

SLAD DATA PROCESSING

December 2001

A. PREPARATION OF INPUT FOR CORRECT (PREP1)

- 1) Raw data files (*name01.raw etc.*) contain intensity data from all 12 detectors written as counts per channels. There are 1000 channels for each detector for each position of the detector box. This data should have been copied automatically from the SLAD instrument PC to the R2EXP1 PC in the data analysis room. Data can then be transferred by ftp to the VMS cluster if desired.
- 2) Depending on preferences:
 - a) Start a session on one of the NT work stations in the users office. Log in as NFLGUEST (password supplied by your local contact). Create your own directory and perform all of your data processing in it. Open the WinNFLP program from the desktop icon and follow the instructions. The raw data files for the current cycle are stored in \\R2EXP1\SLAD1.
 - b) Start a session on one of the ALPHA work stations in the users office. Log in as SLAD_USER (password supplied by your local contact). Open a DECterm window. Alternately, if you are using another terminal, log onto one of the ALPHA workstations, NFL2 or NFL3. Create your own directory and perform all of your data processing in it. The raw data files for the current cycle are stored under the user SLAD in the current directory (rawsep98, for example).
- 3) Type **PREP1** and answer questions. This program reads one or more raw data sets (all files with same name), adds individual runs (files), normalises to the number of monitor counts, recalculates the intensities as a function of scattering angle and writes the data output (*name.pre*) in 24 blocks (1 block for each detector in 2 positions). This program also performs a data quality test and checks the setting of the detector box. The program has an option to skip files that contain faulty data. Detectors may also be skipped , but only for the data quality test. There is a facility to remove data from faulty detectors in the PREP2 program with the PREP2.GRP file. Answer questions given by the program. An answer of (cr) will go on to the next step. The normal output is given in angles A (the default)

B. CORRECT/PREP2

CORRECT and PREP2 can be used to produce the final structure factor $F(Q)$ from a set of data blocks in the *.PRE files created by PREP1. The VMS version of the PREP2 command does both the CORRECT and PREP2 steps. In the Windows version CORRECT and PREP2 are run separately.

1. Correcting data for absorption, multiple scattering etc. with the CORRECT program. A command file for CORRECT should be available before running. Edit a setup "*name.com*"-file for CORRECT which requires details about the sample and experiments. This includes the "*.pre"-files produced by PREP1 for the different measurements (e.g. vanadium rod, empty sample container, background, sample), dimensions of the beam, containers and some information about the sample. By default the output is written as a function of momentum transfer Q . If the output is wanted as a function of scattering angle 2θ , include "XOUT angle" in the CORRECT command file. See the CORRECT manual for details. Remember that the *name* of the CORRECT command file should be the same as in the output "*name.sq*" filename. The output is a file with extension .SQ containing a number of blocks for different detectors and detector-positions on SLAD.

2. Merging the blocks in *name.sq* with the PREP2 program. This second step of the procedure combines intensity data measured at the same value of Q or 2θ from the relevant detectors. The output is written to four data files: *name.sq1*, *name.sq2*, *name.sq3* which refers to the up, middle and down detector banks, respectively, and *name.fq* which is the summed total. The default merging of blocks by PREP2 are given by:

MERGED DETECTOR BANKS	BLOCKS
UP	1 2 3 4 13 14 15 16
MIDDLE	5 6 7 8 17 18 19 20
DOWN	9 10 11 12 21 22 23 24
TOTAL	MERGING BANKS: UP, MIDDLE and DOWN

If you want to change the way PREP2 merges data you need a file in your working directory with extension *.GRP* containing:

```

Line 1      "Number of banks"
Line 2      "Number of blocks in bank 1"  "The block numbers"
Line 3      "Number of blocks in bank 2"  "The block numbers"
...
Last line   "Binning"
```

If binning is 0, a default binning of 0.01\AA^{-1} will be used for momentum transfer and 0.1° for 2θ angle. A PREP2 *.GRP*-file could look like:

```

3
8 1 2 3 4 13 14 15 16
8 5 6 7 8 17 18 19 20
8 9 10 11 12 21 22 23 24
0
```

Use GENIE or some other plotting program to compare the different detectors and then, if necessary rerun PREP2 with the PREP2.GRP file modified to exclude data from faulty detectors. **It is important that all *.PRE files used by CORRECT have the same block structure before using PREP2 or CORRECT!!!**