Data Reduction for the NIST Triple-Axis Spectrometers

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INTRODUCTION

This new triple-axis spectrometer (TAS) data reduction application has been designed so that you can do simple things quickly and easily and perform more sophisticated manipulations with as few mouse clicks as possible. Repetitive tasks such as saving intermediate steps and combining multiple TAS files in a parametric investigation have been automated thus decreasing the amount of time spent on the data reduction phase. Some intelligence has been programmed into this application to facilitate data reduction. For instance, the application automatically selects the independent variable when the file is loaded. Also the user can automatically fit up to 10 Gaussians or 10 Lorentzians to their data at any phase of data reduction without typing in any initial parameter guesses. Originally designed as a simpler alternative to ADDRUN and TASXP this application provides the triple-axis experimentalist with a simple-to-use graphical user interface allowing entry-level users access to rapid data manipulation and processing.

This application allows users to perform fundamental data reduction and processing operations and send the data into the other applications, such as visualization and analysis, that are part of the DAVE software suite. The reduction options include subtraction of fast background, scaling, calibration of an independent variable, addition and subtraction of multiple files, monitor normalization, correction for higher order harmonics present in the incident beam, correction for effects of the resolution volume, and correction for detailed balance.

There are multiple output options. Any plot produced in this application can be sent to a color (encapsulated) postscript file. Moreover the data can be saved as formatted ASCII. The availability of formatted text output for the reduced data in this application ensures that the user has the maximum amount of flexibility in performing more specialized custom analysis and/or producing publication-quality plots.

This manual provides instruction in how to use this data reduction application. In it the user-interface, data reduction options, and summary of the data processing are all described. Furthermore, a complete reduction example is described so that the novice user can gain experience and knowledge of this program's features by following along. Finally a list of frequently-asked questions with answers is provided. If you have a question that does not appear in the list feel free to contact Rob Dimeo via e-mail (robert.dimeo@nist.gov) or telephone ((301) 975-8135).

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OVERVIEW OF THE USER-INTERFACE

The user interface (UI) for this application is file-centric and is relatively sparse in terms of the controls immediately visible (see Fig. 1). This was done on purpose so as not to overwhelm the user with options. As shown in Fig. 1 the UI consists of a tree view on the left side and a data display window on the right side. The tree view provides a means with which the user can organize his/her data files. In order to keep the appearance of the interface clean control of the program is driven largely through context-sensitive menus (CSM). A CSM is made visible by selecting an object such as a data file in the tree view and pressing the right mouse button.

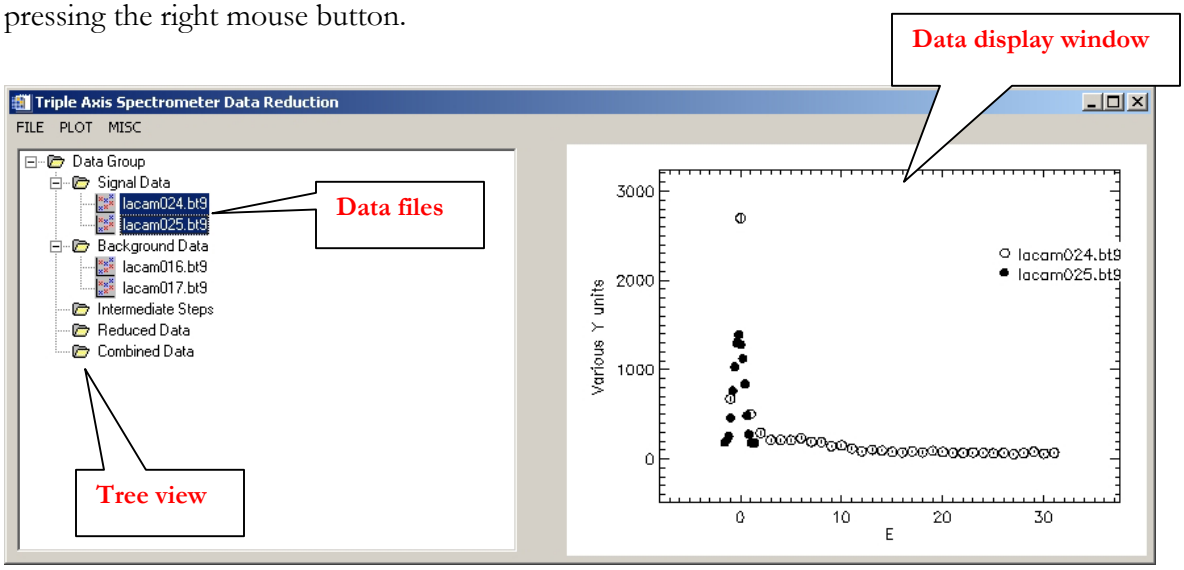

Figure 1 User interface with four data files loaded.

The Menu Bar

The menu bar at the top of the interface contains three menus: **FILE**, **PLOT**, and **MISC**. The menu options under **FILE** are **Load Signal File**, **Add New Data Group**, **Load Example TAS File**, and **Quit**. The first choice allows the user to select multiple TAS data files that will be placed automatically into the **Signal Data** folder. The second choice creates a new root node named **Data Group** which is independent of the original root node. The user can add as many new root nodes as he/she wishes. The third choice loads an example TAS data file into the **Signal Data** folder. An example of the data reduction process will be presented which uses this example file. The last choice exits the program and returning the user to the main DAVE level.

The **PLOT** menu option is Legend plot preferences which launches a dialog with two sliders that control horizontal and vertical placement of the legend and an input text box for the text size. The default size for the legend text is 1.0 and any value between 0.75 and 1.5 should be adequate for postscript output as well as viewing on the screen.

The **MISC** menu options are **Quick-Start Instructions**, **Data Reduction Manual** and **About TAS Data Reduction**. The first choice launches an abbreviated description of this program in PDF format. The second choice launches this document (the *Manual*). The last choice launches a small dialog showing the author and creation date for this application.

The Tree View

The tree view is an interface that facilitates organization of your data. As shown in Fig. 1 the tree view is composed of multiple nodes, branches, and leaves displayed as folders, connecting lines, and scatter plot icons, respectively. The tree view hierarchy is rooted at a node named **Data Group**. Under this root node there are five other nodes named **Signal Data**, **Background Data**, **Intermediate Steps**, **Reduced Data** and **Combined Data**. The user can load data into only two of these folders, **Signal Data** and **Background Data**, which is done using the CSM for those folders. Upon reducing the data, if the user has elected to save the intermediate reduction steps, then new icons appear in the **Intermediate Steps** folder corresponding to the intermediate steps. Moreover at least one new file icon should appear in the **Reduced Data** folder corresponding to the reduced data.

The Data Display Window

The data display window contains a plot of the data reflecting which files are currently selected. Multiple file selection results in multiple symbols and possibly colors whose definitions are seen in the legend. For example, Fig. 1 shows two selected data sets in the tree view and the data display window shows two different data sets with open and filled symbols. The data display window allows zooming using the familiar rubber-band box method. This works by the user holding down the left button while the cursor is in the data display window, dragging the mouse over the region of interest, and releasing the mouse button. The result is a magnified view of the region of interest. In order to autoscale the plot, press the left mouse button while the cursor is anywhere in the data display window.

The Context-Sensitive Menus

Each of the folders and files offer different CSMs to the user. The CSM for the **Data Group** folder is shown in Fig. 2. As the name *context-sensitive menu* implies, choices from this menu affect only those nodes that are derived from this root node. The choices allow the user to specify the reduction preferences, reduce the data, rename the folder labeled **Data Group** to anything the user wishes, change the independent variable of all of the data files contained within this node, and remove all of the data files from the tree hierarchy.

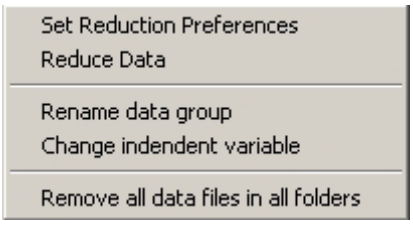

Figure 2 Context-sensitive menu for the **Data Group** folder.

The CSMs for the **Signal Data** and **Background Data** folders are identical and contain two items: **Load file(s)** and **Remove all signal (background) files**. The first choice allows the user to load (possibly) multiple files into the the **Signal** or **Background** folder, depending upon which one was selected when the CSM was invoked. The second choice removes the data from memory (not from disk!) and also deletes the corresponding icons from the tree view. Note that this only applies to the folders from which the CSM was invoked.

There is only one CSM for each of the other folders (**Intermediate**, **Reduced**, **Combined**) and the choice in each of those CSMs is **Remove all Intermediate/Reduced/Combined Files**. The behavior of this selection is identical to that of **Remove all signal files** in the **Signal Data** CSM.

The CSM for the signal data file is shown in fig. 3. The contents of the background data file CSM, Intermediate steps data file CSM, and reduced data file CSM are similar to the elements described below.

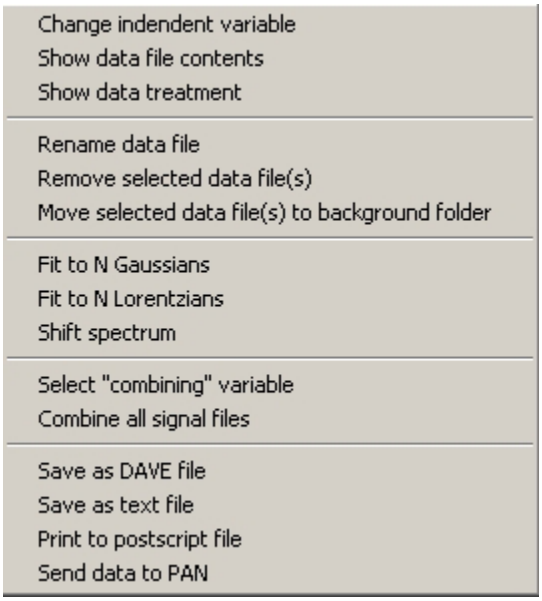

Figure 3 Context-sensitive menu for data files.

The selections in Fig. 3 are summarized below.

- **Change independent variable**: provides the user with a control panel allowing selection of the independent variable from a list of possible choices based on the contents of the data file. Choosing a new variable from the control panel results in an instantaneous update of the data in the data display window.
- **Show data file contents**: launches an ASCII viewer that displays the original raw TAS file, if no reduction steps have been performed, and column-formatted text containing the reduced/processed data if it has been treated (i.e. it is not *raw* data).
- **Show data treatment**: launches an ASCII viewer that displays how the data have been treated.
- **Rename data file**: allows the user to change the name of the file that is displayed next to the file icon.
- **Remove selected data file(s)**: allows the user to remove the selected file from memory (not from the disk!).
- **Move selected data file(s) to background folder**: self-explanatory.
- **Fit to N Gaussians**: Launches a slider control specifying up to 10 Gaussians on a flat background to fit to the data. Note that as soon as you release the left mouse button on the slider a fit will be attempted. The fit appears as a thick purple curve on

top of the data. No initial guesses are needed here becuase an intelligent peak-finding algorithm is used to locate the amplitude, position, and full-width at half-maximum of the peaks.

- **Fit to N Lorentzians**: Same as **Fit to N Gaussians** except that Lorentzian lineshapes are used instead of Gaussians.
- **Shift spectrum**: Launches a text entry where user can specify how much to shift the independent variable (positive or negative increments).
- **Select "combining" variable**: User can select from among all of the independent variables (specifically the mean of all of their recorded values) as well as HFIELD to be used as a second independent variable to combine multiple TAS files. For example, one might want to combine many constant-Q, fixed E_f scans taken at different temperatures and study the temperature-dependence of some peak position. The user should select TACT (e.g. temperature) as the "combining" variable.
- **Combine all signal files**: Combines all of the selected signal files with the default first independent variable and the second independent variable as defined via the "combining" variable discussed previously.
- **Save as DAVE file**: User can save selected files in the standard DAVE format for use in other DAVE applications.
- **Save as text file**: User can save all of the current variables as ASCII.
- **Print to postscript file**: Launches interface allowing extensive control over output format (e.g. color, encapsulated, orientation, size, ...).
- **Send data to PAN**: Data is sent to the data analysis program in DAVE called PAN with no saving necessary.

DATA REDUCTION OPTIONS

There are a number of data reduction options which can be invoked or suppressed based on the needs of the user. All options are chosen using the reduction configuration interface that is launched by selecting **Set Reduction Preferences** from CSM of the **Data Group** folder. The reduction configuration interface is shown in fig. 4 below.

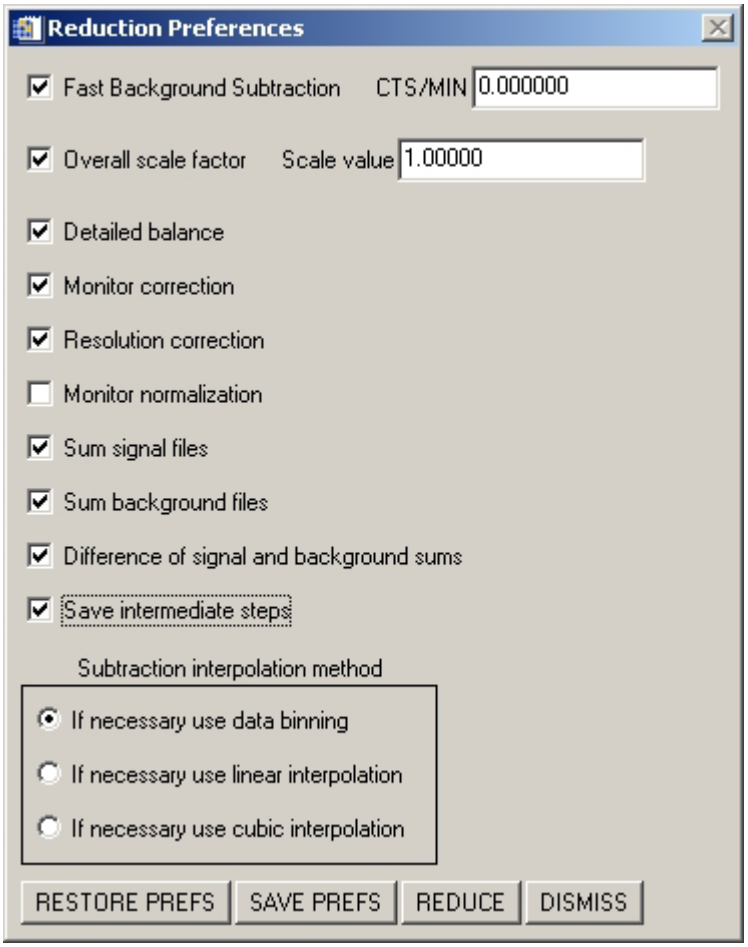

Figure 4 Data reduction preferences interface.

The gory mathematical details of the numerical procedures used in the data reduction are not discussed here but we provide here a summary description of each possible step and how the user-interface shown in Fig. 4 functions.

The Reduction Configuration User-Interface

The user-interface for the reduction is composed of a series of check-boxes and radio buttons. The check-boxes can be "turned on" or "turned off" at will by simply selecting or de-selecting the check-box. For the fast background subtraction the user must make sure that the check-box is "checked" and enter a value in the input labeled CTS/MIN. The overall scale factor functions similarly to the fast background subtraction. The remaining check-boxes behave in a mode in which they are either "on" or "off" depending on their "checked" state. The radio buttons that make up the "Subtraction interpolation method" specify which method is to be used when a subtraction of one file from another is

performed. Data binning, the default, is always recommended but the linear and cubic interpolation methods are also available.

It is important to note that not all of the data reduction steps are applicable to all of the data files. The reduction algorithm is intelligent enough to know when *not* to apply a particular correction even if that particular box was checked by an unknowing user. Inspection of the data treatment via the data file CSM will indicate which reduction steps were *actually* performed.

In order for your customized reduction preferences to take effect you must press the **REDUCE** button. The effect of pressing the **REDUCE** button should be immediate. There is no need to dismiss the configuration UI. If you wish to save your customized data reduction preferences you can save them now and restore them at any time in the future via the **SAVE PREFS** and **RESTORE PREFS** buttons, respectively.

The Data Reduction Steps and Order of Operations

The reduction steps are performed in a specific order as listed in the bullet list below. All possible steps are summarized here but recall that not all of the steps apply to all of the types of TAS files.

- **Summing signal files**: All data files contained in the **Signal Data** folder are combined by summing the intensities weighted by their individual monitor counts.
- **Summing background files**: All data files contained in the **Background Data** folder are combined by summing the intensities weighted by their individual monitor counts.
- **Difference of signal and background sums**: The difference of the summed signal and summed background files is calculated via interpolation (choice of data binning, linear or cubic interpolation) where the background sum is weighted by its monitor prior to performing the difference.
- **Fast background subtraction**: A scalar value (counts/minute) is subtracted off of every data point in the data set after multiplying the scalar value by the time per point. Note that all subsequent reduction operations (except overall scale factor and save intermediate steps) require that a fast background subtraction be performed even if the value of the fast background is zero.
- **Resolution volume correction**: The data and error bars are multiplied by the following factor, $\left(\frac{k_i}{k_f}\right)^3 \frac{\cot(\theta_M)}{\cot(\theta_A)}$, where k_i (k_f) is the wavevector of the incident (scattered) neutron and θ_M (θ_A) is the scattering angle of the monochromator (analyzer). This factor corrects the intensities in a constant-Q scan with fixed incident energy, E_i, since the phase space volume V_f is not constant when one changes the final energy, E_f.[1]

[1] G. Shirane, S.M. Shapiro and J.M. Tranquada, *Neutron Scattering with a Triple-Axis Spectrometer* (Cambridge University Press, 2002).

- **Detailed balance**: The data and error bars are multiplied by a factor $\exp(-\beta E/2)$ where $\beta = 1/k_B T$ and $E=\hbar\omega$ so that the result satisfies the principle of detailed balance: $S(-\mathbf{Q},-\omega) = S(\mathbf{Q},\omega)\exp(-\beta E)$.
- **Monitor correction**: The data and error bars are scaled to account for higher-order harmonics in the beam. This correction is only applied in constant-Q scans when E_f is fixed and E_i varies. The scale factors are read in from a data file collected on BT-2 and the values are interpolated (linearly) to the energy transfers in the data file being reduced.
- **Normalization to beam monitor**: The data and error bars are scaled to the beam monitor as defined by the product of the PRF and MON fields in the original data files. The actual value of the beam monitor used in the multiplication depends on how these quantities have been propagated through the reduction process.
- **Scale factor**: The data and error bars are scaled by the scale factor defined in the reduction configuration UI.

ADDITIONAL DATA PROCESSING AND OPERATIONS

In addition to the data reduction options discussed in the previous section there are a few other operations that do not necessarily fall into the category of data reduction but are available to the user.

- **Shift spectrum**: User can specify how much to shift the independent variable (positive or negative increments, δ). For instance the result of such a shift in the independent variable x is $x_i'=x_i+\delta_i$ where δ can be a positive or negative number.
- **Combine all signal files**: Combines all of the selected signal files with the default first independent variable and the second independent variable as defined via the "combining" variable discussed previously. The combining is performed using linear interpolation for the files so that they all are defined over the same range in the first independent variable. Naturally it is required that all of the first and second ("combining") independent variables be of the same type (e.g. all temperature, or all magnetic field, etc.)

OUTPUT OPTIONS

There are multiple output options for the data files and these options can be accessed via the CSM for those particular files. The choices are listed below:

- **Save as DAVE file**: User can save selected files in the standard DAVE format for use in other DAVE applications.
- **Save as text file**: User can save all of the current variables as ASCII.
- **Print to postscript file**: Launches interface allowing extensive control over output format (e.g. color, encapsulated, orientation, size, ...).
- **Send data to PAN**: Data is sent to the data analysis program in DAVE called PAN with no saving necessary.

A SIMPLE REDUCTION EXAMPLE

A sample data file comes bundled with the DAVE distribution. This data file can be loaded from the **FILE** menu bar with **FILE→LOAD EXAMPLE TAS FILE**. A file icon will appear located under the **Signal Data** folder with the name Lacam025.bt9. You can select this file with the mouse and the data will be displayed in the data display window as shown in fig. 5.

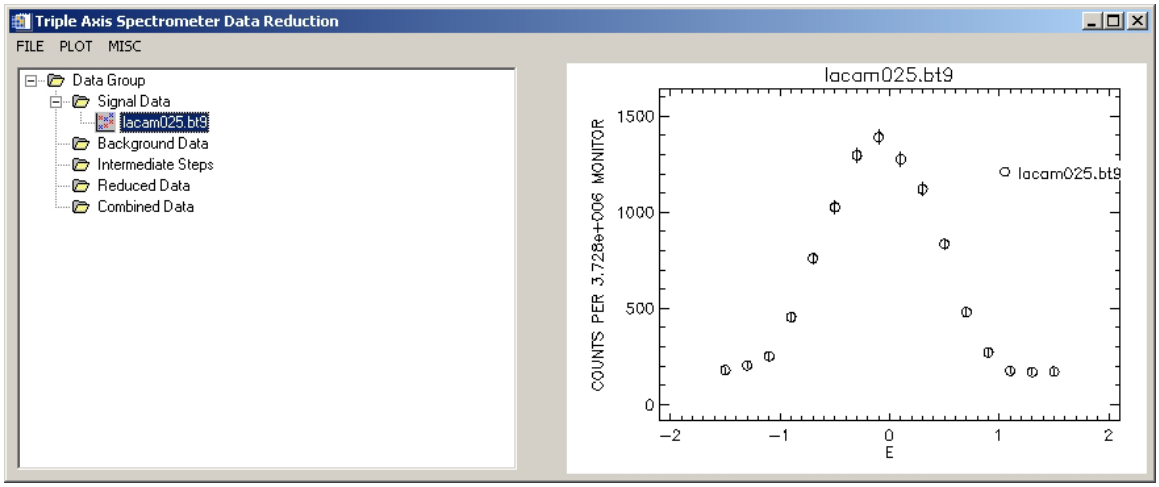

Figure 5 Example TAS data.

Try zooming in and out of the plot using the mouse and the rubber-band box zoom function as described in the description of the data display. Also try examining the contents of the file by invoking the CSM for the file and selecting **Show data file contents**. You should see something similar to what is displayed in fig. 6.

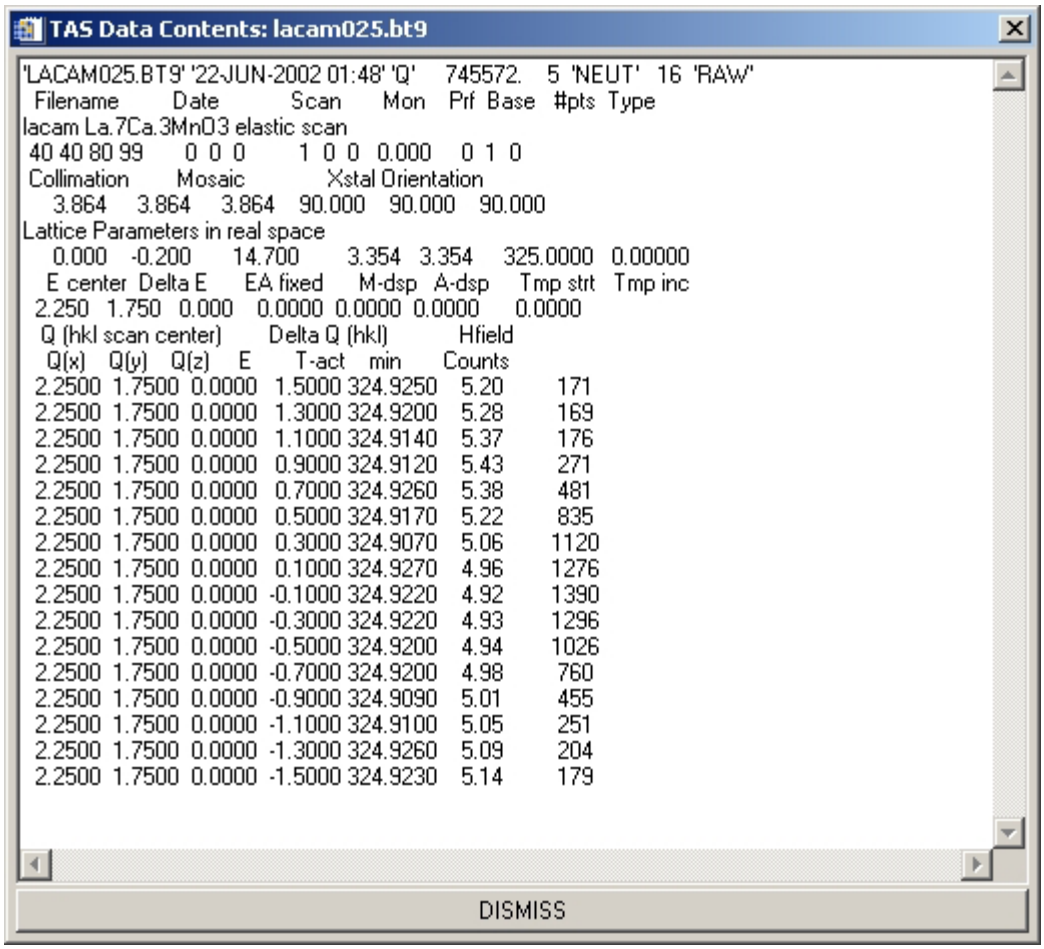

Figure 6 Example data file contents as viewed using the CSM item.

Now examine the reduction preferences by selecting the **Set reduction preferences** item from the **Data Group** CSM. Check off **Save intermediate steps**. Press the **Apply** button and dismiss the interface. Next press the **Reduce data** item from the **Data Group** CSM. After reducing the data the UI should appear like that shown in fig. 7.

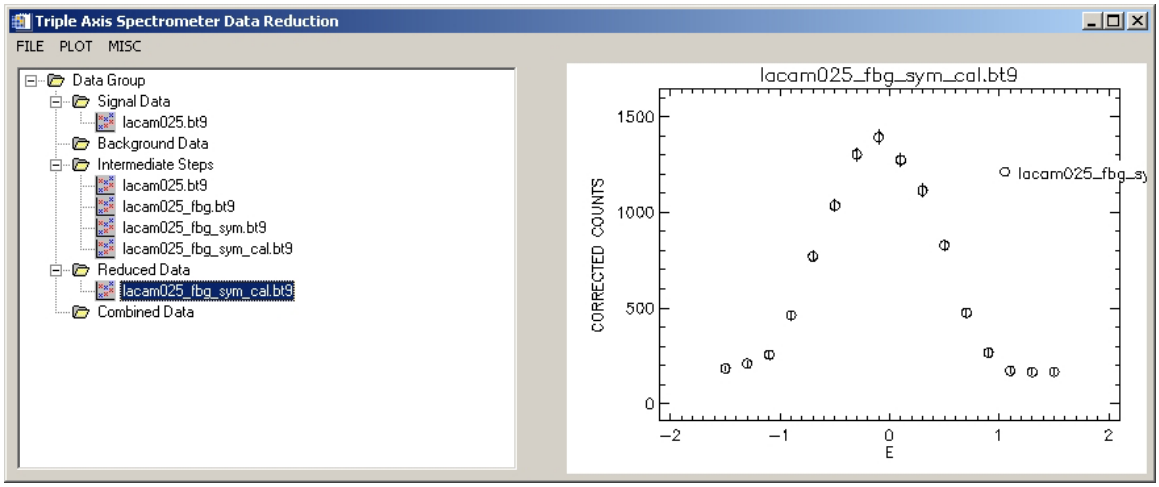

Figure 7 The UI after reducing the data and saving all of the intermediate steps.

Notice that 5 new file icons appear underneath the **Intermediate steps** folder. These can each be inspected individually or they can all be selected for an overplot. Such an overplot provides you with a visual representation of the effects of each reduction step.

You can inspect which data reduction steps were performed on the data set by selecting **Show data treatment** from the CSM of the only file under the **Reduced Data** folder. You should see a display similar to that shown in fig. 8.

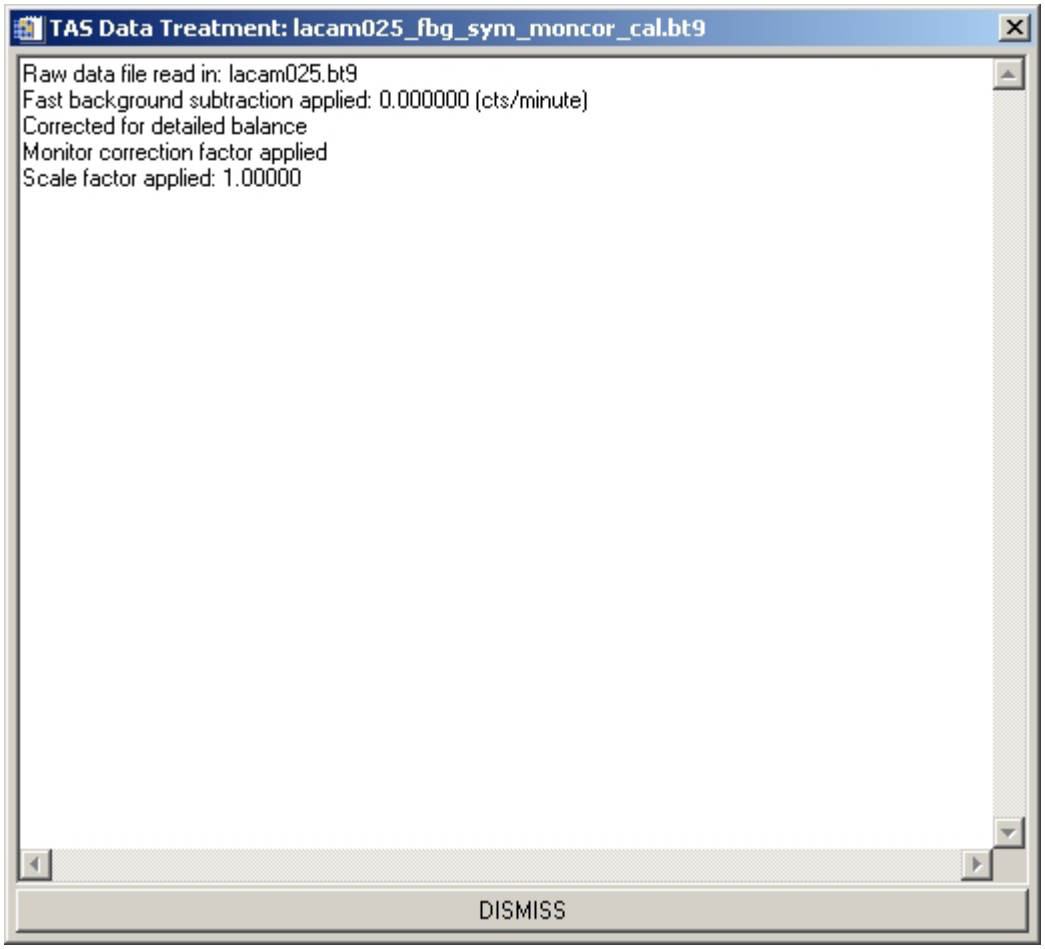

Figure 8 Data treatment for the reduced file.

This is a simple data set for which we can get a quick estimate of the full-width at half maximum of the peak. To do so, select the file icon in the **Reduced Data** folder and select **Fit to N Gaussians** from the CSM. Click once on the slider so that you select one Gaussian for the fit. The results should appear in a dialog box and the resulting fit should also appear superposed in purple on the data in the data display window. See fig. 9.

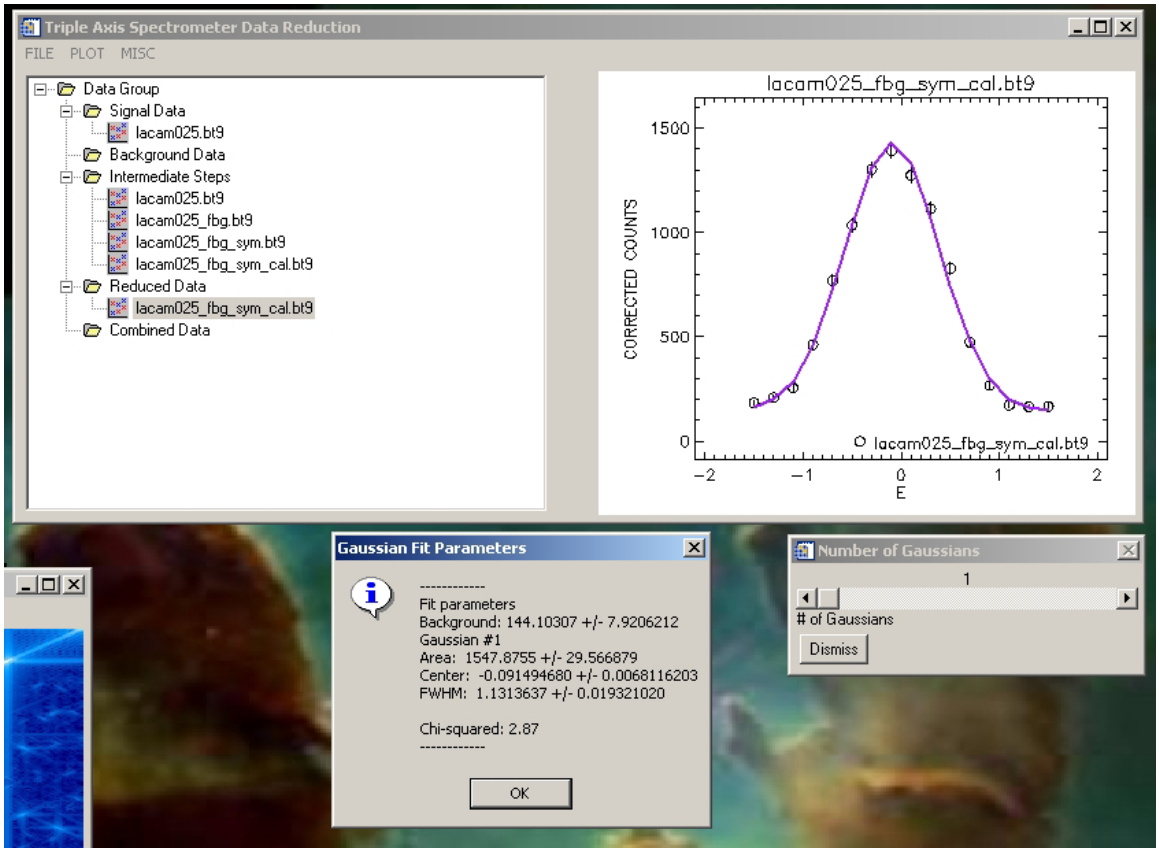

Figure 9 Results of fitting the reduced data to a single Gaussian plus a flat background.

At this point the data reduction is complete and you can do many different things if you wish. You can send the data directly to PAN for more detailed lineshape analysis by selecting **Send data to PAN** from the data file CSM or save the reduced data as a column-formatted text file for instance.

FREQUENTLY-ASKED QUESTIONS

Q: Can I use this software with files that have been processed with ADDRUN?

A: Yes but further processing with this software is not recommended. There are a few reduction operations such as summing that require that the files be expressed in terms of raw counts.

Q: Can I use this software for *alignment* files?

A: Yes and this software is especially useful for fitting multiple peaks to the alignment scan. However the only reduction step available is data scaling.

Q: I get an error message when I read in a data file. What should I do?

A: Check the data file contents. If it has fewer than two data points then there will be an error. If the data file looks fine (for an ICP file), make a note of the error message and send the message contents and a copy of the data file to Rob Dimeo (robert.dimeo@nist.gov).

Q: Can I save my reduced data as formatted text output that can be read into some other software package?

A: Yes. Any step in the reduction process can be saved as text formatted in columns with meaningful titles.