UNITED STATES (DEPARTMENT OF THE INTERIOR)

GEOLOGICAL SURVEY [Reports - Open file series]

# Least-Squares Refinement of Powder Diffraction Data for Unit Cell Parameters

Program Listing for DEC 10 Computer

By

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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

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Program Listing--Continued

## Program Description

This FORTRAN computer program is a time-sharing version of the classic program of Appleman and Evans (1973) and Evans, Appleman, and Handwerker (1963), which indexes powder patterns and refines unit-cell dimensions. The program, originally written to be processed in batch mode for an IBM computer, was modified to run in time-sharing mode on the DEC 10 computer.

This version does not depart philosophically from the original program; however, the input and output formats have been adapted to the time-sharing terminal. These modifications and the actual running of the program are not discussed in detail here, as this report is intended only to make the program itself available. Examples of the input and output formats are shown on pages 3-8.

Input can be entered through the terminal by two methods. An input file may either be independently created and then entered into the program later, or created directly through the interactive mode of the program. With the latter method a file of the input information may also be saved for later use. Both methods allow for the data to be edited after each refinement run.

The output format has been changed to an 80-column width, common to many terminals. Only the last refinement cycle is printed and some of the statistical computations have been surpressed.

Using the "Unit Cell" program from the terminal in a "real time" situation emphasizes the versatility of the program. This ability to interact directly with the computer gives the user a better appreciation of the program, its options, the data, and the problem being solved.

Input and Output Explanations

The following examples are taken directly from a teletype output. They assume familiarity with the DEC computer and therefore no effort has been made to define operational procedures.

User responses to prompting questions from the computer have been underlined.

"CUBIC.DAT" and "CUBIC" are the names of data sets already created and stored on the disk for easy access.

"RUN UNITCS [200,200]" is the command which executes the previously compiled UNITCS program stored in the 200,200 programmer project area of the computer.

The data set used was in the cubic system with a cell edge given as 5.37Å. The maximum two theta value to be calculated was 61 degrees with a wavelength equal to 1.54178 (copper K-alpha radiation). The reflections were entered in angstrom values.

AN EXAMPLE OF A RUN USING A PRE-MADE, DISK STORED DATA SET

```
TYPE CUBIC.DAT
TITLE CUBIC SYSTEM TEST - URANINITE
 $PARAM AO(1)=5.37$
CUBIC$
 $SYSEXT THEMX=61.,PWL=1.54178$
 $DATA D=3.09$
 $DATA D=2.686$
 $DATA D=1.9$
 $DATA D=1.62$
 $DATA D=1.54$
 $DATA ITEST=2$
[0.23  3 0]

*RUN UNITCS [200,200]
ENTER DATA INPUT FILE NAME (MAX 5 CHARS): CUBIC

ENTER SCRATCH FILE NAME (MAX 5 CHARS):CCC



CUBIC SYSTEM TEST - URANINITE

*** SIGNIFICANT FIGURES IN OUTPUT VALUES ARE A FUNCTION OF INPUT DATA ***

    DIRECT CELL  0.53700000E+01  0.53700000E+01  0.53700000E+01
                       90.00000        90.00000        90.00000
                 0.15485415E+03
RECIPROCAL CELL  0.18621974E+00  0.18621974E+00  0.18621974E+00
                       90.00000        90.00000        90.00000
                 0.64576892E-02

1-THETA ANGLES   THTMX =   20.0  NCYC = 2  TOLMN = 0.0200  TOLMX = 0.1000
                 THEMX =   30.5  DMIN =  1.518880  CUBIC SYSTEM

 0 CONDITIONS FOR NON-EXTINCTION CALLED FOR     CLASS CONDITION(S)
```

CYCLE 4
CUBIC SYSTEM TEST - URANINITE
2-THETA TOLERANCE = 0.12760 CUBIC

| N | H K L | D CALC | D.OBS | 2-THETA CALC | 2-THETA OBS | 2-THETA DIF |
|---|---|---|---|---|---|---|
| 1 | 1 1 1 | 3.1009 | 3.0900 | 28.78919 | 28.8934 | -0.10418 |
| 2 | 2 0 0 | 2.6855 | 2.6860 | 33.36367 | 33.3572 | 0.00644 |
| 3 | 2 2 0 | 1.8989 | 1.9000 | 47.90255 | 47.8740 | 0.02859 |
| 4 | 3 1 1 | 1.6194 | 1.6200 | 56.85285 | 56.8305 | 0.02239 |

| | A | B | C |
|---|---|---|---|
| RECIPROCAL CELL | 0.18618529E+00 | 0.18618529E+00 | 0.18618529E+00 |
| R C CORRECTIONS | -0.25821835E-07 | -0.25821835E-07 | -0.25821835E-07 |
| DIRECT CELL | 0.53709936E+01 | 0.53709936E+01 | 0.53709936E+01 |
| D C CORRECTIONS | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 |

| | ALPHA | BETA | GAMMA | VOLUME |
|---|---|---|---|---|
| RECIPROCAL CELL | 90.00000 | 90.00000 | 90.00000 | 0.64541060E-02 |
| R C CORRECTIONS | 0.000 | 0.000 | 0.000 | -0.27357601E-08 |
| DIRECT CELL | 90.00000 | 90.00000 | 90.00000 | 0.15494013E+03 |
| D C CORRECTIONS | 0.000 | 0.000 | 0.000 | 0.66757202E-04 |

LARGEST RESIDUAL REDUCED TO UNIT WEIGHT 0.10418
OBS 1 STANDARD ERROR UNIT WT OBS 0.06381 DEGREES OF FREEDOM 3

| | | | |
|---|---|---|---|
| R C STNDRD ERRS | 0.12898331E-03 | 0.12898331E-03 | 0.12898331E-03 |
| | 0.000 | 0.000 | 0.000 |
| D C STNDRD ERRS | 0.37208555E-02 | 0.37208555E-02 | 0.37208555E-02 |
| | 0.000 | 0.000 | 0.000 |
| | 0.32201294E+00 | | |

CUBIC SYSTEM TEST - URANINITE
HKL LISTING - *** REFERS TO FIXED, R TO REJECTS CUBIC

| N | H | K | L | | D CALC | D OBS | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | | 5.3710 | | 16.50414* | | |
| 2 | 1 | 1 | 0 | | 3.7979 | | 23.42253 | | |
| 3 | 1 | 1 | 1 | | 3.1009 | 3.0900 | 28.78919 | 28.8934 | -0.10418 |
| 4 | 2 | 0 | 0 | | 2.6855 | 2.6860 | 33.36367 | 33.3572 | 0.00644 |
| 5 | 2 | 1 | 0 | | 2.4020 | | 37.43947 | | |
| 6 | 2 | 1 | 1 | | 2.1927 | | 41.16691 | | |
| 7 | 2 | 2 | 0 | | 1.8989 | 1.9000 | 47.90255 | 47.8740 | 0.02859 |
| 8 | 3 | 0 | 0 | | 1.7903 | | 51.00941 | | |
| 9 | 3 | 1 | 0 | | 1.6985 | | 53.98536 | | |
| 10 | 3 | 1 | 1 | | 1.6194 | 1.6200 | 56.85285 | 56.8305 | 0.02239 |
| 11 | 2 | 2 | 2 | R | 1.5505 | 1.5400 | 59.62945 | 60.0765 | -0.44704 |

*IT SHOULD BE NOTED THAT THERE ARE DISCREPANCIES IN THE VARIOUS SETS OF 2-THETA OUTPUT VALUES. THESE ROUNDING ERRORS ARE A FUNCTION OF THE ORIGINAL PROGRAM ALGORITHM AND WELL BEYOND THE ACCURACY OF THE INPUT DATA.

DO YOU WANT TO ALTER VALUES IN THIS EXISTING DATA? YES
WHICH ONES?
LIST
TITLE:CUBIC SYSTEM TEST - URANINITE
SYSTM:CUBIC
A : 5.3700
THEMX: 61.0000
PWL : 1.5418
DSPAC: 1 3.090 0 0 0
DSPAC: 2 2.686 0 0 0
DSPAC: 3 1.900 0 0 0
DSPAC: 4 1.620 0 0 0
DSPAC: 5 1.540 0 0 0

AN EXAMPLE OF A RUN USING THE INTERACTIVE INPUT OPTION

```
RUN UNITCS [200,200]

ENTER DATA INPUT FILE NAME (MAX 5 CHARS):


TITLE : URANINITE   CUBIC SYSTEM TEST DATA

CRYSTAL SYSTEM : CUBIC

ENTER VALUES IN ORDER REQUESTED.  SEPARATE BY COMMAS.
ENTER A : 5.37

ENTER MAX 2-THETA VALUE TO BE CALCULATED:  61

ENTER WAVE LENGTH OF TARGET : 1.54178

ARE THERE CONDITIONS FOR NON-EXTINCTION?  (YES,NO) NO



URANINITE   CUBIC SYSTEM TEST DATA
***SIGNIFICANT FIGURES IN OUTPUT VALUES ARE A FUNCTION OF INPUT DATA***
    DIRECT CELL  0.53700000E+01  0.53700000E+01  0.53700000E+01
                       90.00000        90.00000        90.00000
                 0.15485415E+03
RECIPROCAL CELL  0.18621974E+00  0.18621974E+00  0.18621974E+00
                       90.00000        90.00000        90.00000
                 0.64576892E-02

IS DATA 2-THETA? (YES,NO) NO

ENTER D-SPACING & H K L VALUES.  TERMINATE ENTRY WITH "0" FOR SPACING.
NO. 1       3.09
NO. 2       2.686
NO. 3       1.90
NO. 4       1.62
NO. 5       1.54
NO. 6

1-THETA ANGLES  THTMX =  20.0  NCYC = 2  TOLMN = 0.0200  TOLMX = 0.1000
                THEMX =  30.5  DMIN =  1.518880  CUBIC SYSTEM

 0 CONDITIONS FOR NON-EXTINCTION CALLED FOR     CLASS CONDITION(S)
```

CYCLE 4
URANINITE CUBIC SYSTEM TEST DATA
2-THETA TOLERANCE = 0.12760 CUBIC

| N | H | K | L | D CALC | D OBS | 2-THETA CALC | 2-THETA OBS | 2-THETA DIF |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 3.1009 | 3.0900 | 28.78919 | 28.8934 | -0.10418 |
| 2 | 2 | 0 | 0 | 2.6855 | 2.6860 | 33.36367 | 33.3572 | 0.00644 |
| 3 | 2 | 2 | 0 | 1.8989 | 1.9000 | 47.90255 | 47.8740 | 0.02859 |
| 4 | 3 | 1 | 1 | 1.6194 | 1.6200 | 56.85285 | 56.8305 | 0.02239 |

| | A | B | C |
|---|---|---|---|
| RECIPROCAL CELL | 0.18618529E+00 | 0.18618529E+00 | 0.18618529E+00 |
| R C CORRECTIONS | -0.25821835E-07 | 0.25821835E-07 | -0.25821835E-07 |
| DIRECT CELL | 0.53709936E+01 | 0.53709936E+01 | 0.53709936E+01 |
| D C CORRECTIONS | 0.00000000E+00 | 0.00000000E+00 | 0.00000000E+00 |

| | ALPHA | BETA | GAMMA | VOLUME |
|---|---|---|---|---|
| RECIPROCAL CELL | 90.00000 | 90.00000 | 90.00000 | 0.64541060E-02 |
| R C CORRECTIONS | 0.000 | 0.000 | 0.000 | -0.27357601E-08 |
| DIRECT CELL | 90.00000 | 90.00000 | 90.00000 | 0.15494013E+03 |
| D C CORRECTIONS | 0.000 | 0.000 | 0.000 | 0.66757202E-04 |

LARGEST RESIDUAL REDUCED TO UNIT WEIGHT 0.10418
OBS 1 STANDARD ERROR UNIT WT OBS 0.06381 DEGREES OF FREEDOM 3

| | | | |
|---|---|---|---|
| R C STNDRD ERRS | 0.12898331E-03 | 0.12898331E-03 | 0.12898331E-03 |
| | 0.000 | 0.000 | 0.000 |
| D C STNDRD ERRS | 0.37208555E-02 | 0.37208555E-02 | 0.37208555E-02 |
| | 0.000 | 0.000 | 0.000 |
| | 0.32201294E+00 | | |

URANINITE CUBIC SYSTEM TEST DATA
HKL LISTING - *** REFERS TO FIXED, R TO REJECTS CUBIC

| N | H | K | L | | D CALC | D OBS | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | | 5.3710 | | 16.50414 | | |
| 2 | 1 | 1 | 0 | | 3.7979 | | 23.42253 | | |
| 3 | 1 | 1 | 1 | | 3.1009 | 3.0900 | 28.78919 | 28.8934 | -0.10418 |
| 4 | 2 | 0 | 0 | | 2.6855 | 2.6860 | 33.36367 | 33.3572 | 0.00644 |
| 5 | 2 | 1 | 0 | | 2.4020 | | 37.43947 | | |
| 6 | 2 | 1 | 1 | | 2.1927 | | 41.16691 | | |
| 7 | 2 | 2 | 0 | | 1.8989 | 1.9000 | 47.90255 | 47.8740 | 0.02859 |
| 8 | 3 | 0 | 0 | | 1.7903 | | 51.00941 | | |
| 9 | 3 | 1 | 0 | | 1.6985 | | 53.98536 | | |
| 10 | 3 | 1 | 1 | | 1.6194 | 1.6200 | 56.85285 | 56.8305 | 0.02239 |
| 11 | 2 | 2 | 2 | R | 1.5505 | 1.5400 | 59.62945 | 60.0765 | -0.44704 |

```
DO YOU WANT TO ALTER VALUES IN THIS EXISTING DATA? YES
WHICH ONES?
LIST
TITLE:URANINITE   CUBIC SYSTEM TEST DATA
SYSTM:CUBIC
A    :  5.3700
THEMX: 61.0000
PWL  :  1.5418
DSPAC:  1      3.090   0   0   0
DSPAC:  2      2.686   0   0   0
DSPAC:  3      1.900   0   0   0
DSPAC:  4      1.620   0   0   0
DSPAC:  5      1.540   0   0   0


SAVE
IN FILE : CUB2


STOP
STOP

END OF EXECUTION
CPU TIME: 3.04  ELAPSED TIME: 5:32.72
EXIT
[3.31  114 43]
```

Program Listing

```
C      * * * * * * * * * * * * UNIT CELL PROGRAM * * * * * * * * * * * *
C                          U S GEOLOGICAL SURVEY
C                     GEOLOGIC DIVISION, DENVER, COLORADO
C                      MODIFIED BY GEORGE VAN TRUMP, JR.
C                              ON JAN  5, 1976
C      ------------------------------------------------------------------
C         THIS PROGRAM USES A LEAST SQUARE REFINEMENT WITH INDEXING FOR
C      UNIT CELL ANALYSIS.
C      ------------------------------------------------------------------
C
1           DIMENSION ICLASS(10),ICOND(10),JCLASS(27),JCOND(27),XO(3),
1          1 ICON1(10),IBUF(15),DEG(3)
2           NAMELIST/PARAM/AO,DEG,ITHT,THTMX,NCYC,TOLMN,TOLMX
2          1 /SYSEXT/THEMX,PWL,IOP,SEMULT
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
4          1 IAL1(16)
5           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
6           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
7           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
7          1 E(7),SUM,JA,ITHT,IRSD,MMN
8           COMMON/BLKD/TT(6,6),ST(6,6),SERCE(6),SEDCE(6),DD(3),VCME(6,6),
8          1 SS(21)
9           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
10          COMMON/BLKF/OBSTH(200),SW(200),WL(200),DSP(200),HG(200,3)
11          COMMON/BLKG/IHEAD(14),ICYCLE,IMN,MM,IALF12
12          COMMON/BLKI/Z(6)
13          COMMON/BLKJ/TOLMN
14          COMMON/BLKH/AA(7),DLST(200),THTMX,TOL,NCYC,IOC(200)
15          DATA ICLASS/ 3HHKL,3HHHL,3HOKL,3HHOL,3HHKO,3HHHO,3HHOO,3HOKO,
15         1 3HOOL,3HHLL/,ICOND /4H    H,4H    H,4H    K,4H H+K,4H-H+K,4H     ,
15         24H     ,4H     ,4H  2H,4H  H+/,ICON1/4H+K  ,4H+L  ,4H+L  ,4H+L  ,
15         34H+L  ,4H H  ,4H K  ,4H L  ,4H+L  ,4H2L  / ,IBLK/' '/,
15         4                JCLASS / 6*1,4*2,3*3,3*4,3*5,6,7,8,9,4*10 /,
15         5JCOND / 1,2,3,0,4,5,6,8,2,9,7,8,3,6,8,2,6,7,1,6,6,7,8,6,8,2,10 /
16          DATA IN,IUT/5,1/,IDEV/0/
17          CALL ACCUPD ('XRDCEL')
18          CALL ILL
19       90 IALT=0
20          TYPE 100
21      100 FORMAT (/' ENTER DATA INPUT FILE NAME(MAX 5 CHARS) : ',$)
22          ACCEPT 120,IFLE
23      120 FORMAT (A5)
24          IF (IFLE.EQ.'STOP') GO TO 760
25          IFLAG=0
26          IF (IFLE.NE.'?'.AND.IFLE.NE.' ') GO TO 130
27          IFLAG=1
28          GO TO 140
29      130 ISFILE='SCRAT'
```

```
30     140 IF (IFLAG.EQ.0)  OPEN (UNIT=5,DEVICE='DSKB:',ACCESS='SEQIN',
30        1 FILE=IFLE)
     C FIRST CARD OF DATA SET SHOULD BE A TITLE CARD
31     150 IF (IFLAG.EQ.0) READ (IN,160,END=760) ITES1,ITEST,IHEAD
32     160 FORMAT(A2,A4,14A5)
33         IF (IFLAG.NE.0) GO TO 190
34         IF (ITEST.EQ.IALF(9)) GO TO 190
35         TYPE 170,ITES1,ITEST,IAL1(9),IALF(9)
36     170 FORMAT(1H0,A2,A4,27H IN COLUMNS 1-6 INSTEAD OF ,A2,A4)
37     180 READ (IN,160,END=760) ITES1,ITEST,IHEAD
38         IF (ITEST.NE.IALF(9)) GO TO 180
39     190 TOLMX=0.0
40         TOLMN=0.0
41         THTMX=0.0
42         SEMULT=0.0
43         IF (IALT.EQ.1) GO TO 220
44         PWL=0.0
45         THEMX=0.0
46         DO 200 I=1,3
47         IDG(I)=0
48         FMN(I)=0.0
49     200 AO(I)=0.0
50         DO 210 I=1,27
51     210 IOP(I)=0
52     220 IF (IFLAG.EQ.1) GO TO 240
53         READ (IN,PARAM)
54         READ (IN,230,END=760) ICRYS1,ICRYST
55         READ (IN,SYSEXT)
56     230 FORMAT (A1,A4)
57         CALL SAVE1 (THEMX,DEG)
58         GO TO 250
59     240 CALL INTERA (DEG,THEMX,IALT,&760)
60     250 WRITE (IUT,260) IHEAD
61     260 FORMAT (///1X,14A5)
62         CALL PRMCHK(DEG)
63         IF (ITYP.GE.1.AND.ITYP.LE.7) GO TO 280
64         WRITE (IUT,270) ICRYS1,ICRYST
65     270 FORMAT(36HOCRYSTAL SYSTEM ON SYSEXT GIVEN AS  ,A1,A4)
66         GO TO 315
67     280 SUM=0.0
68         DO 290 L=1,3
69         IF (AO(L).LE.0.0) GO TO 300
70         CALL DGTODM(DEG(L),IDG(L),FMN(L))
71         ALO(L)=FLOAT(IDG(L))*60.0+FMN(L)
72         IF (ALO(L).LE.0.0.OR.ALO(L).GE.10800.0) GO TO 300
73     290 SUM=SUM+ALO(L)
74         IF (SUM.LT.21600.0) GO TO 320
75     300 TYPE 310,(AO(L),L=1,3),(DEG(L),L=1,3)
76     310 FORMAT(26HOGIVEN PARAMETERS IN ERROR,3F11.5,2X,3(F7.3))
```

```
77          IF (IFLAG.NE.0) GO TO 190
78      315 CALL RDHKL (IN,IFLAG,IALT)
79          GO TO 725
80      320 ITHT=MOD(ITHT,2)
81          IF (ITHT.NE.0) GO TO 330
82          THTMX=0.5*THTMX
83          TOLMN=0.5*TOLMN
84          TOLMX=0.5*TOLMX
85          THEMX=0.5*THEMX
86      330 IF (THTMX.LE.0.0) THTMX=20.0
87          IF (NCYC.LT.1) NCYC=2
88          IF (TOLMN.LE.0.0) TOLMN=0.02
89          IF (TOLMX.LE.TOLMN) TOLMX=5.0*TOLMN
90          IF (PWL.LE.0.0) PWL=1.54051
91          IF (SEMULT .LE. 0.0) SEMULT=2.0
92          IALF12=IALF(ITHT+14)
93          CALL OPSET
94          IMN=((N+3)*N)/2
95          DO 340 L=1,3
96          AD(L)=AO(L)
97          ALS(L)=ALO(L)
98          ARAD=0.00029088821*ALO(L)
99          CSA(L)=COS(ARAD)
100     340 SNA(L)=SIN(ARAD)
101         CALL RSCMP
102         DO 350 L=1,3
103         UO(L)=U(L)
104     350 XO(L)=X(L)
105         VRO=VR
106         VCO=VC
107         CALL DCPRN (IUT)
108         CALL RCPRN (IUT)
109         CALL RDHKL (IN,IFLAG,IALT)
110         MM=M
111         IF (M-1) 360,370,370
112     360 THEMXO=0.0
113         GO TO 380
114     370 THEMXO=OBSTH(M)+TOLMX
115     380 THEMX=AMAX1(THEMX,THEMXO)
116         IF (THEMX.LE.0.0.OR.THEMX.GT.90.0) THEMX=90.0
117         DMIN=0.5*PWL/SIN(  0.017453293*THEMX)
118         WRITE (IUT,390) THTMX,NCYC,TOLMN,TOLMX,THEMX,DMIN,ICRYS1,ICRYST
119     390 FORMAT(24H01-THETA ANGLES  THTMX =,F6.1,8H  NCYC =,I2,9H  TOLMN =,
119        1 F7.4,9H  TOLMX =,F7.4/15X,9H  THEMX =,F6.1,8H  DMIN =,F10.6,
119        2 2X,A1,A4,7H SYSTEM)
120         WRITE (IUT,400) NOPT
121     400 FORMAT(1HO,I2,41H CONDITIONS FOR NON-EXTINCTION CALLED FOR,5X,
121        1 18HCLASS CONDITION(S))
122         IF (NOPT .LT. 1) GO TO 450
```

```
      DO 440 L=1,NOPT
      J=JOP(L)
      I=JCLASS(J)
      K=JCOND(J)
      IF (K .GE. 1 .AND. K .LE. 10) GO TO 420
      WRITE (IUT,410) IOP(J),IOP(J),IOP(J)
  410 FORMAT(50X,3HHKL,5X,4HH+K=,I1,6HN,H+L=,I1,6HN,K+L=,I1,1HN)
      GO TO 440
  420 WRITE (IUT,430) ICLASS(I),ICOND(K),ICON1(K),IOP(J)
  430 FORMAT(50X,A5,A4,A2,1H=,I1,1HN)
  440 CONTINUE
  450 CALL HKLGEN (IUT)
      CALL SORTD(NR,DCM,HH,H)
      CALL SKWEZE
      TOL=TOLMX
      ICYCLE=0
  460 OPEN (UNIT=20,DEVICE='DSKB:',ACCESS='SEQINOUT',FILE=ISFILE,
     1 DISPOSE='DELETE')
      CALL SLCR
      IF (MM .LT. N) GO TO 480
      MMN=M-N
      IF (MMN) 470,530,500
  470 IF ((ICYCLE.GE.10).OR.(ICYCLE.GT.NCYC.AND.TOL.LE.TOLMN))GO TO 480
      TOL=0.5*TOL
      IF (TOL .LT. TOLMN) TOL=TOLMN
      NCYC=0
      REWIND 20
      GO TO 460
  480 WRITE (20,490)
  490 FORMAT(12HONO SOLUTION )
      GO TO 700
  500 CONTINUE
  510 FORMAT (14A5,A1)
      J=N+1
      K=J
      DO 520 I=1,N
      AA(I)=A(K)
      J=J-1
  520 K=K+J
  530 CALL PDSQRT(A,N,B,IERR)
      IF (IERR .EQ. 0) GO TO 550
      WRITE (20,540) IERR
  540 FORMAT(38HOSINGULAR NORMAL EQUATION MATRIX - ROW,I2,
     1 36H LINEARLY DEPENDENT ON PREVIOUS ROWS )
      GO TO 470
  550 CALL COORD
      DO 630 J=1,3
      X(J)=X(J)+CR(J)
      U(J)=U(J)+CR(J+3)
```

```
      IF (X(J)) 560,560,580
  560 WRITE (20,570) J
  570 FORMAT(40HOCORRECTED VALUE OF RECIPROCAL CELL EDGE,I2,
     1 27H LESS THAN OR EQUAL TO ZERO )
      GO TO 610
  580 IF (ABS(U(J))-1.0) 630,590,590
  590 WRITE (20,600) J
  600 FORMAT(42HOCORRECTED VALUE OF RECIPROCAL CELL COSINE,I2,
     1 36H EQUALS OR EXCEEDS 1.0 IN ABS VALUE )
  610 DO 620 K=1,J
      X(K)=X(K)-CR(K)
  620 U(K)=U(K)-CR(K+3)
      GO TO 470
  630 CONTINUE
      CALL CMPNUP
      IF (MMN .GT. 0) GO TO 650
      TOL=0.5*TOL
      GO TO 670
  650 DO 660 I=1,N
  660 SUM=SUM-AA(I)*B(I)
      IF (SUM .LT. 0.0) SUM=0.0
      THTSE=SQRT(SUM/FLOAT(MMN))
      CALL RSDPRN
      TOL=SEMULT*THTSE
  670 IF (TOL .LT. TOLMN) TOL=TOLMN
      IF (TOL .GT. TOLMX) TOL=TOLMX
      IF (ICYCLE .LE. NCYC) GO TO 750
      CRMAX=0.0
      DO 680 I=1,N
  680 IF (ABS( B(I)) .GT. CRMAX) CRMAX=ABS( B(I))
      IF (CRMAX .GE. 0.5E-6) GO TO 730
  690 IF (MMN .GT. 0) CALL SESUB
  700 CONTINUE
      REWIND 20
  710 READ (20,510,END=720) IBUF
      WRITE (IUT,510)IBUF
      GO TO 710
  720 CONTINUE
      CALL FNLST (IUT)
  725 CALL FIX (THEMX,IALT,IFLG,IDEV,IUT)
      IFLAG=1
      IF (IFLG) 90,760,150
  730 IF (ICYCLE .LT. 10) GO TO 750
      WRITE (IUT,740)
  740 FORMAT(28HONOT CONVERGENT IN 10 CYCLES)
      GO TO 690
  750 CALL RCMPD
      CALL SORTD(NR,DCM,HH,H)
      REWIND 20
```

```
      GO TO 460
  760 STOP
      END
```

```
1           SUBROUTINE BUILD (DEG,THEMX,ITYPE,DDS,OBSS,IHS,WLCS,NO)
    C       THIS ROUTINE IS USED AN OUTPUT FILE OF THE INPUT INFO ENTERED
    C       THROUGH TIME SHARING.
2           DIMENSION DEG(3),DDS(200),OBSS(200),IHS(200,3),BUF1(16),BUF2(80),
2          1 NAME(2),WLCS(200)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
5           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
5          1 E(7),SUM,JA,ITHT,IRSD,MMN
6           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
7           COMMON/BLKG/IHEAD(14),ICYCLE,IMN,MM,IALF12
8           DATA IT/4/,NAME/'D  =','OBS='/
9           TYPE 100
10     100  FORMAT (' IN FILE : ',$)
11          ACCEPT 110,FNAME
12     110  FORMAT (A5)
13          OPEN (UNIT=IT,DEVICE='DSKB:',ACCESS='SEQOUT',FILE=FNAME)
14          WRITE (IT,120) IHEAD
15     120  FORMAT ('TITLE ',14A5)
16          GO TO (130,150,170,190,150,210,230),ITYP
17     130  WRITE (IT,140) AO(1)
18     140  FORMAT (' $PARAM AO(1)=',F6.3,'$')
19          GO TO 250
20     150  WRITE (IT,160) AO(1),AO(3)
21     160  FORMAT (' $PARAM AO(1)=',F6.3,',AO(3)=',F6.3,'$')
22          GO TO 250
23     170  WRITE (IT,180) AO
24     180  FORMAT (' $PARAM AO=',F6.3,' , ',F6.3,' , ',F6.3,'$')
25          GO TO 250
26     190  WRITE (IT,200) AO,DEG(2)
27     200  FORMAT (' $PARAM AO=',F6.3,' , ',F6.3,' , ',F6.3,
27         1 ', DEG(2)=',F7.3,'$')
28          GO TO 250
29     210  WRITE (IT,220) AO,DEG
30     220  FORMAT (' $PARAM AO=',F6.3,' , ',F6.3,' , ',F6.3,
30         1 ', DEG=',F7.3,' , ',F7.3,' , ',F7.3,'$')
31          GO TO 250
32     230  WRITE (IT,240) AO(1),DEG(1)
33     240  FORMAT (' $PARAM AO(1)=',F6.3,',DEG(1)=',F7.3,'$')
34     250  WRITE (IT,260) ICRYS1,ICRYST
35     260  FORMAT (A1,A4,'$')
36          ENCODE (34,270,BUF1) THEMX,PWL
37     270  FORMAT (' $SYSEXT THEMX=',F7.3,',PWL=',F7.5,',')
38          DECODE (35,280,BUF1) (BUF2(I),I=1,35)
39     280  FORMAT (80A1)
40          LAST=35
41          DO 320 I=1,27
42          IF (IOP(I).EQ.0) GO TO 320
43          LAST=LAST+1
```

```
      IF (LAST.LE.69) GO TO 300
      WRITE (IT,280) (BUF2(J),J=1,LAST-1)
      DO 290 J=1,80
      IF (J.LE.16) BUF1(J)=' '
  290 BUF2(J)=' '
      LAST=2
  300 ENCODE (11,310,BUF1) I,IOP(I)
  310 FORMAT (',IOP(',I2,')=',I2)
      DECODE (11,280,BUF1) (BUF2(J),J=LAST,LAST+10)
      LAST=LAST+11
  320 CONTINUE
      BUF2(LAST)='$'
      WRITE (IT,280) (BUF2(I),I=1,LAST)
      DO 430 I=1,NO
      N=1
      IF (ITYPE.EQ.0) X=DDS(I)
      IF (ITYPE.NE.0) X=OBSS(I)
      DO 330 J=3,1,-1
      IF (IHS(I,J).EQ.0) GO TO 330
      N=J+1
      GO TO 340
  330 CONTINUE
  340 GO TO (350,410,410,410),N
  350 IF (WLCS(I).EQ.0.0) WRITE (IT,360) NAME(ITYPE+1),X
      IF (WLCS(I).NE.0.0) WRITE (IT,365) NAME(ITYPE+1),X,WLCS(I)
  360 FORMAT (' $DATA ',A4,F7.3,'$')
  365 FORMAT (' $DATA ',A4,F7.3,', WLC =',F8.5,'$')
      GO TO 428
  410 IF (WLCS(I).EQ.0.0) WRITE (IT,420)NAME(ITYPE+1),X,(IHS(I,J),J=1
     1,3)
      IF (WLCS(I).NE.0.0) WRITE (IT,425)NAME(ITYPE+1),X,(IHS(I,J),J=1
     1,3),WLCS(I)
  420 FORMAT (' $DATA ',A4,F7.3,',IH=',I2,',',I2,',',I2,'$')
  425 FORMAT (' $DATA ',A4,F7.3,',IH=',I2,',',I2,',',I2,', WLC =',F8.5,
     1 '$')
  428 PWLAST=WLCS(I)
  430 CONTINUE
      WRITE (IT,440)
  440 FORMAT (' $DATA ITEST=2$')
      CLOSE (UNIT=IT)
      RETURN
      END
```

CHKEXT SUBROUTINE

```
1           SUBROUTINE CHKEXT(IH,IK,IL,JEXT)
      C CHECKS MILLER INDICES IH,IK,IL FOR EXTINCTIONS - JEXT SET TO 1
      C IF CURRENT REFLECTION NOT ACCEPTABLE, JEXT SET TO 0 IF IT IS
2           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
2          1 IAL1(16)
3           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
4           JEXT=0
5           DO 130 I=1,NOPT
6           L=JOP(I)
7           IDIV=IOP(L)
8           DO 100 J=1,2
9           IFIJ=IFI(J,L)
10          IF (IFIJ.LT.1.OR.IFIJ.GT.6) GO TO 110
11          IANS=IH*IHKL(IFIJ,1)+IK*IHKL(IFIJ,2)+IL*IHKL(IFIJ,3)
12          IF (IANS.NE.0) GO TO 130
13     100  CONTINUE
14     110  DO 120 K=1,3
15          IFJK=IFJ(K,L)
16          IF (IFJK.LT.1.OR.IFJK.GT.10) GO TO 130
17          IARG=JHKL(IFJK,1)*IH+JHKL(IFJK,2)*IK+JHKL(IFJK,3)*IL
18          IF (MOD(IARG,IDIV).EQ.0) GO TO 120
19          JEXT=1
20          GO TO 140
21     120  CONTINUE
22     130  CONTINUE
23     140  RETURN
24          END
```

```
      SUBROUTINE CMPNUP
C COMPUTES DIRECT CELL PARAMETERS FROM CORRECTED RECIPROCAL CELL
      COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
      COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
      COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
      DIMENSION UOSV(3),FMSV(3),IDGSV(3),FFMN(3),DEG(3)
      WRITE (20,100)
  100 FORMAT (1HO,24X,1HA,15X,1HB,15X,1HC)
      DO 110 J=1,3
      UO(J)=AR(J)
      W(J)=SQRT(1.0-U(J)**2)
      AR(J)=3437.7468*(1.5707963-ATAN2(U(J),W(J)))
      CALL MTDM(AR(J),IDG(J),FMN(J))
  110 UO(J)=AR(J)-UO(J)
      VRO=VR
      VR=SQRT(1.0-U(1)**2-U(2)**2-U(3)**2+2.0*U(1)*U(2)*U(3))*X(1)*X(2)
     1*X(3)
      VRD=VR-VRO
      WRITE (20,130) (X(I),I=1,3)
      DO 120 I=1,3
      UOSV(I)=UO(I)
      IDGSV(I)=IDG(I)
  120 FMSV(I)=FMN(I)
  130 FORMAT(16H RECIPROCAL CELL,1X,3E16.8)
      WRITE (20,140) (CR(J),J=1,3)
  140 FORMAT(16H R C CORRECTIONS,1X,3E16.8)
      DO 170 I=1,3
      J=MOD(I,3)+1
      K=MOD(J,3)+1
      AO(I)=AD(I)
      AD(I)=X(J)*X(K)*W(I)/VR
      ALO(I)=ALS(I)
      IF (ITYP .GT. 5) GO TO 150
      IF (I .EQ. 2 .AND. ITYP .EQ. 4) GO TO 150
      IF (I .EQ. 3 .AND. ITYP .EQ. 2) GO TO 150
      CSA(I)=0.0
      GO TO 160
  150 CSA(I)=(U(J)*U(K)-U(I))/(W(J)*W(K))
  160 ALS(I)=3437.7468*(1.5707963-ATAN2(CSA(I),SQRT(1.0-CSA(I)**2)))
  170 CALL MTDM(ALS(I),IDG(I),FMN(I))
      VCO=VC
      VC=1.0/VR
      WRITE (20,180) (AD(I),I=1,3)
  180 FORMAT(16H      DIRECT CELL,1X,3E16.8)
      DO 190 L=1,3
      FFMN(L)=AD(L)-AO(L)
  190 UO(L)=ALS(L)-ALO(L)
      VCD=VC-VCO
      WRITE (20,200) (FMN(L),L=1,3)
```

```
      200 FORMAT(16H D C CORRECTIONS,1X,3E16.8)
          WRITE (20,210)
      210 FORMAT (//24X,5HALPHA,8X,4HBETA,7X,5HGAMMA,10X,6HVOLUME)
      220 FORMAT (16H RECIPROCAL CELL,1X,3(F12.5),E18.8)
      230 FORMAT (16H R C CORRECTIONS,1X,3F12.3,E18.8)
      240 FORMAT (16H      DIRECT CELL,1X,3(F12.5),E18.8)
      250 FORMAT (16H D C CORRECTIONS,1X,3F12.3,E18.8)
          DO 253 I=1,3
      253 CALL DMTODG(DEG(I),IDGSV(I),FMSV(I))
          WRITE (20,220) DEG,VR
          WRITE (20,230) UOSV,VRD
          DO 256 I=1,3
      256 CALL DMTODG(DEG(I),IDG(I),FMN(I))
          WRITE (20,240) DEG,VC
          DO 260 I=1,3
      260 FMN(I)=FFMN(I)
          WRITE (20,250) UO,VCD
          RETURN
          END
```

```
1           SUBROUTINE COORD
      C COMPUTES CORRECTIONS TO RECIPROCAL CELL ELEMENTS
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           GO TO (100,120,150,170,190,220,240),ITYP
6       100 DO 110 J=1,3
7           CR(J)=B(1)
8       110 CR(J+3)=0.0
9           GO TO 260
10      120 DO 130 J=1,2
11      130 CR(J)=B(1)
12          CR(3)=B(2)
13          DO 140 J=4,6
14      140 CR(J)=0.0
15          GO TO 260
16      150 DO 160 J=1,3
17          CR(J)=B(J)
18      160 CR(J+3)=0.0
19          GO TO 260
20      170 DO 180 J=1,3
21      180 CR(J)=B(J)
22          CR(4)=0.0
23          CR(5)=B(4)
24          CR(6)=0.0
25          GO TO 260
26      190 DO 200 J=1,2
27      200 CR(J)=B(1)
28          CR(3)=B(2)
29          DO 210 J=4,6
30      210 CR(J)=0.0
31          GO TO 260
32      220 DO 230 J=1,6
33      230 CR(J)=B(J)
34          GO TO 260
35      240 DO 250 J=1,3
36          CR(J)=B(1)
37      250 CR(J+3)=B(2)
38      260 RETURN
39          END
```

```
1           SUBROUTINE DCPRN (IUT)
      C PRINTS OUT DIRECT CELL ELEMENTS
2           DIMENSION DEG(3)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
5           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
6           DO 100 L=1,3
7           CALL MTDM(ALS(L),IDG(L),FMN(L))
8       100 CALL DMTODG(DEG(L),IDG(L),FMN(L))
9           WRITE (IUT,110) AD,DEG,VC
10      110 FORMAT(//16H      DIRECT CELL,3E16.8/16X,3F16.5/14X,E18.8)
11          RETURN
12          END
```

DLQOT SUBROUTINE

```
1           SUBROUTINE DLQOT
      C COMPUTES PARTIAL DERIVATIVES OF RECIPROCAL OF D SQUARED
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           DO 100 J=1,3
6           K=MOD(J,3)+1
7           L=MOD(K,3)+1
8           B(J)=FAC*(X(J)*H(J)**2+H(J)*H(L)*X(L)*U(K)+H(J)*H(K)*X(K)*U(L))
9       100 B(J+3)=FAC*H(K)*H(L)*X(K)*X(L)
10          RETURN
11          END
```

```
1           SUBROUTINE DGTODM(DEG,IDG,FM)
      C     CONVERTS DECIMAL DEGREES TO DEGREES AND MINUTES.
2           IDG=DEG
3           FM=60.0*(DEG-IDG)
4           RETURN
5           END
```

```
1           SUBROUTINE DMTODG(DEG,IDG,FM)
      C     CONVERTS DEGREES AND MINUTES TO DECIMAL DEGREES.
2           DEG=IDG+FM/60.0
3           RETURN
4           END
```

FILL SUBROUTINE

```
1           SUBROUTINE FILL (SUB,DD,IH1,IH2,IH3,WLC,NO,DDS,IHS,WLCS)
2           DIMENSION IH(3),DDS(200),IHS(200,3),WLCS(200)
3        90 ISUB=SUB+0.1
4           IH(1)=IH1
5           IH(2)=IH2
6           IH(3)=IH3
7           IF (ABS(SUB-ISUB).GT.0.1) GO TO 160
8           IF (ISUB.LE.NO) GO TO 120
9           NO=NO+1
10          IP=NO
11       100 DDS(IP)=DD
12          WLCS(IP)=WLC
13          DO 110 I=1,3
14       110 IHS(IP,I)=IH(I)
15          GO TO 180
16       120 IF (DD.LE.0.0) GO TO 130
17          IP=ISUB
18          GO TO 100
19       130 DO 140 I=ISUB+1,NO
20          WLCS(I-1)=WLCS(I)
21          DDS(I-1)=DDS(I)
22          DO 140 J=1,3
23       140 IHS(I-1,J)=IHS(I,J)
24          WLCS(NO)=0.0
25          DDS(NO)=0.0
26          DO 150 I=1,3
27       150 IHS(NO,I)=0
28          NO=NO-1
29          GO TO 180
30       160 IP=ISUB+1
31          DO 170 I=NO,IP,-1
32          WLCS(I+1)=WLCS(I)
33          DDS(I+1)=DDS(I)
34          DO 170 J=1,3
35       170 IHS(I+1,J)=IHS(I,J)
36          NO=NO+1
37          GO TO 100
38       180 RETURN
39          END
```

```
1           SUBROUTINE FNLST (IUT)
      C LISTS THEORETICAL REFLECTIONS IN DESCENDING ORDER FOR D-SPACING
      C REFLECTIONS WITH FIXED MILLER INDICES INDICATED BY ***
2           DIMENSION IH(3),JH(3)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
4          1 IAL1(16)
5           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
5          1 E(7),SUM,JA,ITHT,IRSD,MMN
6           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
7           COMMON/BLKF/OBSTH(200),SW(200),WL(200),DSP(200),HG(200,3)
8           COMMON/BLKG/IHEAD(14),ICYCLE,IMN,MM,IALF12
9           COMMON/BLKH/AA(7),DLST(200),THTMX,TOL,NCYC,IOC(200)
10          WRITE (IUT,100) IHEAD,ICRYS1,ICRYST
11     100  FORMAT (///1X,14A5/35H HKL LISTING - *** REFERS TO FIXED,,
11         1 2X,13HR TO REJECTS ,A1,A4)
12          WL1=PWL
13          I2=0
14          IF (MM .LT. 1) GO TO 110
15          WL1=WL(1)
16          I2=IABS(IOC(1))
17          D1=DSP(1)
18     110  WL2=WL1
19          IF (NR .LT. 1) GO TO 120
20          D1=DCM(1)
21     120  D2=D1
22          IGP=1
23          IHP=1
24          WRITE (IUT,130) IALF12,IALF12,IALF12
25     130  FORMAT(4HO  N,5X,1HH,1X,1HK,1X,1HL,4X,6HD CALC,4X,5HD OBS,2X,
25         1    A2,10HTHETA CALC,1X,A2,9HTHETA OBS,1X,A2,
25         2 10HTHETA DIFF)
26     140  IF (IHP .LE. NR) GO TO 150
27          IF (IGP .GT. MM) GO TO 320
28          GO TO 190
29     150  DO 160 L=1,3
30     160  IH(L)=IFIX(HH(IHP,L)+SIGN(0.5,HH(IHP,L)))
31          D=DCM(IHP)
32          IF (IHP .EQ. I2) GO TO 190
33          WLC=WL1
34          IF (ABS(D-D2) .LT. ABS(D1-D)) WLC=WL2
35          THCMP=THETA(0.5*WLC,D)
36          IF (ITHT .EQ. 0) THCMP=THCMP+THCMP
37          WRITE (IUT,170) IHP,(IH(L),L=1,3),D,THCMP
38     170  FORMAT (1H ,I3,4X,3I2,F10.4,9X,F12.5)
39     180  IHP=IHP+1
40          GO TO 140
41     190  DO 200 L=1,3
42     200  JH(L)=IFIX(HG(IGP,L)+SIGN(0.5,HG(IGP,L)))
```

```
      DF=DLST(IGP)
      WT=SW(IGP)**2
      DOBS=DSP(IGP)
      THOBS=OBSTH(IGP)
      WLC=WL(IGP)
      THCLC=THETA(0.5*WLC,DF)
      DIFF=THCLC-THOBS
      IF (ITHT .NE. 0) GO TO 210
      THCLC=THCLC+THCLC
      THOBS=THOBS+THOBS
      DIFF=DIFF+DIFF
  210 JA=IALF(15)
      IF (IOC(IGP) .LT. 0) JA=IALF(16)
      IF (JH(1).NE.0.OR.JH(2).NE.0.OR.JH(3).NE.0) GO TO 260
      WRITE (IUT,220) IHP,(IH(L),L=1,3),JA,DF,DOBS,    THCLC,THOBS,DIFF
  220 FORMAT(1H ,I3,4X,3I2,A2,F8.4,F9.4,F12.5,F12.4,F12.5)
  230 IGP=IGP+1
      D1=D2
      WL1=WL2
      IF (IGP-MM) 240,240,250
  240 IF (IABS(IOC(IGP)) .EQ. I2) GO TO 190
      I2=IABS(IOC(IGP))
      D2=DCM(I2)
      WL2=WL(IGP)
      GO TO 180
  250 I2=0
      GO TO 180
  260 THCMP=THETA(0.5*WLC,D)
      IF (ITHT .EQ. 0) THCMP=THCMP+THCMP
      IF (IGP .LT. 2) GO TO 290
      IF (IABS(IOC(IGP-1)) .NE. I2) GO TO 290
  270 WRITE (IUT,280) (JH(L),L=1,3),JA,DF,DOBS,    THCLC,THOBS,DIFF
  280 FORMAT(4H ***,4X,3I2,A2,F8.4,F9.4,F12.5,F12.4,F12.5)
      GO TO 230
  290 IF (DLST(IGP)-D) 300,300,310
  300 WRITE (IUT,170) IHP,(IH(L),L=1,3),D,THCLC
      GO TO 270
  310 WRITE (IUT,280) (JH(L),L=1,3),JA,DF,DOBS,    THCLC,THOBS,DIFF
      WRITE (IUT,170) IHP,(IH(L),L=1,3),D,THCLC
      GO TO 230
  320 RETURN
      END
```

```
1           SUBROUTINE HKLGEN (IUT)
      C GENERATES MILLER INDICES CORRESPONDING TO PLANES AT DISTANCES FROM
      C DMIN ON UP - MAXIMUM OF 700 REFLECTIONS MAY BE GENERATED
2           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
2          1 IAL1(16)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
5           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
6           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
6          1 E(7),SUM,JA,ITHT,IRSD
7           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
8           COMMON/BLKI/Z(6)
9           QMAX=1.0/(DMIN*DMIN)
10          NR=0
11          DO 100 I=1,3
12          J=MOD(I,3)+1
13          K=MOD(J,3)+1
14          Z(I)=X(I)**2
15     100  Z(I+3)=X(I)*X(J)*U(K)
16          E(1)=Z(1)
17          E(2)=Z(2)
18          E(3)=Z(4)
19          TD=E(1)*E(2)-E(3)*E(3)
20          IL=0
21     110  H(3)=IL
22          E(4)=(Z(5)+Z(5))*H(3)
23          E(5)=(Z(6)+Z(6))*H(3)
24          E(6)=Z(3)*H(3)*H(3)-QMAX
25          TN=E(3)*E(5)-E(1)*E(4)
26          DSCRS=TN*TN-(4.0*E(1)*E(6)-E(5)*E(5))*TD
27          IF (DSCRS.LT.0.0) GO TO 270
28          DSCRM=SQRT(DSCRS)
29          IK1=IFIX((TN-DSCRM)*0.5/TD)
30          IK2=IFIX((TN+DSCRM)*0.5/TD)
31          GO TO (120,130,130,130,130,140,140,130),JTYP
32     120  IF (IK1.LT.    IL) IK1=    IL
33          GO TO 140
34     130  IF (IK1.LT.0) IK1=0
35     140  IK=IK2
36          IF (IK .LT. IK1) GO TO 260
37     150  H(2)=IK
38          GT=(E(3)+E(3))*H(2)+E(5)
39          HT=(Z(5)*H(3)+Z(2)*H(2))*H(2)+(Z(5)*H(2)+Z(3)*H(3))*H(3)-QMAX
40          DEN=Z(1)+Z(1)
41          DSCRS=GT*GT-(DEN+DEN)*HT
42          IF (DSCRS.LT.0.0) GO TO 250
43          DSCRM=SQRT(DSCRS)
44          IH1=IFIX(-(GT+DSCRM)/DEN)
45          IH2=IFIX((DSCRM-GT)/DEN)
```

```
      GO TO (180,180,170,190,180,190,190,160),JTYP
160   IF (MOD(IL,3).EQ.0) GO TO 180
170   IF (IH1.LT.0) IH1=0
      GO TO 190
180   IF (IH1.LT.IK) IH1=IK
190   IH=IH2
      IF (IH .LT. IH1) GO TO 250
200   H(1)=IH
      IF (NOPT.LT.1) GO TO 210
      CALL CHKEXT(IH,IK,IL,JEXT)
      IF (JEXT.NE.0) GO TO 240
210   CALL QCOMP
      IF (Q.LE.0.0) GO TO 240
      NR=NR+1
      DCM(NR)=1.0/SQRT(Q)
      DO 220 J=1,3
220   HH(NR,J)=H(J)
      IF (NR.LT.700) GO TO 240
      CALL SORTD(NR,DCM,HH,FMN)
      CALL SKWEZE
      IF (NR.LT.700) GO TO 240
      WRITE (IUT,230) DMIN
230   FORMAT(43HOMORE THAN 700 REFLECTIONS EXIST FOR DMIN =,F10.5)
      GO TO 270
240   IH=IH-1
      IF (IH.GE.IH1)  GO TO 200
250   IK=IK-1
      IF (IK.GE.IK1) GO TO 150
260   IL=IL+1
      GO TO 110
270   RETURN
      END
```

HKLPR SUBROUTINE

```
1           SUBROUTINE HKLPR
      C PRINTS H,K,L,CALCULATED AND OBSERVED D-S AND THETAS
2           DIMENSION IH(3)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
5          1 E(7),SUM,JA,ITHT,IRSD,MMN
6           WT=SWT*SWT
7           TC=THCMP
8           OB=THOBS
9           TD=DIFF
10          IF (ITHT.NE.0) GO TO 100
11          TC=TC+TC
12          OB=OB+OB
13          TD=TD+TD
14      100 DO 110 L=1,3
15      110 IH(L)=IFIX(H(L)+SIGN(0.5,H(L)))
16          WRITE (20,120) M,(IH(L),L=1,3),JA,D,DOBS     ,TC,OB,TD
17      120 FORMAT(I4,4X,3I2,A2,F8.4,F9.4,F12.5,F12.4,F12.5)
18          RETURN
19          END
```

```
      SUBROUTINE INTERA (DEG,THEMX,IALT,*)
      DIMENSION NAMCRY(8),IH(3),DDS(200),OBSS(200),IHS(200,3),IDAT(16)
     1 ,NAMES(17),AOS(3),IDGS(3),FMNS(3),DEG(3),DEGS(3),IOPS(27),
     2 WLCS(200)
      COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
      COMMON /BLKA/ FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
      COMMON /BLKC/ THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
     1 E(7),SUM,JA,ITHT,IRSD,MMN
      COMMON /BLKE/ DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
      COMMON/BLKF/OBSTH(200),SW(200),WL(200),DSP(200),HG(200,3)
      COMMON /BLKG/ IHEAD(14),ICYCLE,IMN,MM,IALF12
      DATA NAMCRY/'UBIC','ETRA','EXAG','EXAR','RTHO','ONOC','RICL',
     1 'HOMB'/
      DATA NAMES/'TITLE','SYSTM','A','B','C','ALPHA','BETA ',
     1 'GAMMA','THEMX','PWL','IOP','DSPAC','2THET','START','SAVE',
     2 'STOP','TTYNO'/
      ICOME=0
      IF (IALT.EQ.1) GO TO 450
   90 TYPE 100
  100 FORMAT (//' TITLE : ',$)
      ACCEPT 110,IHEAD
  110 FORMAT (14A5)
      IF (IHEAD(1).EQ.' '.OR.IHEAD(1).EQ.'STOP') RETURN 1
  120 TYPE 130
  130 FORMAT (/' CRYSTAL SYSTEM : ',$)
      ACCEPT 140,ICRYS1,ICRYST
  140 FORMAT (A1,A4)
  150 DO 160 I=1,8
  160 IF (ICRYST.EQ.NAMCRY(I)) GO TO 180
      TYPE 170
  170 FORMAT (5X,'ERROR---BAD CRYSTAL SYSTEM.  TRY AGAIN.')
      IF (ICOME.EQ.1) GO TO 700
      GO TO 120
  180 TYPE 190
  190 FORMAT (/' ENTER VALUES IN ORDER REQUESTED.  SEPARATE BY COMMAS.')
      CALL PRMCHK(DEG)
      DO 200 I=1,3
      AO(I)=0.0
      IDG(I)=0
  200 FMN(I)=0
      GO TO (210,240,260,280,240,300,315),ITYP
  210 TYPE 220
  220 FORMAT (' ENTER A : ',$)
      ACCEPT 230,AO(1)
  230 FORMAT (9G)
      GO TO 320
  240 TYPE 250
  250 FORMAT (' ENTER A,C : ',$)
      ACCEPT 230,AO(1),AO(3)
```

```
      GO TO 320
  260 TYPE 270
  270 FORMAT (' ENTER A,B,C : ',$)
      ACCEPT 230,(AO(I),I=1,3)
      GO TO 320
  280 TYPE 290
  290 FORMAT (' ENTER A,B,C,BETA : ',$)
      ACCEPT 230,(AO(I),I=1,3),DEG(2)
      GO TO 320
  300 TYPE 310
  310 FORMAT (' ENTER A,B,C,ALPHA,BETA,GAMMA : ')
      ACCEPT 230,(AO(I),I=1,3),DEG
      GO TO 320
  315 TYPE 316
  316 FORMAT (' ENTER A,ALPHA : ',$)
      ACCEPT 230,AO(1),DEG(1)
  320 IF (ICOME.EQ.1) GO TO 590
      TYPE 340
  340 FORMAT (/' ENTER MAX 2-THETA VALUE TO BE CALCULATED : ',$)
      ACCEPT 230,THEMX
      IF (THEMX.GT.0.0.AND.THEMX.LE.180.0) GO TO 360
      TYPE 350
  350 FORMAT (5X,'ERROR---BAD VALUE.  TRY AGAIN.')
      GO TO 320
  360 TYPE 370
  370 FORMAT (/' ENTER WAVE LENGTH OF TARGET : ',$)
      ACCEPT 230,PWL
      TYPE 380
  380 FORMAT (/' ARE THERE CONDITIONS FOR NON-EXTINCTION? (YES,NO) ',$)
      ACCEPT 390,ANS
  390 FORMAT (A1)
      IF (ANS.NE.'Y') GO TO 450
      TYPE 400
  400 FORMAT (' WHAT ARE THEY?  TERMINATE THIS ENTRY WITH "0".'/
     1 ' FIRST : ',$)
  410 ACCEPT 230,ISUB,IVAL
      IF (ISUB.EQ.0) GO TO 450
      IF (ISUB.GE.1.AND.ISUB.LE.27) GO TO 430
      TYPE 350
      TYPE 420
  420 FORMAT (' AGAIN : ',$)
      GO TO 410
  430 IOP(ISUB)=IVAL
      TYPE 440,ISUB,IVAL
  440 FORMAT (5X,'IOP(',I2,')=',I2,/' NEXT  : ',$)
      GO TO 410
      ENTRY SAVE1 (THEMX,DEG)
  450 DO 330 I=1,3
      DEGS(I)=DEG(I)
```

```
      AOS(I)=AO(I)
      IDGS(I)=IDG(I)
  330 FMNS(I)=FMN(I)
      THEMXS=THEMX
      PWLS=PWL
      DO 455 I=1,27
  455 IOPS(I)=IOP(I)
      RETURN
C
C     ------------------------------------------------------------------
C
      ENTRY INTVAL (MMM,ITEST,IH,DD,OBS,WLC,WT)
      IF (MMM.GT.0) GO TO 470
      NO=0
      ITYPE=0
      TYPE 460
  460 FORMAT (/' IS DATA 2-THETA? (YES,NO) ',$)
      ACCEPT 390,ANS
      IF (ANS.EQ.'Y') ITYPE=1
  470 NO=NO+1
      IF (ITYPE.NE.0) GO TO 510
      IF (MMM.EQ.0) TYPE 480
  480 FORMAT (/' ENTER D-SPACING, H K L, & WLC VALUES.  TERMINATE ENTRY
     1WITH "0" FOR SPACING.')
      TYPE 490,NO
  490 FORMAT (' NO. ',I3,4X,$)
      ACCEPT 230,DD,IH,WLC,WT
      DDS(NO)=DD
      WLCS(NO)=WLC
      DO 500 I=1,3
  500 IHS(NO,I)=IH(I)
      IF (DD.EQ.0.0) ITEST=2
      GO TO 540
  510 IF (MMM.EQ.0) TYPE 520
  520 FORMAT (/' ENTER 2-THETA, H K L, & WLC VALUES.  TERMINATE ENTRY WI
     1TH "0" FOR 2-THETA.')
      TYPE 490,NO
      ACCEPT 230,OBS,IH,WLC,WT
      OBSS(NO)=OBS
      WLCS(NO)=WLC
      DO 530 I=1,3
  530 IHS(NO,I)=IH(I)
      IF (OBS.EQ.0.0) ITEST=2
  540 IF (ITEST.EQ.2) NO=NO-1
      RETURN
      ENTRY SAVE2 (IKDATA)
      ITYPE=IKDATA
      NO=M
      DO 545 I=1,NO
```

```
      WLCS(I)=WL(I)
      DDS(I)=DSP(I)
      OBSS(I)=2.0*OBSTH(I)
      DO 545 J=1,3
  545 IHS(I,J)=HG(I,J)+SIGN(0.0001,HG(I,J))
      RETURN
C
C     ------------------------------------------------------------------
C
      ENTRY FIX (THEMX,IALT,IFLG,IDEV,IUT)
      IFLG=-1
      IALT=0
      TYPE 550
  550 FORMAT (///,' DO YOU WANT TO ALTER VALUES IN THIS EXISTING DATA? '
     1,$)
      ACCEPT 390,ANS
      IF (ANS.EQ.'Y') GO TO 560
      RETURN
  560 IALT=1
      IFLG=1
      THEMX=THEMXS
      PWL=PWLS
      DO 570 I=1,3
      DEG(I)=DEGS(I)
      AO(I)=AOS(I)
      IDG(I)=IDGS(I)
  570 FMN(I)=FMNS(I)
      DO 575 I=1,27
  575 IOP(I)=IOPS(I)
      PWLAST=PWL
      DO 578 I=1,NO
      IF (WLCS(I).EQ.PWLAST) GO TO 576
      PWLAST=WLCS(I)
      GO TO 578
  576 WLCS(I)=0.0
  578 CONTINUE
      TYPE 580
  580 FORMAT (' WHICH ONES?')
  590 ACCEPT 600,IDAT
  600 FORMAT (A5,1X,15A5)
      IF (IDAT(1).EQ.' ') GO TO 880
      IF (IDAT(1).NE.'LIST') GO TO 680
      PWLAST=PWL
      TYPE 610,NAMES(1),(IHEAD(I),I=1,12)
  610 FORMAT (1X,A5,':',12A5)
      TYPE 620,NAMES(2),ICRYS1,ICRYST
  620 FORMAT (1X,A5,':',A1,A4)
  630 FORMAT (1X,A5,':',F9.5)
      TYPE 635,NAMES(17),IDEV
```

```
181    635 FORMAT (1X,A5,':',I2)
182        TYPE 630,NAMES(3),A0(1)
183        IF (ITYP.EQ.3.OR.ITYP.EQ.4.OR.ITYP.EQ.6) TYPE 630,NAMES(4),A0(2)
184        IF (ITYP.NE.1.AND.ITYP.NE.7) TYPE 630,NAMES(5),A0(3)
185        IF (ITYP.EQ.6.OR.ITYP.EQ.7) TYPE 640,NAMES(6),DEG(1)
186    640 FORMAT (1X,A5,':',F8.4)
187        IF (ITYP.EQ.4.OR.ITYP.EQ.6) TYPE 640,NAMES(7),DEG(2)
188        IF (ITYP.EQ.6) TYPE 640,NAMES(8),DEG(3)
189        TYPE 630,NAMES(9),THEMX
190        TYPE 630,NAMES(10),PWL
191        DO 650 I=1,27
192    650 IF (IOP(I).NE.0) TYPE 655,I,IOP(I)
193    655 FORMAT (5X,'IOP(',I2,')=',I2)
194        DO 670 I=1,NO
195        IF (ITYPE.EQ.0) TYPE 660,NAMES(12),I,DDS(I),(IHS(I,J),J=1,3)
196    660 FORMAT (1X,A5,':',I3,F10.3,3I3)
197        IF (ITYPE.NE.0) TYPE 660,NAMES(13),I,OBSS(I),(IHS(I,J),J=1,3)
198    670 IF (WLCS(I).NE.0.0) TYPE 675,WLCS(I)
199    675 FORMAT ('+',29X,F8.5)
200        GO TO 590
201    680 DO 690 I=1,17
202        NT=I
203    690 IF (IDAT(1).EQ.NAMES(I)) GO TO 720
204    700 TYPE 710
205    710 FORMAT (' ITEM NOT IN LIST. TRY AGAIN.')
206        GO TO 590
207    720 GO TO (730,750,700,700,700,700,700,700,770,790,800,
207       1 810,840,862,865,870,785),NT
208    730 DO 740 I=1,14
209    740 IHEAD(I)=IDAT(I+1)
210        GO TO 590
211    750 DECODE (70,760,IDAT) ICRYS1,ICRYST
212    760 FORMAT (5X,A1,A4)
213        ICOME=1
214        GO TO 150
215    770 DECODE (70,780,IDAT) THEMX
216    780 FORMAT (5X,9G)
217        GO TO 590
218    785 DECODE (70,780,IDAT) IDEV
219        IF (IDEV.EQ.0) GO TO 789
220        CLOSE (UNIT=IUT)
221        IF (IDEV.LT.10) ENCODE (5,786,UTNAME) IDEV
222    786 FORMAT ('TTY0',I1)
223        IF (IDEV.GE.10) ENCODE (5,787,UTNAME) IDEV
224    787 FORMAT ('TTY',I2)
225        OPEN (UNIT=IUT,DEVICE=UTNAME,ACCESS='SEQOUT',FILE='PNTFLE')
226        GO TO 590
227    789 CLOSE (UNIT=IUT)
228        OPEN (UNIT=IUT)
```

```
      GO TO 590
  790 PWLAST=PWL
      DECODE (70,780,IDAT) PWL
      DO 795 I=1,NO
  795 IF (WLCS(I).EQ.PWLAST) WLCS(I)=PWL
      GO TO 590
  800 DECODE (70,780,IDAT) ISUB,IVAL
      IOP(ISUB)=IVAL
      GO TO 590
  810 IF (ITYPE.EQ.0 ) GO TO 830
      TYPE 820
  820 FORMAT (' 2-THETA VALUES ENTERED INIT; D-SPACE CHANGES ARE NOT ALL
     10WED.')
      GO TO 590
  830 DECODE (70,780,IDAT) SS,DD1,IH1,IH2,IH3,WLC,WT
      CALL FILL (SS,DD1,IH1,IH2,IH3,WLC,NO,DDS,IHS,WLCS)
      GO TO 590
  840 IF (ITYPE.NE.0) GO TO 860
      TYPE 850
  850 FORMAT (' D-SPACE VALUES ENTERED INIT; 2-THETA CHANGES ARE NOT ALL
     10WED.')
      GO TO 590
  860 DECODE (70,780,IDAT) SS,DD1,IH1,IH2,IH3,WLC,WT
      CALL FILL (SS,DD1,IH1,IH2,IH3,WLC,NO,OBSS,IHS,WLCS)
      GO TO 590
  862 IALT=0
      ICOME=0
      IFLG=-1
      RETURN
  865 CALL BUILD(DEG,THEMX,ITYPE,DDS,OBSS,IHS,WLCS,NO)
      GO TO 590
  870 IFLG=0
  880 RETURN
C
C     ------------------------------------------------------------------
C
      ENTRY GETVAL (MMM,ITEST,IH,DD,OBS,WLC,WT)
      IF (MMM.NE.0) GO TO 890
      ITEST=0
      NUM=0
  890 NUM=NUM+1
      WT=0.0
      IF (NUM.GT.NO) GO TO 930
      IF (ITYPE.NE.0) GO TO 900
      IF (DDS(NUM).EQ.0.0) GO TO 890
      DD=DDS(NUM)
      GO TO 910
  900 IF (OBSS(NUM).EQ.0.0) GO TO 890
      OBS=OBSS(NUM)
```

```
 910  DO 920 I=1,3
 920  IH(I)=IHS(NUM,I)
      WLC=WLCS(NUM)
      RETURN
 930  ITEST=2
      RETURN
      END
```

```
1           SUBROUTINE MTDM(AMN,IDGS,FMNS)
    C CONVERTS MINUTES TO DEGREES AND MINUTES
2           IDGS=AMN/60.0
3           FMNS=ABS(AMN-60.0*FLOAT(IDGS))
4           IF (FMNS-59.995 ) 110,100,100
5       100 IDGS=IDGS+1
6           FMNS=0.0
7       110 RETURN
8           END
```

```
1           SUBROUTINE NORME
      C ACCUMULATES NORMAL EQUATIONS AND SUM OF SQUARES
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
4           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
4          1 E(7),SUM,JA,ITHT,IRSD,MMN
5           EQUIVALENCE (RSMX,RSDMAX),(IRSD,MAXM)
6           L=0
7           NP1=N+1
8           DO 100 J=1,N
9           DO 100 K=J,NP1
10          L=L+1
11       100 A(L)=A(L)+E(J)*E(K)
12          SUM=SUM+E(NP1)**2
13          IF (ABS(E(NP1)).LE.ABS(RSMX)) GO TO 110
14          MAXM=M
15          RSMX=E(NP1)
16       110 RETURN
17          END
```

```
      SUBROUTINE OBSEQ
C FORMS OBSERVATION EQUATION FOR ACCEPTED REFLECTIONS
      COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
      COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
      COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
      COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
     1 E(7),SUM,JA,ITHT,IRSD,MMN
      M=M+1
      DIV=COS(0.017453293*THCMP)
      IF (DIV) 100,100,110
  100 M=M-1
      RETURN
  110 FAC=(57.29578*D*CONST*SWT)/DIV
      EQCNS=SWT*DIFF
      CALL DLQOT
      E(N+1)=-EQCNS
      GO TO (120,130,140,160,180,190,210),ITYP
  120 E(1)=B(1)+B(2)+B(3)
      GO TO 230
  130 E(1)=B(1)+B(2)
      E(2)=B(3)
      GO TO 230
  140 DO 150 J=1,3
  150 E(J)=B(J)
      GO TO 230
  160 DO 170 J=1,3
  170 E(J)=B(J)
      E(4)=B(5)
      GO TO 230
  180 E(1)=B(1)+B(2)
      E(2)=B(3)
      GO TO 230
  190 DO 200 J=1,6
  200 E(J)=B(J)
      GO TO 230
  210 DO 220 J=1,2
  220 E(J)=B(3*J-2)+B(3*J-1)+B(3*J)
  230 RETURN
      END
```

OPSET SUBROUTINE

```
1           SUBROUTINE OPSET
      C DOES BOOKKEEPING FOR SETTING UP EXTINCTION RELATIONS TO USE
2           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
3           NOPT=0
4           IF (JTYP.EQ.8) IOP(6)=3
5           DO 100 L=1,27
6           IF (IOP(L).LT.2.OR.IOP(L).GT.6.OR.IOP(L).EQ.5) GO TO 100
7           NOPT=NOPT+1
8           JOP(NOPT)=L
9       100 CONTINUE
10          RETURN
11          END
```

PDNVRT SUBROUTINE

```
1           SUBROUTINE PDNVRT(A,N,B)
      C COMPLETES THE INVERSION OF POSITIVE DEFINITE SYMMETRIC MATRIX OF
      C ORDER N, STARTING WITH THE TRIANGULARIZED MATRIX RESULTING FROM
      C PDSQRT, THE UPPER TRIANGLE OF THE INVERSE BEING STORED SO THAT ITS
      C ITH ROW AND JTH COLUMN ELEMENT IS A((2*N-I)*(I-1)/2+I-J+1)
      C WITH 1.LE.I.LE.J.LE.N.
2           DIMENSION A(27),B(6)
3           IE=0
4           NP1=N+1
5           NP2=N+2
6           INM=((N+3)*N)/2-1
7           II=1
8           DO 180 I=1,N
9           B(I)=A(II)
10          J=I+1
11      100 IF (J.GT.N) GO TO 120
12          SUM=0.0
13          IJ=II+J-I
14          L=J-1
15          DO 110 K=I,L
16          SUM=SUM-A(IJ)*B(K)
17      110 IJ=IJ+NP1-K
18          B(J)=A(IJ)*SUM
19          J=J+1
20          GO TO 100
21      120 J=N
22          IJ=INM
23      130 SUM=B(J)
24          K=N
25      140 IF (K.LE.J) GO TO 150
26          SUM=SUM-A(IJ)*B(K)
27          IJ=IJ-1
28          K=K-1
29          GO TO 140
30      150 B(J)=A(IJ)*SUM
31          J=J-1
32          IF (J.LT.I) GO TO 160
33          IJ=IJ-2
34          GO TO 130
35      160 DO 170 J=I,N
36          IE=IE+1
37      170 A(IE)=B(J)
38      180 II=II+NP2-I
39          RETURN
40          END
```

```
1           SUBROUTINE PDSQRT(A,N,B,IERR)
      C SOLUTION OF N LINEAR ALGEBRAIC EQUATIONS BY SQUARE ROOT METHOD.
      C UPPER TRIANGLE OF GIVEN POSITIVE DEFINITE SYSTEM STORED SO THAT
      C ELEMENT IN ROW I AND COLUMN J IS A((2*N+4-I)*(I-1)/2+J-I+1), WITH
      C COLUMN N+1 CONTAINING RIGHT HAND SIDE EQUATION CONSTANTS.
      C B() IS SOLUTION VECTOR. IERR=-1 IF N NOT A POSITIVE INTEGER OR IF N
      C EXCEEDS PROGRAMMED LIMIT, IERR=0 IF SOLUTION CARRIED TO COMPLETION,
      C ELSE IERR=ROW FOR WHICH FIRST NON-POSITIVE DIAGONAL PIVOT DETECTED.
2           DIMENSION A(27),B(6)
3           IF (N.GE.1.AND.N.LE.6) GO TO 100
4           IERR=-1
5           GO TO 230
6       100 I2=N+1
7           DO 160 I=1,N
8           J=N
9           K=I
10          SUM=0.0
11          IL=I-1
12          IF (IL.LT.1) GO TO 120
13          DO 110 L=1,IL
14          FAC=A(K)
15          SUM=SUM-FAC*FAC
16          K=K+J
17      110 J=J-1
18      120 SUM=SUM+A(K)
19          IF (SUM.GT.0.0) GO TO 130
20          IERR=I
21          GO TO 230
22      130 FAC=1.0/SQRT(SUM)
23          A(K)=FAC
24          I1=I+1
25          DO 160 J=I1,I2
26          SUM=0.0
27          K=N
28          IJ=J
29          II=I
30          IF (IL.LT.1) GO TO 150
31          DO 140 L=1,IL
32          AI=A(II)
33          SUM=SUM-AI*A(IJ)
34          II=II+K
35          IJ=IJ+K
36      140 K=K-1
37      150 SUM=SUM+A(IJ)
38      160 A(IJ)=FAC*SUM
39          J=((N+3)*N)/2
40          I=N
41      170 IF (I-1) 220,180,180
42      180 SUM=A(J)
```

```
      J=J-1
      K=I+1
      L=N
  190 IF (L-K) 210,200,200
  200 SUM=SUM-A(J)*B(L)
      J=J-1
      L=L-1
      GO TO 190
  210 B(I)=A(J)*SUM
      J=J-1
      I=I-1
      GO TO 170
  220 IERR=0
  230 RETURN
      END
```

PRMCHK SUBROUTINE

```
1           SUBROUTINE PRMCHK(DEG)
      C IMPOSES SYMMETRY CONDITIONS ON DIRECT CELL ELEMENTS,SETS ITYP AND
      C JTYP ACCORDING TO CRYSTAL SYSTEM
2           DIMENSION DEG(3)
3           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
3          1 IAL1(16)
4           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
5           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
6           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
7           ITYP=0
8           IF (ICRYST.NE.IALF(1)) GO TO 130
9           JTYP=1
10          ITYP=1
11          N=1
12          AO(3)=AO(1)
13     100  AO(2)=AO(1)
14     110  DO 120 L=1,3
15          DEG(L)=90.0
16          IDG(L)=90
17     120  FMN(L)=0.0
18          GO TO 240
19     130  IF (ICRYST.NE.IALF(7)) GO TO 160
20          JTYP=2
21     140  ITYP=2
22          N=2
23          AO(2)=AO(1)
24          DO 150 L=1,3
25          DEG(L)=90.0
26          IDG(L)=90
27     150  FMN(L)=0.0
28          DEG(3)=120.0
29          IDG(3)=120
30          GO TO 240
31     160  IF (ICRYST.NE.IALF(8)) GO TO 170
32          JTYP=8
33          GO TO 140
34     170  IF (ICRYST.NE.IALF(3)) GO TO 180
35          JTYP=3
36          ITYP=3
37          N=3
38          GO TO 110
39     180  IF (ICRYST.NE.IALF(4)) GO TO 200
40          JTYP=4
41          ITYP=4
42          N=4
43          DO 190 L=1,3,2
44          DEG(L)=90.0
45          IDG(L)=90
46     190  FMN(L)=0.0
```

```
      GO TO 240
  200 IF (ICRYST.NE.IALF(2)) GO TO 210
      JTYP=5
      ITYP=5
      N=2
      GO TO 100
  210 IF (ICRYST.NE.IALF(5)) GO TO 230
      JTYP=7
      ITYP=7
      N=2
      DO 220 L=2,3
      DEG(L)=DEG(1)
      AO(L)=AO(1)
      IDG(L)=IDG(1)
  220 FMN(L)=FMN(1)
      GO TO 240
  230 IF (ICRYST.NE.IALF(6)) GO TO 240
      JTYP=6
      ITYP=6
      N=6
  240 RETURN
      END
```

QCOMP SUBROUTINE

```
1           SUBROUTINE QCOMP
      C COMPUTES RECIPROCAL OF SQUARE OF DISTANCE FROM ORIGIN FOR PLANE HKL
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/BLKI/Z(6)
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           Q= (Z(1)*H(1)+Z(4)*H(2)+Z(6)*H(3))*H(1)
5          1  +(Z(4)*H(1)+Z(2)*H(2)+Z(5)*H(3))*H(2)
5          2  +(Z(6)*H(1)+Z(5)*H(2)+Z(3)*H(3))*H(3)
6           RETURN
7           END
```

```
1           SUBROUTINE RCPRN (IUT)
      C PRINTS OUT RECIPROCAL CELL ELEMENTS
2           DIMENSION DEG(3)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
5           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
6           DO 100 I=1,3
7           AR(I)=3437.7468*(1.5707963-ATAN2(U(I),SQRT(1.0-U(I)**2)))
8           CALL MTDM(AR(I),IDG(I),FMN(I))
9       100 CALL DMTODG(DEG(I),IDG(I),FMN(I))
10          WRITE (IUT,110) X,DEG,VR
11      110 FORMAT(16H RECIPROCAL CELL,3E16.8/16X,3F16.5/14X,E18.8)
12          RETURN
13          END
```

```
1           SUBROUTINE RCMPD
      C COMPUTES D SPACING FOR GENERATED REFLECTIONS
2           COMMON/BLKI/Z(6)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
6           DO 100 I=1,3
7           J=MOD(I,3)+1
8           K=MOD(J,3)+1
9           Z(I)=X(I)**2
10      100 Z(I+3)=X(I)*X(J)*U(K)
11          DO 130 IC=1,NR
12          DO 110 J=1,3
13      110 H(J)=HH(IC,J)
14          CALL QCOMP
15          IF (Q .GT. 0.0) GO TO 120
16          DCM(IC)=0.0
17          GO TO 130
18      120 DCM(IC)=1.0/SQRT(Q)
19      130 CONTINUE
20          RETURN
21          END
```

```
1           SUBROUTINE RDHKL (IN,IFLAG,IALT)
      C READS HKL CARDS AND STORES OBSERVED DATA
2           DIMENSION H(3),IH(3)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
4          1 IAL1(16)
5           COMMON/BLKC/THCMP,DD,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
5          1 E(7),SUM,JA,ITHT,IRSD,MMN
6           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
7           COMMON/BLKG/IHEAD(14),ICYCLE,IMN,MM,IALF12
8           COMMON/BLKF/OBSTH(200),SW(200),WL(200),DSP(200),HG(200,3)
9           NAMELIST /DATA/ITEST,IH,D,WLC,OBS,WT
10          M=0
11     100  ITEST=0
12          WLC=0
13          WT=0
14          OBS=0
15          DD=0
16          DO 110 I=1,3
17          IH(I)=0
18     110  H(I)=0
19          IF (IFLAG.EQ.0) READ (IN,DATA)
20     120  FORMAT(A2,A4,3I5,F9.6,F8.6,2F9.5)
21          IF (IFLAG.NE.0.AND.IALT.EQ.0) CALL INTVAL(M,ITEST,IH,D,OBS,WLC,WT)
22          IF (IFLAG.NE.0.AND.IALT.NE.0) CALL GETVAL(M,ITEST,IH,D,OBS,WLC,WT)
23          DD=D
24          IF (ITEST.GT.1) GO TO 230
25          IKDATA=0
26          IF (D.EQ.0.0) IKDATA=1
27           IF (WLC.GT.0.0) PWL=WLC
28           IF (WT.LE.0.0) WT=1.0
29          IF (OBS.GT.0.0) GO TO 150
30          IF (DD.GT.0.0) GO TO 160
31     130  WRITE (IUT,140)(IH(L),L=1,3),DD,PWL,OBS,WT
32     140  FORMAT(18HOCARD WITH INDICES,3I5,5H   D =,F10.6,6H   WL =,F9.6,
32         1 13H   OBS ANGLE =,F9.4,8H   WGHT =,F10.5,15H   NOT PROCESSED)
33          GO TO 100
34     150  THOBS=OBS
35          IF (ITHT.EQ.0) THOBS=0.5*THOBS
36          IF (THOBS.GE.90.0) GO TO 130
37          DOBS=0.5*PWL/SIN(0.017453293*THOBS)
38          GO TO 170
39     160  CNST=0.5*PWL
40          THOBS=THETA(CNST,DD)
41          IF (THOBS.LE.0.0.OR.THOBS.GE.90.0) GO TO 130
42          DOBS=DD
43     170  IF (NOPT.LT.1) GO TO 190
44          IF (IH(1).EQ.0.AND.IH(2).EQ.0.AND.IH(3).EQ.0)     GO TO 190
      C CHECKING GIVEN FIXED REFLECTION FOR CONSISTENCY WITH CONDITIONS
```

```
      C FOR NON-EXTINCTION AS GIVEN ON SYSEXT CARD
   45       CALL CHKEXT(IH(1),IH(2),IH(3),JEXT)
   46       IF (JEXT.EQ.0) GO TO 190
   47       WRITE (IUT,180) (IH(L),L=1,3)
   48   180 FORMAT(20HOREFLECTION WITH H =,I5,5H  K =,I5,5H  L =,I5,71H  NOT P
   48      1ROCESSED - SHOULD NOT EXIST ACCORDING TO SYSEXT CARD INFORMATION)
   49       GO TO 100
   50   190 M=M+1
   51       IF (M.LE.200) GO TO 210
   52       WRITE (IUT,200)
   53   200 FORMAT(50HOOVER 200 OBSERVATIONS GIVEN - ONLY FIRST 200 USED)
   54       M=200
   55       GO TO 230
   56   210 OBSTH(M)=THOBS
   57       DSP(M)=DOBS
   58       WL(M)=PWL
   59       SW(M)=SQRT(WT)
   60       DO 220 L=1,3
   61   220 HG(M,L)=IH(L)
   62       GO TO 100
      C SORT GIVEN REFLECTIONS SO AS TO BE IN DECREASING VALUE FOR D-SPACING
   63   230 I=M
   64   240 I=I-1
   65       IF (I.LT.1) GO TO 270
   66       DO 260 J=1,I
   67       IF (DSP(J).GE.DSP(J+1)) GO TO 260
   68       DOBS=DSP(J)
   69       DSP(J)=DSP(J+1)
   70       DSP(J+1)=DOBS
   71       THOBS=OBSTH(J)
   72       OBSTH(J)=OBSTH(J+1)
   73       OBSTH(J+1)=THOBS
   74       WLC=WL(J)
   75       WL(J)=WL(J+1)
   76       WL(J+1)=WLC
   77       SWT=SW(J)
   78       SW(J)=SW(J+1)
   79       SW(J+1)=SWT
   80       DO 250 K=1,3
   81       H(K)=HG(J,K)
   82       HG(J,K)=HG(J+1,K)
   83   250 HG(J+1,K)=H(K)
   84   260 CONTINUE
   85       GO TO 240
   86   270 IF (IFLAG.EQ.0) CALL SAVE2 (IKDATA)
   87       RETURN
   88       END
```

RSCMP SUBROUTINE

```
1           SUBROUTINE RSCMP
      C  COMPUTES RECIPROCAL CELL ELEMENTS FROM DIRECT CELL ELEMENTS
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           DO 100 I=1,3
6           J=MOD(I,3)+1
7           K=MOD(J,3)+1
8           U(I)=(CSA(J)*CSA(K)-CSA(I))/(SNA(J)*SNA(K))
9           W(I)=SQRT(1.0-U(I)**2)
10          X(J)=1.0/(AD(J)*W(I)*SNA(K))
11      100 AR(I)=3437.7468*(1.5707963-ATAN2(U(I),W(I)))
12          VR=X(1)*X(2)*X(3)*SNA(1)*W(2)*W(3)
13          VC=1.0/VR
14          RETURN
15          END
```

```
1           SUBROUTINE RSDPRN
      C PRINTS OUT MAXIMUM RESIDUAL AND STANDARD ERROR OF UNIT WEIGHT
      C OBSERVATION IN TERMS OF THETA OR 2-THETA ACCORDING TO ITHT
2           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
2          1 E(7),SUM,JA,ITHT,IRSD,MMN
3           RM=RSDMAX
4           TSE=THTSE
5           IF (ITHT.NE.0) GO TO 100
6           RM=RM+RM
7           TSE=TSE+TSE
8       100 WRITE (20,110) RM,IRSD,TSE,MMN
9       110 FORMAT (//40H LARGEST RESIDUAL REDUCED TO UNIT WEIGHT,F8.5/3X,
9          1 3HOBS,I4,3X,26HSTANDARD ERROR UNIT WT OBS,F8.5,3X,
9          2 18HDEGREES OF FREEDOM,I3)
10          RETURN
11          END
```

```
1           SUBROUTINE SESUB
      C COMPUTES STANDARD ERRORS AND VARIANCE-COVARIANCE MATRIX
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
4           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
5           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
5          1 E(7),SUM,JA,ITHT,IRSD,MMN
6           COMMON/BLKD/TT(6,6),ST(6,6),SERCE(6),SEDCE(6),DD(3),VCME(6,6),
6          1 SS(21)
7           DO 100 I=1,21
8       100 SS(I)=0.0
9           FACTR=THTSE*THTSE
10          CALL PDNVRT(A,N,B)
11          IEC=((N+1)*N)/2
12          DO 110 I=1,IEC
13      110 A(I)=A(I)*FACTR
14          GO TO (120,140,150,180,220,230,250),ITYP
15      120 DO 130 I=1,3
16      130 SS(I)=A(1)
17          SS(7)=A(1)
18          SS(8)=A(1)
19          SS(12)=A(1)
20          GO TO 310
21      140 SS(1)=A(1)
22          SS(2)=A(1)
23          SS(7)=A(1)
24          SS(3)=A(2)
25          SS(8)=A(2)
26          SS(12)=A(3)
27          GO TO 310
28      150 DO 160 I=1,3
29      160 SS(I)=A(I)
30          DO 170 I=7,8
31      170 SS(I)=A(I-3)
32          SS(12)=A(6)
33          GO TO 310
34      180 DO 190 I=1,3
35      190 SS(I)=A(I)
36          SS(5)=A(4)
37          DO 200 I=7,8
38      200 SS(I)=A(I-2)
39          DO 210 I=7,9
40      210 SS(2*I-4)=A(I)
41          SS(19)=A(10)
42          GO TO 310
43      220 GO TO 140
44      230 DO 240 I=1,21
45      240 SS(I)=A(I)
46          GO TO 310
```

```
47      250 DO 260 I=1,3
48      260 SS(I)=A(1)
49          SS(7)=A(1)
50          SS(8)=A(1)
51          SS(12)=A(1)
52          DO 270 I=4,6
53      270 SS(I)=A(2)
54          DO 280 I=9,11
55      280 SS(I)=A(2)
56          DO 290 I=13,15
57      290 SS(I)=A(2)
58          DO 300 I=16,21
59      300 SS(I)=A(3)
60      310 II=1
61          DO 320 I=1,3
62          SERCE(I)=SQRT(SS(II))
63      320 II=II+7-I
64          DO 330 I=4,6
65          SERCE(I)=3437.7468*SQRT(SS(II))/W(I-3)
66      330 II=II+7-I
67          WRITE (20,340) (SERCE(I),I=1,6)
68      340 FORMAT (//16H R C STNDRD ERRS,3E16.8/16X,3F16.3)
69          DO 350  I=1,3
70      350 SNA(I)=SQRT(1.0-CSA(I)**2)
71          DO 390 I=1,3
72          DO  380 J=1,3
73          IF (I-J) 360,370,360
74      360 TT(I,J)=0.0
75          GO TO 380
76      370 TT(I,J)=-AD(I)/X(I)
77      380 CONTINUE
78      390 CONTINUE
79          DO 400 I=4,6
80          DO 400 J=1,3
81      400 TT(I,J)=0.0
82          DO 410 I=1,3
83          J=MOD(I,3)+1
84          K=MOD(J,3)+1
85      410 DD(I)=-AD(J)*AD(K)*X(J)*X(K)
86          DO 450 I=1,3
87          DO 440 J=4,6
88          IF (I-J+3) 420,430,420
89      420 TT(I,J)=DD(J-3)*AD(I)*CSA(J-3)
90          GO TO 440
91      430 K=MOD(J,3)+1
92          L=MOD(K,3)+1
93          TT(I,J)=DD(J-3)*AD(J-3)*CSA(K)*CSA(L)
94      440 CONTINUE
95      450 CONTINUE
```

```
96          DO 460 I=1,3
97          J=MOD(I,3)+1
98          K=MOD(J,3)+1
99      460 DD(I)=1.0/(W(J)*W(K))
100         DO 500 I=4,6
101         DO 490 J=4,6
102         IF (I-J) 480,470,480
103     470 TT(I,J)=DD(I-3)/SNA(J-3)
104         GO TO 490
105     480 IJ12=12-I-J
106         TT(I,J)=DD(I-3)*CSA(IJ12)/SNA(J-3)
107     490 CONTINUE
108     500 CONTINUE
109         DO 540 I=1,6
110         DO 540 J=1,6
111         SUM=0.0
112         IJ=I
113         DO 530 K=1,6
114         SUM=SUM+SS(IJ)*TT(J,K)
115         IF (I-K) 520,520,510
116     510 IJ=IJ+6-K
117         GO TO 530
118     520 IJ=IJ+1
119     530 CONTINUE
120     540 ST(I,J)=SUM
121         DO 570 I=1,6
122         DO 560 J=1,6
123         SUM=0.0
124         DO 550 K=1,6
125     550 SUM=SUM+TT(I,K)*ST(K,J)
126     560 VCME(I,J)=SUM
127     570 CONTINUE
128     580 FORMAT (1X,6E12.5,I4)
129         DO 590 I=1,6
130     590 SEDCE(I)=SQRT(VCME(I,I))
131         DO 600 I=4,6
132     600 SEDCE(I)=3437.7468*SEDCE(I)
133         FACTR=AD(1)*AD(2)*AD(3)
134         FACTR=FACTR*FACTR/VC
135         DO 610 I=1,3
136         J=MOD(I,3)+1
137         K=MOD(J,3)+1
138         CR(I)=VC/AD(I)
139     610 CR(I+3)=FACTR*SNA(I)*(CSA(I)-CSA(J)*CSA(K))
140         FACTR=0.0
141         DO 620 I=1,6
142         DO 620 J=1,6
143     620 FACTR=FACTR+CR(I)*CR(J)*VCME(I,J)
144         IF (FACTR) 630,630,640
```

```
145    630 FACTR=0.0
146        GO TO 650
147    640 FACTR=SQRT(FACTR)
148    650 WRITE (20,660) (SEDCE(I),I=1,6),FACTR
149    660 FORMAT (//16H D C STNDRD ERRS,3E16.8/16X,3F16.3/14X,E18.8)
150        RETURN
151        END
```

```
1           SUBROUTINE SKWEZE
      C ELIMINATES REFLECTIONS WITH IDENTICAL D-SPACINGS
2           DIMENSION IH(3),JH(3)
3           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
4           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
5           TOL=1.0E-5
6           I=1
7       100 J=I+1
8           IF (J.GT.NR) GO TO 190
9           IF ((DCM(I)-DCM(J)).GE.TOL) GO TO 180
10          DO 110 K=1,3
11          IH(K)=IFIX(HH(I,K)+SIGN(0.5,HH(I,K)))
12      110 JH(K)=IFIX(HH(J,K)+SIGN(0.5,HH(J,K)))
13      120 CALL TSTHKL(ITYP,IH,JH,IEQL)
14          IF (IEQL.NE.0) GO TO 140
15          J=J+1
16          IF (J.GT.NR) GO TO 140
17          IF ((DCM(I)-DCM(J)).GE.TOL) GO TO 140
18          DO 130 K=1,3
19      130 JH(K)=IFIX(HH(J,K)+SIGN(0.5,HH(J,K)))
20          GO TO 120
21      140 JMI=J-I-1
22          J2=NR-JMI
23          J1=I+1
24          IF (J2 .LT. J1) GO TO 170
25          DO 160 K=J1,J2
26          K2= K+JMI
27          DCM(K)=DCM(K2)
28          DO 150 L=1,3
29      150 HH(K,L)=HH(K2,L)
30      160 CONTINUE
31      170 NR=J2
32      180 I=I+1
33          GO TO 100
34      190 RETURN
35          END
```

```
1           SUBROUTINE SLCR
      C SELECTS REFLECTIONS FOR CURRENT CYCLE AND ATTEMPTS TO INDEX
      C REFLECTIONS NOT ALREADY INDEXED
2           COMMON VR,VRO,VC,VCO,Q,FAC,ICRYST,ICRYS1,ITYP,N,M
3           COMMON/ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
3          1 IAL1(16)
4           COMMON/BLKA/FMN(3),AO(3),UO(3),ALO(3),AR(3),A(27),B(6),IDG(3)
5           COMMON/BLKB/U(3),X(3),W(3),AD(3),ALS(3),CSA(3),SNA(3),CR(6),H(3)
6           COMMON/BLKC/THCMP,D,CONST,SWT,DIFF,DOBS,PWL,THTSE,THOBS,RSDMAX,
6          1 E(7),SUM,JA,ITHT,IRSD,MMN
7           COMMON/BLKE/DCM(700),DMIN,HH(700,3),JTYP,IOP(27),JOP(27),NOPT,NR
8           COMMON/BLKF/OBSTH(200),SW(200),WL(200),DSP(200),HG(200,3)
9           COMMON/BLKG/IHEAD(14),ICYCLE,IMN,MM,IALF12
10          COMMON/BLKH/AA(7),DLST(200),THTMX,TOL,NCYC,IOC(200)
11          COMMON/BLKI/Z(6)
12          COMMON/BLKJ/TOLMN
13          ICYCLE=ICYCLE+1
14          TOLP=TOL
15          IF (ITHT .EQ. 0) TOLP=TOLP+TOLP
16          WRITE (20,100) ICYCLE,IHEAD,IALF12,TOLP,ICRYS1,ICRYST
17     100  FORMAT (///6H CYCLE,I3/3X,14A5/3X,A2,17HTHETA TOLERANCE =,F9.5,4X,
17          1A1,A4)
18          M=0
19          IRSD=0
20          SUM=0.0
21          RSDMAX=0.0
22          WRITE (20,110) IALF12,IALF12,IALF12
23     110  FORMAT(4HO  N,5X,1HH,1X,1HK,1X,1HL,4X,6HD CALC,4X,5HD OBS,2X,
23          1A2,10HTHETA CALC,1X,A2,9HTHETA OBS,1X,A2,10HTHETA DIFF)
24          IF (MM .LT. 1) GO TO 300
25          DO 120 L=1,IMN
26     120  A(L)=0.0
27          IHP=1
28          DO 290 IGP=1,MM
29          JA=IALF(15)
30          SWT=SW(IGP)
31          THOBS=OBSTH(IGP)
32          ISUM=0
33          DO 130 L=1,3
34          H(L)=HG(IGP,L)
35          IF (H(L) .NE. 0.0) ISUM=ISUM+1
36     130  CONTINUE
37          PWL=WL(IGP)
38          DOBS=DSP(IGP)
39          DMNDF=ABS(DCM(IHP)-DOBS)
40          JHP=IHP+1
41     140  IF (JHP .GT. NR) GO TO 150
42          IF (ABS(DCM(JHP)-DOBS) .GT. DMNDF) GO TO 150
43          DMNDF=ABS(DCM(JHP)-DOBS)
```

```
      JHP=JHP+1
      GO TO 140
  150 IHP=JHP-1
      IOC(IGP)=IHP
      IF (ISUM .NE. 0) GO TO 250
      D=DCM(IHP)
      DLST(IGP)=D
      CONST=0.5*PWL
      IF (D .LE. CONST) GO TO 280
      THCMP=THETA(CONST,D)
      IF (ABS((THOBS-THCMP)*SWT) .GT. TOL) GO TO 280
      J=IGP-1
      ASSIGN 180 TO JADRS
  160 IF (J .LT. 1 .OR. J .GT. MM) GO TO 170
      IF (ABS(OBSTH(J)-THOBS)*SWT .LT. TOLMN) GO TO 280
      CNST=0.5*WL(J)
      IF (D .LE. CNST) GO TO 170
      THTRY=THETA(CNST,D)
      IF (ABS((OBSTH(J)-THTRY)*SW(J)).LE. TOL) GO TO 280
  170 GO TO JADRS,(180,190)
  180 J=IGP+1
      ASSIGN 190 TO JADRS
      GO TO 160
  190 K=IHP-1
      ASSIGN 220 TO KADRS
  200 IF (K .LT. 1 .OR. K .GT. NR) GO TO 210
      DB=DCM(K)
      IF (DB .LE. CONST) GO TO 210
      THTRY=THETA(CONST,DB)
      IF (ABS(THTRY-THCMP)*SWT .LT. TOLMN) GO TO 280
      IF (ABS(THTRY-THOBS)*SWT .LE. TOL) GO TO 280
  210 GO TO KADRS,(220,230)
  220 K=IHP+1
      ASSIGN 230 TO KADRS
      GO TO 200
  230 IF (THOBS .GT. THTMX .AND. ICYCLE .LE. NCYC) GO TO 290
      DO 240 L=1,3
  240 H(L)=HH(IHP,L)
      GO TO 260
  250 CONST=0.5*PWL
      CALL QCOMP
      IF (Q .LE. 0.0) GO TO 280
      D=1.0/SQRT(Q)
      DLST(IGP)=D
      IF (CONST .GE. D) GO TO 280
      THCMP=THETA(CONST,D)
      IF (ABS((THCMP-THOBS)*SWT) .GT. TOL) JA=IALF(16)
  260 DIFF=THCMP-THOBS
      IF (JA .EQ. IALF(16)) GO TO 270
```

```
      CALL OBSEQ
      CALL HKLPR
      CALL NORME
      GO TO 290
  270 CALL HKLPR
  280 IOC(IGP)=-IOC(IGP)
  290 CONTINUE
  300 RETURN
      END
```

SORTD SUBROUTINE

```
1           SUBROUTINE SORTD(N,D,HH,H)
      C SORTS ARRAY D SO THAT ELEMENTS ARE IN DECREASING ORDER - MILLER
      C INDICES IN ARRAY HH MADE TO CORRESPOND
2           DIMENSION D (700),HH(700,3),H(3)
3           I=N
4       100 I=I-1
5           IF (I.LT.1) GO TO 130
6           DO 120 J=1,I
7           IF (D(J).GE.D(J+1)) GO TO 120
8           FAC=D(J)
9           D(J)=D(J+1)
10          D(J+1)=FAC
11          DO  110 K=1,3
12          H(K)=HH(J,K)
13          HH(J,K)=HH(J+1,K)
14      110 HH(J+1,K)=H(K)
15      120 CONTINUE
16          GO TO 100
17      130 RETURN
18          END
```

```
1           FUNCTION THETA(C,D)
      C COMPUTES ARCSIN(C/D) PROVIDED C.LE.D. ELSE THETA SET TO 90.00
2           FAC=D*D-C*C
3           IF (FAC.GE.0.0 .AND. (D*D+C*C) .GT. 0.0) GO TO 100
4           FAC=90.0
5           GO TO 110
6         100 FAC=57.29578*ATAN2(C,SQRT(FAC))
7         110 THETA=FAC
8           RETURN
9           END
```

```
      SUBROUTINE TSTHKL(ITYP,IH,JH,IEQL)
C TESTS FOR EXACT EQUALITY OF D-SPACINGS FOR TWO REFLECTIONS
      DIMENSION IH(3),JH(3),ITEST(6,7),IHKLC(6,10)
      DATA ITEST / 8,5*0,3,7,4*0,1,2,3,3*0,1,2,3,6,0,0,3,10,4*0,1,2,3,4,
     1 5,6,8,9,4*0 /, IHKLC / 1,1,4*0,2,2,4*0,3,3,4*0,1,2,4*0,2,3,4*0,3,
     2 1,4*0,3*1,3*2,1,1,2,2,3,3,1,2,2,3,3,3*1,2,2,0,0 /
      DO 120 I=1,6
      INTRY=ITEST(I,ITYP)
      IF (INTRY.LT.1.OR.INTRY.GT.10) GO TO 130
      ISUM=0
      J=1
  100 K=IHKLC(J,INTRY)
      IF (K.LT.1.OR.K.GT.3) GO TO 110
      L=IHKLC(J+1,INTRY)
      ISUM=ISUM+IH(K)*IH(L)-JH(K)*JH(L)
      J=J+2
      IF (J.LT.6) GO TO 100
  110 IF (ISUM.EQ.0) GO TO 120
      IEQL=1
      GO TO 140
  120 CONTINUE
  130 IEQL=0
  140 RETURN
      END
```

```
1           BLOCK DATA
2           COMMON /ADATA/IALF(16),IFI(2,27),IFJ(3,27),IHKL(6,3),JHKL(10,3),
2          1 IAL1(16)
3           DATA IALF /   4HUBIC,4HETRA,4HRTHO,4HONOC,4HHOMB,4HRICL,4HEXAG,
3          14HEXAR,4HTLE ,4HRAM ,4HSEXT,4HD   ,4HNISH,4H2-  ,4H    ,4H R  /,
3          2 IAL1(9),IAL1(10),IAL1(11)/2HTI,2HPA,2HSY/, IFI /
3          3 12*0,1,0,1,0,1,0,1,0,4,0,4,0,4,0,5,0,5,0,5,0,6,0,6,0,6,0,1,6,5,6,
3          4 4,6,4,5,2,0,2,0,2,0,2,0 /, IFJ / 1,0,0,2,0,0,3,0,0,1,2,3,4,0,0,5,
3          5 0,0,6,0,0,8,0,0,2,0,0,9,0,0,7,0,0,8,0,0,3,0,0,6,0,0,8,0,0,2,0,0,
3          6 6,0,0,7,0,0,1,0,0,6,0,0,6,0,0,7,0,0,8,0,0,6,0,0,8,0,0,2,0,0,10,0,
3          7 0 /, IHKL / 1,0,1,1,0,0,-1,1,0,0,1,0,0,-1,-1,0,0,1 /, JHKL / 1,1,
3          8 0,1,-1,1,0,0,2,1,1,0,3*1,0,1,4*0,4*1,0,0,1,1,2 /
4           END
```

## References

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Evans, Howard T., Jr., Appleman, Daniel E., and Handwerker, David S., 1963, The least squares refinement of crystal unit cells with powder diffraction data by an automatic computer indexing method: American Crystallographic Association Annual Meeting, 1963, Program and Abstracts, p. 42-43.