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The PRISMA GENIE Data Analysis Manual

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August 1994

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July 29, 1994

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1 Introduction

The GENIE program provides the basic means for analysing data taken on ISIS instruments. In this manual various GENIE macros and some FORTRAN programs which are customised for the analysis of PRISMA data are described. These macros/programs are available to a user who has executed the PRISMA_GENIE_SETUP.COM file and the varous two or three letter abbreviations (listed below) should appear when the user starts GENIE. A point to remember is that since some of these macros create files of their own during data processing it is not wise (safe) for the GENIE program using these macros to be simultaneously run by more than one user in the same subdirectory otherwise conflicts may occur. The macros listed below and the FORTRAN programs are described in more detail in the following pages.

List of GENIE macros

Alignment and Rocking Curve Routines

DD:==	@DSPACE	....	Display spectra in a step scan.
PP:==	@PSPACE	....	Display spectra in a multidetector step scan.
AA:==	@ANALYZ	....	Integrate a step scan for counts vs angle plot.
VA:==	@VANA	....	Transform a vanadium inelastic calibration to E_i.

Analysis of Inelastic Data

MRX:==	@MRX	....	Transform data to energy transfer.

Preparation of Data for PRSPLOT6

CC:==	@CONTOUR	....	Transform inelastic spectra.
VCRS:==	@VCRITICAL	....	Transform diffraction spectra.

Analysis of Temperature During a Run

TP:==	@TPLOT_KNH	....	Temperature plot from a log file.
TPC:==	@TPLOT_KNH_CURR	....	Temperature plot form the current run.
AT:==	@TBAR_KNH	....	Calculates average temperatures from log file.

Transforming and Fitting Workspaces

FF:==	@RUNFIT	....	Peak fitting program.
TT:==	@TRANS	....	Transform a workspace to λ, E_i, d-spacing or Q.
ERR:==	@ERRCOR	....	Rescale error bars which are too small.

2 The NOTICE Program and OLDNOTES.TXT File

The NOTICE program is incorporated into many of the GENIE macros used in the analysis of PRISMA data. It is usually included in these macros as a J/R command where the command string that is run is :

RUN PRISMA_KNH_GEN:NOTICE

This program creates a file OLDNOTES.TXT, the contents of which consists of the angular positions, sample/analyser parameters, the time of flight parameters and the spectra.dat structure for a particular run (.raw file). When the particular run was performed on PRISMA (using the PRISMA operating program) a file called NOTEBOOK.TXT was created into which all of this information was written by the PRISMA operating program. At the point at which the run was ended this file was copied into the .raw file. The NOTICE program simply extracts a copy of the NOTEBOOK.TXT file from the .raw file and names it OLDNOTES.TXT. The information in OLDNOTES.TXT is vital for transforming the time of flight data into energy transfer / wavevector / etc.

Note: The NOTICE program can be run anywhere to obtain the OLDNOTES.TXT file, not just from within GENIE, using the command line given above.

Prompts
The NOTICE program prompts the user for 3 pieces of information The first prompt is :

Enter run number :

which should be the integer run number. The next question is :

Enter directory (INST_DATA) :

This is the directory where the file is to be found. A <return> will use the logical name INST_DATA, which first points to the directory [PRSMGR.DATA] on the ISISE disks and then to the directory [PRSMGR.DATA] on the PRISMA microVax disks when searching for the file. The third and final question is :

Enter extension [.raw] :

Replying with a <return> will mean that NOTICE searches for a file with the extension .RAW. If the file was created with an UPDATE and STORE it has a .SAV extension and you should reply with either SAV or sav to this question.

3 The MODIFY Program

The parameters stored in the OLDNOTES.TXT file produced by the NOTICE program are the parameters that were stored in the PRISMA operating program when the relevant run was performed. In most cases these will be the relevant parameters for transforming a run. However it is possible to conceive of circumstances where this might not be so. For example if the temperature was changed and the user inadvertantly forgot to change the lattice parameters for the sample or if the sample moved on its mount and changed its rotation angle by a small amount. Another possibility is that the user wishes to transform the data using a different set of analyser planes, eg. PG(004) instead of PG(002). Finally, although it is very rare, it is possible for the NOTEBOOK.TXT file to become lost and not recorded with the .raw file (this does require the microVax to crash at a very precise wrong moment, but it has happened on a couple of occassions). Under these circumstances it is possible to analyse the .raw file by using the OLDNOTES.TXT from a run carried out under similar (but not necessarily identical) circumstances. This is done by specifying the "wrong" run number when the NOTICE program is run.

Under all of the circumstances described above, and possibly some as yet unthought of, it would be desirable to be able to modify the parameters in the OLDNOTES.TXT file. This can be done using the MODIFY program. It is run in a number of the macros described later on using the J/R command to execute the command string :

<p align="center">RUN PRISMA_KNH:COLOUR:MODIFY</p>

As in the case of the NOTICE program the MODIFY program need not just be run from within GENIE but can be run on its own by issuing the command above.

The MODIFY program loads the parameters contained in the OLDNOTES.TXT file in the current directory where the program is being run. In most cases this will be the file that has just previously been created by the NOTICE program. The first prompt issued by MODIFY is the question whether the user wishes to modify the parameters contained in the OLDNOTES.TXT file. Since on most occassions no change will be required the default answer is N, which can be selected by just pressing <return>. However if the answer is Y then MODIFY presents the user with a menu of the parameters that can be changed, as follows :

1) Sample parameters
2) Analyser parameters
3) Omega or phi angles
4) Analysing energies

and prompts the user to enter 1, 2, 3 or 4 to select the particular set of parameters for modification or to enter a <return> to exit from MODIFY. If the user selects 1, 2 or 3 they are presented with the current values of the various sample or analyser parameters and omega or phi angles as defaults and asked if they wish to enter a new value. If the value is not to be changed a <return> is sufficient. At the end of the set of values the user is returned to the main menu. The changed set of values can of course be reviewed by simply selecting that set of values again.

The 4th option, analysing energies, alters the analyser and detector angles. It only applies to inelastic measurements. The user is presented with a table of detector numbers and the respective analysing energies. If the analyser detector system was not set up then an analysing energy of 0.0 is presented. The user is then prompted to enter a detector number and a new analysing energy. The appropriate analyser and detector angles are calculated for the new analysing energy and the updated table presented again to the user and the user prompted for a detector and new analysing

energy. This process is continued iteratively until the user has updated all of the necessary analysing energies. In order to return to the main menu the user just enters a <return> at the detector and new analysing energy prompt.

4 Alignment and Rocking Curve Routines

The following routines are usually (but not necessarily always) used at either instrument or sample alignment times. The commands DD, PP and AA are involved with analysing a "scan" ie. where an angle of some description has been stepped and at each step counts recorded as a one or more time of flight spectra. As a precursor a brief description of the structure that a raw file takes during a step scan is given. It isn't of course necessary to follow this to use DD, PP or AA but may explain why these commands are needed to access the data.

4.1 Structure of a RAW file in a Step Scan

When a scan is performed, all of the data (for all detectors and all steps in the scan) is contained in one raw file. The way this is stored is as follows. Consider n detectors being scanned for p steps in the scan. The first (n+3) spectra are stored as follows in the raw file; spectrum S0 is a "junk" spectrum, S1 is the time of flight spectrum for the 1st detector in the spectra.dat list at the 1st point, S2 is the t.o.f. spectrum for the second detector in the spectra.dat list at the 1st point,...., Sn is for detector n at point 1, S(n+1) is for monitor 1 at point 1, S(n+2) is monitor 2 point 1. The spectrum S(n+3) is the equivalent of S0 for point 2, S(n+4) is for detector 1 point 2, and so on for n detectors and p points. Selecting the spectrum corresponding to a particular detector for a certain point in a scan along with the appropriate monitor spectrum with which to normalise the data is therefore not a trivial task. The point about the DD, PP and AA macros is that they do this process for the user and present them with a transformed/integrated and normalised spectrum or spectra.

4.2 The DD:== @DSPACE.COM Macro

The DD command allows the user to select and display a normalised spectrum for a particular detector at a particular point in a scan, and to easily display the same detector for successive points in the scan. This command works on both the PRISMA microVax and ISISE/ISVS5.

Initially the command prompts for a run-number, the answer to this can be (and very often is) DAE, ie. it is possible to view the spectra immediately after they have been taken. The command then prompts for the number of detectors which were or are being scanned. The next question is what units the spectra should be transformed to.:

$$(1) \text{ Lambda, } (2) \text{ Ei, } (3) \text{ D, } (4) \text{ ToF, } (5) \text{ Q}$$

If options 3or 5 are selected the command will then prompt for the PHI value, note that the <u>absolute</u> value of PHI should be entered. Next the command prompts for the lower limit of the display, and then on the next line the upper limit (don't put them both on the same line). It then asks for a bin size, which will be used to rebin the data after it has been transformed to 1, 2,or 3 above. This is all preliminary information which has to be entered when DD is started.

Next the command prompts for the "detector spectrum" to be viewed. Note this refers to the initial step in the scan, ie. the spectra.dat list printed on the LA120. Enter the spectrum number corresponding to the relevant detector in this list. The command then prompts for the point in the scan. After this it will plot the normalised spectrum corresponding to the relevant detector at that point. The normalisation is done by integrating monitor 1, dividing the spectrum by this number and multiplying by 10^5. This removes fluctuations in the ISIS current etc. from the intensities plotted.

When the plot is completed the command then offers 3 options :

$$(1) \text{ Exit, } (2) \text{ Different detector/point, } (\text{return})\text{next point}$$

Option 3 continues to the next point in the scan for the same detector and can be selected just by pressing <return>.

4.3 The PP:== @PSPACE.COM Macro

This macro is in many ways very similar to the DD command. It is however designed for use with a deliberate multi-detector scan. When first aligning a sample it is quite common to use all of the detectors on PRISMA in a scan to "search" for a Bragg peak. The 16 detectors cover a total scattering angle range of 30 degrees, which is equivalent to a rotation of 15 degrees of the crystal. However since the detectors are each 2 degrees apart in scattering angle it is usual to scan the omega angle of the crystal through 1 degree in say steps of 0.1 degrees, 11 points to cover the angular range "between" each detector.

Accessing spectra within such a scan is more easily done with PP than with DD. In order to change from one detector to another with DD it is necessary to exit from DD and re-enter. This isn't necessary with PP, the angular separations of the detectors are "hard programmed" into PP and switching from one detector to another is straightforward.

After starting PP the user is initially prompted for the number of detectors being counted in the scan. The second prompt is for the scattering angle PHI for detector "one" (ie. the angle for whichever detector is stored as spectrum one in the first step of the scan). PP only transforms the spectra to d-spacing and therefore the next three prompts are to do with the display range of the spectra in d-spacing. The first of these three prompts is for the minimum value, second for the maximum and thirdly the bin size into which the d-spacing spectrum should be re-binned. The next prompt is for the run number, which on the PRISMA microVax can also be (and most usually is) DAE. The next prompt is for the detector spectrum, ie. the spectrum number in the first point (spectra.dat list on the LA120) of the desired detector. The final prompt is for the point (step number) in the scan. After this the spectrum is plotted. Once the plot is completed PP offers 4 options :

(1) Exit, (2) Different detector and/or point, (3) Different run number, (CR) Next point

For option 4 a <return> will proceed and plot the same detector for the next point (step) in the scan.

4.4 The AA:== @ANALYZ.COM Macro

This command is used to "analyse" .raw files taken using the SC command. The program will first prompt for a run number to analyse and then run the NOTICE program which will prompt again for the run number and also for the directory and extension of the file to be analysed, as described in section 2.

The program next prints out the range of detectors active in the scan and prompts the user for the range of detectors to analyse. Note there is a maximum limit of 15 detectors which can be analysed at any one time. The range of detectors can be entered on the same line. Next the program prompts the user to see if the analysers were set up (ie. analyser-detector in theta-2theta geometry) or not. Next it prompts for the units in which the data should be integrated (time of flight, wavevector Q, incident energy or energy transfer). Next it prompts for the integration range for the detector and then for the monitor. At this point it starts the calculation. At each stage of the dialogue above a default value or range of values is offered by the program, 9 times out of 10 these default values will be sufficient and just a carriage return can be given. The analysis of the data involves integrating the monitor spectrum between the limits specified and each of the relevant

detector spectra for the limits specified for them at each step in the scan. Normalizing between the steps is done by dividing the detector integrals by the monitor integral and multiplying by 10^5 at each step. The normalized integrated data is then stored in workspaces, one for each detector, where the x-values are the angular positions and the y values the normalized integrated intensities. This data must be displayed in GENIE in point mode. Once the processing is finished a list of which detector is stored in which workspace is printed. This data can be fitted using the FF macro described later on.

4.5   The VA:== @VANA.COM Macro

When the alignment of the angular positions of the analysers and detectors has been completed it is common to run a vanadium calibration measurement in inelastic mode. The analysis of such a run can be done with the VA command. This will transform the time of flight spectrum to the <u>incident</u> neutron energy spectrum and rebin it in 0.1 meV bins. The peaks in the spectra corresponding to the incoherent elastic line from vanadium will therefore be at energies equal to the "true" analyser energies. The VA command initially prompts the user for the run number which is to be analysed. It then runs the NOTICE program and issues a second request for the run number etc. Following the requests from the NOTICE program VA prompts the user for the <u>number</u> of the first detector for analysis (<u>Note:</u> This is really the detector number not the spectrum number). The next prompt is for the number of the last detector for analysis. Following this the program prompts for the energy range over which the data is to be transformed. The first prompt is for the minimum energy and the second prompt for the maximum energy. With this information VA transforms the detector spectra from time of flight to incident energy, normalising them to the monitor spectrum, rebinning the spectra between the minimum and maximum energies in steps of 0.1 meV and finally places the results in workspaces 1 to the number of detectors being analysed.

Once VA has completed its work the workspaces can be plotted and if necessary fitted using the FF command. If the data is to be fitted some care may be needed with the error bars. Vanadium, although a <u>standard</u> incoherent scatterer, should not be mistaken for being a <u>strong</u> incoherent scatterer. Firstly the 0.1 meV bins may be too fine and may need rebinning into 0.2 or 0.5 or even larger (it depends on the value of E_f) bins. Secondly, away from the peak position in the background region, some data points may be zero or extremely small with error bars which are unreasonably small. The ERR command can be used to rectify this problem.

5 Analysis of Inelastic Data

5.1 The MRX:== @MRX.COM Macro

This is now the standard analysis command for data taken in inelastic mode. The command transforms the relevant inelastic spectra from time of flight to energy transfer, normalises it to the incident monitor spectrum and rebins it into units of 0.1 meV. The command will work for any number of spectra from 1 to 16. After entering MRX the program will initially prompt for the run number to be analysed. Following this it runs the NOTICE program which again prompts for the run number etc. Next the MODIFY program is run to allow the user to modify any of the parameters in the OLDNOTES.TXT file if they wish to. After this the final four prompts request, firstly the detector number of the first detector for analysis, secondly the last detector for analysis, thirdly the minimum energy transfer for which the data should be analysed and finally the maximum energy transfer. The data is then transformed and placed in workspaces 1 to the number of detectors analysed.

The MRX command does not work on the PRISMA microVax. If one wishes to look at the data in the DAE then it is necessary to do an UPDATE and a STORE to create a .SAV file. In this case the command SET EXT SAV should be given in GENIE before running MRX.

6 Preparation of Data for PRSPLOT6

6.1 The CC:== @CONTOUR.COM Macro

This macro transforms raw files measured in inelastic mode into a format for plotting in PRSPLOT6. After typing CC the program will prompt the user initially to see if a correction for monitor efficiency is required. The answer to this is almost certainly yes, which is option 1.

Following this the program prompts for the name of a <u>rebin file</u>. In processing data CC transforms each spectrum from time of flight to energy transfer and then uses the parameters in OLD-NOTES.TXT to calculate for each energy transfer the corresponding H,K and L values. These values are written to a file along with the value of the energy transfer E, the counts (per meV) and the error in the counts. After transforming from time of flight to energy transfer, but before calculating H, K and L the data is re-binned in energy transfer. The purpose of the rebin file is to allow the user to define the way in which this re-binning is done. The rebin file should have a reasonably short name with extension .COM and should consist of one line which should be a rebin command for workspace 3 in GENIE. For example ;

> rebin w3 -10 (0.5) 20 (1) 40

The choice of rebin format after w3 is completely up to the user with the proviso that there should be less than or equal to 500 points in the workspace after re-binning. The choice of rebin command depends upon factors such as statistics and resolution.

The next prompt is for the run number to analyse. Following this the NOTICE program is run and again the run number etc. is prompted for. Following this the MODIFY program is run which prompts the user to see if they wish to modify the parameters stored in the OLDNOTES.TXT file. The next two prompts are for the range of detectors to be analysed, the first for the first detector to analyse and the second for the last detector to analyse. The program then prompts for each of the individual detectors between the first and last to see if that particular detector should be included in the analysis or not, 1 to include, 0 to exclude.

CC will then process each of the selected detectors in that particular run. On completion of all of the detectors CC will print out a message telling the user that it has processed the first to last detectors in that particular run and prompt the user to see if another run should be processed. The answers are 0 for no and 1 for yes. If another run is to be processed then control returns to the run number prompt and the whole procedure is repeated.

The output from CC is written to a file CONTOUR.OUT, which is in the appropriate format for loading into PRSPLOT6 with option 5 and for contour plotting. <u>NOTE</u> the CC process always <u>appends</u> data to the file CONTOUR.OUT. If the file already exists in your directory when you type CC whatever you process will be appended to that file. Thus the user must be careful to make sure that CONTOUR.OUT is renamed when they are starting a new contour map. The PRSPLOT6 program will accept any (reasonably short) file name for a contour map file, it doesn't have to be CONTOUR.OUT. Another aspect of this is that it is always possible to add extra runs to a contour map by renaming the file back to CONTOUR.OUT and running CC.

6.2 The VCRS:== @VCRITICAL.COM Macro

This macro transforms raw files measured in diffraction mode into a format for plotting in PRSPLOT6 when loaded with option 6. It offers the option of normalising the data by dividing by a vanadium spectrum. In nearly all cases this is the best option to take, in which case a vanadium calibration must have been (or be) performed for the same detector scattering angles. The data is transformed

from time of flight into wavevector transfer and then using the information from OLDNOTES.TXT the appropriate H, K and L values are calculated and written to a file along with the magnitude in Å^{-1} of the wavevector, the neutron counts (per Å^{-1}) and the error in the counts.

The first prompt after typing VCRS is for a <u>rebin file</u>. This is a one line file where the contents take, for example, the form :

$$> \text{rebin w4 0.5 (0.01) 1.5}$$

and whose name should be reasonably short and should have the extension .COM. After the w4 the choice of rebin structure is up to the user, as long as the total number of points in the workspace after re-binning is less than or equal to 500. The rebin command is used to rebin the workspaces in wavevector transfer in Å^{-1} units.

The next prompts concern the vanadium calibration run. Initially the program prompts to see if a vanadium calibration is required, 1 for yes, 2 for no. Assuming the answer is yes, then the various prompts detailed in the rest of this paragraph are made. If the answer is no then skip to the next paragraph. The program prompts for the run number of the vanadium and then runs the NOTICE program which again prompts for the run number etc. Following this the MODIFY program is run to see if any of the parameters pertaining to the vanadium run need modifying. After this the program prompts for the range of detectors for which the vanadium calibration should be produced. The values in [ ] brackets are default values and may be selected by pressing return. Note it is necessary to have vanadium calibrations for all of the detectors (at the same scattering angles ϕ) as used in the data sets to be processed. Next the program prompts to see if the vanadium run should be smoothed or not, 1 for yes, 2 for no. The answer is on most occasions is yes. Usually a vanadium run will not have been counted for as long as a data run, and the statistics not as good (remember also that vanadium is not a strong incoherent scatterer, just that it has zero coherent scattering). However one is not interested in fine features in the vanadium spectrum, just the overall intensity and a very broad energy/ time of flight dependence. Consequently it is quite valid to fit the vanadium spectrum and to use the fit result rather than the raw data. If the user wishes to see for themselves what the effect of "smoothing" the vanadium is then they can do the following. Read the vanadium spectrum into a workspace, eg. W1 and then type TRANS W1 PRS_KNH_GEN:SMOOTHER W2 and the smoothed vanadium spectrum in time of flight will be written into W2. A comparison of raw data and smoothed data can then be made by overplotting W1 and W2. This smoothing method obviously works well if no analysers were in place in front of the detectors used. However if analysers were in place this smoothing is dubious because it will not take account of dips in the spectra due to scattering by the analysers.

After the vanadium calibration run has been processed or if no vanadium calibration is required the program then prompts for the run number of the data to be transformed and then runs the NOTICE program which again prompts for run number etc. Again this is followed by the MODIFY program to see if the parameters in the OLDNOTES.TXT file should be modified. Next the program prompts for the range of detectors to be analysed. As before the values in [ ] brackets are default values which can be selected by a return. The data is then processed, it is normalised to the incident monitor spectrum, divided by the vanadium for calibration, transformed to wavevector in Å^{-1} and the corresponding H, K and L values calculated. After this the program prints out the run number and range of detectors processed and prompts the user to see if another run is to be processed, 1 for yes and 2 for no. If another run is to be processed then program control returns to the point at which the run number of the data was first prompted for.

The output from VCRS is written to a file called CRITICAL.OUT. This file is always appended to when VCRS is run and thus care must be taken to make sure that this file is appropriately renamed

when all of the relevant processing has been completed. Otherwise detector spectra from unrelated runs will all be mixed together in the same file. Alternatively of course if the user does wish to append an extra run to an existing contour map then the file containing this map should be renamed back to CRITICAL.OUT.

7 Analysis of Temperature during a Run

7.1 The TP:== @TEMP_KNH.COM Macro

This command will use the .LOG file from a run to produce a workspace in GENIE in which a plot of temperature versus real time during the run is given. It can be run on ISISE/ISVS5/etc. or on the PRISMA microVax. It initially prompts the user for the run number and then for the name of the sample environment block. The 3 choices are TEMP, TEMP1 and LAKES. The first two are the two controllers in the Eurotherm and the third is the block appropriate for the Lakeshore controller if it was used. The resulting workspace in GENIE must be plotted in point mode.

7.2 The TPC:== @TEMP_CURRENT_KNH.COM Macro

This is the same as the TP command except that it works for the current run and can only be run on the PRISMA microVax. Note that if you use TPC to look at the temperature change and then a few minutes later use it again to look at the temperature then you may well have to use an L/D command in GENIE. The point is that TPC writes to W1, if you D/L W1 and then use TPC again, and then do D/L W1 again, GENIE will still use the x and y axis limits from the first plot. The L/D command resets the plotting limits.

7.3 The AT:== @TBAR_KNH.COM Macro

This command will calculate the mean and standard deviation of a temperature during a run from the .LOG file. After typing AT the program prompts for the run number. All 3 of the sample environment blocks, TEMP, TEMP1 and LAKES will be processed (assuming they were all being used, otherwise only the active ones) and the relevant average and standard deviation printed out.

8 Transfroming and Fitting Workspaces

8.1 The FF:==@RUNFIT.COM Macro/Program

The FF command is a fitting program which allows up to 301 data points contained in a GENIE workspace to be fitted to up to 5 peaks, plus a flat and a sloping background. These peaks may be any combination of Gaussians (G), Lorentzians (L), Kropf functions (K) and Reversed Kropf functions (R). The Gaussian function is given by :

$$G(x) = H \exp\left(-0.5\left(\frac{x-C}{F/2\sqrt{\log 4}}\right)^2\right)$$

and the Lorentzian function by :

$$L(x) = \frac{H}{(x-C)^2 + (F/2)^2}$$

where H is the height, C is the centre and F is the full width at half maximum. The Kropf function is given by :

$$K(x) = A \exp\left(-\frac{x-O}{\tau}\right)\text{erfc}\left(\frac{1}{\sqrt{2}}\left(\frac{\sigma}{\tau} - \frac{x-O}{\sigma}\right)\right) / \text{erfc}\left(\frac{1}{\sqrt{2}}\left(\frac{\sigma}{\tau}\right)\right)$$

and the reverse Kropf function $R(x)$ can be obtained by changing the minus signs in front of the two $(x - O)$ terms. This function is asymmetric with a sharp edge on one side and a long tail on the other. For $K(x)$ the tail is on the right hand side and for $R(x)$ it is on the left. It should be noted that the A and O parameters are not equivalent to the height and centre of these functions.

The data to be fitted must be contained in a GENIE workspace in a point (not histogram) format. The mode should have been toggled to point plotting mode. Any rebinning of the data has to be done before fitting and the binning has to be set to 1 (ie A B 1). After typing FF the program prompts for the workspace in which the data is held. Next it prompts for a workspace into which the final calculated curve can be written. Following this the program first prompts for the lower x limit for plotting and then for the upper x limit. Note these limits must be given on separate lines. The data is then plotted for the user to view. The next prompt is a request for how many peaks are to be fitted, the answer can be any number from 0 to 5. If the answer is 0 then no peaks will be fitted only a straight line background. Following this a message is printed concerning how to mark the peaks with the cursor and the instruction "Press return to begin". Entering a <return> switches to the graphics screen and activates the cursors. At this point the user should mark the "position" of the peak using the cursors. For the Gaussian and Lorentzian this is the peak centre and maximum height. For the Kropf functions this should be the point of inflection on the sharp edge (quite often about half way up the sharp edge). The marking is done by positioning the cursors and on a Pericom/Falco pressing <return> while on a workstation it is done by clicking the left mouse button. The user is then presented with a menu of various letter choices, enter an E. This process will be repeated for each of the peaks.

The FF program now leaves the GENIE commands and enters the fitting program proper. For all of the following prompts which relate to numerical parameter input a default value is offered which can be selected by just pressing <return>. Also following each parameter a fitting flag is requested, entering a flag of 1 allows the parameter to vary in the fitting while entering a 0 keeps the value fixed. The first two parameters prompted for are the flat level and the (linear) slope of

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the background. Then for each peak in turn the various parameters are requested. Firstly the type of peak is requested, the answer should be one of the letters G, L, K or R. For the Gaussian and Lorentzian these are the values H, F and C and for the Kropf functions the values A, σ, τ and O. Finally the program prompts for an upper limit to the number of fitting iterations it should carry out.

The fitting program then proceeds to carry out the non-linear least squares fit. At each step of the iteration it prints out to the screen the agreement factor. This is defined as :

$$\sqrt{\frac{1}{N-k} \sum_i \left(\frac{I_i^{obs} - I_i^{cal}}{e_i} \right)^2}$$

where I_i^{obs} are the experimental values, I_i^{cal} are the calculated values from the fit, the e_i are the errors in the observed values, N is the number of data points and k is the number of parameters being varied. At the end of the fitting the program prints to the screen the final fit parameter results and plots a calculated curve through the data on the graphics screen. Note this calculated curve is contained in the workspace selected for the calculated results at the beginning and can therefore be replotted by the user if necessary. The program also creates two files in the current directory, PRGFIT.OUT and PRGFIT.RES. The first of these contains the parameter results at each iteration during the fit and is overwritten each time a fit is performed. The second file PRGFIT.RES contains the final fit results along with other information such as the fit time, integrated area of the fitted peak and for the Kropf functions their peak height, centre of mass and peak position. This file is always <u>appended</u> to. So if a series of fits is performed then all of the fit results will be saved in the same file. Some care must be taken therefore to make sure that PRGFIT.RES files are deleted or renamed when they are finished with.

8.2   The TT:==@TRANS.COM Macro

This GENIE command will transform a workspace from time of flight into either, wavelength (lambda), incident neutron energy (E_i), or d-spacing. It will perform the time shift to account for the DAE counting error, set the parameters for the workspace and carry out the units command. The resulting transformed data is contained in the same workspace. It is not rebinned after the units command.

The command prompts initially for the workspace number and then for the type of counter :

<center>1) Detector, 2) Monitor 1, 3) Monitor 2</center>

Next the command prompts for the choice of units to which the workspace is to be transformed :

<center>1) Lambda, 2) EI, 3) E-transfer, 4) Q</center>

For options 3 and 4 the command will then prompt for the PHI angle. Note the input should be the <u>absolute</u> value of PHI.

8.3   The ERR:== @ERRCOR.COM Macro

This command can be used to set a lower limit to the size of error bars in a workspace. It is quite often a problem when processing vanadium energy calibration runs (but also on other occasions) that data points in the background region have unreasonably small error bars. This can cause problems when trying to fit the data. The ERR command can be used to search through a workspace and replace

error bars smaller than a preset value to the preset value. After typing ERR the user is prompted for the number of the workspace to be processed. Next the user is prompted for the minimum value for the error bar. After this ERR processes the workspace.