THE FOLLOWING VALUES ARE RECOMMENDED                                 000028
C  FOR ON-LINE PLOT: RADIUS=09.00, HT=.070, NPERM=0 ,SEP=04.0           000029
C  FOR OFF-LINE PLOT, RADIUS=15.00, HT=.100, NPERM=0, SEP=04.0          000030
C  TO DRAW THE ENCLOSING RECTANGLE, RET=1.                              000031
C  IF A RECTANGLE IS NOT DESIRED, RET=2                                 000032
      READ *, RADI, HT, NPERM,SEP,RET                                   000033
      IF (RET.NE.1)  RET=0                                              000034
      PRINT 59, RADI, HT, NPERM,SEP                                     000035
 59   FORMAT (T2, *PLOT RADIUS IS *, F6.3,* CM*,/ T2,*HT OF NUMBERS IS*,000036
     AF5.3, / T2,*NPERM IS *, I2  /                                     000037
     BT2,*SEPERATION BETWEEN PLOTS IS *,F4.1, * INCHES*)                000038
      IF (RET.EQ.0) PRINT 143                                           000039
 143  FORMAT (//T2,*NO ENCLOSING RECTANGLE*)                            000040
C  RADPL IS THE SPACING BETWEEN CENTERS OF THE PLOTS                    000041
      RADPL=RADI*2.0/2.54+SEP                                           000042
C  HI,WI ARE THE PARAMETERS USED IN PR07 TO DRAW THE ENCLOSING SQUARE    000043
      H1=(RADI+0.50)/2.54                                               000044
      W1=H1                                                             000045
C  INITIALIZE ORIGIN AT BOTTOM OF PAGE                                  000046
      READ 5000,YORIG                                                   000047
 5000 FORMAT(F5.1)                                                      000048
      CALL PLOT(0.0,YORIG,-3)                                           000049
C  MOVE ORIGIN TO CENTER OF PAGE                                        000050
      CALL PLOT (6.0,14.75,-3)                                          000051
C  READ IN PARAMETERS OF CRYSTAL LATTICE                                000052
C  A,B,C ARE THE LENGTHS OF THE 3 CRYSTALLOGRAPHIC AXES                 000053
C  ALPHA,  BETA, GAMMA ARE THE THREE CRYSTALLOGRAPHIC ANGLES            000054
C  NN SPECIFIES THE TYPE OF PLOT DESIRED                                000055
C   NN=1 PROVIDES A PLANE PROJECTION                                    000056
C   NN=2 PROVIDES A DIRECTION PROJECTION                                000057
C   NN=3 PROVIDES A DIRECTION PROJECTION SUPERIMPOSED                   000058
C    ON A PLANE PROJECTION                                              000059
      READ *,  A,B,C,ALPHA,BETA,GAMMA,NN                                000060
      NSS=1                                                             000061
C  TEST FOR AN HEXAGONAL CRYSTAL STRUCTURE.                             000062
C    IF HEXAGONAL STRUCTUR, USE 4-INDEX NOTATION                        000063
```

```
      IF (ABS(ALPHA+BETA+GAMMA-360.0).LE.(0.001) ) NSS=2                000064
      IF(NN.EQ.1.AND.NSS.EQ.1) PRINT 40                                 000065
      IF(NN.EQ.1.AND.NSS.EQ.2) PRINT 41                                 000066
      IF(NN.EQ.2.AND.NSS.EQ.1) PRINT 42                                 000067
      IF(NN.EQ.2.AND.NSS.EQ.2) PRINT 43                                 000068
      IF(NN.EQ.3.AND.NSS.EQ.1) PRINT 45                                 000069
      IF(NN.EQ.3.AND.NSS.EQ.2) PRINT 46                                 000070
40    FORMAT(//T2,*PLOT PLANE PROJECTIONS- NON-HEXAGONAL CRYSTAL STRUC*) 000071
41    FORMAT(//T2,*PLOT PLANE PROJECTIONS- HEXAGONAL CRYSTAL STRUCT*)    000072
42    FORMAT(//T2,*PLOT DIRECT PROJECTIONS-NON-HEXAGONAL CRYSTAL STRUC*) 000073
43    FORMAT(//T2,*PLOT DIRECT PROJECTIONS- HEXAGONAL CRYSTAL STRUC*)    000074
45    FORMAT(//T2,* PLOT PLANE & DIRECTION PROJECTIONS- NON-HEXAGONAL *) 000075
46    FORMAT(//T2,*PLOT PLANE & DIRECTIONS - HEXAGONAL*)                000076
C  PRO1 CALCULATES SOME BASIC QUANTITIES USED LATER                     000077
      CALL PRO1                                                         000078
C     NPERM CAN BE USED TO PROVIDE PERMUTED INDICES.                    000079
C     THIS WOULD ELIMEINATE THE NEED FOR DATA CARDS WITH  THE INDICES.  000080
C     HOWEVER THIS ASPECT OF THE PROGRAM IS NOT DEVELOPED.              000081
C     SET  NPERM=0                                                      000082
      IF (NPERM.NE.0) GO TO 130                                         000083
C  THIS PART OF THE PROGRAM READS THE INDICES, COUNTS THEM,             000084
C    AND STORES THEM IN ARRAYS.                                        000085
C  NOTE: HEXAGONAL INDICES MUST BE GIVEN IN   4-INDEX NOTATION         000086
      I=0                                                               000087
      GO TO (201,202), NSS                                              000088
 201  I=I+1                                                             000089
      READ 2,IH(I),K(I),L(I), M                                         000090
    2 FORMAT(3I3,I2)                                                    000091
      IF (M.LT.0) GO TO 4                                               000092
      GO TO 201                                                         000093
 202  I=I+1                                                             000094
      READ 22, IH(I),K(I),IT(I),L(I),M                                  000095
 22   FORMAT (4I3,I2)                                                   000096
      IF (M.LT.0) GO TO 4                                               000097
      GO TO 202                                                         000098
 4    I=I-1                                                             000099
      IF (I.GT.NMAX) PRINT 9,NMAX                                       000100
 9    FORMAT ( 3(/),3H***,3X,*YOU HAVE EXCEEDED ARRAY DIMENSIONS FOR *,  000101
     A*THE INDICES*,  /, T3, *THE ARRAY DIMENSIONS ARE SET FOR *,I4,    000102
     B  3(/)  )                                                         000103
 25   PRINT 44,I                                                        000104
44    FORMAT(/,T2,*NO. OF INDICES USED WAS *,I5)                        000105
C  THIS PART OF THE PROGRAM CALCULATES THE APPROPRIATE COORDINATES      000106
C    AND PLOTS THEM.                                                   000107
      NNO=1                                                             000108
      NN1=0                                                             000109
C  READ IN NUMBER OF PLOTS DESIRED (1 TO 9)                             000110
120   READ 5,I9                                                         000111
5     FORMAT (I1)                                                       000112
C  THIS BRANCH TRANSFERS THE PROGRAM TO THE APPROPRIATE PLACE           000113
C    DEPENDING ON  THE TYPE OF PROJECTION REQUIRED.                    000114
      GO TO (20,21,52) ,NN                                              000115
C  PRO2 CALCULATES PARAMETERS FOR PLANE PROJECTIONS                     000116
   20 CALL PRO2(I,NSS)                                                  000117
C  A TRANSFER TO STATEMENT 50 BELOW IS DONE IF A PLANE PROJECTION IS    000118
C    REQUESTED                                                         000119
      GO TO (50,51),NNO                                                 000120
C  PRO6 CALCULATES PARAMETES FOR DIRECTIONS                             000121
21    CALL PRO6 (I,U,V,W,NSS)                                           000122
C    REQUESTED.                                                        000123
      GO TO (50,51),NNO                                                 000124
C  THIS SECTION PROVIDES FOR PLOTTING PLANES AND DIRECTIONS ON THE      000125
C    SAME PLOT.                                                        000126
 52   NN1=3                                                             000127
      DO 10  II=1,I9                                                    000128
C  READ TITLE.  NEW LINES BEGIN WITH CC1,CC21,CC+1,AND CC61 OF THE      000129
C    DATA CARD.                                                        000130
```

```
C  NOTE: THERE MUST BE AS MANY TITLE CARDS AS PLOTS DESIRED              000131
      READ  450, ((NT(KA,JA),JA=1,20),KA=1,4)                           000132
 450  FORMAT (80A1)                                                     000133
      IF (II.GT.1)  GO TO 111                                           000134
C  PRO7 DRAWS THE CIRCLE OF THE PROJECTION AND THE ENCLOSING SQUARE.     000135
C    ALSO  IT PRINTS THE TITLE.                                         000136
  8   CALL PRO7(W1,H1,NT,RADI,RET)                                      000137
      NNO=NNO+1                                                         000138
C  THIS SECTION ACTUALLY CALC POSITION COORDS, AND PLOTS PLANES         000139
C    AND DIRECTIONS ON THE SAME PLOT.                                   000140
      DO 99  I3T=1,2                                                    000141
      NN=I8T                                                            000142
      GO TO(20,21),NN                                                   000143
C  PRO3 READS THE CENTER INDEX AND CALC SEVERAL PARAMETERS              000144
 51   CALL PRO3(NN,U,V,W,NSS)                                           000145
C  PLOTTING OF THE INDICES IS DONE IN THIS DO-LOOP                      000146
      DO 100  N=1,I                                                     000147
C  PRO4 CALC PLOTTING COORD AND DETERMINES IF INDEX IS WITHIN           000148
C    THE PROJECTION FIELD.                                              000149
C   ACCURACY IS  0.10 RADIAN                                            000150
      CALL PRO4(N,NSW)                                                  000151
      GO TO (11,100),NSW                                                000152
C   PRO5 DOES THE PLOTTING OF ALL INDICES                               000153
11    CALL PRO5(N,NSS,NN)                                               000154
100   CONTINUE                                                          000155
 39   CONTINUE                                                          000156
      NNO=1                                                             000157
 10   CONTINUE                                                          000158
C  END OF SECTION FOR SUPER-IMPOSED PLOTS                               000159
C                                                                       000160
C  THIS TERMINATES THE PROGRAM                                          000161
 57   CALL PLOT (RADPL,0.0,-3)                                          000162
      CALL PLOTE(999)                                                   000163
      GO TO 30                                                          000164
C                                                                       000165
C  BEGIN SECTION FOR PLOTTING PLANE OR DIRECTION PROJECTION             000166
 50   DO 310  II=1,IB                                                  000167
C  READ TITLE.  NEW LINES BEGIN WITH CC1,CC21,CC41,AND CC61 OF THE      000168
C    DATA CARDS.                                                        000169
C  NOTE: THERE MUST BE AS MANY TITLE CARDS AS PLOTS DESIRED.            000170
      READ  450, ((NT(KA,JA),JA=1,20),KA=1,4)                           000171
      IF (II.GT.1)  GO TO 111                                           000172
C  PRO7 DRAWS THE CIRCLE OF THE PROJECTION AND THE ENCLOSING SQUARE.     000173
C    ALSO  IT PRINTS THE TITLE.                                         000174
 38   CALL PRO7(W1,H1,NT,RADI,RET)                                      000175
C  PRO3 READS THE CENTER INDEX AND CALC SEVERAL PARAMETERS              000176
      CALL PRO3(NN,U,V,W,NSS)                                           000177
C  PLOTTING OF THE INDICES IS DONE IN THIS DO-LOOP                      000178
      DO 311  N=1,I                                                     000179
C  PRO4 CALC PLOTTING COORD AND DETERMINES OF INDEX IS WITHIN           000180
C    THE PROJECTION FIELD.                                              000181
C   ACCURACY IS  0.10 RADIAN                                            000182
      CALL PRO4(N,NSW)                                                  000183
      GO TO (311,310), NSW                                              000184
C   PRO5 DOES THE PLOTTING OF ALL INDICES                               000185
 311  CALL PRO5(N,NSS,NN)                                               000186
 310  CONTINUE                                                          000187
C  END OF SECTION FOR PLOTTING PLANE OR DIRECTION PROJECTIONS           000188
      GO TO 57                                                          000189
30    STOP                                                              000190
 111  CALL PLOT (0.0,0.0,3)                                             000191
      CALL PLOT (RADPL,0.0,-3)                                          000192
      IF  (NN1.EQ.3)  GO TO 8                                           000193
      GO TO 38                                                          000194
C  PRO8 NOT OPERATIONAL. BE SURE NPERM=0                                000195
```

```
 150  CALL PRO8 (NPERM,NSS)                                                  000196
      I=NPERM**3                                                             000197
      GO TO 25                                                               000198
      END                                                                    000199
C                                                                            000200
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$  000201
C                                                                            000202
      SUBROUTINE PRO1                                                        000203
C  THIS PROGRAM CALCULATES BASIC QUANTITIES FROM THE CRYSTAL LATTICE         000204
C    DATA AND PLACES THEM IN COMMON.                                         000205
      COMMON NB,ND,       P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,   000206
     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SM,         000207
     2SK,SL,E,X2,Y2,Z2,X,Y                                                   000208
     3,A,B,C,ALPHA,BETA,GAMMA                                                000209
      COMMON /A/ PI                                                          000210
      P=COS(ALPHA*PI/180.0)                                                  000211
      Q=COS(BETA*PI/180.0)                                                   000212
      R=COS(GAMMA*PI/180.0)                                                  000213
      RS=SQRT(1.-R*R)                                                        000214
      VOL=A*B*C*SQRT(1.-P*P-Q*Q-R*R+2.0*P*Q*R)                               000215
      S11=B*B*C*C*(1.-P*P)                                                   000216
      S22=A*A*C*C*(1.-Q*Q)                                                   000217
      S33=A*A*B*B*(1.-R*R)                                                   000218
      S12=A*B*C*C*(P*Q-R)                                                    000219
      S23=A*A*B*C*(Q*R-P)                                                    000220
      S31=A*B*B*C*(R*P-Q)                                                    000221
      WD=(C*SQRT(1.0-Q*Q-((P-Q*R)/RS)**2))                                   000222
      W=A/WD                                                                 000223
      V=-((W*C*(P-Q*R))/(B*RS*RS))                                           000224
      U=-((W*C*Q)+(V*B*R))/A                                                 000225
      R2=((RADI*RADI)+0.5)                                                   000226
      RETURN                                                                 000227
      END                                                                    000228
C                                                                            000229
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$  000230
C                                                                            000231
      SUBROUTINE PRO2(IC,NSS)                                                000232
C  THIS PROGRAM QUANTITIES FROM THE INDEX VALUE OF PLANE AND PLACES          000233
C    THEM IN COMMON FOR USE IN  PRO4.                                        000234
      COMMON NB,ND,       P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,   000235
     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SM,         000236
     2SK,SL,E,X2,Y2,Z2,X,Y                                                   000237
     3,A,B,C,ALPHA,BETA,GAMMA                                                000238
      COMMON /C/ IH(250),K(250),IT(250),L(250)                               000239
      DO 5 I=1,IC                                                            000240
      H(I)=IH(I)                                                             000241
      G(I)=K(I)                                                              000242
      F(I)=L(I)                                                              000243
      D(I)=VOL/SQRT((S11*H(I)*H(I))+(S22*G(I)*G(I))+(S33*F(I)*F(I))+(2.*     000244
     1S12*H(I)*G(I))+(2.*S31*H(I)*F(I))+(2.*S23*G(I)*F(I)))                  000245
      X1(I)=RADI*H(I)*D(I)/A                                                 000246
      Y1(I)=RADI*D(I)*((G(I)/B)-(H(I)*R/A))/RS                               000247
      Z1(I)=RADI*D(I)*(H(I)*U+G(I)*V+F(I)*W)/A                               000248
 5    CONTINUE                                                               000249
      RETURN                                                                 000250
      END                                                                    000251
C                                                                            000252
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$  000253
C                                                                            000254
      SUBROUTINE PRO3(NN,UZ,VZ,WZ,NSS)                                       000255
C  THIS PROGRAM READS IN THE INDEX OF CENTER OF THE PROJECTION AND           000256
C    CALCULATES VARIOUS PARAMETERS WHICH ARE PLACED IN COMMON.               000257
C  NOTE: A HEXAGONAL SYSTEM REQUIRES 4-INDEX NOTATION                        000258
C  ALSO : A NEGATIVE NUMBER ON THE DATA CARD AFTER THE INDEX DATA            000259
C    WILL TERMINATE THE INPUTING OF DATA.                                    000260
      COMMON NB,ND,       P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,   000261
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     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SH,    000262
     2SK,SL,E,X2,Y2,Z2,X,Y                                              000263
     3,A,B,C,ALPHA,BETA,GAMMA                                           000264
      GO TO (4,31), NSS                                                 000265
    4 READ 2,  NH,NK,NL,M                                               000266
    2 FORMAT(3I3,I2)                                                    000267
      IF(M)7,6,6                                                        000268
7     CALL PLOT(10.0,0.0,-3)                                            000269
      PRINT 5                                                           000270
 5    FORMAT (T2,*PROGRAM TERMINATED FROM PRO3*)                        000271
      CALL PLOTE (999)                                                  000272
      GO TO 3                                                           000273
    6 CONTINUE                                                          000274
      GO TO (1,9),NN                                                    000275
    1 SH=-NH                                                            000276
      SK=-NK                                                            000277
      SL=-NL                                                            000278
      E=VOL/SQRT((S11*SH*SH)+(S22*SK*SK)+(S33*SL*SL)+(2.*S12*SH*SK)+(2.*000279
     1S23*SK*SL)+(2.*S31*SL*SH))                                        000280
      X2=RADI*SH*E/A                                                    000281
      Y2=RADI*E*((SK/B)-(SH*R/A))/RS                                    000282
      Z2=RADI*E*(SH*U+SK*V+SL*W)/A                                      000283
      GO TO 3                                                           000284
    9 SU=-NH                                                            000285
      SV=-NK                                                            000286
      SW=-NL                                                            000287
43    E=SQRT(A*A*SU*SU+B*B*SV*SV+C*C*SW*SW+2.*B*C*SV*SW*P+2.*C*A*SW*SV*Q000288
     1+2.*A*B*SU*SV*R)                                                  000289
      X2=RADI*(SU*A+SV*B*R+SW*C*Q)/E                                    000290
      Y2=RADI*((SV*B*RS)+((SW*C*(P-Q*R))/RS))/E                         000291
      Z2=RADI*(A*A*UZ*SU+B*B*VZ*SV+C*C*WZ*SW+B*C*P*(VZ*SW+WZ*SV)+A*C*Q*(000292
     1WZ*SU+SW*UZ)+A*B*R*(UZ*SV+VZ*SU))/(E*A)                           000293
    3 RETURN                                                            000294
31    READ 30,NH,NK,NI,NL,M                                             000295
30    FORMAT (4I3,I2)                                                   000296
       IF (M.LT.0)  GO TO 7                                             000297
      GO TO (1,42), NN                                                  000298
42    SU=-(NH-NI)                                                       000299
      SV=-(NK-NI)                                                       000300
      SW=-NL                                                            000301
      GO TO 43                                                          000302
      END                                                               000303
C                                                                       000304
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$ 000305
C                                                                       000306
      SUBROUTINE PRO4(N,NSW)                                            000307
C  THIS PROGRAM CALCULATES THE PLOTTING CORRDINATES OF THE INDICES      000308
C    (IN INCHES)                                                        000309
C  AND DETERMINES IF THE INDEX IS WITHIN THE FIELD OF PROJECTION        000310
C  ACCURACY IS  0.10 RADIAN                                             000311
C  THE INDEX COORDS, X&Y, ARE PLACES IN COMMON FOR USE IN PRO5          000312
      COMMON N3,ND,       P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,000313
     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SH,    000314
     2SK,SL,E,X2,Y2,Z2,X,Y                                              000315
     3,A,B,C,ALPHA,BETA,GAMMA                                           000316
       NSW=1                                                            000317
      DENOM=X2*(X1(N)-X2)+Y2*(Y1(N)-Y2)+Z2*(Z1(N)-Z2)                   000318
      IF(DENOM)21,10,21                                                 000319
   10 NSW=2                                                             000320
      GO TO 14                                                          000321
   21 X3=(X2*(Y1(N)*Y2+Z1(N)*Z2)-X1(N)*(Y2*Y2+Z2*Z2))/DENOM             000322
      Y3=(Y2*(X2*X1(N)+Z2*Z1(N))-Y1(N)*(X2*X2+Z2*Z2))/DENOM             000323
      Z3=(Z2*(X2*X1(N)+Y2*Y1(N))-Z1(N)*(X2*X2+Y2*Y2))/DENOM             000324
      T=X3*X3+Y3*Y3+Z3*Z3                                               000325
      IF(T-R2)9,8,10                                                    000326
    8 IF(SH)9,11,9                                                      000327
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   11 IF(SK)9,12,9                                                          000328
   12 X=X3                                                                  000329
      Y=Y3                                                                  000330
      GO TO 14                                                              000331
    9 S=SQRT(X2*X2+Y2*Y2)                                                   000332
      A11=-(X2*Z2)/(RADI*S)                                                 000333
      A12=-(Y2*Z2)/(RADI*S)                                                 000334
      A13=S/RADI                                                            000335
      A21=Y2/S                                                              000336
      A22=-X2/S                                                             000337
      X=-(A11*X3+A12*Y3+A13*Z3)                                             000338
      Y=A21*X3+A22*Y3                                                       000339
   14 RETURN                                                                000340
      END                                                                   000341
C                                                                           000342
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$ 000343
C                                                                           000344
      SUBROUTINE PRO5(N,NSS,NNA)                                            000345
C  THIS PROGRAM DOES THE PLOTTING OF THE INDICES                            000346
      COMMON NB,ND,       P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,    000347
     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SH,        000348
     2SK,SL,E,X2,Y2,Z2,X,Y                                                  000349
     3,A,B,C,ALPHA,BETA,GAMMA                                               000350
      COMMON /B/  HT                                                        000351
      COMMON /D/ IB,I                                                       000352
      DIMENSION NN(4),NJ(4),NAST(4),RDIFF(4)                                000353
C  ND IS USED TO PLOT A LINE OVER AN INDEX INDICATING A NEG VALUE           000354
C  NB IS USED TO PLOT A BLANK SPACE OVER AN INDEX  INDICATING A             000355
C    POSITIVE VALUE.                                                        000356
      ND=80                                                                 000357
      NB=72                                                                 000358
C  NSYM SPECIFIES THE SYMBOL USED TO PLOT THE POINT                         000359
C   PLANES HAVE AN X                                                        000360
C   DIRECTIONS HAVE A DIAMOND                                               000361
      IF (NNA.EQ.1)  NSYM=4                                                 000362
      IF (NNA.EQ.2)  NSYM=5                                                 000363
      KH=H(N)                                                               000364
      KK=G(N)                                                               000365
      KL=F(N)                                                               000366
      IND=3                                                                 000367
      GO TO (201,202),NSS                                                   000368
C  THIS SECTION DETERMINES HEXAGONAL 4-INDICES. THE INPUTTED                000369
C    4-INDICES WERE CONVERTED TO 3-INDICES FOR                              000370
C    COMPUTATIONAL REASONS.                                                 000371
202   IND=4                                                                 000372
      GO TO  (2001,2002), NNA                                               000373
C   HEXAGONAL PLANES                                                        000374
2001  NJ(1)=KH                                                              000375
      NJ(2)=KK                                                              000376
      NJ(3)=-(KH+KK)                                                        000377
      NJ(4)=KL                                                              000378
      GO TO 203                                                             000379
C   HEXAGONAL DIRECTIONS                                                    000380
2002  RDIFF(1)=(2*KH-KK)/3.                                                 000381
C   HEXAGONAL DIRECTION TEST FOR TRUNCATION OF INDEX DUE TO                 000382
C    RECOMPUTATION.                                                         000383
C   PROGRAM WILL PLOT AN ASTERISK ABOVE TRUNCATED INDEX                     000384
      RDIFF(2)=(2*KK-KH)/3.                                                 000385
      RDIFF(3)=-(KH+KK)/3.                                                  000386
      RDIFF(4)=KL                                                           000387
      DO 45  IL=1,4                                                         000388
      NJ(IL)=RDIFF(IL)                                                      000389
      NAST(IL)=1                                                            000390
      IF (ABS( NJ(IL)-RDIFF(IL)).GE.1.E-3)  NAST(IL)=2                      000391
45    CONTINUE                                                              000392
      GO TO 203                                                             000393
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C  THIS SECTION DETERMINES NON-HEXAGONAL 3 INDICES                        000394
  201 NJ(1)=KH                                                           000395
      NJ(2)=KK                                                           000396
      NJ(3)=KL                                                           000397
C  TEST FOR SIGN OF INDEX                                               000398
203   DO 44  J=1,IND                                                    000399
      IF(NJ(J))55,66,66                                                 000400
   55 NN(J)=ND                                                          000401
      NJ(J)=-NJ(J)                                                      000402
      GO TO 44                                                          000403
   66 NN(J)=NB                                                          000404
   44 CONTINUE                                                          000405
C  CONVERT X,Y COORDS FROM INCHES TO CM                                 000406
      X=X/2.54                                                          000407
      Y=Y/2.54                                                          000408
C  DRAW SPECIAL SYMBOL IN CENTER FOR PLANE  PROJECTION (SQUARE)         000409
      IF (X.EQ.0.0.AND.Y.EQ.0.0.AND.NNA.EQ.1) CALL SYMBOL(X,Y, HT ,     000410
     A0,0.0, -1)                                                        000411
C  DRAW SPECIAL SYMBOL IN CENTER FORDIRECTION PROJECTION (TRIANGLE) AND  000412
C  PRINT INDEX BELOW SYMBOL AT CENTER                                   000413
      IF (X.EQ.0.0.AND.Y.EQ.0.0.AND.NNA.EQ.2)  GO TO 95                 000414
C  DRAW THE INDEX SYMBOL                                                000415
      CALL SYMBOL (X,Y,HT,NSYM,0.0,-1)                                  000416
C  POSITION PEN ABOVE INDEX THAT WILL BE LABELED                        000417
      PY1=Y+HT                                                          000418
 96   DO 30  II=1,IND                                                   000419
C  MOVE PEN TO SPACE NUMBERS                                            000420
      BBX=X+(II-2)*(HT+0.01)-0.03                                       000421
C  CALC ARRAY VALUE FOR TABLE FOR THE INDEX INTEGERS                    000422
      NSYB=NJ(II)+54                                                    000423
C  TEST FOR INDEX INTEGER EXCEEDING 9                                   000424
      IF (NSYB.GT.63)  GO TO 12                                         000425
C  DRAW THE INDEX INTEGERS                                              000426
 13   CALL SYMBOL (BBX,PY1,HT,NSYB,0.0,-1)                              000427
30    CONTINUE                                                          000428
C  POSITION PEN ABOVE NUMBER TO DRAW LINE INDICATING NEG                000429
      PY2=PY1+HT+0.02                                                   000430
C  DRAW NEG LINE OR BLANK                                               000431
      DO 31  IJ=1,IND                                                   000432
      BX=X-0.03+(IJ-2)*(HT+0.01)                                        000433
      HTT=HT+0.01                                                       000434
      CALL SYMBOL (BX,PY2,HTT,NN(IJ),0.0,-1)                            000435
31    CONTINUE                                                          000436
      IF (NSS.EQ.2.AND.NNA.EQ.2)  GO TO 70                              000437
      RETURN                                                            000438
C  DRAW ASTERISK FOR HEX DIRECTIONS TO INDICATE TRUNCATION              000439
 70   PY3=PY2+0.05                                                      000440
      DO 46  ILL=1,4                                                    000441
      DX=X+(ILL-2)*HTT -0.03                                            000442
      IF (NAST(ILL).EQ.1) CALL SYMBOL(DX,PY3,HTT,72,0.0,-1)             000443
      IF (NAST(ILL).EQ.2) CALL SYMBOL (DX,PY3,.03,11,0.0,-1)            000444
46    CONTINUE                                                          000445
      RETURN                                                            000446
 95   CALL SYMBOL(X,Y,HT,2,0.0,-1)                                      000447
      PY1=Y-2.10*HT                                                     000448
      GO TO 96                                                          000449
 12   NSYB=32                                                           000450
      IF (NSS.EQ.1)  PRINT 10,NJ                                        000451
      IF (NSS.EQ.2) PRINT 11,NJ                                         000452
 10   FORMAT (T2,3(1X,I6)  )                                            000453
 11   FORMAT (T2,4(1X,I6)  )                                            000454
      PRINT 16,I9,I                                                     000455
 16   FORMAT (T2,I3, I5)                                                000456
      GO TO 13                                                          000457
      END                                                               000458
C                                                                       000459
```

```
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C
      SUBROUTINE PRO6 (IC,UZ,VZ,WZ,NSS)
C  THIS PROGRAM CALCULATES QUANTIES FROM INDEX VALUES OF DIRECTIONS
C    AND PLACES THEM IN COMMON FOR USE IN PRO4.
      COMMON N3,ND,         P,Q,R,RS,VOL,S11,S22,S33,S12,S23,S31,WD,W,V,U,
     1RADI,R2,H(250),G(250),F(250),D(250),X1(250),Y1(250),Z1(250),SH,
     2SK,SL,E,X2,Y2,Z2,X,Y
     3,A,B,C,ALPHA,BETA,GAMMA
      COMMON /C/ IH(250),K(250),IT(250),L(250)
      IF (NSS.EQ.2)  GO TO 20
      DO 6 I=1,IC
      H(I)=IH(I)
      G(I)=K(I)
      F(I)=L(I)
 6    CONTINUE
 21   DO 7 I=1,IC
      D(I)=SQRT(A*A*H(I)*H(I)+B*B*G(I)*G(I)+C*C*F(I)*F(I)+2.*B*C*G(I)*F(
     1I)*P+2.*C*A*F(I)*H(I)*Q+2.*A*B*H(I)*G(I)*R)
      X1(I)=RADI*(H(I)*A+G(I)*B*R+F(I)*C*Q)/D(I)
      Y1(I)=RADI*((G(I)*B*RS)+((F(I)*C*(P-Q*R))/RS))/D(I)
      Z1(I)=RADI*(A*A*H(I)*UZ+B*B*G(I)*VZ+C*C*F(I)*WZ+B*C*P*(VZ*F(I)+WZ*
     1G(I))+A*C*Q*(F(I)*UZ+WZ*H(I))+A*B*R*(UZ*G(I)+H(I)*VZ))/(D(I)*A)
 7    CONTINUE
      RETURN
 20   DO 5 I=1,IC
      H(I)=IH(I)-IT(I)
      G(I)=2.*K(I)-IH(I)
      F(I)=L(I)
 5    CONTINUE
      GO TO 21
      END
C
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C
      SUBROUTINE PRO7(W1,H1,NT,RADI,RET)
C  THIS PROGRAM DRAWS THE PROJECTION CIRCLE, THE ENCLOSING SQUARE, AND
C  PRINTS THE TITLE
      DIMENSION NT(4,20)
      COMMON /A/ PI
      INTEGER RET
      RAD=RADI /2.54
C  HH1,WW1 ARE THE HEIGHT AND WITH OF THE RECTANGLE
C  REC MUST EQUAL 1 IN ORDER TO GET RECTANGLE
      HH1=H1*2.0
      WW1=W1*2.0
C  CALL RECT USES A SPECIAL CALCOMP ROUTINE- MUST USE SPECIAL
C    CONTROL CARDS TO ACCESS IT.
      IF (RET.EQ.1) CALL RECT(-H1,-W1,HH1,WW1,0.0,3)
C  THIS SECTION OF THE PROGRAM DRAWS THE PROJECTION CIRCLE
C  DRAW CIRCLE USES A SPECIAL CALCOMP ROUTINE- MUST USE SPECIAL
C    CONTROL CARDS TO ACCESS IT.
      CALL CIRCLE (RAD,0.0,0.0,360.0,RAD,RAD,0.0)
C  PRINT TITLE FROM NT ARRAY.  TITLE WILL BE PLACES IN LOWER
C    LEFT-HAND CORNER  BETWEEN SQUARE AND CIRCLE.
C  LETTER HT FIXED AT 0.100 INCH
      CALL PLOT (0.0,0.0,3)
      DO 90  LR=1,4
      YY=-(RAD-0.50)-(0.2000)*(LR-1)
      DO 90  LS=1,20
      XX=-(RAD+0.12)+(.075)*( LS-1)
      CALL SYMBOL(XX,YY,.100,NT(LR,LS),0.0,1)
90    CONTINUE
      RETURN
      END
C
```

```
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C
      SUBROUTINE PROB (NPERM,NSS)
C  THIS SUBROUTINE COULD BE DEVELOPED TO PERMUTE INDICES IN ORDER TO
C    AVOID READING IN THE CARD DATA.
      RETURN
      END
```


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