Single Crystal Diffractometer
User's Guide
and
Reference Manual

Web page for links to software and manuals:

http://www.pns.anl.gov/SCD/scd2.html

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Introduction

Welcome to IPNS. This document has been created to aid you in your use of the single crystal diffractometer (SCD). To page someone on the public address system in the 360/375/399 area, dial 2-7448.

The data acquisition system is described in the *User Manual for the IPNS Data Acquisition System - Vaxstation version* by R. K. Crawford. A copy of the manual should be on the desk next to the SCD Vaxstation terminal. The node name of the SCD Vaxstation is "SCD" and its TCP/IP address is "**scd.pns.anl.gov**". The Username for the main directory is "**SCD**". See Art for the Password. Programs are executed by issuing a **program__name** command at the console. All programs prompt the user for input. Type **PHELP** for online help with the data acquisition command system.

Programs for SCD data analysis are also run by simply typing the name of the program. All programs prompt the user for input and either run interactively or create a **program_name.COM** command file to submit to a batch queue. All executable files are stored in the [SCD.EXE] directory.

A histogram run file consists of a header, which contains the title, the user's name, goniometer angles, etc., and the actual histogram data with 2 bytes for each histogram bin. The histogram represents a three-dimensional array of counts with channel numbers corresponding to a position on the detector face (X,Y) and the time-of-flight (T or Z). Histogram run files are named "SCD0**NRUN**.RUN" where **NRUN** is a number from 0000 to 9999. A typical histogram array of 85x85x120 channels consists of 867,000 "bins", which requires more than 1.6 Mbyte of disk space.

Some interesting facts and figures are:

The position-sensitive scintillation area detector contains a 2-mm. thick sheet of ^{6}Li loaded glass, behind which is a 7 X 7 array of 2-inch square photomultiplier tubes. The detector has nominal active area of 30 X 30 cm. and an effective active area of 28 x 28 cm with a spatial resolution of 3 mm.

The moderator-to-sample distance is 950 cm. And the sample to detector distance is 32 cm. The time-of-flight for a 1 Å neutron to scatter off the sample and reach the detector is approximately 2.5 msec.

The monitor detector is a low efficiency BF_3 proportional counter located at the end of the collimator, which is about 45 cm. upstream from the sample.

Data Collection Procedure

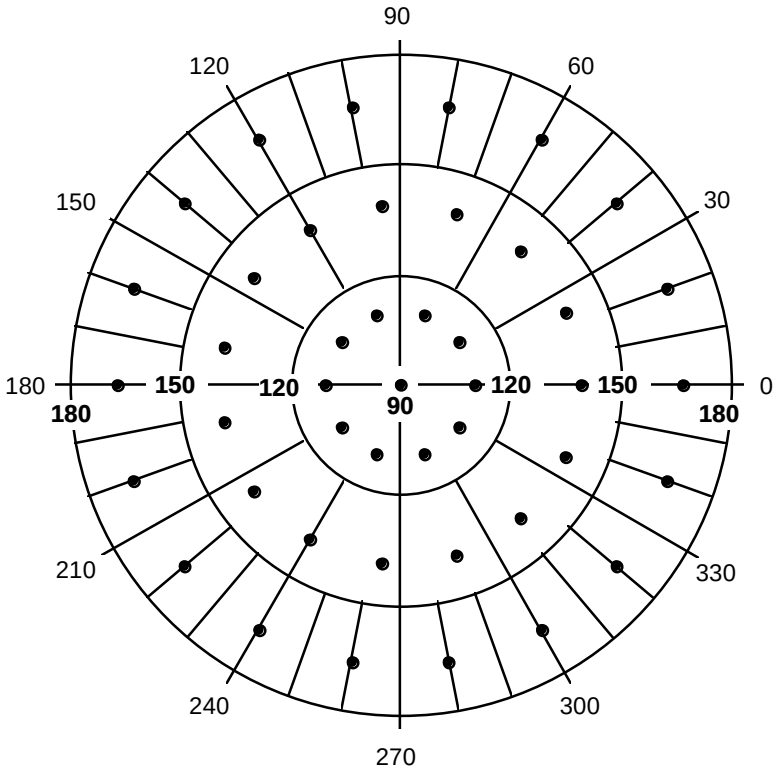
After the crystal has been mounted and centered in the beam, you will probably want to obtain one, two or possibly three histograms at different chi and phi settings angles to examine the crystallinity of the sample and obtain an orientation matrix. If you wish to obtain several histograms, run **TABLE** to create a file of settings angles for automatic data collection mode. When the Displex refrigerator is in place, settings for DETA (detector angle), OMEGA and DETD (detector distance) are 90.0 and 45.0 degrees and 32.0 cm., respectively, and cannot be changed.

Use **NEWRUN**, **SCHEDULE** and **START** to collect the data (see "How to Get Started"). The histogrammed data can be examined using DISPLAY COMMANDS for data displays on the color CRT screen.

PEAKS can be run to search the histograms for peaks, interpolate and integrate them. The results of this are written on a EXPNAM.PEAKS file, where EXPNAM is an experiment name chosen by the user. In addition, a file named EXPNAM.EXP contains general information about the experiment and information about each histogram as it is processed. Then **BLIND** may be run to index the data and provide a preliminary orientation matrix. **INDEX** is then used to index all the reflection data and **LSQRS** to perform a unit cell least squares on the indexed data. At this point the user can apply his or her crystallographic wisdom to determine whether or not to collect data. However, it is important to emphasize that it is not necessary to know the unit cell, space group or orientation matrix in order to collect data, although it can be useful. At a later stage, this information will be required for data analysis procedures.

If you have determined the cell dimensions (orientation matrix), you may run **SIM** to simulate data. This helps you to chose a wavelength range to best match the resolution of the instrument. You may also wish to run **SETANG** to obtain the chi and phi angles for the (100), (010) and (001) reflecting positions. Note that only chi angles between 90° and 180° are feasible, so that it may be necessary to calculate the Friedel pair of a reflection. The setting angles can be located on the following figure, which contains chi and delta phi angles for a sample-to-detector distance of 32 cm., and appropriate histogram settings can be selected to obtain a complete unique set of data based on the Laue symmetry of the crystal.

Histogram Setting Angles



χ	Δφ
167	20
139	24
110	36

Routine automatic data collection should be preceded by executing **TABLE** again to generate a new table of settings to be used in covering reciprocal space. Or, you can use tables previously stored as INSTDIR:*.CTL files. **NEWRUN** and **START** can be used as before to collect the data.

Data reduction is accomplished with **ANVRED** (Argonne National Laboratory Variable Wavelength Data Reduction program). For the least-squares refinement of the structural parameters use the program **ANVLS** (Argonne National Laboratory Variable Wavelength Least Squares).

Data Collection on the SCD

Bold face type is the user input followed by RETURN. The characters CR indicates that only the RETURN key is typed. Italic text in boxes or in brackets are comments.

Log on if necessary.

```
        Welcome to VAX/VMS V5.5

Username: SCD
Password: IPNSSCD
        Welcome to VAX/VMS version V5.5 on node SCD
    Last interactive login on Tuesday, 13-JUL-1993 16:09
    Last non-interactive login on Tuesday, 13-JUL-1993 14:17
Good afternoon!
Today is Tuesday, 13-JUL-1993.  The time is 16:20:07 on node SCD.
******************** IPNS NEWS *******  9-July-1993  *****************

                *****   IPNS Lunch Talk Schedule   *****
     7/15 - BUMPED - no lunch!
     7/22 - BUMPED - no lunch!
     7/29 - Adam Ellison (ANL/MSD):  GLAD:  We Can Analyze Data Now!
                ****************************************

IPNS will run until July 28.

***************************** Operator's Message ****************************
 7-14-93 WED. 0900 - ? C MODERATOR GAS WILL BE CHANGED,HE COMPRESSOR BREAKER
 CHANGED AND C MODERATOR TEMP VS SPECTRUM RUNS WILL BE DONE AFTER BEAM
 RESEARCH.

*****************************     SCD NEWS     ******************************

***  PEAKS can now search for peaks in "live" histograms.  10/21/92

***  PLOTHIST is a new program that can plot contour and/or 3D surface
     plots of time-slices from live or file histogram data. 10/21/92

***  SCAN will now plot on the terminal in addition to writing files
     for input to EASYPLOT or KaleidaGraph.                  2/14/93

*******************************************************************************

SCD>
```

Next, calibrate the angles if necessary and position the crystal at the desired angles.

```
SCD> STEP
   *** STPDRV ***
 SCD0 USING SCD MOTORS       -- DEVICE    6
ENTER MOTOR POSITIONS ONLY (P), CHANGE LIMITS (L),
 CALIBRATE (C), CHANGE OTHER PARAMETERS (O),
 OR EXIT (E) ?
C
USE <CR> FOR NO CHANGE
 CHI NOW   ?   (   180.000 )     CR
 PHI NOW   ?   (   114.000 )     0.0
```

```
 OMEGA NOW ?   (    45.000 )     CR
 DETA NOW  ?   (    90.000 )     CR
 DETD NOW  ?   (    32.000 )     CR
ENTER MOTOR POSITIONS ONLY (P), CHANGE LIMITS (L),
 CALIBRATE (C), CHANGE OTHER PARAMETERS (O),
 OR EXIT (E) ?
```

NEWRUN will actually get the current angles from the numbers in the parentheses below rather than the "NOW" angle, so make sure they are the same as shown for PHI.

```
P
USE <CR> FOR NO CHANGE
 CHI NOW     180.000     CHI LOW      90.000     CHI HI      180.000
 CHI       ?   (   180.000 )     CR
 PHI NOW       0.000     PHI LOW     -90.000     PHI HI      360.000
 PHI       ?   (   114.000 )     0.0
 OMEGA NOW    45.000     OMEGA LOW     0.000     OMEGA HI    360.000
 OMEGA     ?   (    45.000 )     CR
 DETA NOW     90.000     DETA LOW      0.000     DETA HI     180.000
 DET ANG   ?   (    90.000 )     CR
 DETD NOW     32.000     DETD LOW      0.000     DETD HI      50.000
 DET DIST  ?   (    32.000 )     CR
```

Now set-up the first RUN file.

```
SCD> NEWRUN
```

Enter the appropriate input for NEWRUN. The default histogram has a minimum wavelength of 0.7 Å and a maximum wavelength of 4.2 Å.

```
SCD> PEAKS
Live or File data (L,<F>)? L

RUN number =  587
TMin =  1730   TMax = 10382
XNum = 85   YNum = 87   WLNum = 120
It is assumed that DETD = 32 cm and (delta t)/t = 0.015

Do you want to index the peaks (Y,<N>)? CR
Number of peaks per histogram to be found? 30

Do you want to limit the search to a range of
time-slices (Y,<N>)? CR
SUBROUTINE OPNRUN:  NRUN =     587
Reading time-slice 119

 No.    X    Y    T    XCM    YCM    WL   Count

   1   27   28   57  -5.91  -5.21  1.576   732
   2    7   48   60 -12.13   0.78  1.645  1392
   3   24   69   62  -6.84   7.06  1.696  1086
   4   32   84   65  -4.35  11.56  1.771  1069
   5   48   79   66   0.63  10.06  1.799   612
   6    7   82   67 -12.13  10.96  1.821   831
   7   29    3   69  -5.29 -12.70  1.878   738
   8   28   77   70  -5.60   9.46  1.908   696
   9   60   65   71   4.36   5.87  1.938  1956
  10   39   32   75  -2.17  -4.01  2.057  1874
  11   11   25   76 -10.89  -6.11  2.083   789
  12   18    7   79  -8.71 -11.50  2.177   816
```

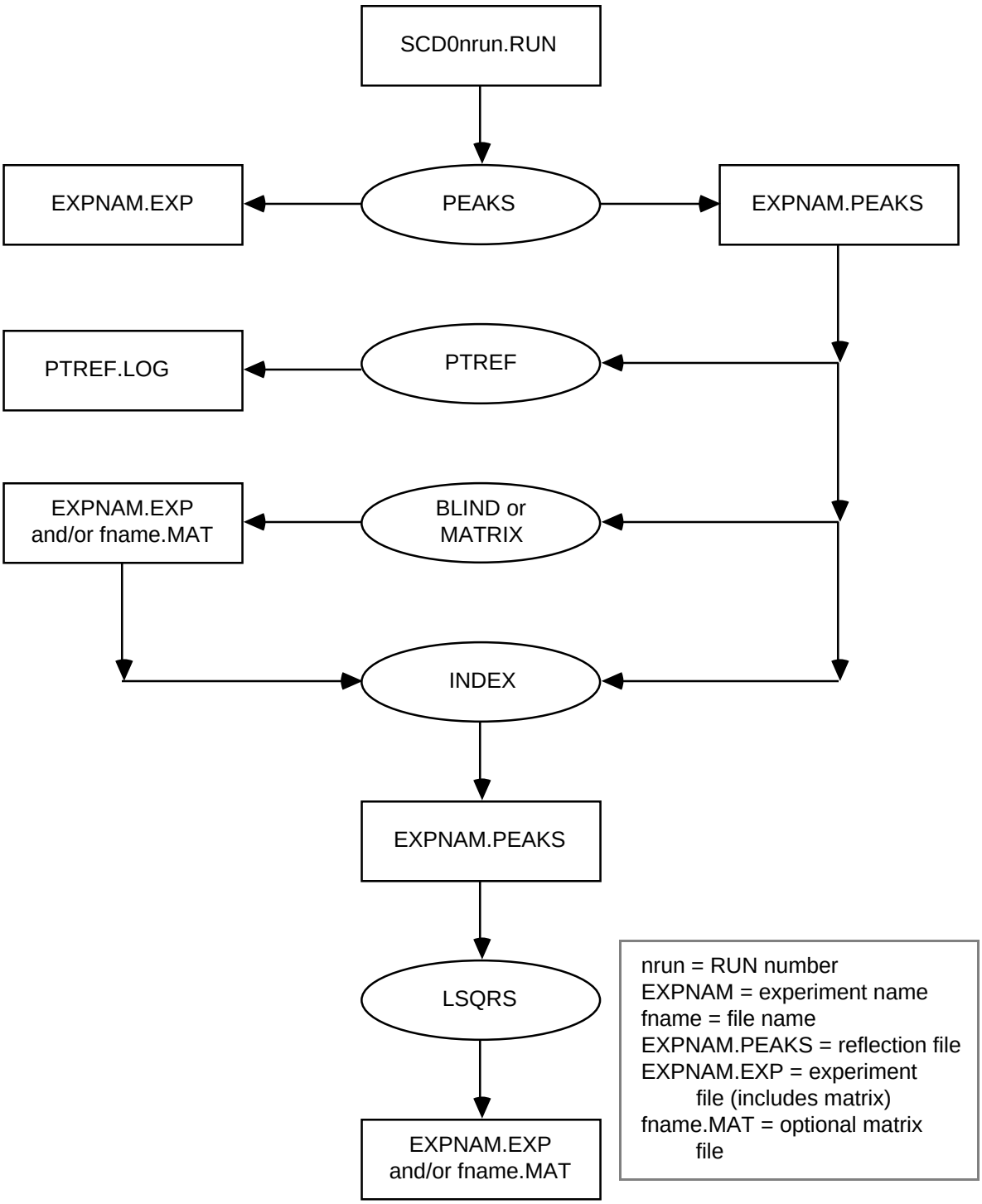
```
  13   54   46   81   2.49   0.18  2.249  1118
  14   37   51   81  -2.80   1.68  2.248   593
  15   81   56   82  10.90   3.17  2.278  2006
  16    5   46   83 -12.76   0.18  2.311  1128
  17   64   27   84   5.61  -5.51  2.349   627
  18   29   40   86  -5.29  -1.62  2.421  1310
  19   48   34   86   0.63  -3.41  2.421  1255
  20   78   83   87   9.96  11.26  2.450   840
  21   79   43   88  10.27  -0.72  2.491  1128
  22   18   27   89  -8.71  -5.51  2.528  3090
  23   39   20   89  -2.17  -7.61  2.530  1028
  24   21   65   91  -7.78   5.87  2.604   751
  25   26    5   91  -6.22 -12.10  2.601   656
  26   59   37   97   4.05  -2.52  2.850   806
  27   77   58  103   9.65   3.77  3.111   587
  28   28   77  104  -5.60   9.46  3.157  1545
  29   74   42  111   8.72  -1.02  3.504  1270
  30   18   61  112  -8.71   4.67  3.556   925

Peaks are also listed in the PEAKS.LOG file.
 NORMAL PROGRAM TERMINATION
```

Data Analysis Flow Diagrams and Examples

The following pages contain flow diagrams and examples representing how to process and analyze data. In the flow diagrams, the names of programs are within ovals and files are in rectangles. The arrows indicate input and output data files. By no means do these diagrams include all programs you may wish to use to analyze and display your data. Therefore, it is highly recommended that you familiarize yourself with the descriptions of the programs in PROGRAMS ON THE VAX.

Determining the Unit Cell and Orientation Matrix

INDEXING AND UNIT CELL LEAST-SQUARES



In the following examples, user input is in **bold face** *type.*

For a new experiment, run KEY to create the expnam.EXP file with the correct instrument calibration parameters.

```
ANLPNS UD1:SCD> KEY
\\\\\\\      KEY      ///////

This program will create a key indexed file containing
data presently stored in the histogram files which is
compatible with similar files used by Los Alamos
National laboratory; one such file contains all of the
header information for every histogram relating to one
experiment


Experiment name? MYCRYSTAL
Enter number of histograms to be copied: 1
EXP file does not exist. A NEW FILE IS BEING OPENED.
Do you want to create/update orientation matrix (Y/N)? N

Do you want to
   (1) choose a set of default instrument parameters;
or (2) input parameters manually from the console?
1

( 1)  NACL DISK          JAN. 1984
 660.15    2.70    3.21    3.11    0.04   -0.05
( 2)  NACL 2 X 2 X 2 CRYSTAL  MARCH 1984
 655.66   -2.10    3.23    3.13    0.31   -0.13
( 3)  NACL 2 X 2 X 2 XTAL    MAY 1984
 658.15    5.00    3.14    3.06   -0.87    0.17
( 4)  NACL 2 X 2 X 2 XTAL  JUNE 1984
 659.11    0.50    3.16    3.10    0.29   -0.20
( 5)  NACL 2 X 2 X 2 XTAL  FEB. 1985
 658.26    0.00    3.23    3.09   -0.74    0.18
( 6)  NaCl 2 X 2 X 2 Xtal  Feb. 1986
 662.06    7.90    3.23    3.12   -0.89    0.11
( 7)  NaCl 2 X 2 X 2 Xtal  May  1986
 660.71    5.10    3.23    3.12   -0.80    0.11
( 8)  NaCl 2 X 2 X 2 mm Xtal  Dec. 1986
 947.46    6.30    3.21    3.10   -0.41    0.36
( 9)  NaCl 2 x 2 x 2 mm Xtal  March 1987
 946.19    6.30    3.22    3.11   -0.40    0.33
(10)  Quartz crystal              August 1989
 944.71    5.60    3.19    3.12   -0.10    0.41

Input a number from 1 to 10? 10

     0 Channels Overflowed for RUN 1601
```

The file MYCRYSTAL.EXP has been created with the instrument calibration parameters and parameters from RUN 1601. Next run PEAKS to locate Bragg peaks.

```
ANLPNS UD1:SCD> PEAKS
PEAKS (1) finds peaks in histograms;
      (2) finds and interpolates
A PEAKn.REF file is created which contains this data appended
to the end of the existing data.  The "old" REF file
can be deleted at the users option.  Select path by entering
number 1 or 2: 2
EXPNUM? 16
Starting and ending HSTNUM? 1,1
Number of peaks per histogram to be found? 30
```

```
Do you want to limit the search to a range of
time-slices (Y/N)? N

************************************************************

       To submit to batch, type:

              MEDIUM program_name

       where "program_name" is the name of the program.

       The LOG file will be in your current directory.

************************************************************

FORTRAN STOP
ANLPNS UD1:SCD> MEDIUM PEAKS
Job PEAKS (queue MEDIUM, entry 51) started on PNS_MEDIUM
```

PEAKS created a PEAK16.REF file with the list of peaks. This is a binary file so it is necessary to run PTREF to examine the list of peaks.

```
ANLPNS UD1:SCD> PTREF
PEAKn.REF(1) or EXPTn.REF(2) file (1 or 2)? 1
EXPNUM? 16
Starting SEQNUM: 1
Starting HSTNUM: 1
Print on  line printer(1) or console(2)? 1
FORTRAN STOP
```

The line printer option actually outputs to a PRINT.LOG file which can be examined using the EDT editor.

```
ANLPNS UD1:SCD> EDT PRINT.LOG
Input file does not have standard text file format
    1       1  RUN NUMBER =  1601
*C
```

SEQ, or SEQNUM = the sequence number of the peak.
H,K,L = the Miller indices which are not known at this point.
X,Y,Z = the histogram channel numbers.
XCM,YCM = the horizontal and vertical detector position in centimeters measured from the center of the detector.
WL = the wavelength in Angstroms.
IPKOBS = the actual number of neutron counts in the peak height.

```
1  RUN NUMBER =  1601
     CHI     PHI    OMEGA   DETA    DETD     MONCNT
   167.00    0.00   45.00   90.00   32.00      53275
   SEQ   H   K   L     X      Y      Z      IPKOBS    GENTXT    HSTNUM    REFLAG
                       XCM    YCM    WL         IT       BKG       INI       SIG

     1   0   0   0  33.95   4.80   6.11       102         0      1601        11
                    -3.21 -11.96 0.6491         0      0.00      0.00      0.00
     2   0   0   0   5.61  36.97  14.89       221         0      1601        11
                   -12.01  -1.61 0.7394         0      0.00      0.00      0.00
     3   0   0   0  15.32  58.98  15.12       322         0      1601        11
                    -9.00   5.47 0.7422         0      0.00      0.00      0.00
```

SEQNUMs 4 to 24 are not shown.

```
    25   0   0   0  40.35  69.02  74.19      1178         0      1601        11
                    -1.22   8.70 1.7907         0      0.00      0.00      0.00
    26   0   0   0  18.27  16.37  74.44       530         0      1601        11
                    -8.08  -8.24 1.7960         0      0.00      0.00      0.00
    27   0   0   0  23.79  61.66  85.30       682         0      1601        11
```

```
                    -6.36   6.33 2.1148         0      0.00      0.00      0.00
[EOB]
Command: QUIT
```

Run BLIND to auto-index the peaks and obtain the reduced cell and the orientation matrix. If the cell parameters are known and the unit cell is small, another option is to run MATRIX.

```
ANLPNS UD1:SCD> BLIND

 *******LAUE INDEXER*******

(OUTPUT ALSO SENT TO PRINT FILE)


INPUT FROM REFLECTION FILE (Y,N)? Y
EXPNUM? 16
PEAKn.REF (1) OR EXPTn.REF (0) FILES? 1
SEQUENCE NUMBERS?(MAX=17,END WITH ZERO(0)
20            ! Normally input the 6 to 8 peaks with the longest
21            ! wavelengths since they will have the smallest hkl indices
22            ! as in this example.  However, if that fails, sometimes the
23            ! reflections with shorter wavelengths will succeed, or
24            ! some random selection of peaks.  See also MULTI_BLIND
25            ! and MATRIX.
26
27
0

   #  SEQ       XCM       YCM      WL
   1   20    -1.052   -10.196    1.2506
   2   21     4.294     1.376    1.2732
   3   22     4.046    11.618    1.3242
   4   23     1.818    -0.930    1.4451
   5   24    -1.911    -3.828    1.6336
   6   25    -1.222     8.704    1.7907
   7   26    -8.078    -8.238    1.7960
   8   27    -6.364     6.333    2.1148

*****************

ERROR LIMIT=0.03

REDUCED CELL

CELL VOLUME=   112.7

** CELL SCALARS ***              ! These are the reduce cell scalars:
   23.96   29.34   23.91         !      r11    r22    r33
   -0.01  -11.83    0.12         !      r23    r31    r12

A=   4.895   B=   5.416   C=   4.889
ALPHA=  90.03   BETA= 119.62   GAMMA=  89.75

     #   SEQ     H     K     L
     1    20    -3    -5     2
     2    21    -2    -6     1
     3    22    -1    -6     0
     4    23    -2    -5     1
     5    24    -2    -4     1
     6    25    -1    -4     0
     7    26    -2    -3     1
     8    27    -1    -3     0

ORIENTATION MATRIX
```

```
 0.20462    0.06625   -0.09473
-0.05064    0.17678    0.01642
 0.18529    0.03966    0.13946
STORE THE MATRIX(Y,N)?
Y
ON SEPARATE FILE(1), EXPERn.EXP(2) OR BOTH(3)?
1
Name of file?
BLIND.MAT
OPENING FILE BLIND.MAT
```

Examination of the cell scalars show that r11 = r33 ≠ r22, r23 = r12 = 0, and r31 = -(1/2)r11. Locate this set of relationships in the table in the BLIND section of the black loose leaf binder.

Now use INDEX to index the peaks in the PEAK16.REF file with the reduced cell.

```
ANLPNS UD1:SCD> INDEX
INDEX reads from a PEAKx.REF;n or EXPTx.REF;n file and
writes indexed data on a PEAKx.REF:n+1 or EXPTx.REF;n+1
file (n is the file version number).

PEAKx.REF(1), EXPTx.REF(2) or PEAKINT(3) file?
  Enter 1, 2 or 3: 1
EXPNUM? 16
Restrictions on the SEQNUMs (Y/N)? N
Restrictions on the histograms (Y/N)? N
Input matrix at console(1), from a matrix file(2) or from an EXPERn.EXP file(3)?
   Enter 1, 2 or 3: 2
Enter the "filename.filetype" of the matrix file: BLIND.MAT
 MATRIX
      0.204620  0.066250 -0.094725
     -0.050643  0.176782  0.016423
      0.185295  0.039659  0.139464

 4.895000  5.416000  4.889000 90.029999119.623001 89.749001  112.6860
Indices will be listed on the PRINT.LOG file.
DO YOU WISH TO RETAIN THE NEW FILE (Y,N)?Y
FORTRAN STOP
```

If you wish, you can examine the PRINT.LOG file to see how well the peaks are indexed. Now run LSQRS to get the best unit cell parameters and orientation matrix using all the peaks in the PEAK16.REF file.

```
ANLPNS UD1:SCD> LSQRS
Is input on a
      (1) PEAKn.REF file?
      (2) EXPTn.REF file?
or a  (3) PEAKINT output file?
Enter 1, 2 or 3: 1
Enter EXPNUM: 16

Do you want to select individual HSTNUMs (Y/N)? N
Minimum and maximum wavelengths: 0.5,5.0
Minimum peak count: 1

List reflections (1) on the terminal
                 (2) in a PRINT.LOG file
                 (3) or both?
Input 1, 2 or 3: 3


INDEX TRANFORMATION MATRIX:

 |     1.0     0.0     0.0| |hOLD|       |hNEW|
```

```
 |     0.0     1.0     0.0| |kOLD|   =   |kNEW|
 |     0.0     0.0     1.0| |lOLD|       |lNEW|

INPUT NEW TRANSFORMATION MATRIX (Y,N)?
Y
INPUT NEW TRANSFORMATION MATRIX
ROW 1: 0.,0.,1.                  ! This is the transformation matrix from
ROW 2: 1.,0.,0.                  ! the table of cell scalars.
ROW 3: 0.,1.,0.


INDEX TRANFORMATION MATRIX:

 |     0.0     0.0     1.0| |hOLD|       |hNEW|
 |     1.0     0.0     0.0| |kOLD|   =   |kNEW|
 |     0.0     1.0     0.0| |lOLD|       |lNEW|

INPUT NEW TRANSFORMATION MATRIX (Y,N)?
N
Input individual SEQNUMs (Y/N)? N
LATTICE PARAMETERS:
   4.8758    4.9387    5.4205   90.0313   90.3433  118.9134    114.25
LEAST SQUARES OUTPUT FOR EXPERIMENT  16 HISTOGRAM     1
  #    H    K    L       X      Y      Z      XCM     YCM      WL      IPK

     1  4.  -6.  -9.   33.9    4.8    6.1   -3.21  -11.96   0.649      102
  ----                 33.6    4.3    6.0   -3.32  -12.11   0.648
       3.98  -5.98  -9.02     DELHKL =    0.07
```

SEQNUMs 2 to 26 not shown.

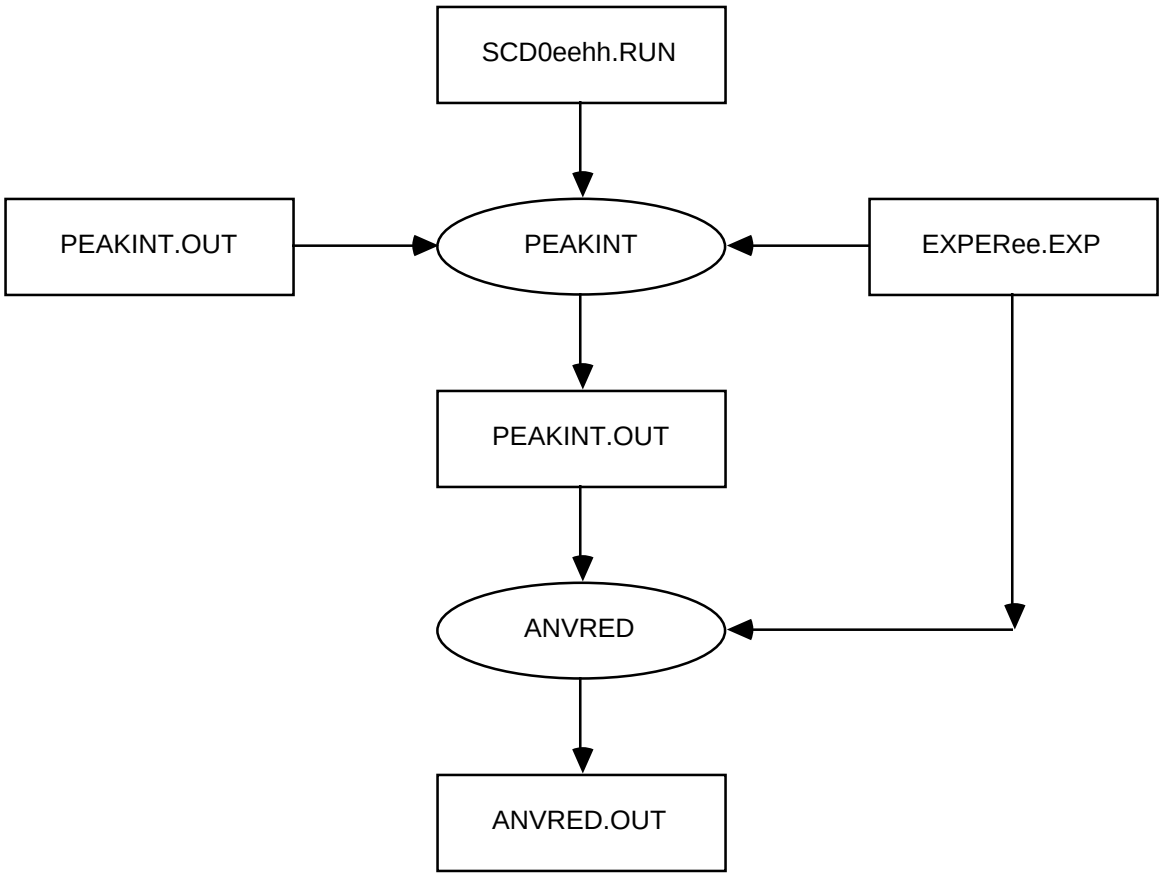
```
    27  0.  -1.  -3.   23.8   61.7   85.3   -6.36    6.33   2.115      682
  ----                 23.8   61.8   85.4   -6.37    6.37   2.117
       0.00  -1.00  -3.00     DELHKL =    0.01
LEAST SQUARES SUMMARY:



ORIENTATION MATRIX:
  0.18214   0.04038   0.14176
  0.20134   0.06616  -0.09269
 -0.04994   0.17688   0.01596
LATTICE PARAMETERS:
   4.8758    4.9387    5.4205   90.0275   90.3476  118.9134    114.25
LATTICE PARAMETER STANDARD DEVIATIONS:
   0.0129    0.0149    0.0084    0.1944    0.1760    0.2318      0.55
MINCNT      1    TOTAL NUMBER OF REFLECTIONS      27
WLMIN, WLMAX   0.5000   5.0000
STORE MATRIX AND CELL PARAMETERS IN MATRIX FILE(Y/N)?
Y
ENTER filename.filetype (15 CHARACTERS)
LS1601.MAT
Save matrix and cell parameters in the EXPERn.EXP file (Y/N)? Y
Orientation matrix and unit cell dimensions already
stored in EXPERn file
 0.204550  0.185028  0.050453
 0.066270  0.041051 -0.177062
-0.093718  0.137533 -0.014767

  4.9360   4.9440   5.4142   90.082   89.923  120.260
Replace them with new parameters (Y/N)? Y
FORTRAN STOP
```

The hkl indices were only transformed for the LSQRS calculations, but the PEAK16.REF file still contains the indices for the reduced cell. To transform them to the above unit cell, run INDEX again.

```
ANLPNS UD1:SCD> INDEX
INDEX reads from a PEAKx.REF;n or EXPTx.REF;n file and
writes indexed data on a PEAKx.REF:n+1 or EXPTx.REF;n+1
file (n is the file version number).

PEAKx.REF(1), EXPTx.REF(2) or PEAKINT(3) file?
  Enter 1, 2 or 3: 1
EXPNUM? 16
Restrictions on the SEQNUMs (Y/N)? N
Restrictions on the histograms (Y/N)? N
Input matrix at console(1), from a matrix file(2) or from an EXPERn.EXP file(3)?
   Enter 1, 2 or 3: 3
 MATRIX
      0.182137  0.040381  0.141757
      0.201344  0.066157 -0.092685
     -0.049940  0.176883  0.015958

 4.875800  4.938700  5.420500 90.028000 90.348000118.913002  114.2529
Indices will be listed on the PRINT.LOG file.
DO YOU WISH TO RETAIN THE NEW FILE (Y,N)?Y
FORTRAN STOP
```

Data Integration and Reduction

DATA INTEGRATION AND REDUCTION



ee = EXPNUM
hh = HSTNUM
PEKINT.OUT = reflection file
ANVRED.OUT = reflection file
EXPERee.EXP = experiment file (includes matrix)

Examples of peak integration

The first choice for peak integration is the program **PEAKINT** which integrate each peak with both 3x3x3 and 5x5x5 integration dimensions. In the latter case, the time channels which are integrated range from -1 to +3 relative to the peak maximum. The second choice for integrating is **INT85Z** which permits the user the set the integration volume limits.

If **PEAKINT** and **INT85Z** are not suitable for integration because of a large mosaic, twinning or multidomains resulting in broad or multiple peaks, then the alternative is **INTSCD** written by (in alphabetical order) Bruce Forsyth, Rob Stansfield, Andy Stringer, Clive Wilkinson and Chick Wilson. The following is an example of the INTSCD.DAT file read by subroutine PINPUT.

```
Printing flags (IPRNTS, IPRNT1,2,3,4,5,0).
  0  4
First pass (IMD1, ITBG, XSD); box limits (ACC1AN, ACC1CA, ACC1FR).
 0      3      3.0
 0.4  0.4  0.4
Second pass (IMD2, VOLFAC, NCONT, NUSE); FRHT(I); box; ELPS(I,J).
 0      4.0    4     3
 0.20   0.10   0.05   0.02
 0.4    0.4    0.4
     0.092      0.0608    0.0389
     0.0456    -0.0550   -0.0394
Third pass XVOLBG; NVOLMX; (NUMELM(I)); NCONM; (NUMMDL(I))
  2.5
 18
              1220  1060   930
   800   690   580   490   410
   340   270   220   170   130
   100    70    50    30    20
 15
    50    80   100   150   250
   300   400   500   600   700
   800  1000  1500  2000  2500
Weak peaks (PSIGWP, PSGSHP, NWPKS, DVOL1, DVOL2).
   0.5  3.   3  500  500
Normalisation constants (XMONST, XANGST).
 10000.   0.1
```

The following definitions of input parameters are based on written comments by Clive. Numbers which have to be changed most often are in bold face.

IMD1	box type (0 = rectangular, 1 = ellipsoidal).
ITBG	number of iterations of background calculation in first pass (normally 3).

XSD — points which are more than this number of S.D.'s from mean in background calculation are rejected (normally 3).

ACC1AN, ACC1CA, ACC1FR — multipliers in X,Y,T for "first pass box." ["Reflection box" of data read from file is bigger than this (unless numbers are 1.0).]

IMD2 — box type (see IMD1 above).

VOLFAC — only relevant if previous number is 1 for ellipsoid (unusual).

NCONT — numbers of levels at which peak will be contoured.

NUSE — contour level number which is used as "standard."

FRHT(I) — fractional contours for peak modelling (I=1,3).

box — multiplies X,Y,T for second pass box limits (when modelling).

ELPS(I,J) — default shape ellipsoid parameters ($1/a^2$ = 0.3, $1/b^2$ = 0.3, $1/c^2$ =0.5 here).

XVOLBG — factor by which $\sigma(I)/I$ is multiplied to define peak boundary. 2.5 is about correct for Frank Rotella's vesuvianite data as his $\sigma(I)/I$ minimum is fairly far out (~250). A bigger number will be required for other SCD "typical" peaks as $\sigma(I)/I$ occurs very close to the centre of the peak (~50 or less).

NVOLMX — number of volume steps.

NUMELM(I) — volume (cells) steps for modelling (I=1,NVOLMX).

NCONM — number of volume steps.

NUMMDL(I) — volume (cells) steps for peak integrations (I=1,NCONM).

PSIGWP — signal/noise ratio I_0/pB for "strong/weak" decision. Having decided on the appropriate volume for DVOL1 and DVOL2 from XVOLBG above (say 500 in Frank's case), this number decides how many strong peaks (and therefore models) you get. Typically ~0.5 is OK, but may need to lower it if very few "strong" peaks around.

PSGSHP — if (max peak count) X fractional height chosen above (3) as standard < PSGSHP X SQRT(B) ??? add to library ("intermediate"). [Not clear (AJS).]

MWPKS — n.a.

DVOL1, DVOL2 — default volumes for peak if no models available. (Peak measured inside DVOL1, Bg outside DVOL2. I (CW) make these the same. DVOL1 is also used as the value of p in the I_0/pB strong/weak decision.) Default volume should be roughly value given by XVOLBG (say 500 here).

XMONST, XANGST n.a.

Display Commands

Commands are available for making X, Y or T histogram plots and sum-channel plots of live or file area detector data. The type of plot data is set with the TYPE command:

TYPE=FD ---> density plot of file data

TYPE=LD ---> density plot of multibus (live) data

TYPE=FH ---> histogram plot of file data

TYPE=LH ---> histogram plot of multibus (live) data

The density plot time-slice range is set with the ZMIN and ZMAX, or the ZLIM commands. Type PAGE to show successive individual plots: for example, if ZLIM=15,21, PAGE would show 15 then 16 etc. to 21. Alternatively, typing ADD with the same ZLIM would give a single plot which is the sum of the histograms 15 through 21.

You must have UNIT=C to use the density plot. This is the default.

One-dimensional histogram plots are set up using the XPT, YPT, TPT and HST commands:

HST=X ---> vary X; Y and T constant

HST=Y ---> vary Y; X and T constant

HST=T ---> vary T; X and Y constant

XPT, YPT and TPT are used to select the X,Y,T point through which the plot must pass. For example, XPT=17 means the plot must pass through X=17, measured in channels from the left edge of the density plot. Limits on the 1-D histogram plots are set using XMIN and XMAX, or XLIM.

The sum-channels are plotted by setting UNIT=S and TYPE=LH or TYPE=FH. This is a plot of the total number of counts in a time-slice vs. the time channel number. To plot the monitor spectrum, set UNIT=T, TYPE=L or F, and ID=1.

Once all the parameters are set, enter D to initiate the plot. The plot will appear on the color CRT terminal. Enter CVS to clear the screen and exit for the display program.

Programs on the VAX

Programs with an asterisk following their name exist as executable images on the [SCD] directory. They can be run, or set-up, interactively simply by typing the name of the program without "RUN [SCD]" preceding the name. Many of the programs automatically prepare a COM file for the user to submit to one of the batch queues. All source codes (except for structure analysis programs such as ANVLS) are stored in [SCHULTZ.PROGRAMS]. They can be compiled using the **FOR** command and can be linked to all subroutine object libraries using the **LLIB** command.

ANALYZE	Summarizes intensity distribution of all histogram data for a given experiment. It prints out the intensity distributions in terms of I(integrated)/sig(I) and of I(integrated). Required data file is EXPTn.REF .
ANVLS	Argonne National Laboratory Variable Wavelength Least Squares performs least squares fit of the data to positional and thermal parameters. This program is the ORXFLS3 program adapted to variable wavelength data. See [SCHULTZ.ANVLS]ANVLS.MEM for a detailed description.
ANVRED*	Argonne National Laboratory Variable Wavelength Data Reduction performs data reduction on EXPTn.REF or PEAKINT output files. An interactive program on the VAX system, it corrects the reflection data for absorption, a source spectrum, detector efficiency, sin(theta)**2/wl**4 and a monitor count. This program generates two files, one of which is compatible with ANVLS.
BKG	Program to determine peak and background limits around Bragg peaks.
BLIND*	Given reflection data (from the PEAKn.REF file of input by the user) BLIND indexes the data and presents for the user the unit cell parameters and an orientation matrix. The user has the option of storing this data on the EXPERn.EXP file or a file_name.MAT file for future use. (See also **MULTI_BLIND** and **MATRIX**.)
CANTFOUR	Canterbury Fourier program.
CONTOUR	Performs contour plots of histogram data or Fourier maps.
DECAL	Program to calculate instrument parameters using data from a NaCl crystal. Calibrated parameters are the X and Y detector conversion values (channel number to position in centimeters), the location of the "center" of the detector, the sample-to-moderator distance, and the shift in t-zero.
DIFFPEAK	This program will subtract a "background" histogram from a "data" histogram and search for a list of "difference" peaks.
DLIST	Calculate and list d-spacings of reflections on EXPTn.REF file.

* Currently available as an executable image on [SCD].

DSPACE	Calculate d-spacing for each histogram wavelength channel for a specified X,Y position.
EDREF*	Allows the user to delete reflections from the reflection file (see also PEAKEDTEDT).
EDTREF	Allows the user to change parameters within a reflection record in the EXPTn.REF file, or to delete the reflection from the file.
FOURIER	Fourier and Patterson synthesis program. See [SCHULTZ]HIRO.MEM for details.
FRIEDEL	Calculates the position of the Friedel pair of an input reflection for general chi and phi angles. Useful for centering crystals in the Displex vacuum shroud.
HKLCAL*	Calculates the h,k,l value of the detector center (WL = 1.0) given the orientation matrix, DETA, DETD, OMEGA, CHI, PHI.
HTOX*	Calculates the detector space coordinates corresponding to an entered value of h,k,l. Useful for locating specific peaks in a histogram, particularly if they correspond to incommensurate values of h,k,l.
INDEX*	Given an orientation matrix, indexes reflections on a PEAKn.REF or EXPTn.REF file.
INDEX2	Given an orientation matrix, program calculates h,k,l with user input histogram positions (x,y,z).
INT85	Calculates the position of peaks in a histogram using an orientation matrix, integrates the region around the calculated peak position and writes the result on a EXPTn.REF file. Input files are SCDOnnnn.RUN files and possibly a xxxxxx.MAT file. The program is capable of handling histograms with variable time channel widths and is compatible with other keyfile access programs. The time width of a reflection is defined by minus and plus delta values from the peak position.
INT85Z*	Same as INT85, but the time width of a reflection is defined by a minus number of channels and a plus number of channels from the peak position. (See also **PEAKINT.**)
KEY*	Creates a key-access file (see PROGRAMMING GUIDE) containing instrument parameters, cell parameters and experimental data, excluding the actual histogram. The file is named EXPERn.EXP, where 'n' is the experiment number.
LEVY	Calculates setting angles to obtain a hemisphere of data with minimum overlap.

* Currently available as an executable image on the [SCD].

LINEPL — For a given histogram, displays the variation of intensity across (constant Y) or up-and-down (constant X) the face of the detector for a given time layer. Will also perform plots of intensity versus wavelength and reciprocal d-spacing. (See also **QPLOT.**)

LSQRS* — Using indexed data from a reflection file, performs a unit cell least squares to obtain the best cell parameters and orientation matrix. The user has the option of storing the matrix and cell constants for future use.

MATRIX* — User inputs cell parameters and a list of peaks. Program tries to index peaks and obtain an orientation matrix. (See also **BLIND** and **MULTI_BLIND**.)

MONITOR — Obtains the beam monitor spectrum from a RUN file. The output contains wavelength, intensity and time-of-flight.

MULTI_BLIND* — This program creates a COM file containing a series of BLIND runs for every possible combination of four reflections in a list of SEQNUMs from a PEAKn.REF file. After submitting to a batch queue, the user should examine the LOG file to identify any successful runs. The user should then run BLIND interactively to input those four reflections and obtain an orientation matrix. (See also **BLIND** and **MATRIX**.)

PEAKEDT* — Deletes reflections from a **PEAKINT** output file.

PEAKINT* — Integrates Bragg peaks. Two integrated intensities are obtained for each peak, a small one based on a 3x3x3 integration envelope, and a large one based on a 5x5x5 envelope. Use **PEAKPRT** to list the output reflection file.

PEAKPRT* — Program to list contents of a **PEAKINT** output file. Also calculates average ratios of small to large integration envelopes for the strong peaks.

PEAKS* — Searches histograms for peaks, interpolates and stores the results on a PEAKn.REF file. Use **PTREF** to print the reflection file.

PEKPLV — Plots peaks from a EXPTn.REF file in x,y, and z direction. The histogram run file is also needed.

PLOT3D* — This program reads input data files (in binary format) created by either RLPLN or SUMHST and produces a plot file (PLT2.dat) which can be displayed on various graphic devices. Given the PLT2.DAT file, a user simply issues the **POSTPLOT** command on a terminal.

PTHIST* — Prints portions of the raw histogram data on the console and/or screen for examination. There is also an integration option.

PTREF* — Prints the contents of EXPTn.REF or PEAKn.REF on the line printer. Use **PEAKPRT** for a reflection file created by PEAKINT.

---

* Currently available as an executable image on the [SCD].

QPLOT* Plot any q-vector defined by two hkl points. Use **EASYPLOT** to plot the results on the output file.

RLPLN* Calculates the variation in intensity across a reciprocal lattice plane (one Miller index constant) for one histogram. The user specifies a reflection corresponding to the desired h, k or l value to be kept constant. The results are written on a binary data file. This data file is read by program PLOT3D which displays the results.

RLROW Plots the variation in intensity across a reciprocal lattice vector (two Miller indices constant) for one histogram. The user either specifies a reflection number corresponding to the desired constant hkl values, or inputs directly the values of the indices. A file named ROW.NUM is also created containing the numerical values (intensity vs. hkl) calculated by the program. (See also **QPLOT.**)

SCAN* Obtains data from a histogram for a scan of X, Y or T with the other 2 coordinates constant. T scans are also obtained as wavelength and d-spacing scans. The output is compatible with **EASYPLOT**.

SCNPLT This program displays the reciprocal space coverage of the area detector for goniometer angles specified by the user. The version of the program in [SCD] produces hardcopy, whereas the version in [SCD.LARSON.SCD] runs interactively using the VS11 color display.

SEPD_SPEC Calculates an incident spectrum based on a fit to vanadium data from the SEPD. To get the current SEPD incident intensity parameters for the type 1 function of equation 3 on page 1-2 of the Users Manual FOR RIETVELD ANALYSIS AT IPNS, **RUN DRA1:[ROTELLA]TOFPARM**.

SETANG* Calculate the setting angles CHI and PHI given an orientation matrix (on the matrix file), H,K,L, DETA, DETD and OMEGA.

SIM* Simulates a histogram of Bragg data.

SORTAV Sorting and averaging program. See [SCHULTZ]HIRO.MEM for details.

SORTD Program for sorting reduced TOF SCD data. Multiple and equivalent reflections are listed together along with statistical information.

SPECTRUM Obtains a one-dimensional spectrum file for correcting data for the wavelength dependence of the incident spectrum and the detector efficiency. It is used periodically by the Instrument Scientist to analyze a histogram from a spherical vanadium sample. (See also **SEPD_SPEC**.)

---

* Currently available as an executable image on the [SCD].

STATS* For each histogram, this program summarizes the number of reflections with intensity > 3*sigma, > 5*sigma and > 10*sigma and gives the total number of reflections found. The program works on reflection files EXPTn.REF or a PEAKINT output file. The program also output a file compatible with **EASYPLOT** of the number of reflections above 3 sigma per 0.1 Angstroms in the wavelength range.

SUBBKG This program subtracts one histogram (usually background) from a second histogram (data) and stores the result in a third histogram. (See also **DIFFPEAK**.)

SUMHST* This program creates a file (with user supplied filename.filetype) which is the input to the plot program PLOT3D.

TRACER* Lattice transformation and cell reduction program.

TRANS3* Calculated detector coordinates (XCM,YCM,WL) from channel numbers (X,Y,Z) using instrument parameters input by the user. Writes to the VDU only: for output file creation use XTOXCM.

UMAT3* Calculates an OM using three reflections from the same histogram.

XTOD* Input channel numbers for a point in a histogram and obtain XCM, YCM, WL, and the reciprocal and read d-spacing.

XTOH* Program to calculate hkl values from XYZ channel numbers input by the user (inverse of HTOX).

XTOXCM Program to read reflection file and write a new file with updated values for XCM,YCM,WL based on instrument parameters input by the user. For screen output only, use TRANS3.

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* Currently available as an executable image on the [SCD].

VAX Subroutines

Subroutines on the VAX reside in the [SCHULTZ]SCDLIB.OLB library. The exceptions are the GETxxx and READ2D subroutines, which are stored in the [PNSLIB]RUNLIB2.OLB library. Use the LLIB command to link to these libraries and also PNS_LIB:TOOLS/LIB and VIDEO/OPT.

ABC (U,A,B,C,ALPHA,BETA,GAMMA,VOL)
Given the matrix U(3,3), ABC calculates the unit cell constants.

AXT (AV,T,CV)
Performs matrix multiplication AV*T = CV, where T is 3x3 and AV and CV are column matrices.

CALDET (AMAT)
This is a function, not a subroutine. It calculates the determinant of the 3x3 matrix AMAT.

CENTER (H,K,L,ICELL,IEX)
Tests for extinctions due to a centered lattice.

CTAU (XCM,YCM,WL,TAU,DETA,DETD)
Calculates TAU (2sin(theta)/lamda) given the other quantities.

DEAD (NRUN)
Reads in the dead-time spectra and averages.

DVTODET (XD,YD,ZD,XCM,YCM,WL)
Convert diffraction vector (XD,YD,ZD) in units of reciprocal Angstroms to detector coordinates (XCM,YCM,WL). The diffractometer angles are stored in COMMON/SET/.

EFFMAP
Calculates a three-dimensional detector efficiency map (X,Y,T) for a histogram and stores values in array DETEFF.

EZCODE (NRUN)
A function that converts an integer (NRUN) to an ASCII code.

GETxxx (RUN,IERR,var1[,var2...])
Various subroutines from [PNSLIB]RUNLIB2.OLB that get data from the run file. Most of these values are stored in the DATACOM common by subroutine KEYWRITE.

GETCHI	CHI
GETCST	ICST,ITNUM
GETDAT	IHIST,NUMB,OFFSET [IHIST is INTEGER*2] **(see READ2D)**
GETDTA	DETA
GETDTD	DETD
GETELN	ELAPSD
GETLI	L1

---

* Currently available as an executable image on [SCD].

GETLNG	IHIST,NUMB,OFSET [IHIST is INTEGER*4] **(see READ2D)**
GETNAM	USER
GETOMG	OMEGA
GETPHI	PHI
GETPLS	PULSES
GETSDT	STRDAT
GETSTM	STRTIM
GETTTL	DESCR
GETWMI	TMIN
GETWMA	TMAX
GETWNM	WLNUM
GETXNM	XNUM
GETYNM	YNUM

GHIST (IHIST,IYMIN,IYMAX,LAYER)
Retrieves histogrammed data from disk. Time layer = LAYER, minimum and maximum values for the y channels are IYMIN, IYMAX respectively. The data are placed in the 1-dimensional array IHIST(7395). The calling routine must contain the following statement: COMMON/ALL/ XNUM,YNUM,WLNUM, RUN,I84
(see READ2D)

GHIST2 (IHIST,LAYER)
Gets a all data for one time-slice. If you need data from more than one Y channel per time-slice, use this subroutine rather than GHIST to decrease the number of disk-reads. The calling routine must contain values for XNUM and YNUM in "COMMON/ALL/XNUM,YNUM,WLNUM,RUN,I84" **(see READ2D).**

GTIMOD (IMODE,PRGNAM,LPRGNM)
If job is running in batch mode, return IMODE = 0. If job is running in interactive mode, opens a COM file (UNIT=41) to submit to batch and returns IMODE = 1. Programs which call this subroutine must link to PNS_LIB:TOOLS/LIB.

HUX (XH,XK,XL,U,XCM,YCM,WL)
Calculate detector coordinates (XCM,YCM,WL) from the indices XH,XK,XL and the U matrix. "COMMON/SET/CHI,PHI,OMEGA,DETA,DETD" must also be provided.

INFO (NRUN,IERR)
Given the run number INFO retrieves the following data from disk: CHI,PHI,OMEGA,DETA,DETD,MONCNT. This data is transferred with the following common statements: "COMMON /SET/CHI,PHI,OMEGA,DETA,DETD /MONI/MONCNT". IERR is returned as .LT. 0 if an error is encountered.

INSCAL
Obtains calibrated instrument parameters from file [SCD]INSPAR.DAT or from user. Requires "COMMON /INSPAR/ XLENG, TZERO, XBOX85, YBOX85, XBIAS, YBIAS, XLEFT, XRIGHT, YLOWER, YUPPER".

INTERP (XOBS,YOBS,ZOBS,REFLAG,X,Y,Z,IPK,INTRP,IDIM,IHIST)
Calculate interpolated histogram peak position coordinates X,Y,Z.

INTG (XOBS,YOBS,ZOBS,IPKOBS,REFLAG,DELTAX,DELTAY,DELTAZ,I,IT,BKG,SIG,IHIST)
Determine the integrated intensity of a Bragg peak.

INTGT

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* Currently available as an executable image on the [SCD].

Peak integration subroutine called by REFGEN.

INVERT (AMAT,N,DET)
Invert the NxN matrix AMAT, which is defined as REAL*8. The maximum value of N is 100. The routine also returns the determinant DET.

JINDEX
Transforms H,K,L indices using a transformation matrix input by the user.

KEYWRT (IUNIT,ITYPE,IWRT,IVANA)
Subroutine to read, transfer of update data on the EXPERn.EXP file, where

```
IUNIT =     unit number of EXPERn.EXP file (usually 45)
ITYPE =     1 -- update/create/read orientation matrix and cell
      dimensions.
            2 -- update/create/read detector parameters.
            3 -- create/read histogram parameters.
IWRT  =     0 -- create/read only; no update option.
            1 -- update/create/read all allowed.
IVANA =     0 -- normal data.
            1 -- vanadium spectrum (HSTNUM set to 90).
            2 -- background spectrum (HSTNUM set to 80).
```

LAUE (XCM,YCM,WL,DIFFXX,DIFFYY,DIFFZZ)
Calculates the diffraction vector in reciprocal Angstrom units from XCM,YCM,WL. The calling routine also must contain the diffractometer angles in "COMMON/SET/CHI,PHI,OMEGA,DETA,DETD".

MAT2EXP (BA,SIGA,U)
Writes lattice constants and orientation matrix on the EXP file for the first time. The parameters are passed to the subroutine from an interactive main program, and are not obtained from a matrix file. BA and SIGA are arrays of dimension (7) containing A,B,C,ALPHA,BETA,GAMMA,VOL and their sigmas. U is the (3,3) orientation matrix. The EXP file must be opened and assigned to unit 45.

MATIN2 (AMAT,BMAT)
Second version of MATINV. The original matrix and its inverse are AMAT and BMAT, respectively.

MATINV (AMAT)
Inverts the 3x3 matrix AMAT.

MATMUL (AM,BM,CM)
Performs the multiplication CM=AMxBM, where AM,BM,CM are all 3x3 matrices.

MONPLT (EXPNUM)
Saves a smoothed dead-time spectrum on a DTS file for data reduction.

NEWROT (U,CHI,PHI,OMEGA)
Rotates a 3x3 matrix (U) for which all angles are zero to a 3x3 matrix at CHI,PHI,OMEGA

NTERP
Version of INTERP used in HNTINT.

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* Currently available as an executable image on the [SCD].

OPNCOM (PRGNAM,LPRGNM)
Creates a COM file to submit to batch after interactive session.

OPNEXP (IU,EXPNUM)
Opens existing or new EXP file. The unit number IU is usually 45.

OPNMAT (IUNIT,U)
Routine to open and read a filnam.MAT file. The orientation matrix is U(3,3) and the cell parameters and sigmas are entered into COMMONs labeled /CELL/ and /SIG/.

OPNREF (EXPNUM,IUNIT)
Routine to open existing EXPTn.REF file (n = EXPNUM, IUNIT = unit number).

OPNRUN (EXPNUM,HSTNUM)
Routine to open histogram run file.

PEAK (NOPK,MINCT,NSEARC,IDIM,IHIST,LAY1,LAY2)
Searches the histogram for Bragg peaks.

PHIST2 (IHIST,LAYER)
Puts an entire WL layer of data into a histogram RUN file.

QUAD
Determines the coefficients of a quadratic formula to fit a Bragg peak to Interpolate its maximum position.

READ2D (IHIST,LSUM,RUN,85,87,LAYER,1,IERR)
The data for one time-slice is returned in IHIST and the time-slice sum is returned as LSUM. The number of the time-slice is LAYER. IHIST is defined as INTEGER*4 IHIST(7424), where 7424 is an integer multiple (29) of 256 which is greater than or equal to 7395.

RECIP (REL,REC)
Calculate reciprocal cell parameters from real parameters, or vice versa. The arrays REC(7) and REC(7) contain real or reciprocal A,B,C,ALPHA,BETA,GAMMA,VOL In units of angstroms, degrees and angstroms**3, respectively.

RECIPR
Calculate reciprocal cell parameters and cell volumes from real cell parameters. The parameters are transmitted through COMMON/CELL/.

REFFIL (EXPNUM,BREFL,IFILE)
Builds and stores the name of the reflection file for experiment EXPNUM In the byte array BREFL. IFILE = 0 for PEAKn.REF file and otherwise for EXPTn.REF file.

REFGEN (JMN,JMX,CURMAT,ICELL,L1,TMIN,TMAX)
For a particular crystal orientation and instrument setting, predicts the indices (H,K,L) and positions (XCM,YCM,WL) of reflections in the histogram.

REFGN2
Second version of REFGEN.

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* Currently available as an executable image on the [SCD].

REFNAM (EXPNUM,BREFL)
Builds and stores the name of the reflection file for experiment EXPNUM in the CHARACTER*11 variable BREFL.

REFSET (JMX)
Set-up routine for REFGEN.

SAVMAT (U,A,B,C,ALPHA,BETA,GAMMA,SIGA,SIGB,SIGC,SIGALP,SIGBET,SIGGAM)
Save U matrix, cell parameters and sigmas on a filnam.MAT file.

SMOOTH
Spline smoothing routine.

SORTMAT (N,AA,BB,CC,DD)
Subroutine to sort four arrays (AA,BB,CC,DD) with respect to ascending values of DD.

SPECTR (EXPNUM,WLNUM,WLMIN,WLMAX,CSPCT)
Uses the uncorrected vanadium incoherent scattering spectrum and corrects it for background, absorption and detector efficiency.

TMAT (T)
Routine to calculate the T matrix from the real unit cell parameters in the labeled common /CELL/. The routine also calculates the real and reciprocal cell volumes and the reciprocal unit cell parameters.

TRANS2 (X,Y,Z,IFOR,SCM,YCM,WL)
Same as TRANSF, except most parameters are passed using the COMMONs in COMMON.FOR.

TRANSD (X,Y,Z,IFOR,XCM,YCM,WL)
Transforms between histogram and detector coordinates (see TRANSF). This subroutine is capable of handling time channel doubled histogram data.

TRANSF (X,Y,Z,FORWRD,XCM,YCM,WL,XNUM,YNUM,TMIN,TMAX,WLNUM)
Transforms between histogram and detector coordinates. When FORWARD = 1, histogram ---> detector; when FORWARD = 0, detector ---> histogram.

TRNSFR (XNUM,YNUM,WLNUM)
Transfers a portion of the histogram run file to the array ISTOR(15,15,15).

TRNSPO (AMAT,BMAT)
Transpose 3x3 matrix AMAT and return as BMAT.

TXB (T,B,C)
Perform matrix multiplication T*B = C, where T is 3x3 and B and C are column matrices.

UPSET (EXPNUM)
Set-up routine for DCOL.

UPSET2
Second version of UPSET.

---

* Currently available as an executable image on the [SCD].

UTF (UOBS,UCALC,RA)
Calculate a new U matrix (UCALC) using the observed U matrix (UOBS)and the known cell parameters (RA).

VNOC (TMIN,TMAX,WLMIN,WLMAX,RUN,DETD,L1)
Convert TMIN and TMAX to WLMIN and WLMAX.

WEIGHT (X,Y,Z,WF,WI)
Uses a weighted sum technique to calculate the interpolated intensity WI at nonintegral histogram coordinates X,Y,Z. W is the exponential weighting factor and is usually set to 2.0 or 1.5.

WLCONV (TMIN,TMAX,WLMIN,WLMAX,RUN,DETD)
Second version of VNOC.

XUH (XCM,YCM,WL,U,XH,XK,XL)
Converts detector coordinates to nonintegral hkl coordinates.

---

* Currently available as an executable image on the [SCD].

Programming Guide

COMMON.FOR

The FORTRAN statement

```
      INCLUDE 'INC:COMMON.FOR/LIST'
```

was used in old programs to include the following lines

```
      INTEGER*2 EXPNUM,FORWRD,GENTXT,H,HSTNUM,INTDIM
      INTEGER*2 K,L,NRUN,REFLAG,SEQNUM,WLNUM,XNUM,YNUM
      INTEGER*4 ELAPSD,IT,MONCNT,OFFSET,TMAX,TMIN,IPK
      REAL*4    INTI,L1
      BYTE      BREFL(20),BTEST(4),BUFF(80),DESCR(80),IDATE(9)
      BYTE      ITIME(8),STRDAT(9),STRTIM(8)
      COMMON    /ALL/    XNUM,YNUM,WLNUM,RUN
      COMMON    /CELL/   A,B,C,ALPHA,BETA,GAMMA,VOL,
     &                   AS,BS,CS,ALPHAS,BETAS,GAMMAS,VOLS
      COMMON    /INSPAR/ L1,TZERO,XBOX85,YBOX85,XBIAS,YBIAS,
     &                   XLEFT,XRIGHT,YLOWER,YUPPER
      COMMON    /MONI/   MONCNT
      COMMON    /RFIL/   BUFF,NLEN
      COMMON    /SET/    CHI,PHI,OMEGA,DETA,DETD
      COMMON    /SIG/    SIGA,SIGB,SIGC,SIGALP,SIGBET,SIGGAM
      COMMON    /TIMES/  TMIN,TMAX
      DATA      RAD /57.29577951/
```

This should not be used for programs which involve key-access files.

DATACOM.FOR

For new programs which involve key-access files, the FORTRAN statement

```
      INCLUDE 'INC:DATACOM.FOR/LIST'
```

will include the following lines in the program:

```
         INTEGER*2 EXPNUM,FORWRD,GENTXT,H,HSTNUM,INTDIM
         INTEGER*2 K,L,NRUN,NRUN1,NTIME(256),REFLAG,SEQNUM
         INTEGER*2 WLNUM,XNUM,YNUM
         INTEGER*4 ELAPSD,DEDSUM,MNCT(256),NSUM(256),OFFSET,PLS
         INTEGER*4 SUMTOT,TMAX,TMAXH,TMIN,TMINH,IDTIME(256)

         REAL*4    INTI,L1

         BYTE      BTEST(4),BUFF(80),DESCR(80)
```

---

* Currently available as an executable image on [SCD].

```
      BYTE      ENDDAT(9),ENDTIM(8),IDATE(9)
      BYTE      ITIME(8),STRDAT(9),STRTIM(8),USER(80)

      CHARACTER BREFL*20,PRGNAM*10,crun*4,EXPNAM*14,RVRS*4,OFF*4

      DIMENSION U(3,3),VCONT(5)

      COMMON    /ALL/    XNUM,YNUM,WLNUM,RUN,I84
      COMMON    /CELL/   A,B,C,ALPHA,BETA,GAMMA,VOL,
     &                   AS,BS,CS,ALPHAS,BETAS,GAMMAS,VOLS
      COMMON    /INSPAR/ L1,TZERO,XBOX85,YBOX85,XBIAS,YBIAS,
     &                   XLEFT,XRIGHT,YLOWER,YUPPER
      COMMON    /INSTR/  INAME
      COMMON    /LIMITS/ WLMIN,WLMAX,ITMIN,ITMAX,XBOXCM,YBOXCM
      COMMON    /MONI/   MONCNT
      COMMON    /RFIL/   BUFF,NLEN
      COMMON    /SET/    CHI,PHI,OMEGA,DETA,DETD
      COMMON    /SIG/    SIGA,SIGB,SIGC,SIGALP,SIGBET,SIGGAM,
      1                       SIGVOL
      COMMON    /TIME/   NTIME,NDMIN,NDMAX
      COMMON    /TIMES/  TMIN,TMAX

      COMMON    /DATA1/  U,ELAPSD,DESCR,USER
      COMMON    /DATA2/  PLS,NCH,CTSPLS,PDEDAV
      COMMON    /DATA3/  STRDAT,STRTIM,ENDDAT,ENDTIM
      COMMON    /DATA4/  MNCT,IDTIME,NSUM,NMON,MNNUM
      COMMON    /DATA5/  MNSUM,DEDSUM,SUMTOT
      COMMON    /DATA6/  L1D,L2D,LOF
      COMMON    /DATA7/  XDS,YDS
      COMMON    /DATA8/  EXPNUM,HSTNUM,SEQNUM
      COMMON    /DATA9/  IMODE,RVRS,OFF
      COMMON    /DATA10/ CRUN
      COMMON    /DATA11/ EXPNAM,NRUN,NRUN1

      DATA      RAD /57.29577951/
      DATA      HOM /0.39559974/
      DATA      INAME /'SCD0'/
```

Reflection files

Reflection files PEAKn.REF and EXPTn.REF (n = EXPNUM) have file attributes

```
     RECORDTYPE='SEGMENTED' and FORM='UNFORMATTED'.
```

To open an existing file:

```
     CALL OPNREF (EXPNAM,IUNIT)
```

Each record is read using an unformatted READ statement:

```
     READ (IUNIT) SEQNUM,INTDIM,NRUN,H,K,L,X,Y,Z,XCM,YCM,WL,
    &     IPK,IT,BKG,INTI,SIG,REFLAG,CHI,PHI,OMEGA,DETA,DETD,
```

---

* Currently available as an executable image on the [SCD].

```
    &     MONCNT
```

Reflection files created by PEAKINT are different than those created by PEAKS or INT85Z. The following is an example of how to read a reflection file created by PEAKINT:

```
     INCLUDE 'INC:DATACOM.FOR/LIST'
     CHARACTER*15 REFNAM
          .
          .
          .
     TYPE 100
 100 FORMAT('$Enter "filename.filetype" : ')
     ACCEPT 110,REFNAM
 110 FORMAT (A)
     OPEN(UNIT=1,NAME=REFNAM,TYPE='OLD',FORM='UNFORMATTED')
          .
          .
          .
     READ (1,END=1000) SEQNUM,NRUN,H,K,L,X,Y,Z,XCM,YCM,WL,IPK,
    &  REFLAG,CHI,PHI,OMEGA,DETA,DETD,ELAPSD,
    &  XINT1,XSIG1,IDIM1,XINT2,XSIG2,IDIM2
```

Matrix files

Matrix and unit cell parameters are now stored on the EXPERn.EXP file. However, independent matrix files may sometimes be used. Matrix files file_name.MAT have the attributes FORM='FORMATTED', RECORDTYPE='FIXED', RECORDSIZE=80, and BLOCKSIZE=400.

To open and read an existing file:

```
     CALL OPNMAT (IUNIT,U)
```

The orientation matrix is stored in U(3,3) and the cell parameters and their standard deviations are entered into the labelled COMMONs /CELL/ and /SIG/.

Run files

Histogram, or run files, have names SCD0nrun.RUN, where nrun is the RUN number.

To open an existing RUN file:

```
     CALL OPNRUN (NRUN)
```

Data are obtained from the run files with:

```
     CALL READ2D (IHIST,LSUM,RUN,85,87,LAYER,1,IERR)
```

---

* Currently available as an executable image on the [SCD].

where LSUM is the sum of the counts on time-slice LAYER. IHIST is defined as INTEGER*4 IHIST(7424), where 7424 = 29*256, which is an integer value times 256 and is greater than 7395 = 85*87.

Data can also be obtained with:

```
CALL GETLNG (RUN,IERR,IHIST,NUMB,OFFSET)
```

Within each time-slice, the OFFSETs are as follows:

Symbol	Description	Offset	
S	Sum of 2-d data	0	
D	2-d data		2
E1	Neutron events outside of XY array	7355	
E2		"	7356
E3		"	7357
E4		"	7358
Q1	Neutron events out of bounds	7359	
Q2		"	7360
P	Sum of pulser counts inside window	7227	
R	Pulser pulses rejected by ADC deadtime	7353	
L	Neutron events lost due to deadtime	7354	

The total number of words in each time-slice (with XNUM = YNUM = 85) is 85*87 = 7395. Therefore, to obtain the 85x85 array for time-slice 10, the code would be:

```
DATA NUMB/7225/                              ! 85*85 = 7225
DATA NUMB2/7395/                             ! 85*87 = 7395
LAYER=10
OFFSET = (LAYER - 1)*(NUMB2 + 2) + 2
CALL GETLNG (RUN,IERR,IHIST,NUMB,OFFSET)
```

Key-access files

Key-access files have been introduced into the SCD program library. They contain the matrix file, the dead time spectrum file, the vanadium and background spectra files, and alleviate the need for reading the histogram header to obtain experimental parameters. They may be printed out in order to obtain an easily read record of experimental and instrumental data. The file will also be compatible with LANL software, and vice verse.

The file name is EXPNAM.EXP and has the attributes RECORDTYPE='VARIABLE', ACCESS='KEYED', ORGANIZATION='INDEXED', KEY=(1:12), FORM='FORMATTED' and CARRIAGECONTROL='LIST'. A particular record is read by defining the appropriate twelve character keyword and adding the specifier KEY=keyword to the corresponding READ statement; the format for any such READ command must skip over the key field before attempting to read a record:

```
FORMAT (12X,...).
```

---

* Currently available as an executable image on the [SCD].

To write a new record on the file, use a WRITE statement of form

```
     WRITE (unit,mm) keyword,...
  mm FORMAT (A12,...).
```

To change an existing record in the file first READ the record, then use a REWRITE statement with the same format as the above WRITE statement.

Subroutine KEYWRT may be used to read,write or update the data from an existing EXPNAM.EXP file; [SCDSOFT.INCLUDES]DATACOM.FOR must be included in the main program. KEYWRT may also be used to transfer data from a run file or a matrix file to the EXPNAM.EXP file.

The program KEY will create a new EXPNAM.EXP file or add run file to an existing file. It can be used to (i) create/update the orientation matrix and unit cell parameters; (ii) update instrument parameters.

EXPNAM.EXP files can be edited using EDT. However, after EXITing from EDT, the file must be converted back to a key-access format by typing

```
@[SCD]CNVRTEXP
```

Key definitions:

	DESCR	Title.
	USER	User name.
CRS0	VSIGV	Unit cell volume and sigma.
CRS1	ABC	Unit cell axes in Angstroms.
"	ABCSIG	Sigmas for unit cell axes.
"	ANGLES	Unit cell angles.
"	ANGSIG	Sigmas for unit cell angles.
CRS11	UBMAT1-3	Orientation matrix.
HSTnnnCHI		Chi angle for histogram nnn.
"	CTSPLS	Average counts per pulse for 3-d histogram.
"	DEAD 1-m	Dead time loss spectrum.
"	DEDSUM	Sum of dead time loss spectrum.
"	DETA	Detector angle.
"	DETD	Detector distance (cm.).
"	ELAPSD	Elapsed monitor counts.
"	ENDDAT	Date of histogram completion.
"	ENDTIM	Time of histogram completion.
"	L1D	
"	L2D	
"	LOF	Offset for start of overflow table. = NCH + 2*(WLNUM+2)
"	MNCT 1-m	Monitor spectrum.
"	MNNUM	Number of monitor time channels
"	MNSUM	Sum of monitor spectrum.
"	NCH	Number of 3-d histogram channels. = (XNUM*YNUM+2)*WLNUM
"	OMEGA	Omega angle.
"	PDEDSAV	Average percent dead time loss for histogram.
"	PHI	Phi angle.
"	PLSNUM	Total number of pulses.
"	STRDAT	Start date for histogram.
"	STRTIM	Start time for histogram.
"	SUM 1-m	Time-slice sum spectrum.

---

* Currently available as an executable image on the [SCD].

```
            "  SUMTOT                  Total number of counts in the
               histogram.
            "  TMAX                    Maximum TOF (microseconds).
            "  TMIN                    Minimum TOF (microseconds).
            "  TOF  1-m                Starting TOF for each time channel.
            "  WLMAX                   Maximum wavelength (Angstroms).
            "  WLMIN                   Minimum wavelength (Angstroms).
            "  WLNUM                   Number of wavelength channels.
            "  XNUM                    Number of horizontal detector
               channels.
            "  YNUM                    Number of vertical detector
               channels.
         INST  BCHI                    CHI offset.
            "  BDETA                   DETA offset.
            "  BOMGA                   OMEGA offset.
            "  DETA                    Detector angle.
            "  DETD                    Detector distance.
            "  L1                      Moderator-to-sample distance (cm.).
            "  TMAX                    Maximum TOF (microseconds).
            "  TMIN                    Minimum TOF (microseconds).
            "  TZERO                   Time-zero offset (microseconds).
            "  XBIAS                   Horizontal offset of detector
               origin.
            "  XBOX85                  Horizontal channels per cm. assuming
               XNUM = 85.
            "  XDIS
            "  XLEFT                   Distance from detector left border
               to origin.
            "  XRIGHT                  Distance from detector right border
               to origin.
            "  XWDTH                   Detector width (cm.).
            "  YBIAS                   Vertical offset of detector origin.
            "  YBOX85                  Vertical channels per cm. assuming
               YNUM = 85.
            "  YDIS
            "  YHGT                    Detector height (cm.).
            "  YLOWER                  Distance of lower detector edge to
               origin.
            "  YUPPER                  Distance of upper detector edge to
               origin.
```

Creating COM files interactively

It is often necessary to submit programs to batch rather than run them in interactive mode. Programs can be written to create a COM file interactively and then to stop before the actual analysis begins and instruct the user to submit the COM file to batch. The following is an example for the hypothetical program called XAMPLE:

```
      INCLUDE 'INC:DATACOM.FOR/LIST'
      DATA PRGNAM/'XAMPLE'/,LPRGNM/6/
           .
           .
      CALL GTIMOD (IMODE,PRGNAM,LPRGNM)
           .
           .
      TYPE 1
    1 FORMAT('$EXPNUM? ')
      ACCEPT *,EXPNUM
        IF (IMODE.EQ.1) WRITE (41,*) EXPNUM
           .
           .
```

---

* Currently available as an executable image on the [SCD].

```
IF (IMODE.EQ.1) THEN
  TYPE *,'Type MEDIUM XAMPLE'
  STOP
END IF
     .
     .
```

* Currently available as an executable image on the [SCD].

Glossary of Variable Names and Terms

NAME	TYPE	DEFINITION
A	R*4	a-axis unit cell length
ALPHA	R*4	unit cell angle between B and C
ANGL(5)	R*4	array containing CHI,PHI,OMEGA,DETA,DETD
B	R*4	b-axis unit cell length
BETA	R*4	unit cell angle between A and C
BKG	R*4	integrated background
BREFL	CH*11	reflection file name "EXPTx.REF" (x=EXPNUM)
C	R*4	c-axis unit cell length
CHI	R*4	chi goniometer angle
CTSPLS	R*4	counts/pulse
DEDSUM	I*4	total dead-time counts
DELT	R*4	time channel width in microseconds
DESCR(80)	BYTE	experimental description (80 characters)
DETA	R*4	detector angle (TTH)
DETD	R*4	detector distance
DIFFXX	R*4	diffraction vector x-direction
DIFFYY	R*4	diffraction vector y-direction
DIFFZZ	R*4	diffraction vector z-direction
ELAPSD	I*4	elapsed monitor counter
ENDDAT(9)	BYTE	histogram end date "dd-mo-yr"
ENDTIM(8)	BYTE	histogram end time "hh:mm:ss"
EXPNUM	I*2	experiment number
FORWRD	I*2	= 0, transform from detector (XCM,YCM,WL) to histogram (X,Y,Z) coordinate in SR TRANSF; = 1, histogram to detector
GENTXT	I*2	INTPKX*100+INTPKY*10+INTPKZ
H	I*2	Miller index.
HSTNUM	I*2	histogram number (maximum 99)
I84	I*4	= 0 for "old" histograms (85x85, pre 9/84) = 1 for "new" histogram (85x87) with Zilog Z8001 = 2 for 85x87 with N32016 microprocessor, post 9/86
ICELL	I*2	number corresponding to P, A, B, C, F or I centered cell
ICST	I*2	time channel start times in microseconds
IDATE(9)	BYTE	current date from subroutine DATE(IDATE)
IDIM1	I*4	in PEAKINT, dimensions of small integration envelope
IDIM2	I*4	in PEAKINT, dimensions of large integration envelope
IDTIME(256)	I*2	dead-time spectrum
IEX	I*2	flag (1,0) indicating whether a reflection is or is not extinct due to centering
IHIST(7395)	I*2	1-D array containing histogram data from 1 time layer. The x and y data are stored as follows: (Y=n), X=1,2,...,XNUM, (Y=n+1), X=1,2,...,XNUM Data obtained with GETDAT.
IHIST(7424)	I*4	same as above, except larger word size accommodates overflows. Data obtained with GETLNG or READ2D.
IMODE	I*4	from GTIMOD, = 0 if batch job, = 1 if interactive job
INTDIM	I*2	same as GENTXT

---

* Currently available as an executable image on [SCD].

```
      INTPKX      I*2         peak integration limit in x
      INTPKY      I*2         in y
      INTPKZ      I*2         in z
      INTI        R*4         see XINT
      IPKOBS      I*4         observed or interpolated peak intensity
      IPK         I*4         same as IPKOBS
      IT          I*4         integrated intensity including background
      ITIME(8)    BYTE        current time from TIME(ITIME)
      IUNIT       I*4         unit number of reflection file in FORTRAN code
      K           I*2         Miller index.
      L           I*2         Miller index.
      L1          R*4         moderator-to-sample distance in centimeters
      LOF         I*4         overflow pointer
      LPRGNM      I*4         number of characters in PRGNAM
      LSUM        I*4         time-slice sum returned by READ2D
      MNCT(256)   I*2         monitor spectrum converted to 3-D time channels
      MNNUM       I*4         number of monitor time channels (= (NCI/NDE)-2)
      MNSUM       I*4         total monitor counts
      MONCNT      I*4         monitor count (usually = MNSUM)
      NCH         I*4         number of histogram channels (= 7424*WLNUM)
      NCI         I*4         total number of channels used for 1-D detectors
                  (= (MNNUM+2)*NDE)
      NDE         I*4         number of 1-D detectors (= NMON)
      NMON        I*4         number of 1-D detectors (= NDE)
      NRUN        I*2         100*EXPNUM + HSTNUM
      NSUM(256)   I*4         spectrum of time-slice sums
      NTIME(256)  I*2         time-channel starting times (microsec)
      OFFSET      I*4         number of histogram channels which are skipped
                  over before reading data.
      OMEGA       R*4         goniometer angle
      ORGMAT(3,3) R*4         the 3X3 orientation matrix when all goniometer
                  angles are zero
      PDED(256)   R*4         the percent dead-time spectrum
      PDEDAV      R*4         average percent dead-time
      PHI         R*4         goniometer angle
      PLS         I*4         number of pulses during collection of histogram
      PRGNAM      CH*10       program name
      REFLAG      I*2         l*100 + m*10 + n, where
                                    "n" is the overlap flag in PEAKINT:
                                          0 -- PEAKINT: normal integration
                                          1 -- PEAKINT: overlapping peaks
                                               PEAKS: normal
                                          2 -- delayed neutron correction
                                          3 -- PEAKINT: 1 + 2
                                    "m" is the interpolation flag:
                                          1 -- 3-d interpolation OK
                                          2 -- interpolation routine not
                                     called; in PEAKINT, centroid not
                           determined due to negative
intensity
                                    "l" is the integration flag:
                                          1 -- integrated peak OK
                                          4 -- integration routine not called
                                404 -- calculated overlapping integration
envelopes
                                405 -- peak position not highest count in
integration envelope
      RUN         R*4         NRUN stored as an ASCII code
      SEQNUM      I*2         sequence number in reflection file
      SIG         R*4         estimated standard deviation in peak intensity
      SIGA        R*4         standard deviation for A
```

---

* Currently available as an executable image on the [SCD].

SIGALP	R*4	standard deviation for ALPHA
SIGB	R*4	standard deviation for B
SIGBET	R*4	standard deviation for BETA
SIGC	R*4	standard deviation for C
SIGGAM	R*4	standard deviation for GAMMA
STRDAT(10)	BYTE	histogram start date "dd-mon-yr"
STRTIM(8)	BYTE	histogram start time "hh:mm:ss"
SUMTOT	I*4	total counts in histogram
T(3,3)	R*4	T matrix as defined by Hamilton, International Tables, Vol. IV, p. 280.
TAU	R*4	2.0 * sin(theta)/WL
THETA	R*4	Bragg angle
TMAX	R*4	maximum time-of-flight in microseconds
TMIN	R*4	minimum time-of-flight in microseconds
TTH	R*4	two-theta
TZERO	R*4	value added to TOF when converting to WL
U(3,3)	R*4	U matrix based on observed rotation matrix and known cell parameters
UOBS(3,3)	R*4	U matrix based on least-squares fit of triclinic cell to observed data
USER(80)	BYTE	user's name
WL	R*4	wavelength in angstroms
WLMAX	R*4	maximum WL
WLMIN	R*4	minimum WL
WLNUM	I*4	number of wavelength channels
X	R*4	x histogram coordinate
XBIAS	R*4	zero point of detector in x direction
XCM	R*4	x position on detector (cm)
XINT	R*4	net intensity
XINT1	R*4	in PEAKINT, net intensity from small integration envelope
XINT2	R*4	in PEAKINT, net intensity from large integration envelope
XLEFT	R*4	leftmost detector limit (cm)
XNUM	I*2	number of x channels
XRIGHT	R*4	rightmost detector limit (cm)
XSIG1	R*4	in PEAKINT, standard deviation for XSIG1
XSIG2	R*4	in PEAKINT, standard deviation for XSIG2
XTALD	R*4	source to crystal distance
Y	R*4	histogram y-coordinate
YBIAS	R*4	zero point of the detector in the y direction
YCM	R*4	y position on detector (cm)
YLOWER	R*4	lowest detector limit (cm)
YNUM	I*2	number of y channels
YUPPER	R*4	upper detector limit (cm)
Z	R*4	histogram z coordinate

---

* Currently available as an executable image on the [SCD].