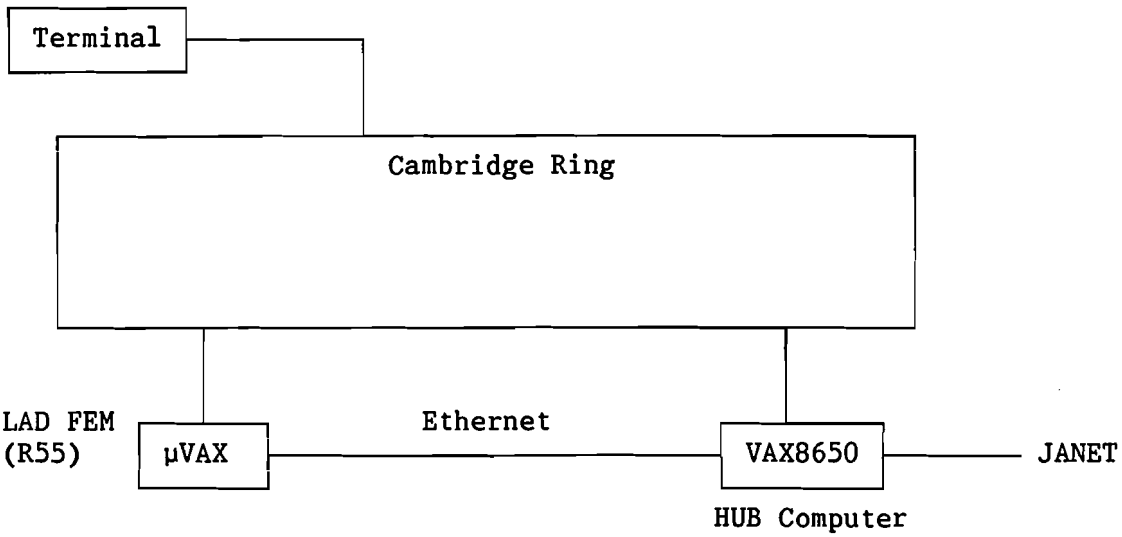
SECTION 3

HOW TO RUN THE PROCEDURES

3.1 THE ISIS COMPUTING SYSTEM

3.1.1 The computers

The current ISIS computing system (sometimes referred to as PUNCH - PUlsed Neutron Computer Heirarchy) is illustrated below and is fully described in the PUNCH User Manual.



Each instrument is controlled by a Front End Mini (FEM) computer which in the case of LAD is a Micro-VAX 2. The central mainframe, referred to as the HUB, is a VAX8650.

The FEM and the HUB are connected by two network systems - the Cambridge Ring and Ethernet. The HUB is also the node for other wide area networks such as JANET, for UK universities, and DECnet, EARN and BITNET for world-wide access.

Users will be assigned their own username on the HUB (see Local Contact for details) for use in analysing data. The username will be of the form ABC01 where the letters are the initials of the user and the numerals take into account several users with the same initials. The same username may also be used to log on to the LAD FEM.

3.1.2 Getting started

>>>Note : any command typed into the computer should be followed by pressing the RETURN key (sometimes referred to as Carriage Return CR). This will be assumed throughout the manual.

To log on to the HUB ...

1. Press the BREAK key on the terminal until the prompt

DNS:

appears

2. Type CALL HUB
3. Press RETURN to make the prompt Username: appear
4. Type the username (eg ABC01)
5. In response to the prompt Password: type password
6. A short command routine will then be executed, setting the system ready for analysing LAD data, and then the user will be logged on to the HUB and able to commence data analysis. The command routine must be setup by the Local Contact during the first use of the username.

Periodically the user will be required to change the password. This is done by use of the command SET PASS.

Once logged on, the user ABC01 will have access to an area of disk space for storing files in the directory [ABC01] and any sub-directories of it. In these areas there are full access rights ie read,write,execute,delete. The user has limited rights usually read only to areas within [LADMGR]. Initially, when the data is collected, it is stored in the directory [LADMGR.DATA] on the FEM and automatically transferred to the HUB in the same directory. However, due to space restrictions the data is archived onto optical disk and deleted within a few days. Data files are restored by issuing the command RESTLAD when logged onto the HUB. This restores the raw data

files to the area [LADMGR.RESTORE], with the restore process taking a maximum of about 10 minutes. The data files are held in this area for a period of 3 days. Both these areas can be referred to by the logical name 'inst_data' - for example a directory listing can be obtained by DIR inst_data.

Programs and command files are stored in the area [LADMGR.PROGS] which has the logical name 'g_f'. (Note: a 'logical name' is simply a convenient synonym used to stand for a string of characters)

The user may wish to make use of sub-directories to help organise the files within his own area. In this case the following commands are useful:

CREATE/DIR [ABC01.ANA]	- create a sub-directory named [ABC01.ANA]
SET DEF [ABC01.ANA]	- set the default directory to be [ABC01.ANA]. This has the effect that subsequently the computer will assume that a file is in the directory [ABC01.ANA] unless another directory is specified.
SH DEF	- show the default directory.

3.2 DATA FILES AND BATCH SYSTEM

3.2.1 Data File Structure

The data on the FEM can be in 3 locations - the DAE, the CRPT or disk (either as a .SAV file or a .RAW file). On the HUB it is either .SAV or .RAW.

The convention used to name files involves 3 parts : a filename, an

extension and a version number. For data the filename is constructed from the instrument name (3 characters) and a 5 digit run number. The type of file is specified by the extension - for example SAV or RAW. The full name of the raw data file (version 1) for run 1234 for example is LAD01234.RAW;1 . In our programs we continue to use this form of nomenclature so that data for a specific sample can be recognised by its run number and the type of data by the extension name. Within the programs the instrument name and leading zeros in a run number need not be specified.

In all the above cases the file structure is the same. There is a header section which contains information supplied by the instrument control program (ICP) on the FEM.

There are sections on :

- -instrument parameters; for example detector angles, flight paths, spectrum numbers for detectors and monitors.
- -run parameters; for example date/time of start and end, number of protons, neutrons and frames.
- -sample parameters; for example title of run, dimensions.

These are followed by arrays containing :

- -time of flight which is stored as the time boundaries for the channels as specified by the ICP.
- -each spectrum as counts per channel.

Files are in binary format but ASCII versions of parts of the data can be provided.

The GENIE program can also create files in binary format but with a different layout. The file starts with a selection of parameters from the RAW data header section such as scattering angle and flight paths and is followed by arrays containing the values of x, y and error on y. Such binary files will be used extensively by our programs with the

type of data denoted by the extension.

Programs are available for converting these binary files to ASCII format.

3.2.2 Batch System

The batch system enables a program to be run non-interactively so as not to tie up the terminal. It is of most use for long programs, such as those used to calculate the absorption correction and the multiple scattering correction. Some useful batch related commands are as follows;

SUBMIT VAN01234.COM - submit the command file VAN01234.COM to be run by batch.

SHOW QUE *$BATCH - show the status of all batch queues.

DELETE/ENTRY=999 RLDE$BATCH - delete batch job 999 (the entry number 999 may be obtained by use of the SHOW QUE command) from queue RLDE$BATCH (for example).

SHOW SYS/BAT - shows all the batch jobs currently executing in the current processor and how much CPU time each has used. Note that if a job has been submitted to a different CPU from the current one the amount of time in that job can only be obtained by logging on to the appropriate CPU. This is not normally possible for HRPD, POLARIS and CRISP unless you know the password because these FEM's have limits on who can log on.

3.3 INSTRUMENT INFORMATION

3.3.1 Calibration

On a time-of-flight instrument the data must be converted from stored counts in channels to counts in other units such as wavelength, d-spacing and Q-vector. These conversions are determined by two standard equations :

$$t + \Delta = (m/h)\, L\lambda$$

$$\lambda = 2d \sin\theta \qquad \text{(Bragg's equation)}$$

where t is the time of flight
Δ is the origin in time determined by the electronics
L is the total flight path equal to the sum of the initial (l_1) and final (l_2) flight paths
λ is the wavelength
2θ is the scattering angle
d is the d-spacing of the powder peak

These parameters are determined with calibration experiments of two types. The first equation can be used with neutron absorption resonances which occur at fixed energy or wavelength. By measuring many resonances from different foils placed in the incident beam, values for Δ and L can be determined. Most resonances occur at high energies (~eV) (short times-of-flight) so these calibrations give good values for Δ.

The second equation of course leads to the familiar calibration using standard powders such as Ni, Al_2O_3 and MgO. These experiments will give values of Δ and the product $L\sin\theta$. At short times there are either no Bragg peaks or they cannot be resolved so that the value of Δ by this technique is not as reliable as that from resonances.

As pointed out in Appendix A the Bragg peaks have an asymmetric

shape which varies with scattering angle, so the peaks have to be analysed to take this into account.

The instrument calibrations are carried out by the Instrument Scientists and do not normally need to be repeated by the user. Nonetheless it is wise to look for discrepencies between the results from different scattering angles to determine if the supplied calibration is correct. The header sections of the .RAW data files should contain the correct values. On the FEM they are stored in a file called DETECTOR.DAT. If that file does not contain all the values or if they need changing a similar file can be created on the HUB to be used by our programs.

3.3.2 Spectrum numbering

All detectors and monitors are allocated a spectrum number. The physical detectors are mapped to spectrum numbers by software via a file called SPECTRA.DAT. These can be changed by the user at the start of an experiment, but in most cases a standard setup is used. The number of spectra and the number of channels per spectrum are defined on the FEM by the ICP and their product defines the storage capacity required and the maximum value is determined by the hardware in the FEM.

In the data analysis programs the spectra can be further combined for example according to scattering angle. This will in general be neccessary to reduce the volume of data and is particularly true for the scintillator modules which have a large number of detector elements. Subsequently a combined spectrum from several detectors is treated as though being at the average angle. In the case of LAD the detectors occur in groups at scattering angles of approximately 5°, 10°, 20°, 35°, 58°, 90° and 150° and the default way of combining the detectors is based on these groups.

Two of the spectra are always the monitors - one in the incident beam and the second in the transmitted beam.

The header section of the data files also keeps a record of the spectrum numbering and in our programs we make use of this data so that the user does not need to know them.

3.3.3 Time channels

The time channel structure is set up by the ICP and three basic structures are available : channel width constant with time, channel width proportional to time-of-flight and width proportional to the square of the time-of-flight. There can be up to five ranges of time-of-flight each with a choice of structure.

The constant channel width is the simplest but has the disadvantage that on converting to Q the data becomes squashed into the low Q region with the high Q region having widely spaced points. The second choice has the advantage that the channel widths are proportional to the resolution over the whole range since the resolution is constant in $\Delta t/t$ and $\Delta Q/Q$. For this option the distribution of points in Q is still on constant increment but not as bad as the first option. The last choice would provide constant increments in Q.

On LAD we have chosen the second option - that is the channel width is proportional to time-of-flight. There is only one region staring at 200 μs ending at 19500 μs just before the next pulse which arrives at 20 ms. The constant of proportionality is 0.002 which allows for about ten points across a Bragg peak at the backward angle (150°), highest resolution detectors. Since the resolution worsens as the scattering angle decreases and the constant does not change with angle, the number of points at the lower angles are higher than necessary.

The combination of unequal Q increments and the increments in general being smaller than neccessary for liquid and amorphous work means that rebinning of data in Q is always required.

TABLE 3.1

Example of DETECTOR.DAT file

LAD February 1989

Number of detectors, Number of user table parameters/detector
84 5

Det	Delta	Len2	Code	2theta	ut1	ut2	ut3	ut4	ut5
1	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
2	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
3	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
4	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
5	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
6	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
7	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
8	4.4	1.128	150	145.6	1.0	1.25	10.0	0.006	0.
9	4.6	1.047	150	9.6	1.0	1.25	10.0	0.016	0.
10	4.6	1.047	150	9.6	1.0	1.25	10.0	0.016	0.
11	5.4	1.033	150	4.8	1.0	1.25	10.0	0.02	0.
12	5.4	1.033	150	4.8	1.0	1.25	10.0	0.02	0.
13	-0.7	-1.092	150	180.0	2.0	0.00244	44.0	0.001	0.
14	-0.95	1.260	150	0.01	2.0	0.00244	44.0	0.001	0.
15	-1.0	1.039	150	88.4	2.0	1.25	1.0	0.014	0.
16	-1.0	1.039	150	88.8	2.0	1.25	1.0	0.014	0.
17	-1.0	1.039	150	89.1	2.0	1.25	1.0	0.014	0.
18	-1.0	1.039	150	89.5	2.0	1.25	1.0	0.014	0.
19	-1.0	1.039	150	89.7	2.0	1.25	1.0	0.014	0.
20	-1.0	1.039	150	90.0	2.0	1.25	1.0	0.014	0.
21	-1.0	1.039	150	90.3	2.0	1.25	1.0	0.014	0.
22	-1.0	1.039	150	90.55	2.0	1.25	1.0	0.014	0.
23	-1.0	1.039	150	90.9	2.0	1.25	1.0	0.014	0.
24	-1.0	1.046	150	57.0	2.0	1.25	1.0	0.008	0.
25	-1.0	1.046	150	57.2	2.0	1.25	1.0	0.008	0.
26	-1.0	1.046	150	57.45	2.0	1.25	1.0	0.008	0.
27	-1.0	1.046	150	57.8	2.0	1.25	1.0	0.008	0.
28	-1.0	1.046	150	58.0	2.0	1.25	1.0	0.008	0.
29	-1.0	1.046	150	58.3	2.0	1.25	1.0	0.008	0.
30	-1.0	1.046	150	58.7	2.0	1.25	1.0	0.008	0.
31	-1.0	1.046	150	59.0	2.0	1.25	1.0	0.008	0.
32	-1.0	1.046	150	59.3	2.0	1.25	1.0	0.008	0.
33	-1.0	1.043	150	34.1	2.0	1.25	1.0	0.012	0.
34	-1.0	1.043	150	34.4	2.0	1.25	1.0	0.012	0.
35	-1.0	1.043	150	34.7	2.0	1.25	1.0	0.012	0.
36	-1.0	1.043	150	34.9	2.0	1.25	1.0	0.012	0.
37	-1.0	1.043	150	35.3	2.0	1.25	1.0	0.012	0.
38	-1.0	1.043	150	35.6	2.0	1.25	1.0	0.012	0.
39	-1.0	1.043	150	35.9	2.0	1.25	1.0	0.012	0.
40	-1.0	1.043	150	36.1	2.0	1.25	1.0	0.012	0.
41	-1.0	1.043	150	36.4	2.0	1.25	1.0	0.012	0.
42	-1.0	1.04	150	19.1	2.0	1.25	1.0	0.013	0.
43	-1.0	1.04	150	19.5	2.0	1.25	1.0	0.013	0.
44	-1.0	1.04	150	19.8	2.0	1.25	1.0	0.013	0.

45	-1.0	1.04	150	20.1	2.0	1.25	1.0	0.013	0.
46	-1.0	1.04	150	20.4	2.0	1.25	1.0	0.013	0.
47	-1.0	1.04	150	20.7	2.0	1.25	1.0	0.013	0.
48	-1.0	1.04	150	21.0	2.0	1.25	1.0	0.013	0.
49	-1.0	1.04	150	21.2	2.0	1.25	1.0	0.013	0.
50	-1.0	1.04	150	19.1	2.0	1.25	1.0	0.013	0.
51	-1.0	1.04	150	19.5	2.0	1.25	1.0	0.013	0.
52	-1.0	1.04	150	19.8	2.0	1.25	1.0	0.013	0.
53	-1.0	1.04	150	20.1	2.0	1.25	1.0	0.013	0.
54	-1.0	1.04	150	20.4	2.0	1.25	1.0	0.013	0.
55	-1.0	1.04	150	20.7	2.0	1.25	1.0	0.013	0.
56	-1.0	1.04	150	21.0	2.0	1.25	1.0	0.013	0.
57	-1.0	1.04	150	21.2	2.0	1.25	1.0	0.013	0.
58	-1.0	1.043	150	34.1	2.0	1.25	1.0	0.012	0.
59	-1.0	1.043	150	34.4	2.0	1.25	1.0	0.012	0.
60	-1.0	1.043	150	34.7	2.0	1.25	1.0	0.012	0.
61	-1.0	1.043	150	34.9	2.0	1.25	1.0	0.012	0.
62	-1.0	1.043	150	35.3	2.0	1.25	1.0	0.012	0.
63	-1.0	1.043	150	35.6	2.0	1.25	1.0	0.012	0.
64	-1.0	1.043	150	35.9	2.0	1.25	1.0	0.012	0.
65	-1.0	1.043	150	36.1	2.0	1.25	1.0	0.012	0.
66	-1.0	1.043	150	36.4	2.0	1.25	1.0	0.012	0.
67	-1.0	1.046	150	57.0	2.0	1.25	1.0	0.008	0.
68	-1.0	1.046	150	57.2	2.0	1.25	1.0	0.008	0.
69	-1.0	1.046	150	57.45	2.0	1.25	1.0	0.008	0.
70	-1.0	1.046	150	57.8	2.0	1.25	1.0	0.008	0.
71	-1.0	1.046	150	58.0	2.0	1.25	1.0	0.008	0.
72	-1.0	1.046	150	58.3	2.0	1.25	1.0	0.008	0.
73	-1.0	1.046	150	58.7	2.0	1.25	1.0	0.008	0.
74	-1.0	1.046	150	59.0	2.0	1.25	1.0	0.008	0.
75	-1.0	1.046	150	59.3	2.0	1.25	1.0	0.008	0.
76	-1.0	1.039	150	88.4	2.0	1.25	1.0	0.014	0.
77	-1.0	1.039	150	88.8	2.0	1.25	1.0	0.014	0.
78	-1.0	1.039	150	89.1	2.0	1.25	1.0	0.014	0.
79	-1.0	1.039	150	89.5	2.0	1.25	1.0	0.014	0.
90	-1.0	1.039	150	89.7	2.0	1.25	1.0	0.014	0.
81	-1.0	1.039	150	90.0	2.0	1.25	1.0	0.014	0.
82	-1.0	1.039	150	90.3	2.0	1.25	1.0	0.014	0.
83	-1.0	1.039	150	90.55	2.0	1.25	1.0	0.014	0.
84	-1.0	1.039	150	90.9	2.0	1.25	1.0	0.014	0.

The first column is the detector number; delta, l_2 and 2theta are as defined above; Code defines the instrument (150 is LAD); the parameters ut1-ut5 are user defined and in this case are :

ut1	detector type code 1=gas 2=scintillator
ut2 and ut3	parameters to calculate detector efficiency
ut4	resolution
ut5	spare

The calibration determines $L=l_1+l_2$, l_1 is taken to be the nominal value of 10.0m. If l_1 is not defined in the parameter section of the data files then l2 can be set to L for the purposes of unit conversion to wavelength.

3.4 OVERVIEW OF GENIE

For more details of this program the user should consult the GENIE Manual. We will restrict ourselves to comments on the general principles and the more important points in its operation.

The overall program structure is command driven, not by menu. However where possible the individual routines called by the commands will include a menu or question/answer structure for ease of use.

Workspaces are used for data manipulation. The number of workspaces and their size (array length) can be chosen by the user. However there is a limited memory space available so the product of the number of workspaces and their length must be within this limit. There must always be enough space for the graphics area and buffer areas. This will normally be set for you.

Command files can be used for repetitive operations and can also include terminal input. A command file is program run within GENIE which executes commands from a .COM file instead of the user typing in at the keyboard. Command files are run in GENIE by typing @ followed by the name of the .COM file which is to be run. The name must be prefixed by a directory name if the command file does not reside in the current default directory.

There is an initialisation command file that is automatically read on entering GENIE. This sets up values for the number of spectra and their size and the default disk directories.

The data in Workspaces can be written to binary files for subsequent reading back into workspaces.

External programs can be run to manipulate data in workspaces - these are the FUNCTION and TRANSFORM commands and are used in our programs for example to read in corrections parameters. Data in non-GENIE type files (usually ASCII) can be read into workspaces using

the Load command.

The units of x in the workspace can be changed provided that the workspace contains instrument parameters which are input via the SET PAR command. The y-values of the data in the workspaces are stored in the form of 'per unit of x' eg per microsec or per $Å^{-1}$. Care must be taken when changing units and dividing - for example the correct order is to change unit then divide. The option of scaling x to the y-unit can be removed with the SET Yunit command.

3.4.1 Simple Example of GENIE commands

In order to read in a sample and vanadium spectrum, divide and display as S(Q) the following operations are necessary :

```
>ASS 1234                    assign run number for sample
>W1=S1                       read spectrum 1 into workspace 1
>Set PAR 1 10 1. 150. 0 0    set parameters
>U/Q W1                      change units to Q
>ASS 1235                    assign run number for vanadium
>W2=S1
>Set PAR 2 10 1. 150. 0 0
>U/Q W2
>W3=W1/W2                    divide S by V to give S(Q)
>D W3                        display S(Q)
>L/X 0 20                    change range of X (ie Q)
>D/E                         display new Q range and with error bars
```

3.4.2 GENIE command files

Operations can be stored as a command file and such a file is provided for calculating the 'crude' S(Q), i.e. (sample-can)/vanadium, with no other corrections. The routine is started in GENIE with the command @g_f:SQRAW, that is, the command file is called SQRAW.COM in directory g_f. It prompts for sample, can and vanadium run numbers and

for the angle. The resulting "raw" S(Q) is displayed.

3.5 OVERVIEW OF PROGRAMS

The package provides a series of stand-alone Programs and GENIE routines which are to be run in a particular order :

Program NORM normalises RAW data and produces output files with extensions .MON and .NRM.

TRANSMISSION Routines calculate cross-sections from the transmission data with extension .MON and creates files with extension .MUT.

Program CORAL calculates the corrections using the files with extension .MUT and produces corrections files with extensions .ABS, .MUL or .REF.

Routine VANSM treats the reference or vanadium spectra using files with extensions .NRM and .REF and creates files with extension .SMO.

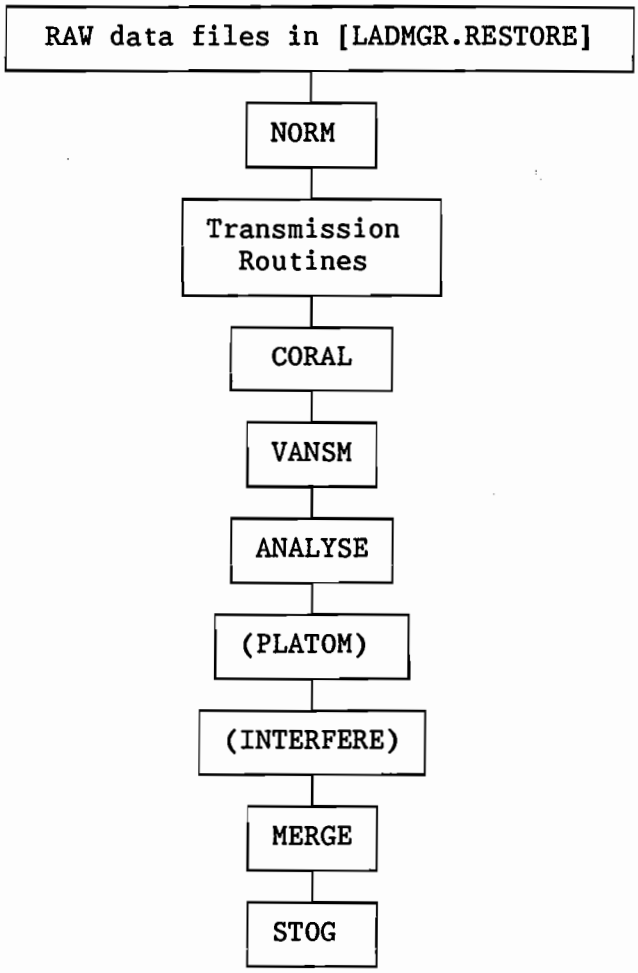
Routine ANALYSE takes the files with extensions .NRM, .ABS, .MUL and .SMO to produce the corrected S(Q) at each angle as an output file with extension .DCS.

Routine PLATOM calculates the self scattering at each angle, creating an output file with extension .SLF. Routine INTERFERE subtracts the self scattering in the .SLF file from the total scattering in the .DCS file to yield the interference scattering which is placed in a file of extension .INT.

Routine MERGE combines the individual angles in a file with extension INT or DCS to produce a single S(Q) in a file with extension .SOQ.

Routine STOG transforms S(Q) to g(r) and GTOS transforms g(r) to S(Q).

The diagram below shows the normal sequence of operations, and Appendix D summarizes the filename extensions which are produced.



The operations in brackets are optional and can be skipped if necessary. This will typically happen when the inelasticity correction is either not needed or not calculable.

3.6 PROGRAM NORM

Version 4.1 March 1989

3.6.1 Introduction

This program NORMalises the RAW data - that is it takes detector spectra, corrects for deadtime, divides by the monitor spectrum, converts from time-of-flight to Q-vector, combines spectra and outputs results to files.

The following operations are carried out on all spectra :

- the time-of-fight is converted to wavelength using the parameters contained in the RAW file. Each spectrum has the same range of time-of-flight so because each spectrum may have a different flight path the wavelength range will differ. Before manipulating spectra they must therefore be rebinnned onto a common wavelength range (this also includes the same increment in wavelength).
- the counts are corrected for detector dead time. This requires the total frames for the run which is taken from the parameter section.
- the error is taken to be the square root of the count.

The program is in two sections each producing an output file which can subsequently be read into GENIE using the REad command.

3.6.2 Monitor files

This section creates a file with the extension .MON containing the two monitor spectra.

The incident monitor is just converted to wavelength. The transmission monitor is converted to wavelength, rebinned to the wavelength range of the incident monitor and divided by the incident monitor spectrum. The purpose of dividing by the incident monitor

spectrum is to allow for the possibility of variations in moderator temperature leading to changes in the flux wavelength distribution as well as scaling all runs to a same neutron flux. It is therefore in a form suitable for calculating the transmission cross-section.

3.6.3 Detector files

This section deals with the detector spectra and creates a file with the extension .NRM. The spectra can be 'grouped' together in a manner defined in a data file. A default version called GROUPS.DAT is available for LAD in the instrument program directory (G_F:).

The operations are :

- the individual spectra are read, converted to wavelength and normalised to the incident monitor spectrum as outlined above. This must be done on the individual detectors in wavelength and not after addition or converting to Q in order to take correct account of the shape of the monitor spectrum.
- the individual detectors are converted into counts per Q - each spectrum is rebinned onto a specified Q range and constant Q increment and the spectra within a defined group are added.

The default grouping for LAD creates a file of 14 groups corresponding to the 7 scattering angles on either side. The groups are in pairs in increasing angle.

3.6.4 Operation

The program is a stand-alone program similar in operation to GENIE and is started with the command NORM.

The program prompt is n> .

The command RUN defines run numbers to be used.
The command GRoup defines the spectra group structure.
The command BEGIN starts the program looping over all groups.

The command CALib initialises reading of the detector table (optional).

The sequence of commands is as follows :

>SET DIR or DISK	)	default values on
>SET INST	)	entry to program
>SET EXT	)	
>CAL		if required
>GR		
>RUN		
>BE		to begin operation
>EX		to exit program

The HELP facility is also available within the program. The command Help will provide brief comments on the NORM commands whilst Help GENIE gives information on GENIE commands.

***** IMPORTANT NOTE: At the time of writing NORM contains a bug which ***** means it can only be run on one set of data, i.e. one sequence ***** of commands as above. On completion it must be exitted and ***** restarted with the NORM command again for each set of .RAW ***** files.

3.6.5 Description of Commands

A full description of the commands now follows :

B E g i n

This command begins the automatic looping over all the groups as defined by the Group command.

The routine prompt is begin>

The routine will ask for :
increment in Q (delta_q) default is 0.02
maximum Q value (q_max) default is 50.

Alternatively the two parameters can be included with the command in the form BE delta_q q_max.

Each spectrum/group will be rebinned at constant delta_q where the q_values are integer multiples of delta_q ie N*delta_q. The minimum rebinned q_value is the first multiple of delta_q greater than the minimum q_value of the raw data. The maximum rebinned q_value is the last multiple of delta_q less than the maximum q_value of the raw data or the defined maximum q_value whichever is the smaller.

If the CAL command has previously been issued the values of the calibration constants will be changed.

There is an error message if a run number has not been given or if the groups have not been defined and the command is aborted.

C A L i b

This command initiates the changing of the values of the calibration constants. The new values must be in the file DETECTOR.DAT which must exist in the current directory. The new values are displayed as they are read in.

The command must be issued before both the RUN and BEgin commands. The monitor data is read during RUN so its parameters will not be changed unless CALib is issued before it.

There is an error message if the number of detectors is wrong or if the detector numbers are out of sequence and the parameters are not changed.

The option can be removed with the qualifier /N.

G R o u p

The group command defines the group structure of the spectra.
The routine prompt is group>

There will be a request to input a filename. A <CR> will default to the file G_F:GROUPS.DAT in the LADMGR program area, otherwise type the name of the file to be read (with directory if necessary).

The group structure (as in the file) is as follows :
first line : number of groups
subsequent lines (one for each group) :
number of spectra, the spectra numbers
Up to 25 groups are allowed, each with up to 25 spectra.
The spectra should be in increasing angle.

There is one qualifier /TYPEIN which allows the group structure to be typed in directly. There will be prompts for input ; the structure is similar to that in the file.

If the group file does not exist or if more than 25 groups are defined there is an error message and the command is aborted.

R U N

Defines the run numbers. The command is :

RU <run1> <run2> ...

Up to 8 runnumbers may be specified.

The output file will take the name of the first run number specified and will contain a sum over all the runs.

3.6.6 Example of GROUPS.DAT file

Standard Groups.dat file for LAD
corresponding to detector layout on February 1989

14	number of groups
1 11	5° gas L
1 12	5° gas R
1 9	10° gas L
1 10	10° gas R
8 42 43 44 45 46 47 48 49	20° scintillator L
8 50 51 52 53 54 55 56 57	20° scintillator R
9 33 34 35 36 37 38 39 40 41	35° scintillator L
9 58 59 60 61 62 63 64 65 66	35° scintillator R
9 24 25 26 27 28 29 30 31 32	60° scintillator L
9 67 68 69 70 71 72 73 74 75	60° scintillator R
9 15 16 17 18 19 20 21 22 23	90° scintillator L
9 76 77 78 79 80 81 82 83 84	90° scintillator R
4 1 2 3 4	150° gas Left
4 5 6 7 8	150° gas Right

The average angles produced by these groupings are :

4.8°, 9.6°, 20.23° , 35.27° , 58.08° , 89.69° and 145.6°.

3.6.7 Batch operation

The program can also be run in batch mode. A command file must be created in the following format :

```
$ norm
> gr
<return>
> run n1 n2 ....
> be delta_q q_max
> ex
$ exit
```

The job is submitted to the batch queue with the SUBMIT command, for example if the command file is called TEST.COM the job is started with SUBMIT TEST.

3.6.8 Reading output files

The data in the .MON and .NRM files can be read into a workspace using a standard READ command. For example, to read the fifth group of NRM into the second workspace type

Read W2 LAD01234.NRM 5 after the prompt >.

The following GENIE command files carry out the standard operations similar to SQRAW ie calculating a 'crude' S(Q) (see section 3.4.2). There are 2 versions:

SQGRP	operates on individual groups
SQANG	operates on angles as in the default grouping

The routines prompt for sample, can and vanadium run numbers and for the group number or angle, as appropriate.

3.7 TRANSMISSION ROUTINES

The transmission cross-section of a sample in a t-o-f experiment (and thus the absorption correction) cannot be calculated from the individual atomic cross-sections (eg. by assuming a 1/v dependence of the absorption cross-section) because of the effect of S(Q). Hence the transmission is calculated from the experimental data (for both sample and vanadium) - see section 2.4

These command files for GENIE calculate the transmission cross-section from the monitor data in either the .RAW files or in .MON files. The former is useful for checking the sample during the run whilst the latter is for the subsequent analysis. Two forms of sample geometry can be treated : cylindrical and flat plate. So the corresponding 2 routines are :

TCR	cylindrical geometry	.RAW data
TFR	flat plate geometry	.RAW data
TCM	cylindrical geometry	.MON data
TFM	flat plate geometry	.MON data.

To run these GENIE command files the user should go into GENIE and type @g_f:tcr for example.

The routines prompt for the sample and background run numbers and then divide sample by background to give the transmission. NOTE: if the sample is in a container then the correct background to use is the empty container run number, NOT the 'nothing in the beam' background. The next prompt is for the binning parameters - default values or input values. Then a Function program is entered to calculate the cross-section - TRANSCYL for cylindrical geometry or TRANSFLAT for flat plate geometry.

The result is displayed and the routine prompts for a choice of recalculating or outputting the result to an ASCII file suitable for the corrections programs - this file has the sample runnumber and

extension .MUT. See section 2.4 for further information on the calculation of the total cross-section.

The program TRANSCYL can take into account 2 concentric cans or 1 can plus a furnace, i.e. there are 4 radii defining 3 annuli. The routine will calculate the cross-section of annulus 1 and requires the cross-sections for annuli 2 and 3 as input. The following input is required :

- beam width
- radius 1 default=0. (ie =0 for solid sample)
  (= inner radius for empty can)
- radius 2 (= outer radius of sample)
- radius 3 default=0. (ie no can)
  (= outer radius of can)

if can is defined (ie non-zero value for radius 3)

- radius 4 default=0. (ie no furnace or second can)
  (= furnace/second can outer radius)

- sample number density in atom or mol per $Å^3$
  if can is defined can number density
  filename for cross-section data
  if furnace is defined furnace number density
  filename for cross-section data

The cross section file consists of the total scattering and absorption cross-sections at a series of wave-lengths. A file can be created using the program CSFILE. Standard files for vanadium (VAN.MUT) and titanium-zirconium (TIZR.MUT) are available in the program directory (g_f). If a cross-section data file does not exist there is an error message and the routine is aborted.

A subtlety occurs on LAD associated within the transmission monitor which does not sample the transmitted beam uniformly, but instead samples the beam on a square grid with 5mm between elements. This means the cross section determined from the transmission monitor

readings can be significantly in error, particularly if the sample does not attenuate the beam very much or if the sample is much thinner than the beam. This effect is also pronounced when the transmission of a thin sample container is being measured. In such cases the beam width can be regarded as an adjustable parameter, which is altered until the cross section of the vanadium rod comes out as expected: this should then be used as the "effective" beam width for the samples. If the container attenuation is so small to make the transmission readings unreliable then one of the standard .MUT files should be used for the container cross section

The program TRANSFLAT requires the following input :

- sample thickness
- sample number density in atom or mol per $Å^3$

The .MUT files can be read into GENIE with the command

```
LO W1 LAD*****.MUT g_F:read_cs
```

which puts the cross section into workspace 1

A straight line fitting program is available to fit a straight line through the cross section data. This is accessed by typing

```
FU w1 g_F:fit_line w2
```

which puts the straight line fit to the data in w1 into w2. This is useful for determining the asymptotic values of the measured cross sections.

3.8 PROGRAM CORAL

Version 4.1 March 1989

3.8.1 Introduction

The stand-alone program CORAL is used to set up a calculation of either an absorption correction or a multiple scattering correction. The actual calculations use several minutes of computer time and so they are performed in batch, with the program CORAL setting up the necessary input.

The scheme described in section 2.5 is used to perform the calculations. They may be performed for either a cylindrical or a flat plate sample, with or without a container.

The corrections calculated by CORAL may be performed for either a .NRM file or a .RAW file, although in the recommended sequence of analysis it is a .NRM file which is corrected. In order to perform either calculation a file containing the total cross-section is required. In normal use the .MUT file calculated by the TRANSmission programs may be used for this.

The absorption and multiple scattering corrections for a sample may be performed in either order. In the case of vanadium the recommended sequence of analysis involves performing only a multiple scattering correction at this stage, using the special CORAL command VA.

The program CORAL uses the following file naming conventions (for correcting the run LAD01234.NRM for example):

	Absorption Correction	Multiple Scattering Correction	Vanadium Correction
(Created before Batch Job)			
File Containing Commands to Run Batch Job:	ABS01234.COM	MUL01234.COM	VAN01234.COM
File Containing Input Parameters for Batch Job:	LAD01234.AIN	LAD01234.MIN	LAD01234.MIN
(Created during Batch Job)			
File Containing Log of Batch Job:	ABS01234.LOG	MUL01234.LOG	MUL01234.LOG
File Containing Batch Job Result:	LAD01234.ABS	LAD01234.MUL	LAD01234.REF

(Files named CYLMUL.IN and CYLMUL.OUT are also used during the multiple scattering calculation, but are deleted after successful operation.)

As well as the usual input parameters such as dimensions, this program requires a description of the beam profile and the total cross section as a function of wavelength. This cross-section data is in a data file with extension MUT as produced by the TRANSmission program. It can also take into account several annuli surrounding a sample (eg can and furnace) and masked beams (e.g. beam width smaller than sample diameter).

The location of the input run is defined using the SET commands. The default directory is set on entry to the instrument data area, e.g. [LADMGR.DATA] for LAD, and the default extension is RAW. All output goes to the current directory.

3.8.2 Operation

The program is a stand-alone program similar in operation to GENIE but without any display options and is started with the command CORAL.

The program prompt is c>

The sequence of commands is as follows :

```
SET EXT              (if required - default is RAW)
SET DISK or DIR      (if required - default is [LADMGR.DATA])
SET INS              (if required - default is LAD)
SET GEOM C or F      (if required - default is C)

RUN  <runnumber>

SA or VA

CA                   if required

BE
OUT [option]
SUB
```

In the program some of the parameters have fixed values while others are set to default values. When a default can be changed its value is printed and <RETURN> keeps the default - otherwise type in the new value.

The HELP facility is also available within the program. The command Help on its own will provide brief comments on the CORAL commands whilst Help Genie gives information on Genie commands.

When running CORAL it is important to type the full sequence of the above commands from RU to BE before typing OUT, otherwise errors in the output files can occur. Thus if when in SAMPLE or CAN or VANADIUM or

BEAM a typing error occurs, then the whole sequence from RUN (inclusive) should be typed again to ensure the output files are correct

3.8.3 Hints on running

The cylindrical input file format in 3.8.4 is used for both the absorption and the multiple scattering programs. The only change neccessary to the parameters is the step size (line 4). The MS calculation can have a larger step size than the absorption (by up to an order of magnitude). Typically, for MS use 0.1 and for absorption 0.02.

The flat plate input file is also used for both correction programs but line 3 is only nesseccary for the multiple scattering and default values have been set at 0.001 for accuracy and 100 planes.

The MS program assumes an input file with extension MIN and creates an output file with extension MUL and a lineprinter listing with extension LIS. The filename for all three files is the same.

The corrections programs are called CYLABSTOF, CYLMULTOF, FLTABSTOF and FLTMULTOF and are in the instrument program directory, ie [ladmgr.progs] or logical name g_F on LAD.

There are command files also in [ladmgr.progs] for running the programs called RUNABS and RUNMUL with one parameter - the filename. All created files will be in the current directory.

The programs take up to 15 mins of CPU time (especially the cylindrical multiple scattering program), so submitting to batch processing is highly recommended. Two further command files are available to make this easier and they assume that the filenames have the form LAD{runnumber} where {runnumber} is 5 digits - the same format as .RAW files. These commands in [ladmgr.progs] are SUBABS and SUBMUL and assume that the runnumber only has 3 digits. When running from the

[lad] area the abbreviations SUBA and SUBM can be used eg SUBA 123 or SUBM 234. All created files will be in the current directory.

If a program runs out of CPU time the problem is probably due to a step size that is too small. Resubmit with a larger step size - say a factor two larger. This should only occur for samples of large radius eg greater than 10mm.

The use of CORAL removes all these complications and avoids detailed knowledge of the operating system.

Do not run two versions of the same option at the same time - for example, wait for an ABS or MUL program to finish before starting a new version. ABS and MUL can be run at the same time.

If you are logged on at a terminal there will be a message from CORAL when a batch job has finished.

In the course of setting up the input files to run the corrections programs you will need to specify the capture cross section at 1.8Å. The value needed should be checked by looking at the measured cross sections since the SCATTERING cross section is determined from the TOTAL cross section by means of the relation

$$\sigma_s(\lambda) = \sigma_t(\lambda) - \sigma_a(\lambda).$$

Therefore IF for some reason the capture cross is LESS than its barn book value, e.g. due to an error in the sample composition, then simply using the 'barn book' value could lead to a NEGATIVE scattering cross section in the multiple scattering routines. In other words the capture cross section typed into CORAL must be consistent with the total cross section values in the .MUT files used.

Finally note that when running the multiple scattering for a container on its own the multiple scattering run is set up with the SA command (and not the CA command), i.e. the container must be treated as

a sample in this case.

3.8.4 Description of commands

A full description of the commands now follows :

Inputs parameters associated with the neutron beam and the instrument.

The routine prompt is beam>.

If neither a SA or VA command has previously been issued an error message is printed and the routine is aborted.

For **CYLINDRICAL** geometry the parameters are (in cm):

Incident beam width

Incident beam height default 4.0

The following assumptions are made concerning the beam, although the programs are designed to accept more general cases. If alternative conditions are known to exist then the input .AIN and .MIN files must be modified outside of CORAL and before the jobs are submitted to batch

a) The collimation to the detector is set to 4cm wide - this will be wider than the sample in most cases.

b) The neutron beam height (defaulted to 4cm) will in general be less than the sample height (defaulted to 6cm). The neutron beam is centred on the centre of the sample.

c) The profile across the beam is constant and the beam is symmetric about the sample centre.

For **FLAT** plate geometry the only parameter is :

The angle between the incident neutron beam and a line perpendicular to the sample plane. The default value is 0., that is sample perpendicular to the beam. It is assumed that the sample is an infinite plate.

The routine also reads the data file (RAW or NRM) to obtain the number of angles and their values. The angle for each group will be printed.

Inputs parameters associated with a can and other annuli such as radiation shields.

The routine prompt is can>

For **CYLINDRICAL** geometry the parameters are :

Outer radius of annulus (cm) (for single can radius 3)

For **FLAT** plate geometry the parameters are :

Thickness of can at front (cm)

Thickness of can at back - default front value

COMMON parameters are :

Number density in atom or mol per $Å^{-3}$

Absorption cross-section @1.8Å in barns

File name for cross-section data - there is NO default file name.

If the file does not exist an error message appears and the routine is aborted.

There is one qualifier - MANY - which is invoked for more than one annulus . [At present restricted to 2 annuli]. This would be used for cases involving shields etc. When used the routine prompts for the number of annuli and the above set of parameters is repeated for each annulus. If not specified the default is one annulus.

The routine reads the number of wavelengths in the cross-section data file and if this differs from that in the sample file an error message is printed.

G E o m

The sample geometry can be changed using the SET command.

The command SET Geom Cyl

invokes cylindrical geometry whereas

the command SET Geom Flat

invokes flat plate geometry.

On entering the program the default is Cylindrical.
This command must be issued before any of the SA, VA or CA commands.

O U t p u t

This initiates output of parameters to a file.

The command O {option}

creates a file with the extension AIN or MIN (as specified by the option parameter) and the name will be that specified in the RUN command. If the option is not specified the routine prompts for a value.

{option} can take the values :
- Van for vandium corrections
- Abs for absorption correction
- Mul for multiple scattering correction

The routine prompt is out>

For **CYLINDRICAL** geometry the parameter is :

step size (cm) the default values are :
- 0.1 for VAN and MUL
- 0.02 for ABS

For **FLAT** plate geometry the parameters are :

for multiple scattering only		
accuracy	default	0.001
number of planes	default	100

The name of the data file created is also printed.

If a run number has not been given an error message is printed and the routine is aborted. The same happens if the option value is incorrect.

R U n

The output filename is defined with the command

RUN {run number}

If the runnumber is not specified, its value is asked for.

For the Vanadium it would be the vanadium run number. The sample run number is used for absorption and multiple scattering in the sample. If a can is present its run number is used for the can multiple scattering

S A m p l e

Inputs parameters associated with the sample.

The routine prompt is sam>

For **CYLINDRICAL** geometry the parameters are :

Sample height (cm) default 6.0

First radius (cm) default 0.0 for solid rod

Second radius (cm)

For **FLAT** plate geometry the parameters are :

Sample thickness (cm)

COMMON parameters are :

Number density in atom or mol per $Å^3$

Absorption cross-section @1.8Å in barns

File name for cross-section data - if only <RETURN> is typed itdefaults to a file with runnumber and extension .MUT eg LAD00123.MUT.

The routine checks that the data file exists ; if it does, the routine reads the number of wavelengths in the cross-section data file and uses that value. If the file does not exist it prompts for a value.

The job is submitted to the batch queue to run the corrections programs with the command

SUB {runnumber}

If {runnumber} is not specified the value given in the RU command is used and the correction option is that defined by the last Output command issued.

If {runnumber} is specified it refers to a file with that runnumber, not that given by the RUn command. The routine will ask for the correction option. This will normally be used to submit a job using a file created in a previous session on Coral.

There will be a LOG file with a name of the form ABS{runnumber} or MUL{runnumber} with extension .LOG.
The output from the programs will be in files with name LAD{runnumber} and extension .MUL, .ABS or .REF (for the VAN).
Lineprinter output will have extension .LIS.

Inputs parameters associated with vanadium.

The routine prompt is van>

For **CYLINDRICAL** geometry the parameters are :

Beam height (cm) default = 6.0

Vanadium radius (cm) assumes a solid rod

For **FLAT** plate geometry the parameter is :

Vanadium thickness (cm)

COMMON parameters are :

Number density default = 0.072 atoms/Å^3

Absorption cross-section @1.8Å default = 5.04 barns

File name for cross-section data - if <RETURN> is typed it defaults to file with runnumber and extension .MUT eg LAD00123.MUT.

The routine checks that the data file exists ; if it does, the routine reads the number of wavelengths in the cross-section data file and uses that value. If the file does not exist it prompts for a value.

3.8.5 Format of data files

For **CYLINDRICAL** geometry the format for the input data file to the programs is :

line	parameters
1	title
2	number of profile values
3	the profile values
4	step size for calculation (cm)
5	number of detector angles
6	the angle values
7 .1	height of sample
7 .2and.3	position of incident beam edges
7 .4and.5	position of detected beam edges
7 .6and.7	bottom and top of incident beam
7 .8and.9	bottom and top of scattered beam
8	number of annuli in sample (na)
9	radii of annuli (na+1) values
10 .1	number density in atom or mol/Å^3
10 .2	absorption c/s at 1.8Å
11	filename of total (scat+abs) c/s data
12	as 10 for next annulus
13	as 11 " " "

and so on.

For **FLAT** plate geometry the format for the input data file to the programs is :

line	parameters
1	title
2	angle between sample and beam

3		accuracy and number of planes calculation
4		number of detector angles
5		the angle values
6		number of cans plus sample
7		thicknesses of sample and can (front and back)
8	.1	number density atom or mol/$Å^3$ for sample
8	.2	absorption c/s at 1.8Å for sample
9		filename of sample total (scat+abs) c/s data
10		as 8 for can
11		as 9 for can

3.8.6 Format of output files

The .ABS files consist of a tabulation of the absorption factors, such as $A_{S,SC}$ for example, for every wavelength and scattering angle specified in the input file. The format is:-

no. of wavelengths
bank no. (not necessarily group no.), scattering angle of bank

then for each wavelength the values of

$\lambda(Å)$ $A_{S,S}$ $A_{S,SC}$ $A_{C,SC}$ $A_{C,C}$

This is repeated for each bank (normally 7 banks for LAD)

The .MUL files have a similar format. Using the notation of section 2.8 it is:-

no. of wavelengths
bank no. (not necessarily group no.), scattering angle of bank

then for each wavelength the values of

λ(Å) SINGLE(λ) M(λ) TOTAL(λ)

3.9 ROUTINE VANSM

This is a GENIE command file that removes the Bragg peaks from the vanadium spectra, puts a smooth line through the data, and divides by the calibration correction as described in section 2.7. This calibration correction is obtained by combining the results of the single and multiple scattering correction in the file with extension .REF with a vanadium Placzek correction estimated using the program g_F:N_PLAVAN, which uses the same formalism as that used for the sample Placzek correction described in section 3.11.

The routine reads the vanadium data from the file with extension .NRM and smooths using Chebyshev polynomials. The Bragg peaks are removed at the same time by ignoring the region around the peaks in the fitting procedure. The fitting routine defaults to 10 polynomials but this can be changed if required.

The routine is run from GENIE by typing @G_F:VANSM .

The routine just simply for the vanadium run number and a corresponding background run number and automatically loops through the groups. It requires a file with extension .REF to exist in the current directory, as produced by the VA command in CORAL. The smoothed result is output to a file with extension .SMO. Spectra from the SMO file can be read using the standard GENIE READ command.

It is recommended that users check that a satisfactory smooth line has been put through the vanadium data. This can be done by displaying the contents of workspaces 1 - n (n is the number of groups) after running VANSM. These workspaces contain the difference between the original .NRM data for each detector group and the smoothed version,

original .NRM data for each detector group and the smoothed version, but BEFORE the calibration correction has been applied. The command for this would be:

D/L W5 to display the difference for detector group 5

The user may wish to experiment with fitting Chebyshev polynomials of order other than the default 10:
-Before running VANSM diagnostic output may turned on by typing (in GENIE) v19=1.
-Similarly typing v20=15 sets the polynomial order to 15 for example.
The ideal polynomial order is selected so that the residual given in the diagnostic output has settled down to a value almost independent of polynomial order. Thus a suitable procedure for selecting an appropriate polynomial order involves first doing a test fit with diagnostic output on a very large (~50→100) polynomial order.

3.10 ROUTINE ANALYSE

This GENIE command file takes the spectra data and applies the corrections to produce the differential scattering cross section. The routine is invoked with the command

@g_F:ANALYSE

The routine reads sample and can data from the NRM files, the smoothed vanadium from the SMO file and corrections from the ABS and MUL files. It carries out the following operations as described in section 2.8:

- subtract background from sample
- divides sample by vanadium
- subtracts multiple scattering from sample
- if can is present :
  - subtract background from can

- divide can by vanadium
- subtract multiple scattering from can
- apply absorption correction to can
- subtract can from sample

- apply absorption correction to sample
- divide by sample calibration constant.

This is done on all groups specified and the results written to a file with extension .DCS. (Note that the sequence of operations given above is necessary in order that the corrections be performed properly.)

The ANALYSE routine requires the following input :

- option of can or no can
- sample, background and can run numbers
- range of groups to be used
- sample calibration constant which :

**** for CYLINDRICAL samples is the number of atoms or scattering units in the beam x 10^{-24}

**** for FLAT PLATE samples is the product of atomic number density (in atoms per $Å^3$) and the thickness of the sample in cm.

Spectra from the .DCS file can be read using the standard GENIE READ command.

(Note DCS stands for Differential Cross Section.)

3.11 ROUTINES PLATOM AND INTERFERE

PLATOM is a GENIE function to evaluate the self scattering from the sample. This routine uses the approach described by Powles [6] and extended by Howe, McGreevy and Howells [20] (see section 2.9) which

involves an expansion in powers of M^{-1} and derivatives of the detector efficiency and flux distribution. The user should decide whether or not this approach is acceptable for his particular experiment. It is intended to eventually offer programs implementing other alternative approaches to inelasticity correction. The routine PLATOM is executed by entering GENIE and typing:-

@g_f:PLATOM

A .NRM file is required for input so as to obtain the required Q-scale. (The default directory must be set to that of the .NRM file before entering GENIE.)

The GENIE function PLATOM can be applied to a multi-component system and requires the following input :

- number of atom species and for each one :
  - its fractional concentration (these should add to one)
  - its atomic weight. (in atomic mass units, ^{12}C=12.0)
  - its total scattering cross-section (in barns)
  - sample temperature (in units of Kelvin - used to calculate mean atomic kinetic energy in sample)

The user should check that the calculation of the self scattering is acceptable by using GENIE plots to check whether the corrected differential cross section oscillates about the calculated self scattering. At high Q the differential cross section (LAD01234.DCS) should tend to the average level given by the self scattering (LAD01234.SLF). This check may be performed by using GENIE to DISPLAY the self scattering and then to PLOT the differential cross-section on top (or vice versa). For example:

```
> READ W1 LAD01234.DCS 5
> READ W2 LAD01234.SLF 5
> D W1
> P W2
```

(Programming note: If the user makes changes to the routine PLATOM.COM to suit his own requirements he should be aware that it makes use of the GENIE variable v18.)

The GENIE routine INTERFERE is used to calculate the interference (or distinct as it is otherwise known) scattering by subtracting the self scattering (in the .SLF file) from the differential scattering cross-section (in the .DCS file). This routine is invoked by entering GENIE and typing:-

```
@g_f:INTERFERE
```

3.12 ROUTINE MERGE

This GENIE command file combines selected areas of spectra from different groups into one composite S(Q) as defined in section 2.10. For input it requires the sample .DCS or .INT file, the vanadium .SMO file and the vanadium .MON file to be present in the user's area. The output is in the file with extension .SOQ. Before running this command file the user must determine by plotting the results from ANALYSE or INTERFERE to determine which groups and which Q ranges for each group he or she wishes to merge. The routine is invoked by typing:-

```
@g_F:MERGE
```

3.13 ROUTINES STOG AND GTOS

These GENIE functions carry out the Fourier Transform of S(Q) to g(R) and its inverse g(R) to S(Q). They are invoked with the GENIE TRANSFORM command. Otherwise the required input by the user should be fairly straightforward. The command is for example, after the GENIE

```
TR W1 g_f:STOG W2
```

etc. Note that for these routines to work correctly it essential for both S(Q) and g(r) to oscillate about unity.