ANVLS

ANL Variable Wavelength Least-Squares Program

Modified version of ORXFLS3 by Busing, Martin and Levy

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USING ANVLS ON THE SCD VAX

Creating your ANVLS.EXE file

On the SCD VAX, the program is stored in directory [SCDSOFT.ANVLS]. Subroutines are stored in an object library called [SCDSOFT.ANVLS]ANVLS.OLB.

To create an ANVLS.EXE file in your subdirectory, type

```
$ LINK [SCDSOFT.ANVLS]ANVLS,ANVLS/LIB
```

If you need to modify one of the user subroutines, copy [SCDSOFT.ANVLS]USER.FOR into your subdirectory and edit it as required. Then type

```
$ FORTRAN USER
$ LINK USER,[SCDSOFT.ANVLS]ANVLS,ANVLS/LIB
$ RENAME USER.EXE ANVLS.EXE
```

Submitting ANVLS to batch

An example of a COM file for a batch job is a follows:

```
$ RENAME [SCD]ANVLS.LOG [SCD.name]ANVLS.LOG
$ SET DEFAULT [SCD.name]
$ ASSIGN ANVRED.OUT     FOR001   ! Reflection data file.
$ ASSIGN ANVLS.DAT      FOR005   ! Control cards, etc.
$ ASSIGN ANVLS.RES      FOR006   ! "Printed" output.
$ ASSIGN COORD.IN       FOR014   ! Input parameters.
$ ASSIGN COORD.OUT      FOR015   ! Output parameters.
$ ASSIGN USER.FOR       FOR016   ! USER.FOR file.
$ ASSIGN ORFFE.DAT      FOR003   ! Output for ORFFE (optional).
$ ASSIGN FOFC.DAT       FOR012   ! Output for CANTFOUR (optional).
$ RUN ANVLS
```

To submit the COM file to the MEDIUM batch queue, type:

```
$ MEDIUM ANVLS
```

Input files

The three input files are as follows:

ANVLS.DAT -- This file contains all the input described in Chapter 2 except the reflection data and the parameters.

ANVRED.OUT -- This file contains the reflection data in "card" format. Therefore, IWHRT on the first control card should be set to -1.

COORD.IN -- This file contains the parameters as described in parts 7 to 10 in Chapter 2. It may contain more than one set of parameters if the file was written by a previous run of 2 or more cycles. Therefore, be sure to set IP to the correct value on the first control card.

Output files

ANVLS.RES -- This file contains the "printed" output.

COORD.OUT -- Parameters output after each cycle of refinement. These parameters can be refined further by renaming COORD2.DAT to COORD1.DAT and running ANVLS again.

FOFC.DAT -- Output for Fourier programs (optional).

ORFFE.DAT -- Output for the function and error program (optional).

User subroutines

The most commonly modified user subroutines are included in the file [SCDSOFT.ANVLS]USER.FOR, which can be copied into your subdirectory and edited (see Section 1.1). The following is an example listing of USER.FOR file:

```
C
C
C    SUBROUTINES FOR USERS
C
      SUBROUTINE WEIGHT

        INCLUDE '[SCDSOFT.ANVLS]ANVCOM.FOR/LIST'

        ILOGIC=1

        SIGYO = SQRT(SIGYO**2 + (0.02*YO)**2)

        IF (YO .LT. 3.0*SIGYO) THEN
          ILOGIC=0
          RETURN
        END IF

        RETURN
        END

C-----------------------------------------------------------------------

      SUBROUTINE RESETP

        INCLUDE '[SCDSOFT.ANVLS]ANVCOM.FOR'

        DO I=2,NQ
        SC(I) = SC(1)
        END DO

      RETURN
      END
```

```
C-----------------------------------------------------------------------

      SUBROUTINE LOGIC

        INCLUDE '[SCDSOFT.ANVLS]ANVCOM.FOR'

        ILOGIC = 1

        L = X(3)
        L = MOD(L,2)
        IF(L.EQ.0) RETURN
        ILOGIC = 0

        RETURN
        END

C-----------------------------------------------------------------------

        SUBROUTINE CSTRAN

        INCLUDE '[SCDSOFT.ANVLS]ANVCOM.FOR'

        DO I=2,NQ
        DFDS(1) = DFDS(1) + DFDS(I)
        CONTINUE

        RETURN
        END
```

Labelled common

The file [SCDSOFT.ANVLS]ANVCOM.FOR contains the labelled commons with dimensions for the arrays. A listing of the file follows:

```
C       The following COMMON statements contain all the COMMON blocks
C       in the entire ANVLS program.

C     DIMENSIONED FOR 150 ATOMS, 200 VARIABLES, 1200 PARAMETERS, AND
C     100 SCALE FACTORS

      COMMON /C1/ AM( 20100)
     1/C2 /ATOM  (    150) /C3 /AI    (    150) /C4 /BETA  ( 6, 150)
     2/C5/DADAI  (    150) /C6 /DADB  ( 6, 150) /C7 /DADC  (10, 150)
     3/C8 /DADFI ( 2, 150) /C9 /DADX  ( 3, 150) /C10/DBDAI (    150)
     4/C11/DBDB  ( 6, 150) /C12/DBDC  (10, 150) /C13/DBDFI ( 2, 150)
     5/C14/DBDX  ( 3, 150) /C15/DFDAI (    150) /C16/DFDB  ( 6, 150)
     6/C17/DFDC  (10, 150) /C18/DFDFI ( 2, 150) /C19/DFDX  ( 3, 150)
     7/C20/GAMMA (10, 150) /C21/SF    ( 2, 150) /C22/IGM   (    150)
     8/C23/IDL   (    150) /C24/ITA   (    150) /C25/ITC   (    150)
     9/C26/XYZ   (  3,150) /C27/DIAG  (    200) /C28/DV    (    200)
     A/C29/V     (    200) /C30/DC    (   1200) /C31/KI    (   1200)
     B/C32/P     (   1200) /C33/DFDS  (    100) /C34/DFDZE ( 6, 100)
     C/C35/IKE   (    100) /C36/SC    (    100) /C37/ZEXT  ( 6, 100)
     D/C38/NDATE           /C39/STI   (    150) /C40/PS    (   1200)
     E/C41/DR    (   1200) /C42/DP    (   1200) /C43/IKI   (   1200)

      COMMON /COMDL/DADD(15,95), DELTA(15,95), DFDD(15,95), DBDD(15,95)
```

```
 COMMON /OTHER/ A, AA(6), AP, B, BB(6), BP, CA, CB, CHG(12), COSIJ,
1 COSWH, DAMP(12), DFDPX(20), DFDTO, DY, EXPIJ, F, FI(2), FK, FKSQ,
2 FMU(6), FRACPT, FS(3,3,24), FSQ, FTA(2), FTACOI, FTACOS, FTASII,
3 FTASIN, FX(32,10), GEXT, HHB, HHHJ(10), HHJ(6), HJ(3), HX, IC,
4 ICENT, IFSQ, IHKL(4), II, IID, IJ, IJD, IPCA, ISENT, IT, ITF,
5 ITIP, ITOP, IW, IWBCD, IWHET, IWHPK, ILOGIC, ITO, IN, INTIME,
6 IOUT, IP, IPT, IQ, ISING, ISTOP, ISYM, IWHRT, IWHTF, IXFE, JK,
7 IEXT, MMM, NA, NC, NCY,        NF, NM, NNA, NNN, NO, NP, NPX,NQ,
8 NS, NT, NV, NVT, PDI, PIFI(2), PRCP(6), PT, PX(20), Q, RCP(6),
9 RHO, SCLOUT, SIG, SINIJ, SINTHL, SINWH, SQRTAB, SQRTW, SQSIG(2),
A SQTO, TFI, TITLE(18), TJ, TO, TS(3, 24), VARI, VOLSQ, YOSC, DYSC,
B YCSC, WDY, WL, YC, YEXT, YMIN, TFO, FCSQ, TBAR, TWTH, OMG, CHI,
C PHI, EFPIP1, EFPIP2, SIGYO, SIGYOS, X(4), ERR(12), YO,
D XCM, YCM, HSTNUM, SEQNUM,IDATA

   DIMENSION ROW(200),PD(200)
   EQUIVALENCE (DV(1),ROW(1),PD(1))
   REAL*8 ATOM,NDATE
```

ANVLS INSTRUCTIONS

ANVLS -- ANL Variable Wavelength Least Squares Program

```
**************************************************************
 Original ORXFLS3 Comments:
 ORXFLS3 CRYSTALLOGRAPHIC STRUCTURE-FACTOR LEAST-SQUARES PROGRAM
 OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE  37830
 BASED ON ORFLS BY W R BUSING, K O MARTIN, AND H A LEVY
 WITH CONTRIBUTIONS FROM R D ELLISON, W C HAMILTON, J A IBERS,
 C K JOHNSON, AND W E THIESSEN
 APRIL, 1971 VERSION
**************************************************************

 *** PROG:XFLSAX*** ADAPTED ANL 360/75 SEPT. 1971 J. M. WILLIAMS

 ANVLS  --  Adapted from ORXFLS3 by A. J. Schultz, Nov. 1980.
            Contributions by R. A. Jacobson (Sept., 1982) and
            W. Jauch (July, 1987) to extinction corrections.


1) TITLE CARD
    COLS
    1-72  TITLE, ANY 72 HOLLERITH CHARACTERS

2) FIRST CONTROL CARD
    COLS
    1- 3  NC, NUMBER OF CYCLES IN THIS JOB. 0 FOR STR FACT CALC.
    4- 6  NVT, TOTAL NUMBER OF VARIABLES. USED FOR CALC OF SQSIG.
             WILL BE RESET IF SMALLER THAN NV, THE NUMBER OF
             PARAMETERS VARIED IN THIS RUN. MAY BE LEFT 0
    7- 9  IW, WEIGHT INDICATOR
             0 - WEIGHT ACCORDING TO SIGYO
             1 - UNIT WEIGHTS
   10-12  IP, PARAMETER INPUT INDICATOR
             0 - INPUT FROM CARDS
             POSITIVE - INPUT FROM PREVIOUS CYCLE IP ON TAPE ITIP
             NEGATIVE - INPUT FROM PREVIOUS CYCLE -IP ON TAPE ITOP
   13-15  IT, PARAMETER OUTPUT INDICATOR
             0 - PARAMETER OUTPUT ON PRINTER ONLY
             1 - PARAMETERS WRITTEN ON TAPE ITOP AFTER EACH CYCLE
             2 - PARAMETERS PUNCHED ON CARDS AFTER EACH CYCLE
   16-18  IWBCD, STRUCTURE FACTOR PRINT INDICATOR
             0 - NO STRUCTURE FACTOR LISTING
             1 - COMPLETE STR FACT OUTPUT FOR EACH CYCLE
             2 - COMPLETE STR FACT OUTPUT FOR FIRST AND LAST CYCLE
             3 - SAME AS 2 WITH ABBREVIATED OUTPUT ON OTHER CYCLES
             4 - COMPLETE STR FACT OUTPUT ON FINAL CYCLE ONLY
             5 - SAME AS 4 WITH ABBREVIATED OUTPUT ON OTHER CYCLES
             6 - ABBREVIATED OUTPUT FOR EACH CYCLE
   19-21  ICMO, CORRELATION MATRIX OUTPUT INDICATOR
             0 - PRINT ABBREVIATED CORRELATION MATRIX ONLY
             1 - PRINT BOTH ABBREVIATED AND FULL MATRIX
   22-24  IWHTF, TEMPERATURE-FACTOR EXIT INDICATOR
             0 - EXIT ON NON-POSITIVE DEFINITE TEMPERATURE FACTOR
             1 - DO NOT EXIT ON NON-POSITIVE DEFINITE TEMP FACTOR
```

25-27 IWHPK, PARAMETER SELECTION INTEGER INDICATOR
0 - VARY SAME PARAMETERS ON EACH CYCLE
1 - READ NEW PARAMETER SELECTION INTEGERS EACH CYCLE
28-30 IWHRT, REFLECTION DATA INDICATOR
-1 - DATA FROM CARDS. TO BE WRITTEN ON TAPE ITRD
0 - DATA FROM CARDS. NO TAPE TO BE WRITTEN. (DO NOT USE UNLESS NC=0.)
1 - DATA FROM TAPE ITRD WRITTEN PREVIOUSLY
2 - NO REFLECTION DATA. INDICES COMPUTED BY SUB GENER
31-33 IXFE, INDICATOR FOR TAPE FOR OR FFE3 PROGRAM
0 - NO TAPE WRITTEN
1 - OUTPUT WRITTEN ON TAPE ITFFE
34-36 IANTP, INDICATOR FOR TAPE FOR ANALYZE AND EDIT PROGRAMS
0 - NO TAPE WRITTEN
1 - OUTPUT WRITTEN ON TAPE ITAN
35-39 IWHET, INDICATOR FOR TAPE FOR FOURIER PROGRAM
0 - NO TAPE WRITTEN
1 - OUTPUT WRITTEN ON TAPE ITFR
40-42 IPCA, PRINCIPAL COMPONENT ANALYSIS INDICATOR
IRRELEVANT AT PRESENT
43-45 JOB, MULTIPLE JOB INDICATOR
0 - ONLY ONE JOB OR FINAL JOB OF SEQUENCE
1 - ANOTHER COMPLETE SET OF INPUT DATA FOLLOWS
46-48 ITIP, TAPE NUMBER FOR PARAMETER INPUT. 0 RESET TO 4
49-51 ITOP, TAPE NUMBER FOR PARAMETER OUTPUT. 0 RESET TO 5
52-54 ITRD, TAPE NUMBER FOR REFLECTION DATA. 0 RESET TO 11
55-57 ITFFE, TAPE NUMBER FOR OR FFE3 PROGRAM. 0 RESET TO 3
58-60 ITAN, TAPE NUMBER FOR ANALYZE OR EDIT. 0 RESET TO 2
61-63 ITFR, TAPE NUMBER FOR FOURIER PROGRAM. 0 RESET TO 12

3) SECOND CONTROL CARD
COLS
1- 3 NF, NUMBER OF SETS OF SCATTERING FACTOR TABLES
0 - INDICATES NEUTRON PROBLEM
4- 6 IFSQ, F OR F**2 INDICATOR
1 - INPUT OBS AND CALC VALUES ARE MAGNITUDE OF F
2 - INPUT OBS AND CALC VALUES ARE SQUARE OF F
7- 9 ICENT, CENTROSYMMETRIC INDICATOR
1 - CENTROSYMMETRIC WITH CENTER AT ORIGIN
2 - NON-CENTROSYMMETRIC
10-12 NS, NUMBER OF SYMMETRY CARDS, I.E. THE NUMBER OF EQUIVALENT POSITIONS USED IN THE CALCULATION. OFTEN NS IS THE NUMBER OF GENERAL POSITIONS IF ICENT=2 OR HALF THAT NUMBER FOR ICENT=1
13-15 ISYM, INDICATOR FOR USERS SUBROUTINE SYMTRY WHICH TREATS CONSTRAINTS FOR ATOMS IN SPECIAL POSITIONS.
0 - CALL SYMTRY
1 - SYMTRY NOT REQUIRED. BY-PASS IT
16-18 NQ, NUMBER OF SCALE FACTORS. THIS IS THE MAXIMUM VALUE OF IQ, THE INTEGER WHICH DIVIDES REFLECTIONS INTO GROUPS WITH COMMON SCALE AND EXTINCTION PARAMETERS
19-21 IEXT, EXTINCTION INDICATOR
0 - NO EXTINCTION CORRECTION TO BE APPLIED
1 - EITHER ISOTROPIC OR ANISOTROPIC EXTINCTION

```
   22-24  ITO, INDICATOR FOR OVERALL TEMPERATURE FACTOR
             0 - SET COEFFICIENT AT 0. OMIT FROM INPUT AND OUTPUT
             1 - INCLUDE OVERALL TEMPERATURE FACTOR IN CALCULATION
   25-27  ITF, INDICATOR FOR ATOM TEMPERATURE FACTORS. IF ITC(I)
             IS SPECIFIED FOR AN ATOM IT OVERRIDES ITF
             1 - ISOTROPIC TEMPERATURE FACTOR ON EACH ATOM
             2 - ANISOTROPIC TEMPERATURE FACTOR ON EACH ATOM
             3 - INPUT IS ISOTROPIC. CONVERT TO ANISOTROPIC FORM
   28-30  NA, NUMBER OF ATOMS IN ASYMMETRIC UNIT
   31-33  NNA, NUMBER OF ATOMS INCLUDED IN STRUCTURE FACTOR FOR
             PARTIAL DIFFERENCE FOURIER. THE FIRST NNA ARE USED
   34-36  NPX, NUMBER OF EXTRA PARAMETERS PX TO BE INCLUDED IN
             INPUT AND OUTPUT. THESE ARE DEFINED BY USER
   37-39  MMM, INDICATOR FOR STANDARD OR CRYM DATA
             NEGATIVE - STANDARD "CARD" INPUT ON UNIT -MMM
             0 - IPNS DATA
             POSITIVE - DATA FROM CRYM ON UNIT MMM
   40-42  NNN, INDICATOR FOR IPNS DATA
             0 - STANDARD DATA
             POSITIVE - IPNS DATA ON UNIT NNN, IQ WILL NOT
                        BE SET TO HSTNUM
             NEGATIVE - IPNS DATA ON UNIT -NNN, IQ WILL BE
                        SET TO HSTNUM FOR EACH REFLECTION
   43-45  IRRELEVANT
   46-54  YMIN, IRRELEVANT IF IW=0. THRESHOLD USED TO DIVIDE
             REFLECTIONS INTO WEAK AND STRONG FOR R FACTOR
             CALCULATION WHEN IW=1

4) SCATTERING FACTOR TABLES. NF SETS OF FOUR CARDS EACH. OMIT
      FOR NEUTRON PROBLEMS (NF=0). SINTHL IS SIN(THETA)/LAMBDA.
      ENTRIES MAY BE LEFT BLANK FOR SINTHL BEYOND THE RANGE USED
   FIRST CARD
    COLS
    1- 9  FX(1,I), SCATTERING FACTOR FOR SINTHL=0.00
   10-18  FX(2,I) FOR SINTHL=0.05
     .    ETC                .
   64-72  FX(8,I) FOR SINTHL=0.35
   SECOND CARD
    COLS
    1- 9  FX(9,I) FOR SINTHL=0.40
     .    ETC                .
   THIRD CARD
    COLS
    1- 9  FX(17,I) FOR SINTHL=0.80
     .    ETC                 .
   FOURTH CARD
    COLS
    1- 9  FX(25,I) FOR SINTHL=1.20
     .    ETC                 .
   64-72  FX(32,I) FOR SINTHL=1.55

5) SYMMETRY INFORMATION. NS CARDS EACH OF WHICH DESCRIBES ONE
      SYMMETRY TRANSFORMATION. INCLUDE THE BASIC POSITION X,Y,Z.
      FOR CENTROSYMMETRIC SYMMETRY WITH THE ORIGIN AT A CENTER
      INCLUDE ONLY ONE OF EACH CENTROSYMMETRIC PAIR AND SET
      ICENT=1
```

THE TRANSFORMED COORDINATES ARE IN THE FORM
X(NEW)=T(X)+M(XX)*X+M(XY)*Y+M(XZ)*Z
Y(NEW)=T(Y)+M(YX)*X+M(YY)*Y+M(YZ)*Z
Z(NEW)=T(Z)+M(ZX)*X+M(ZY)*Y+M(ZZ)*Z

FORMAT(3(F15.10,3F3.0))

COLS	
1-15	T(X)
16-18	M(XX)
19-21	M(XY)
22-24	M(XZ)
25-39	T(Y)
40-42	M(YX)
43-45	M(YY)
46-48	M(YZ)
49-63	T(Z)
64-66	M(ZX)
67-69	M(ZY)
70-72	M(ZZ)

6) DIRECT CELL PARAMETERS AND WAVELENGTH.
FORMAT(7F9.6) IN THE ORDER
A,B,C,COS(ALPHA),COS(BETA),COS(GAMMA),WAVELENGTH
OR
A,B,C,ALPHA,BETA,GAMMA,WAVELENGTH.
WAVELENGTH MUST NOT BE ZERO IF NNN=0.

7) SCALE FACTOR AND EXTINCTION PARAMETERS. NQ CARDS.

COLS	
1- 9	SC(IQ), SCALE FACTOR FOR GROUP IQ
10-18	IKE(IQ), KIND OF EXTINCTION INDICATOR
0	ZACHARIASEN TYPE I ISOTROPIC
1	-"- TYPE I ANISOTROPIC
2	-"- TYPE II ANISOTROPIC
-1	-"- ISOTROPIC --> TYPE I ANISOTROPIC
-2	-"- ISOTROPIC --> TYPE II ANISOTROPIC
10	BECKER & COPPENS TYPE I GAUSSIAN PARAMETER G
11	-"- TYPE I LORENTZIAN PARAMETER G
12	-"- TYPE II PARAMETER R
20	-"- GENERAL GAUSSIAN PARAMETERS G AND R
21	-"- GENERAL LORENTZIAN PARAMETERS G AND R
22	KULDA (RANDOM ELASTIC DEFORMATION) PARAMETERS G AND A

FOR ZACHARIASEN ISOTROPIC EXTINCTION, COLS 19-27 CONTAIN THE COEFFICIENT G AND COLS 28-72 ARE IRRELEVANT. FOR ANISOTROPIC EXTINCTION,

COLS	
19-27	Z(1,1)
28-36	Z(2,2)
37-45	Z(3,3)
46-54	Z(1,2)
55-63	Z(1,3)
64-72	Z(2,3)

FOR ZACHARIASEN, G AND Z AS DEFINED AND SCALED BY P. COPPENS AND W. C. HAMILTON, ACTA CRYST. A26, 71 (1970).

FOR BECKER & COPPENS:

COLS
19-27 G - ISOTROPIC MOSAIC SPREAD PARAMETER IN RAD*-1 * 10**-4
28-36 R - DOMAIN SIZE RADIUS IN MICROMETERS

FOR KULDA:

COLS
19-27 G - AS IN BECKER & COPPENS
28-36 A - PATH LENGTH RATIO

NOTE: AT PRESENT, B&C AND KULDA ARE IMPLEMENTED ONLY FOR NEUTRONS WITH REFINEMENT BASED ON F**2.

THE BECKER & COPPENS FORMALISM OF EXTINCTION CORRECTION (ACTA CRYST.(1974) A30,129 & 148 ; ACTA CRYST.(1975) A31,417)

THE TOTAL EXTINCTION CORRECTION FACTOR Y, WHICH IS APPLIED TO FC**2 IS DEFINED AS

Y = YP(XP) * YS(YP(XP)*XS)

WHERE YP AND YS ARE THE CONTRIBUTIONS TO Y FROM PRIMARY AND SECONDARY EXTINCTION RESP. THEY ARE DETERMINED FROM THE PARAMETERS XP AND XS WHICH ARE FUNCTIONS OF THE REFINABLE PARAMETERS R AND/OR G. YP SOLELY DEPENDS ON THE PARAMETER R AND IS CALCULATED ONLY IN THE GENERAL CASE (SIMULTANEOUS REFINEMENT OF R AND G). IN THE OTHER CASES YP IS SET TO 1.

INPUT/OUTPUT OF THE REFINABLE PARAMETERS:

R (DOMAIN SIZE PARAMETER) IN MICROMETERS
G (MOSAIC SPREAD PARAMETER) IN RAD*-1 * 10**-4
GAUSSIAN MOSAIC SPREAD DISTRIBUTION: FWHM [RAD] = 0.6643/G
LORENTZIAN -"- : FWHM [RAD] = 0.3183/G

KULDA'S RED (RANDOM ELASTIC DEFORMATION) MODEL OF EXTINCTION CORRECTION (ACTA CRYST.(1987) A43,167)

THE RED MODEL RELIES ON TWO PARAMETERS, G AND A. G IS EQUIVALENT TO THE MOSAIC SPREAD PARAMETER FOR A GAUSSIAN DISTRIBUTION. THE PARAMETER A REPRESENTS A MEASURE OF PROPORTION BETWEEN PRIMARY AND SECONDARY EXTINCTION (A -> 0 : NO PRIMARY EXTINCTION ; A -> 1 : PRIMARY EXTINCTION DOMINATES).

8) OVERALL TEMPERATURE FACTOR CARD. OMIT IF ITO=0

COLS
1- 9 TO, OVERALL ISOTROPIC TEMPERATURE FACTOR COEFFICIENT

9) ATOM PARAMETERS. TWO(OR MORE) CARDS PER ATOM FOR NA ATOMS.
FIRST CARD
COLS

1- 6 ANY 6 HOLLERITH CHARACTERS INDENTIFYING ATOM I. THESE WILL BE PRINTED WITH THE PARAMETER OUTPUT.

7- 9 BLANK

10-18 X-RAY SCATTERING FACTOR IDENTIFIER OR NEUTRON SCATTERING FACTOR. FOR X-RAY PROBLEMS THIS IS AN INTEGER FROM 1 TO NF INDICATING THE SERIAL NUMBER(IN THE ORDER READ) OF THE SCATTERING FACTOR TABLE TO BE USED FOR ATOM I. FOR NEUTRON PROBLEMS (NF=0) THIS IS THE SCATTERING FACTOR ITSELF. IN EITHER CASE A DECIMAL POINT MUST BE INCLUDED.

19-27 A MULTIPLIER, A(I), APPLIED TO THE SCATTERING FACTOR OF ATOM I. THIS NUMBER WILL BE 1.0 UNLESS SYMMETRY CONDITIONS OR DISORDER DICTATE OTHERWISE.

28-36 THE COORDINATE X(I) FOR ATOM I.

37-45 THE COORDINATE Y(I) FOR ATOM I.

46-54 THE COORDINATE Z(I) FOR ATOM I.

55-63 THE IMAGINARY PART OF THE SCATTERING FACTOR.

64-72 THE REAL PART OF THE ANOMOLOUS SCATTERING (FOR X RAY PROBLEMS).

SECOND CARD
FOR ISOTROPIC TEMPERATURE FACTORS COLS 1-9 CONTAIN THE COEFFICIENT B AND COLS 10-63 ARE IRRELEVANT

FOR ANISOTROPIC TEMPERATURE FACTORS,
COLS
1- 9 BETA(1,1)
10-18 BETA(2,2)
19-27 BETA(3,3)
28-36 BETA(1,2)
37-45 BETA(1,3)
46-54 BETA(2,3)
55-63 NOT USED
FOR EACH ATOM,
COLS
64-66 ITC(I), INDIVIDUAL ATOM TEMPERATURE FACTOR INDICATOR
0 USES ITF FROM SECOND CONTROL CARD
1 THIS ATOM IS ISOTROPIC
2 THIS ATOM IS ANISOTROPIC
3 THIS ATOM INPUT AS ISOTROPIC - CONVERT TO ANISOTROPIC.

67-69 IGM(I), GAMMA TENSOR INDICATOR
0 NO GAMMA TENSOR FOR THIS ATOM
1 GAMMA TENSOR USED FOR THIS ATOM

70-72 IDL(I), DELTA TENSOR INDICATOR - IRRELEVANT AT PRESENT
THIRD AND FOURTH CARDS. GAMMA TENSOR COEFFICIENTS. OMIT IF IGM(I)=0.

THIRD CARD
1-14 C(1,1,1)
15-28 C(2,2,2)
29-42 C(3,3,3)
43-56 C(1,1,2)
57-70 C(1,2,2)

FOURTH CARD
1-14 C(1,1,3)
15-28 C(1,3,3)
29-42 C(2,2,3)
43-56 C(2,3,3)
57-70 C(1,2,3)

10) EXTRA PARAMETER CARDS. OMIT IF NPX=0
NPX EXTRA PARAMETERS WHICH CAN BE DEFINED BY THE USER IN SUBROUTINE RESETP. FORMAT(8F9.0)

11) PARAMETER SELECTION CARDS. OMIT IF NC=0. THESE CARDS SPECIFY THE PARAMETERS TO BE VARIED. EACH COLUMN SPECIFIED BELOW CONTAINS AN INTEGER KI(I)
IF KI(I)=0, PARAMETER I WILL BE HELD CONSTANT. OTHERWISE PARAMETER I WILL BE ADJUSTED.
NON-ZERO VALUES OF KI(I) ARE OF TWO TYPES. KI(I)=1 SIGNIFIES THAT THE FULL PARAMETER CORRECTIONS WILL BE APPLIED. KI(I)=2 THROUGH 9 SIGNIFIES THAT THE FRACTION KI(I)/10 OF THE CALCULATED CORRECTION WILL BE APPLIED.

FOR SCALE FACTOR AND EXTINCTION PARAMETERS. NQ CARDS.
COL
1 KI FOR SCALE FACTOR

FOR ISOTROPIC EXTINCTION, KI FOR G IS IN COLUMN 4,COLS 5 THROUGH 9 ARE IRRELEVANT

FOR ANISOTROPIC EXTINCTION,
COL
4 KI FOR Z(1,1)
5 KI FOR Z(2,2)
6 KI FOR Z(3,3)
7 KI FOR Z(1,2)
8 KI FOR Z(1,3)
9 KI FOR Z(2,3)

FOR OVERALL TEMPERATURE FACTOR. ONE CARD. OMIT IF ITO=0.
COL
1 KI FOR OVERALL TEMPERATURE FACTOR

FOR ATOM PARAMETERS. NA CARDS.
COL
1 KI FOR REAL PART OF SCATTERING FACTOR (SF(1,I))
2 KI FOR IMAGINARY PART OF SCATTERING FACTOR (SF(2,I))
3 KI FOR ATOM MULTIPLIER (AI(I))
7 KI FOR X COORDINATE OF ATOM I
8 KI FOR Y COORDINATE OF ATOM I
9 KI FOR Z COORDINATE OF ATOM I

IF ATOM I HAS AN ISOTROPIC TEMPERATURE FACTOR, KI FOR B IS

IN COLUMN 13, AND COLS 14-18 ARE IRRELEVANT

IF ATOM I HAS AN ANISOTROPIC TEMPERATURE FACTOR,
COL
13 KI FOR BETA(1,1)
14 KI FOR BETA(2,2)
15 KI FOR BETA(3,3)
16 KI FOR BETA(1,2)
17 KI FOR BETA(1,3)
18 KI FOR BETA(2,3)

IF IGM=0, COLS 22 THROUGH 31 ARE IRRELEVANT, OTHERWISE,
COL
22 KI FOR C(1,1,1)
23 KI FOR C(2,2,2)
24 KI FOR C(3,3,3)
25 KI FOR C(1,1,2)
26 KI FOR C(1,2,2)
27 KI FOR C(1,1,3)
28 KI FOR C(1,3,3)
29 KI FOR C(2,2,3)
30 KI FOR C(2,3,3)
31 KI FOR C(1,2,3)

FOR EXTRA PARAMETERS. OMIT IF NPX=0
FORMAT(37I1)

12) REFLECTION DATA CARDS. THESE CARDS ARE OMITTED IF IWHRT IS GREATER THAN ZERO. ONE CARD IS NEEDED FOR EACH REFLECTION OBSERVED OR FOR EACH STRUCTURE FACTOR TO BE COMPUTED.

THE DATA ARE READ ACCORDING TO THE 'REVISED STANDARD FORMAT' (I1,F3.0,2F4.0,2F9.0,F3.0,F11.0,4F7.0)

COLS
1 BLANK
2- 4 THE INDEX H. NO DECIMAL POINT NEEDED IF RIGHT ADJUSTED.
5- 8 THE INDEX K. NO DECIMAL POINT NEEDED IF RIGHT ADJUSTED.
9-12 THE INDEX L. NO DECIMAL POINT NEEDED IF RIGHT ADJUSTED.
13-21 THE OBSERVED VALUE OF /F/ OR F**2, WHICHEVER IS BEING REFINED. FOR STRUCTURE FACTOR CALCULATIONS THIS FIELD MAY BE LEFT BLANK.
22-30 THE STANDARD ERROR OF THIS OBSERVATION. IF IW=1,THIS FIELD IS IRRELEVANT.
31-33 IQ, THE SCALE FACTOR IDENTIFIER HAVING A VALUE BETWEEN 1 AND NQ. THE SCALE FACTOR SC(IQ) AND THE CORRESPONDING EXTINCTION PARAMETERS WILL BE USED IN COMPUTING THIS REFLECTION.
34-44 TBAR, THE ABSORPTION-AVERAGED MEAN PATH LENGTH FOR THIS REFLECTION. TBAR= -(1/T)(D T/D MU), WHERE T IS THE FRACTIONAL TRANSMISSION AND MU IS THE LINEAR ABSORPTION COEFFICIENT (N.B. TBAR IS A POSITIVE NUMBER). THIS FIELD IS IRRELEVANT IF NO EXTINCTION CORRECTION IS BEING APPLIED.

THE NEXT FOUR FIELDS CONTAIN THE DIFFRACTOMETER SETTING ANGLES FOR THE REFLECTION AND ARE IRRELEVANT IF AN ANISOTROPIC EXTINCTION CORRECTION IS NOT BEING APPLIED.

COLS	
45-51	TWO THETA
52-58	OMEGA
59-65	CHI
66-72	PHI

IPNS DATA. THE FORMAT IS THE SAME ALTHOUGH THE CONTENTS OF SOME FIELDS HAVE BEEN CHANGED. EACH CARD CONTAINS THE FOLLOWING DATA:

ISENT,H,K,L,YO,SIGYO,IQ,TBAR,WL,XCM,YCM,HSTNUM,SEQNUM

13) OBSERVATION TERMINATION CARD. OMIT IF IWHRT .GT. 0

COL	
1	1 AS A SENTINEL FOR THE END OF THE OBSERVATION DECK

14) CHANGE OF PARAMETER SELECTION INTEGERS. OMIT IF IWHPK=0.
IF IWHPK=1, A NEW SET OF PARAMETER SELECTION CARDS MUST BE SUPPLIED HERE FOR EACH CYCLE OF REFINEMENT AFTER THE FIRST.

USER SUBROUTINES

THE FOLLOWING SUBROUTINES ARE AVAILABLE TO BE MODIFIED BY THE USER FOR EACH PARTICULAR PROBLEM. IN GENERAL IT WILL BE NECESSARY TO ADD THE COMMON STATEMENTS FOR THE VARIABLES TO WHICH REFERENCE IS MADE.

SUBROUTINE CSTRAN

PURPOSE- TO MODIFY THE CALCULATED DERIVATIVES TO PROVIDE FOR ANY DESIRED CONSTRAINT BETWEEN PARAMETERS. ANY EXTRA PARAMETERS PX MAY IN EFFECT BE DEFINED BY THIS SUBROUTINE.

CALLED ONCE FOR EACH REFLECTION AT THE END OF SUBROUTINE CALC WHICH CALCULATES THE STRUCTURE FACTOR AND ITS DERIVATIVES. IT IS CALLED BEFORE SUBROUTINE SBTOP STORES THESE DERIVATIVES IN ARRAY DC. IT IS CALLED DURING EACH CYCLE OF REFINEMENT BUT NOT FOR THE FINAL STRUCTURE FACTOR CALCULATION.

SUBROUTINE MUST SET CERTAIN DERIVATIVES IN TERMS OF OTHERS.

EXAMPLE- THE NEUTRON SCATTERING FACTOR OF ATOM 3 IS CONSTRAINED TO BE THE SAME AS THAT OF ATOM 2 AND ONLY THE LATTER IS VARIED. CSTRAN INCLUDES THE STATEMENT

```
DFDFI(2)=DFDFI(2)+DFDFI(3)
```

NOTE 1- SUBROUTINE RESETP MUST ALSO BE PREPARED WHENEVER SUBROUTINE CSTRAN IS USED.

NOTE 2- A GENERAL SUBROUTINE CSTRAN IS AVAILABLE WHICH AUTOMATICALLY SETS THE DERIVATIVES TO CORRESPOND TO CONSTRAINTS DEFINED BY SUBROUTINE RESETP. SUBROUTINE SYMTRY SHOULD NOT BE USED IF THIS GENERAL CSTRAN IS USED.

SUBROUTINE GENER(NOW)

PURPOSE- TO GENERATE INDICES FOR STRUCTURE FACTOR CALCULATION WHEN NO OBSERVATION CARDS ARE USED.

CALLED ONCE FOR EACH REFLECTION ON FIRST CYCLE INSTEAD OF READING OBSERVATION IF IWHRT=2.

ON ENTRY NOW=2 IF FIRST ENTRY.

SUBROUTINE MUST ON FIRST ENTRY-
SET NOW=0, ISENT=0, YO=0.0, SIGYO=0.0, X(4)=1.0, AND INITIALIZE LOOPS TO GENERATE INDICES X(1)=H, X(2)=K, X(3)=L.

ON SUBSEQUENT ENTRIES-
SET X(1), X(2), AND X(3).

ON ENTRY AFTER FINAL REFLECTION-
SET ISENT=1.

SUBROUTINE LOGIC

PURPOSE- TO SELECT THE OBSERVATIONS TO BE INCLUDED.

CALLED ONCE FOR EACH OBSERVATION ON EVERY CYCLE ON RETURN FROM
SUBROUTINE CALC WHICH COMPUTES THE STRUCTURE FACTOR BUT
BEFORE THE OBSERVED AND CALCULATED QUANTITIES ARE PRINTED.

ON ENTRY ILOGIC=1 UNLESS IT HAS BEEN CHANGED BY SUBROUTINE WEIGHT.

SUBROUTINE MAY SET ILOGIC AS FOLLOWS-

1	INCLUDE REFLECTION.
0	PRINT REFLECTION BUT OMIT IT FROM REFINEMENT AND FOURIER TAPE.
-1	PRINT REFLECTION AND INCLUDE IT ON FOURIER TAPE (IF USED) BUT OMIT FROM REFINEMENT.

NOTE THAT THE EFFECT OF SETTING ILOGIC IN SUBROUTINE LOGIC
IS DIFFERENT THAN THAT OF SETTING IT IN SUBROUTINE WEIGHT.

SUBROUTINE MASTER

PURPOSE- TO ENABLE THE USER TO REDIMENSION ARRAYS BY
RECOMPILING ONLY THIS ONE SUBROUTINE.

METHOD- THOSE ARRAYS WITH DIMENSIONS MOST LIKELY TO BE CHANGED
BY THE USER HAVE BEEN PLACED IN LABELED COMMON, ONE ARRAY
PER BLOCK. IN ALL ROUTINES EXCEPT MASTER THESE ARRAYS ARE
DIMENSIONED AM(1), ETC. THE DESIRED DIMENSIONS ARE SPECIFIED
IN MASTER AND THESE WILL OVERRIDE THE SMALLER ONES GIVEN IN
THE REST OF THE PROGRAM.

NOTE- THIS METHOD WORKS SUCCESSFULLY WITH THE IBM 360 OPERATING
SYSTEM. THE USER MAY HAVE TO MAKE MODIFICATIONS TO USE IT
WITH OTHER COMPUTER SYSTEMS.

SUBROUTINE OBSIN

PURPOSE- TO READ OR SET THE DATA FOR EACH OBSERVATION WITH
THE FORMAT AND SEQUENCE OF THE INFORMATION UNDER CONTROL
OF THE USER.

CALLED ONCE FOR EACH OBSERVATION (UNTIL ISENT=1) DURING
THE FIRST CYCLE PROVIDED THAT IWHRT=0 OR -1.

SUBROUTINE MUST- READ OR SET
ISENT, X(1)=H, X(2)=K,X(3)=L,
YO SIGYO X(4)=IQ

- READ OR SET TBAR IF AN EXTINCTION CORRECTION IS TO BE MADE.
- READ OR SET TWTH, OMG, CHI, PHI IF AN ANISOTROPIC EXTINCTION CORRECTION IS TO BE MADE.

NOTE THAT A STANDARD SUBROUTINE OBSIN HAS BEEN PROVIDED.

SUBROUTINE RESETP

PURPOSE- TO SET CERTAIN PARAMETERS WHICH HAVE NOT BEEN ADJUSTED BY LEAST SQUARES IN TERMS OF OTHERS WHICH HAVE. ANY EXTRA PARAMETERS PX ARE IN EFFECT DEFINED BY THIS SUBROUTINE.

CALLED ONCE NEAR THE START OF THE PROBLEM AFTER THE PARAMETERS HAVE BEEN READ AND ONCE ON EACH CYCLE AFTER THE PARAMETERS HAVE BEEN REFINED BY LEAST SQUARES. IN EACH CASE RESETP IS CALLED BEFORE THE PARAMETERS ARE COPIED INTO ARRAY P BY SUBROUTINE SBTOP, BEFORE THEY ARE PRINTED, AND BEFORE THE TEMPERATURE FACTORS ARE TESTED FOR POSITIVE-DEFINITE CHARACTER.

SUBROUTINE MUST SET DEPENDENT PARAMETERS IN TERMS OF THOSE WHICH HAVE BEEN VARIED.

EXAMPLE FOR THE CONSTRAINTS USED AS EXAMPLES FOR SYMTRY AND CSTRAN WE WOULD INCLUDE-

```
SF(1,3)=SF(1,2)
XYZ(2,4)=XYZ(1,4)
XYZ(3,4)=0.333333
XYZ(2,5)=XYZ(1,5)
XYZ(3,5)=0.333333
XYZ(2,6)=XYZ(1,6)
XYZ(3,6)=0.333333
```

SUBROUTINE SYMTRY(I)

PURPOSE- TO CONSTRAIN ATOMIC PARAMETERS WHICH ARE RELATED TO EACH OTHER BECAUSE THE ATOM IS IN A SPECIAL POSITION. ALTERNATIVELY, THE SAME RESULT CAN BE ACCOMPLISHED BY USING SUBROUTINE CSTRAN.

CALLED NA TIMES FOR EACH OF THE NS SYMMETRY POSITIONS IN THE CALCULATION OF EACH STRUCTURE FACTOR.

ON ENTRY- I=1, 2, 3...NA ON SUCCESSIVE ENTRIES FOR EACH SYMMETRY POSITION.
- IF I=1 THEN TJ, HJ, AND HHJ HAVE BEEN SET FOR THIS SYMMETRY POSITION.
- IF I=2, 3, ETC. THEN TJ, HJ, AND HHJ RETAIN THE VALUES SET PREVIOUSLY BY THIS SUBROUTINE.

SUBROUTINE MUST SET TJ, HJ, AND HHJ AS DESCRIBED IN ORNL-TM-305.

EXAMPLE- IF NA=6 AND ATOMS 4, 5, AND 6 ARE IN THE SPECIAL POSITION X, X, 1/3 THE STATEMENTS INCLUDED ARE

```
GO TO (20,20,20,10,20,20),I
```

```
          10 TJ=TJ+HJ(3)/3.0
             HJ(1)=HJ(1)+HJ(2)
             HJ(2)=0.0
             HJ(3)=0.0
          20 RETURN
```

NOTE 1- SUBROUTINE RESETP MUST BE PREPARED WHENEVER SUBROUTINE SYMTRY IS USED.

NOTE 2- SUBROUTINES SYMTRY AND CSTRAN MAY BOTH BE USED IN THE SAME PROBLEM, BUT SYMTRY MUST NOT BE USED IF THE GENERAL CSTRAN IS USED.

SUBROUTINE WEIGHT

PURPOSE- TO COMPUTE WEIGHTS AND SELECT THE OBSERVATIONS TO BE INCLUDED.

CALLED ONCE FOR EACH OBSERVATION ON EVERY CYCLE AFTER THE OBSERVATION HAS BEEN READ FROM CARDS, TAPE, OR DISK (OR AFTER ITS INDICES HAVE BEEN GENERATED) BUT BEFORE THE CORRESPONDING STRUCTURE FACTOR IS CALCULATED.

ON ENTRY RHO AND SINTHL HAVE BEEN CALCULATED AND ILOGIC=1.

SUBROUTINE MAY- CALCULATE SIGYO TO SET WEIGHT.
- SET ILOGIC AS FOLLOWS-
  1 INCLUDE REFLECTION
  0 OMIT THIS OBSERVATION FROM LISTING AND REFINEMENT.
  -1 OMIT THIS AND ALL SUBSEQUENT OBSERVATIONS.

NOTE- THE EFFECT OF SETTING ILOGIC IN SUBROUTINE WEIGHT IS DIFFERENT FROM THAT OF SETTING IT IN SUBROUTINE LOGIC.

GLOSSARY OF SYMBOLS

A	REAL COMPONENT OF STRUCTURE FACTOR
AA(6)	DIRECT LATTICE METRIC TENSOR
AABB	A*A+B*B
*AI(NA)	ATOM MULTIPLIERS
AM(NM)	MATRIX OF NORMAL EQUATIONS
AMO(--)	SECOND PART OF MATRIX FOR 360/91
AP	CONTRIBUTION OF FIRST NNA ATOMS TO A. FOR DIF FOURIER
*ATOM(NA)	ALPHANUMERIC ATOM NAMES
B	IMAGINARY COMPONENT OF STRUCTURE FACTOR
BB(6)	RECIPROCAL LATTICE METRIC TENSOR
*BETA(6,NA)	ANISOTROPIC TEMPERATURE FACTOR COEFFICIENTS
BP	CONTRIBUTION OF FIRST NNA ATOMS TO B. FOR DIF FOURIER
CA	COEFFICIENT USED IN CALCULATING DERIVATIVES
CALC SUB C	COMPUTE YC AND ITS DERIVATIVES
CB	COEFFICIENT USED IN CALCULATING DE
CCHI	COS(CHI)
CDG	COEFFICIENT USED TO CALCULATE ANIS EXTINCTION DERIVS
CED SUB C	SET CHG, ERR, AND DAMP FOR PARAMETER OUTPUT
CHG(12)	PARAMETER CHANGES FOR ONE LINE OF OUTPUT
CHI	DIFFRACTOMETER ANGLE CHI
CMEDIT SUB C	PRINT EDITED CORRELATION MATRIX
CNU	COS(OMEGA+THETA)
COSIJ	CONTRIBUTION OF ATOM I IN SYMMETRY POSITION J
COSWH	COS OF CALCULATED PHASE FOR FOURIER INPUT
CPHI	COS(PHI)
*CSTRAN SUB C	USERS ROUTINE TO SET DERIVATIVES FOR CONSTRAINTS
CSTTSQ	(COS(2.0*THETA))**2
DADAI(NA)	D A/D AI
DADB(6,NA)	D A/D BETA. ALSO SUM OVER J OF HHJ*COSIJ
DADC(10,NA)	D A/D GAMMA. ALSO SUM OVER J OF HHHJ*SINIJ
DADD(15,NA)	D A/D DELTA
DADFI(2,NA)	D A/D FI. ALSO SUM OVER J OF COSIJ*EXPIJ
DADX(3,NA)	D A/D XYZ. ALSO SUM OVER J OF HJ*SINIJ
DAMP(12)	DAMPING FACTORS FOR ONE LINE OF PARAMETER OUTPUT
DBDAI(NA)	D B/D AI
DBDB(6,NA)	D B/D BETA. ALSO SUM OVER J OF HHJ*SINIJ*EXPIJ
DBDC(10,NA)	D B/D GAMMA. ALSO SUM OVER J OF HHHJ*COSIJ*EXPIJ
DBDD(15,NA)	D B/D DELTA
DBDFI(2,NA)	D B/D FI. ALSO SUM OVER J OF SINIJ*EXPIJ
DBDX(3,NA)	D B/D XYZ. ALSO SUM OVER J OF HJ*COSIJ*EXPIJ
DC(NP)	DERIVATIVES OF YC WITH RESPECT TO ALL PARAMETERS
DELTA(15,NA)	DELTA TENSOR. COEFFICIENTS OF FOURTH CUMULANT
DEXT	DIAGONAL ELEMENT OF ZEXT
DFDAI(NA)	D YC/D AI
DFDB(6,NA)	D YC/D BETA
DFDC(10,NA)	D YC/D GAMMA
DFDD(15,NA)	D YC/D DELTA
DFDFI(2,NA)	D YC/D FI. REAL AND IMAG
DFDGX	D YC/D GEXT
DFDPX(NPX)	D YC/D PX. TO BE SET BY USERS SUBROUTINE CSTRAN
DFDS(NQ)	D YC/D SC
DFDTO	D YC/D TO
DFDX(3,NA)	D YC/D XYZ
DFDZE(6,NQ)	D YC/D ZEXT.
DIAG(NV)	DIAGONAL ELEMENTS OF INVERSE MATRIX
DMP	DAMPING FACTOR APPLIED TO PARAMETER CHANGES

DOT FUN	OBTAIN INNER PRODUCT OF TWO VECTORS
DV(NV)	DERIVATIVES OF YC WITH RESPECT TO VARIABLES
DY	YO-YC
DYSC	DY SCALED TO REMOVE EXTINCTION AND SCALE FACTOR
EFPIP1	EXTRA VARIABLE FOR EACH REFLECTION. AVAILABLE TO USER
EFPIP2	EXTRA VARIABLE FOR EACH REFLECTION. AVAILABLE TO USER
ERR(12)	PARAMETER ERRORS FOR ONE LINE OF OUTPUT
EXPIJ	TEMPERATURE FACTOR FOR ATOM I IN SYMMETRY POSITION J
F	SCALED STRUCTURE FACTOR MAGNITUDE WITH EXTINCTION
FACT	FACTOR WHICH MODIFIES DERIVATIVES FOR EXTINCTION
FCSQ	UNSCALED CALCULATED STRUCTURE FACTOR SQUARED
FFYYG	FCSQ*GMXT*YEXT**2
FI(2)	REAL AND IMAGINARY PARTS OF ATOMIC SCATTERING FACTOR
FK	SCALED STRUCTURE FACTOR MAGNITUDE WITHOUT EXTINCTION
FKSQ	SCALED STRUCTURE FACTOR SQUARE WITHOUT EXTINCTION
FMU(6)	MEAN SQUARE THERMAL DISPLACEMENTS, ANGSTROMS SQUARED
FRACPT	FRACTIONAL PART OF PT
FS(3,3,NS)	MATRICES FOR SYMMETRY TRANSFORMATIONS
FSQ	SCALED STRUCTURE FACTOR SQUARE INCLUDING EXTINCTION
FTA(2)	REAL AND IMAGINARY PARTS OF AI*FI*TFI
FTACOI	AI*FI*TFI*SUM OVER J OF COSIJ. FOR IMAGINARY FI
FTACOS	AI*FI*TFI*SUM OVER J OF COSIJ. FOR REAL PART OF FI
FTASII	AI*FI*TFI*SUM OVER J OF SINIJ. FOR IMAGINARY FI
FTASIN	AI*FI*TFI*SUM OVER J OF SINIJ. FOR REAL PART OF FI
*FX(32,NF)	X-RAY SCATTERING FACTOR TABLES
GAMMA(10,NA)	GAMMA TENSOR. COEFFICIENTS OF THIRD CUMULANT
*GENER SUB C	GENERATE INDICES IF NO OBSERVATIONS ARE AVAILABLE
GEXT	EXTINCTION COEFFICIENT. ISOTROPIC OR ANISOTROPIC
GGEXT	QUADRATIC FORM FOR ANISOTROPIC EXTINCTION
GMXT	GAMMA OF COPPENS AND HAMILTON EXTINCTION FORMULA
HHB	ARGUMENT FOR EXP IN ANISOTROPIC TEMPERATURE FACTOR
HHHJ(10)	TRANSFORMED INDEX PRODUCTS FOR GAMMA TENSOR
HHJ(6)	TRANSFORMED INDEX PRODUCTS
HJ(3)	TRANSFORMED INDICES
HX	ARGUMENT FOR SIN OR COS
*HSTNUM	HISTOGRAM NUMBER OF IPNS REFLECTION
I	INDEX FOR LOOPS
*IANTP	1 TO WRITE TAPE FOR ANALYZE AND EDIT, 0 FOR NO TAPE
IC	INDEX WHICH COUNTS LEAST-SQUARES CYCLES
*ICENT	1 FOR CENTROSYMMETRIC, 2 FOR NON-CENTROSYMMETRIC
*ICMO	1 PRINT COMPLETE CORRELATION MATRIX, 0 OMIT
*IDL(NA)	DELTA TENSOR INDICATOR. 0 NOT USED, 1 USED
*IEXT	0 FOR NO EXTINCTION, 1 FOR EXTINCTION
*IFSQ	1 TO REFINE ON STRUCTURE FACTOR, 2 FOR ITS SQUARE
*IGM(NA)	GAMMA TENSOR INDICATOR. 0 NOT USED, 1 USED
IHKL(4)	ARRAY X STORED IN INTEGER FORM FOR OUTPUT
II	INDEX WHICH LOCATES DIAGONAL ELEMENT OF AM
IID	INCREMENT ADDED TO II TO STEP DOWN DIAGONAL OF AM
IJ	INDEX WHICH LOCATES AN ELEMENT OF AM
IJD	INCREMENT USED TO STEP IJ ALONG ROW-COLUMN OF AM
*IKE(NQ)	0 ISO EXT, 1 OR 2 ANIS TYPE 1 OR 2, -1 -2 ISO TO ANIS
ILAST	IC-NCY. 0 ON FINAL STRUCTURE FACTOR CALCULATION
ILOGIC	INDICATOR SET BY LOGIC. 1 FOR YO INCLUDED, 0 OMITTED
IN	TAPE NUMBER FOR STANDARD INPUT
INTIME	INITIAL TIME, SEC/100
IOUT	TAPE NUMBER FOR STANDARD OUTPUT
*IP	PARAMETER INPUT INDICATOR. 0 FROM CARDS, ELSE TAPE
*IPCA	0 LEAST SQUARES. 1 PRINCIPAL COMPONENT ANALYSIS
IPT	INTEGRAL PART OF PT
IQ	SCALE FACTOR IDENTIFIER. READ AS X(4)
*ISENT	SENTINEL SET TO 1 TO END OBSERVATION INPUT

```
 ISING         1 IF MATRIX IS SINGULAR, 0 IF NOT
 ISTOP         INDICATOR SET BY TEST. NON-ZERO TERMINATES JOB
*ISYM          NON-ZERO TO BY-PASS SYMTRY FOR GREATER SPEED
*IT            0 NO PARAMETER OUTPUT, 1 FOR TAPE, 2 FOR CARDS
 ITA(NA)       TEMPERATURE FACTOR INDICATOR FOR EACH ATOM
*ITAN          TAPE NUMBER FOR ANALYZE AND EDIT. 0 CHANGED TO 2
*ITC(NA)       TEMPERATURE FACTOR INDICATOR AS READ. IF 0 ITF USED
 ITEMP         ABS(IP) FOR OUTPUT
*ITF           1 FOR ISOTROPIC, 2 ANISOTROPIC, 3 CHANGE ISO TO ANISO
*ITFFE         TAPE NUMBER FOR FFE. 0 CHANGED TO 3
*ITFR          TAPE NUMBER FOR FOURIER. 0 CHANGED TO 12
 ITIME  FUN    READ COMPUTER CLOCK
*ITIP          TAPE NUMBER FOR PARAMETER INPUT. 0 CHANGED TO 4
 ITMP          ITIP FOR IP NEGATIVE, ITOP FOR IP POSITIVE
*ITO           1 USE OVERALL TEMPERATURE FACTOR. 0 DO NOT USE IT
*ITOP          TAPE NUMBER FOR PARAMETER OUTPUT. 0 CHANGED TO 5
*ITRD          TAPE NUMBER FOR REFLECTION DATA. 0 CHANGED TO 11
 IVTIME        TIME FOR MATRIX INVERSION, SECONDS
*IW            0 WEIGHT USING ERRORS, 1 UNIT WEIGHTS
*IWBCD         0 NO REFLECTION OUTPUT, 1 COMPLETE OUTPUT, 2-6 OTHER
*IWHET         1 TO WRITE TAPE FOR FOURIER PROGRAM, 0 FOR NO TAPE
*IWHPK         1 NEW INPUT OF KI EACH CYCLE, 0 KI INPUT ONLY ONCE
*IWHRT         -1 DATA CARDS TO TAPE, 0 CARDS, 1 TAPE, 2 USE GENER
*IWHTF         1 PREVENTS STOP ON NON-POS-DEF TEMP FACTOR, 0 TO STOP
*IXFE          1 WRITE TAPE FOR OR FFE, 0 NO OR FFE TAPE
 J             INDEX FOR LOOPS
 JJ            INDEX WHICH LOCATES AN ELEMENT OF AM.
 JK            INDEX WHICH LOCATES AN ELEMENT OF AM
*JOB           1 ANOTHER COMPLETE JOB FOLLOWS, 0 THIS IS LAST JOB
 K             INDEX FOR LOOPS
 KI(NP)        VARIABLE SELECTION INDICATORS. 0 FIXED, NON-ZERO VARY
 KIREAD SUB C  READ PARAMETER SELECTION INTEGERS KI. COMPUTE NV
 LC            LINE COUNT
 LK            IWHRT+2
 LN            NUMBER OF LINES ABOUT TO BE PUT OUT
 LNCT   SUB    COUNT LINES OF OUTPUT AND ADVANCE PAGE WHEN NEEDED
*LOGIC  SUB C  SET ILOGIC OR MODIFY RESULTS AFTER CALC IS CALLED
 MATIME        TIME FOR MATRIX SET UP, SECONDS
 MATINV SUB    CHOLESKI INVERSION OF SYMMETRIC MATRIX
 MATSTO SUB C  STORE MATRIX AM AND VECTOR V OF NORMAL EQUATIONS
*MMM           UNIT NUMBER FOR CRYM DATA, OTHERWISE 0
 N             NV+1
*NA            NUMBER OF ATOMS IN ASYMMETRIC UNIT
*NC            NUMBER OF REFINEMENT CYCLES TO BE PERFORMED
 NCY           NC+1
 NDATE         ALPHANUMERIC DATE OF CALCULATION
*NF            NUMBER OF X-RAY SCATTERING FACTOR TABLES. 0 NEUTRON
 NFPX          NUMBER OF FULL LINES OF EXTRA PARAMETER OUTPUT
 NLPX          NUMBER OF EXTRA PARAMETERS IN LAST LINE OF OUTPUT
 NM            NV*(NV+1)/2, THE NUMBER OF ELEMENTS IN THE MATRIX
*NNA           NUMBER OF ATOMS INCLUDED IN AP AND BP FOR DIF FOURIER
*NNN           0 FOR STANDARD DATA, NONZERO FOR IPNS DATA
 NO            NUMBER OF OBSERVATIONS
 NOW           ARGUMENT FOR GENER.
 NP            TOTAL NUMBER OF PARAMETERS
 NPX           NUMBER OF EXTRA PARAMETERS DEFINED BY USER
*NQ            NUMBER OF SCALE FACTORS IN PARAMETER LIST
*NS            NUMBER OF SYMMETRY CARDS
 NT            TAPE NUMBER FOR PARAMETER OUTPUT
 NV            NUMBER OF VARIABLES
*NVT           TOTAL NUMBER OF VARIABLES. USED FOR GOODNESS OF FIT
```

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*OBSIN  SUB C READ REFLECTION DATA IN ANY FORMAT
 OBSTO  SUB   STORE OBSERVATIONAL EQUATIONS FOR SINGULAR VALUES
 OMG          DIFFRACTOMETER ANGLE OMEGA
 P(NP)        LIST OF ALL PARAMETERS SOME OF WHICH WILL BE VARIED
 PAROUT SUB C PRINT PARAMETER OUTPUT
 PD(NV)       CALCULATED PARAMETER CHANGES FOR VARIABLES
 PDI          PD(I)
 PEXT         POLARIZATION FACTOR INCLUDING SCALING
 PHI          DIFFRACTOMETER ANGLE PHI
 PIFI(2)      REAL AND IMAGINARY PARTS OF + OR -6.28*AI*FI*TFI
 PRCP(6)      PRODUCTS OF RECIPROCAL LATTICE PARAMETERS
 PRELIM SUB C READ STRUCTURAL INPUT DATA AND DO INITIAL CALCULATION
 PT           LOCATION OF FI IN SCATTERING FACTOR TABLE FX
 PTOSB  SUB   COPY VARIOUS PARAMETERS FROM ARRAY P
 PX(NPX)      EXTRA PARAMETERS DEFINED BY USERS SUBROUTINE RESETP
 Q            CALCULATED INTENSITY OF REFLECTION. FOR OUTPUT ONLY
 RAD          CONSTANT PI/180
*RCP(6)       DIRECT LATTICE PARAMETERS
*RESETP SUB C USE VARIED PARAMETERS TO RESET THOSE CONSTRAINED
 RFAC   SUB C ACCUMULATE AND PRINT AGREEMENT FACTORS
 RHO          (SIN(THETA)/LAMBDA)**2
 RNU          DIFFRACTOMETER ANGLE NU=OMEGA+THETA IN RADIANS
 ROW(NV)      ROW OF CORRELATION MATRIX FOR OUTPUT
 SBTOP  SUB   SET UP ARRAY P FROM VARIOUS PARAMETERS
 SC(NQ)       SCALE FACTORS WHICH MULTIPLY CALC STRUCTURE FACTOR
 SCHI         SIN(CHI)
 SCLOUT       DIVISOR FOR OBSERVATION OUTPUT. INCLUDES SC AND YEXT
*SEQNUM       SEQUENCE NUMBER OF IPNS REFLECTION
 SF(2,NA)     NEUTRON SCATTERING FACTOR OR X-RAY IDENTIFIER
 SFOUT  SUB C PRINT STRUCTURE FACTOR OUTPUT ACCORDING TO OPTIONS
 SIG          SUM OF (SQRTW*(YO-YC))**2
*SIGYO        STANDARD ERROR OF YO.
 SIGYOS       SIGYO SCALED TO REMOVE EXTINCTION AND SCALE FACTOR
 SINIJ        CONTRIBUTION OF ATOM I IN SYMMETRY POSITION J
 SINTHL       SIN(THETA)/LAMBDA
 SINTT        SIN(2.0*THETA)
 SINWH        SIN OF CALCULATED PHASE FOR FOURIER INPUT
 SNU          SIN(OMEGA+THETA)
 SPHI         SIN(PHI)
 SQRTAB       SQRT(A**2+B**2)
 SQRTW        SQUARE ROOT OF WEIGHT OF OBSERVATION
 SQSIG(2)     SQRT(SIG/NO-NV) AND SAME SAVED FROM PREVIOUS CYCLE
 SQTO         SC(IQ)*EXP(-TO*RHO)
 SQTOSQ       (SC(IQ)*EXP(-TO*RHO))**2
 SQYEXT       SQRT(YEXT)
 SVDLS  SUB   SINGULAR VALUE DECOMPOSITION LEAST-SQUARES SOLUTION
*SYMTRY SUB C CONSTRAIN PARAMETERS OF ATOMS IN SPECIAL POSITIONS
*STI(NA)      SCATTERING FACTOR TABLE IDENTIFIER FOR X-RAY PROBLEMS
 TBAR         ABSORPTION AVERAGED PATH LENGTH FOR EXTINCTION
 TEST   SUB C TEST FOR NON-POSITIVE-DEFINITE TEMPERATURE FACTORS
 TFI          ISOTROPIC TEMPERATURE FACTOR
 TITLE(18)    ALPHANUMERIC TITLE OF JOB
 TJ           TRANSLATIONAL TERM FOR TRIGONOMETRIC ARGUMENT HX
*TO           OVER-ALL TEMPERATURE FACTOR COEFFICIENT
 TS(3,NS)     TRANSLATIONAL PART OF SYMMETRY TRANSFORMATIONS
 TWTH         DIFFRACTOMETER ANGLE TWO THETA
 V(NV)        VECTOR OF NORMAL EQUATIONS
 VARI         SQSIG(1)**2
 VEXT(3)      VECTOR WHICH DEFINES ANISOTROPIC EXTINCTION
 VOLSQ        DIRECT CELL VOLUME SQUARED
 VVEXT(6)     PRODUCTS OF ELEMENTS OF VEXT
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WDY	(YO-YC)/SIGYO
*WEIGHT SUB C	CALCULATE SIGYO OR SET ILOGIC BEFORE CALC IS CALLED
WL	X-RAY OR NEUTRON WAVELENGTH
*X(4)	INDICES H,K, AND L, AND SCALE FACTOR IDENTIFIER IQ
*XCM	DETECTOR X COORDINATE FOR IPNS REFLECTION
*XYZ(3,NA)	FRACTIONAL COORDINATES X, Y, AND Z FOR NA ATOMS
YC	CALCULATED SCALED STRUCTURE FACTOR OR ITS SQUARE
*YCM	DETECTOR Y COORDINATE FOR IPNS REFLECTION
YCSC	YC SCALED TO REMOVE EXTINCTION AND SCALE FACTOR
YEXT	EXTINCTION FACTOR APPLIED TO STRUCTURE FACTOR SQUARED
*YMIN	USED TO CLASSIFY REFLECTIONS FOR R FACTORS IF IW=1
YO	OBSERVED STRUCTURE FACTOR OR ITS SQUARE
YOSC	YO SCALED TO REMOVE EXTINCTION AND SCALE FACTOR
YYONE	0.5*(YEXT**2+1.0)
*ZEXT(6,NQ)	ANISOTROPIC EXTINCTION COEFFICIENTS