GFit, A Computer Program to Determine Peak Positions and Intensities in Experimental Spectra.

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PROGRAM GFit v 3.03 (1998-04-01)

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GFit is a highly interactive program to perform the basic scientific task of determining peak parameters in a spectrum. The program performs a weighted non-linear least-squares fit of a sum of Gaussian or Lorentzian functions to an experimental spectrum (X,I,ΔI) under manual supervision. The program has unrestricted size of input data, a selection of input formats and fit functions (documented below). Input "X-values" need not be equidistant. Also included is the possibility to handle several different input materials simultaneously $\{(X_i, I_i, \Delta I_i)\}$ i=1,...n, and to work efficiently with the same spectral range contained in a number of consecutively numbered files.

Windows 95 / NT version written in FORTRAN-90 as a QuickWin application for Digital Visual Fortran 5.0 A.

Updated documentation and information about new versions may be obtained from: http://kurslab-atom.fysik.lth.se/Lars/Gfit/html/index.html

GFit has evolved from a program called CARATE by Lars Carle'n, Internal Report LUNFD/6 (NFFK-7014) 1982. The current version is completely rewritten over the years by Lars Engström, Department of Atomic Spectroscopy, University of Lund, Sweden.

CURRENT DIMENSIONS:

The present version uses the FORTRAN 90 concept of dynamically allocated storage. Thus, number of data points, number of different data sets and number of fit parameters (directly related to number of peaks) are not restricted in the program. However, due to programming convenience some limits - hopefully of no practical concern - have been set. Thus, you may only input up to 150 different data sets, and fit up to 100 peaks. Furthermore, only 7 different colors have been implemented, i.e. all data sets from number 7 will be white in the plots.

INSTALLATION:

1. Create a folder named either C:\Leforprog\GFIT\ or C:\Program Files\GFIT\
2. Copy the following files to the chosen folder: GFit.exe, GFit.ini, GFit.path, GFit.doc, GFtext.bmp, GFit.bmp and GFmulti.bmp (and Demo-1.dat)

FILE STRUCTURE:

The program is completely contained in the file GFit.exe. GFit starts by reading 2 files that must have the names GFit.ini and GFit.path and be stored in either C:\Leforprog\GFit\ or C:\Program Files\GFit\. The .ini file is used to set the default values of some parameters and the .path file is used to specify

the (default) names of input/output files. Self-explaining samples of these files are included at the end of this documentation.
GFit also reads 3 bitmap files that must be named GFtext, GFit and GFmulti.bmp and stored in C:\Leforprog\GFIT\ or C:\Program Files\GFIT\. If you rename (or delete) these files, no images will appear initially.

KNOWN PROBLEMS:
The choice of building GFIT as a QuickWin application rather than as a full Windows program introduces several limitations and problems. Unfortunately these are due to limitations in the QuickWin library and thus beyond my control!

1a. GFit is optimized for the following settings: Video mode 1024*768, or higher, with "large fonts" (see My Computer/Display) and more than 256 colors, or video mode 800*600 with "small fonts" and more than 256 colors. The video mode 600*480 is not supported.

1b. In addition to these general settings you may design your Windows environment in very many ways, mostly using the “Appearance” dialog under “Display” in “My Computer”. However, the different sizes you may select are not accessible to a QuickWin application. Hence with some settings the message field at the bottom of the GFit window, used to display instructions to the user, may be off center and difficult to read. Solution: test with different settings in “Appearances”, e.g. change "Scheme" from "Windows Standard" to "Windows Large"

2. If you run (permanently) with your computer set to 256 colors, you should rename or delete the files GFtext, GFit., GFmulti.bmp, since these images will cause erroneous colors on the "input section" page the first time you run.

3. GFit may run extremely slow if you have some particular programs active at the same time. This includes some SCREEN SAVERS!! Solution: Close these programs. You may have to experiment. Word, Netscape, other QuickWin programs,.... are OK

MENUES.

GFit is completely controlled via menu selections. Below is a list and comments on the various options menu by menu.

File

Input New Data Set.

Terminates the current session and transfers control to the input section. If you have saved fit results either on the "log" or the "lsqr" file, new output file names are automatically created by concatenating a number to the end. If you have written to the "lsqr" file, you will be asked whether to append new results or to create a new file.

Save Fit in Lsqr Format

Saves fitting results (peak position, intensity and fitfunction number and, with input format 2 and 8, also FWHM) on a file with the name given in the GFit.path file. Note that here any polynomial calibration is not used, thus peak positions are always in "input units". A dialog window allows you to edit the peak list before saving to file. This can be used to write comments to the line list or to enter reference wavelengths. To enter references, press "TAB". This will write an "R" in position 55 (as required by a program called LSQR used to create wavelength lists through a polynomial calibration function) and then allow you to enter the reference wavelength and its uncertainty following the "R".

Enable Saving to Log File

This is a checked/unchecked menu item. Default unchecked, except after input option -1. If checked, a full log of the fit results, including all estimated uncertainties in the parameter values, are automatically written to the "log" file specified in the .path file.

Write Plot Data to File

This is a checked/unchecked menu item. This option will dump the data (X,I,ΔI) to a file. (File Open Dialog will allow you to select it's name.) Only data within the present plot limits will be dumped. X-values will be calibrated, if this option is set. Subsequent plots of fitted functions will also be dumped. Close this option by selecting it again.

Select Text

This command pauses the program and prepares the current window so that you can mark a block of output text for copying. When you select this command, a highlight marker is placed at the first character position of the text layer in the window, and the phrase Mark Text is prepended to the windows title. To mark text for copying, drag through a block of text with the left mouse button pressed. The selected text is shown in reverse black and white. Note, due to a bug in this QuickWin function the reverse mode only works with a black background, however the selection process itself works even though you can't see it against a white background! Once you have

marked a block of text, use the Copy command to place it on the Clipboard for pasting.

Select Graphics

This command pauses the program and prepares the current window so that you can mark a rectangular portion of the image for copying. When you select this command, the phrase Mark Graphics is prepended to the windows title. To select a portion of the window, drag across it with the left mouse button pressed. A rectangle marks the borders of the current selection. Once you have marked a portion of the window, use the Copy command to place it on the Clipboard for pasting. The same bug makes the rectangle invisible against a white background.

Select All

This command pauses the program and selects the entire contents of the active window, including any text in the screen buffer but not visible in the window, for copying as a bitmap.

Copy

Note, Ctrl+C does not work, you must the this copy option or (Ctrl+Insert)
Copy the selected text or graphics to the Clipboard. After the selected text or graphic has been transferred, the title of the current window is restored to its original name, and the application resumes execution.
Note, some menus may appear gray - i.e. not activated - after a copy or "select" operation, this is also a bug! All menus are, however, active, just click on them as usual!

Print

Use this command to print a graphic image of the current window. The Print Setup dialog enables you to select a printer, to specify the paper orientation, and to select other printer-specific characteristics. Remember to change to a black and white plot before printing to a non-color printer!

Save

Use this command to save a copy of the current window as a bitmap (.bmp) graphics file. (File Open Dialog will allow you to select it's name.)

About GFit

Presents a message with the current version of GFit

Quit

Terminates GFit. If you have written to either the "log" or the "lsqr" file the output filename(s) used is shown.

Get Next Input File

This, and the following two, options appear only if you have selected to work with consecutively numbered files (input option -1). Use the first file as a prototype to select the X-range and other options, then this option brings in the same region (i.e. same index range) from the next file. If you have

performed a fit the parameters are still active, thus the new file may be fitted directly using the previous results as start values.

Get Previous Input File
As above, but decreases file number.

Continue with Automatic Fits
Once you have made a fit, this option will allow you to make identical fits to a number of data files without user intervention. This mode is automatically terminated if an error condition occurs during the fit.

Lsqr.

This is a single item menu copy of "Save Fit in Lsqr Format" above, thus working like a button, just click (or use the quick access Alt+q) to obtain this action.

Main.

Clear and Redraw Plot
This does not affect the fit parameters. This very frequent option is also available as a single item menu, which thus works as a "button", marked "Clear".

Select X-range
All 5 options reset the fit parameters.
When using "X-units" you define the plot limits by giving X-min and X-span. Note, X is in " calibrated units " if a linear calibration is in effect, otherwise use "input units".

Select Y-range
This does not affect the fit parameters. Y-values are always given in a linear scale even if you make a log-plot.

Publication Quality Plot
This opens a dialog box with all the possible options available. All options have default values. If you use this option a second time, the values from the first run is used as defaults.

Add Text to Plot.
This opens a dialog where you may specify the text string you want printed and it's font size. In the plot window you are now prompted (message field below plot) to point with the mouse to where you want the upper left corner of the text string. Click the LEFT mouse to see the result, if you want another position just point and click again. When you are satisfied click RIGHT mouse. The program stores the text, it's font size and position. You may now repeat the process with another text string. A maximum of 40 strings can be used. Note that only normal alphanumeric characters can be written. Use the

"Clear Last" button to erase the last string entered, or "Clear All" to erase all text entered. After any of the clear commands you will remain in the text option to enter new strings or press "Quit" to exit.

Restore working plot.

Cancels the Publication Quality Plot option.

Color Plot on/off.

Select a black graph on a white background (necessary before you print to a non-color printer) or a color plot

Smoothing.

Checked/unchecked menu item. Performs a three-point binomial smoothing, y(i) = [y(i-1) + 2*y(i) + y(i+1)] / 4. Restore by selecting this option again. Note that the smoothing is automatically removed if you select any of the X-range options, or change active set in a multiple data set application. The smoothing option is disabled if you work with "consecutively numbered data sets" (input option -1)

Log (base e) Plot.

Checked/unchecked menu item. Doesn't affect the actual input data. Default is a linear plot.

Calibrate X-Scale.

Defines a 3:de degree polynomial for the conversion of input X-values to "physical units". The derivative is used to convert FWHM and peak position uncertainties. If you make a calibration there will be a third line under the X-axis in the plot, giving start and end value in calibrated units. Note that fitted peak positions written to the "lsqr" file are not affected by any calibration, but always in "input X-units"

Toggle Intensity/Area.

Toggles between output of peak intensity (default) or peak area. Area of a Gaussian is calculated as fac*(FWHM)*I. fac = 0.5*sqrt(pi/ln(2)), FWHM is in channels (not the printed value of FWHM which is in input units) to give the area the dimension of summed intensity. For accurate comparisons over a whole spectrum the input data should thus be equidistant. With Lorentzian shapes the area is calculated as FWHM*I*pi/2, with FWHM again in channels

Get Info Using Mouse.

Activates mouse. Left or right mouse for information, right to quit. The X and Y values printed refer to closest input data.

Plot type

Select to plot data either as histogram, line, "+" sign, errorbars with or without a horizontal line at the top and bottom. For the last three types the symbol size can be either 2, 3 or 5 pixels. Note that a histogram plot is not a true histogram since the data is actually at the left corner, rather than in the center. To make the plot of the fitted functions appear truer to the eye the functions are shifted by half the separation between the first two points in the fit interval. However, if the step size between these particular points happens

to be very non-representative the shifted curves may look erroneous. The default plot type may be set in the .ini file

Peaks

Select Start Point, Select Peak(s), Select End Point

Start/End points may be selected using any mouse button. When selecting start values for the peaks you must use the left mouse for all but the last peak. Right mouse for last/only peak. The actual data values at indicated indices are used as limits and start values in the fit. Thus the vertical position of the mouse is not important.
These very frequent options are also available as single item menus, which thus works as "buttons", marked Start, Peak and End.
If you don't select a start/end point, the low and high plot limit is used as start and end, respectively, by default

Delete Last Peak.

During peak selection, last peak is the last entered, irrespective of position. After a fit the peaks are sorted in increasing position, and hence the last peak is now the highest position peak.

Delete Selected Peak

Use the mouse to point at any peak (within +- 2 channels), click to remove this peak from the fit.

Fit Func.

1.

Trial function consists of a sum of Gaussians with a constant background, and a common FWHM for all components within each structure, i.e. between the start and end points selected. The common FWHM may, of course, vary from one structure to another.

$$f(x) = Bcg + \sum_i I_{0i} e^{-c\cdot\left(\frac{x-x_{0i}}{FWHM}\right)^2} \quad \text{where } c = 4\cdot\ln(2).$$

2.

As 1 but with a quadratic background:

$$f(x) = b_0 + b_1 x' + b_2 x'^2 + \sum_i I_{0i} e^{-c\cdot\left(\frac{x-x_{0i}}{FWHM}\right)^2}, \text{ with } x' = x - x(\text{start index})$$

Note, the value and uncertainty of b_1 and b_2 are only given on the screen. Only b_0 and its uncertainty is written to the log file. Initial values for the background terms are automatically derived from a linear fit (b_2=0) through the two end points. The use of x' means that the background coefficients are local for each structure.

3.

As 1 but with fixed, given, peak separations:

$$f(x) = Bcg + I_{01}e^{-c\cdot(\frac{x-x_{01}}{FWHM})^2} + \sum_{i>1} I_{0i}e^{-c\cdot(\frac{x-(x_{01}+\Delta_i)}{FWHM})^2}$$

Prior to selecting this function you should select the start/end interval and one reference peak. You will be asked for the number of additional peaks and their separations Δ_i. If you have already performed a fit involving several peaks prior to this selection, the first (i.e. lowest position) peak is automatically used as the reference.

4.

As 3 but now also with fixed, given, relative intensities ($R_i = I_i / I_{ref}$):

$$f(x) = Bcg + I_{01}\left\{e^{-c\cdot(\frac{x-x_{01}}{FWHM})^2} + \sum_{i>1} R_i e^{-c\cdot(\frac{x-(x_{01}+\Delta_i)}{FWHM})^2}\right\}$$

5.

Combination of 1 and 3. Select Start/End interval and the reference peak for the fixed structure prior to selecting this function. You will be asked for the number of additional peaks in the fixed structure and their separations. After this you select additional free peaks in the normal way. Selecting this function a second time produces the fit.

6.

As 1 but with each component with its own FWHM.

$$f(x) = Bcg + \sum_i I_{01}e^{-c\cdot(\frac{x-x_{0i}}{FWHM_i})^2}$$

7.

As 3 but with each component with its own FWHM.

$$f(x) = Bcg + I_{01}e^{-c\cdot(\frac{x-x_{01}}{FWHM_1})^2} + \sum_{i>1} I_{0i}e^{-c\cdot(\frac{x-(x_{01}+\Delta_i)}{FWHM_i})^2}$$

8.

This trial function consists of a sum of Lorentzians with a constant background, and a common FWHM for all components within each structure.

$$f(x) = Bcg + \sum_i I_{0i}\frac{a}{4(x-x_{0i})^2 + a} \quad \text{where } a = \frac{Fwhm^2}{4}.$$

9.

As 8 but with each component with its own FWHM.

$$f(x) = Bcg + \sum_i I_{0i}\frac{a_i}{4(x-x_{0i})^2 + a_i} \quad \text{where } a_i = \frac{(Fwhm_i)^2}{4}.$$

Fit Control.

Reset Fit Parameters.

Fit parameters are start and end points of the fit interval, the number and estimated positions of the peaks, i.e. what you give using the "Select Peaks" menu. During a fit to a given structure you may change these parameters by selecting new values, e.g. keep adding more and more peaks. However, if you want to restart or move to another structure you must first reset the parameters with this option and then start over with the selection. Some options reset the parameters automatically, for example all 5 X-range options. A reset sets all fit parameters free by default, see next option.

Set, Fix or Unfix Parameters.

Opens a dialog window where all fit parameters are given with their current values and status (fixed or free). You may edit this table to set new values and status (0 = fix, 1 = free). When you are finished, "ESC" ends this options and sets the new values and status. If you are using the fit functions 3, 5 or 7, the fixed separations are also given and possible to change. To use this option you must first make a fit with the desired fit function, i.e. you can't set parameter values in advance.

Select Start Value BCG.

Use the mouse to define the start value of a constant background. In this case the value corresponding to the vertical mouse position is used, not any actual input data value.

List Fitted Uncertainties.

The calculated one-standard deviation error estimates in the peak positions and intensities are listed on the screen. Note! Calculated error estimates are only reliable and meaningful if correct weights are used in the fit. This, in turn, depends on the error estimates in the input intensity data, see the discussion below about the different input formats

Set Parameters Auto Start Values

GFit may generate start values for the peaks using an automatic peak-finding algorithm, based on tests on the first and second derivatives of the experimental data. The peak-finding is controlled by the 4 parameters that may be set using this dialog box. The default parameter values may be set in the .ini file. The peak-finding itself is invoked using the single item menu "Auto Start Values" described below.

1. "Number of intervals used to calculate derivatives"

   Suggested value is the number of channels corresponding to the half width at half maximum (HWHM not FWHM). The first derivative in point x(j) is calculated as (y(j+1)-y(j-1))/(x(j+1)-x(j-1)) if number of intervals is 1, otherwise the derivative is the average value of the differences obtained using j±1, j±2,...,j±n, where n is the number of intervals. This acts like a smoothing process.

2. "Percent above background to accept peak"

   This parameter is used to reject peaks with too low intensity. A peak with a maximum intensity of I_{max} is rejected unless:

I_{max}-Bcgr > Max((1.+P/100.)*Bcgr,10.), where P is the percentage given. The current value of a constant background (Bcgr) is taken from the previous fit or may be given using the option "Select Start Value BCG", above.
If the option "Absorption spectrum" below is checked, this parameter should instead represent the absolute intensity relative to the background to accept a peak (as stated by the altered text in the dialog).

3. "Bad peak parameter"
Let R be the ratio of the first derivatives in the high and low inflection point. For a perfectly symmetric peak R should be -1.
If p < Abs(R) < 1/p, where p is the "Bad peak parameter" a fitting procedure is used to obtain the peak position, otherwise the position is taken as the average value of the two inflection points. The latter case is clearly less reliable.
4. "Minimum points within FWHM".
A peak with less than this number of points is rejected.

Absorption spectrum

Checked/unchecked item. If selected, this option changes the test normally performed against negative intensity in any fitted peak to a similar test of no positive intensities. Furthermore, as stated above, the minimum intensity parameter in the automatic peak-finding algorithm is redefined. Note the printed intensities on the screen and in the "lsqr" file is the absolute value, while the actual fit parameters are negative.

Start, Peak, End, Fit 1 and Clear

All these menus are single item menus, thus working like "buttons", just click to obtain the desired action. These options are copies of available menu items in other menus. Note also that you may have "quick access" by the key combination Alt + underlined character, e.g. Alt + s to initiate selection of start point.

Plot Func.

This opens a dialog where you may select to plot one or more of the individual peaks fitted as well as the total function, i.e. the sum, or just the fitted background.

Multiple Sets.

(This menu is present only in input mode 0, work with multiple input data)

Select Active Set.

If you have read multiple data sets, this option selects which set number (in input order) is to be active. Note that all sets are plotted, but any quantitative information and the fit results refer only to the active set. An exception is the X-value scale in the plots, which is common to all sets. It is possible to plot a section of the active set (index1 to index2) where one or more other sets do not have data points, i.e. no X-values. These sets are, of course, not visible.

Using the checkbox you may make a particular set active and let this set be the only one plotted, i.e. make use of the full plot area.

Whether the fit parameters are reset or not depends on if the data sets are "identical" or not. If all sets contain the same number of points and the first and last X-values are the same in all sets, they are considered to be "identical", e.g. several sets of CCD measurements or JET spectra. In this case the fit- parameters are not reset when changing the active set. Thus after a fit to one set you may change the active set and directly fit the same spectral structure in another set. If the sets are not considered "identical" the fit parameters are reset when changing the active set.

Set Next Set Active, Set Previous Set Active.

Set Offset.

This option change the offset applied to shift the different sets vertically. Note that this is for display purposes only. Default is 100/(number of sets) percent, i.e. the whole y-range is divided equally between the sets. You may test different values by clicking OK and then Exit when you are satisfied.

Arithmetic Operations.

This option appears only if the sets are "identical" (as defined above), and allows you to combine different sets by arithmetic operations, i.e.
SetA = SetA (operator) SetB, where operator is +, -, x or / and A and B represent any of the sets read. E.g. Set1 = Set1 - Set2, could represent a background subtraction of the data in Set 1 by the measured background in Set2. **Warning**: the actual data in Set1 are changed by this option and the weights, related to. the uncertainties, of each point in Set1 is irreversibly altered. (E.g. if you make the reverse operation Set1 = Set1 + Set2 the data in Set1 would be restored, but the uncertainty of each point in Set1 has now been increased by twice the uncertainty in the corresponding data point in Set2)

Auto Start Values

This is a single item menu, producing start values of the peaks through an automatic peak-finding algorithm. The search is performed within the interval specified by "Start" and "End" (above), or between the current plot limits. Suggested peak positions are marked in the plot. The peak-finding process is controlled by parameters that may be given in a dialog box under the menu "Fit Control". The current value of a constant background (Bcgr) is taken from the previous fit or may be given using the option "Fit Control/Select Start Value BCG", above. Once preliminary peak positions have been found you may:

1. Accept these and directly perform a fit using a selected fit function.
2. Add more peaks using "Peak", above
3. Delete one or more suggestions, using "Delete selected peak", above

SOME COMMENTS:

1. If you want to fit a larger number of peaks it is usually better to start with a more limited number and then add on a few at a time. If you want fit function 6 (with free FWHM), it is sometimes better to first make a fit using function 1 (common FWHM) to obtain improved start values, and then use number 6.

2. Current fit convergence criteria is that all parameters should change by less than the estimated uncertainty/10 between two iterations. Max 10 iterations will be performed. However, repeated selection of any fit function give 10 iterations each time. (Note that repeated use of functions 3,4,5 and 7 in the same fit does not require reentering the fixed peak separations and relative intensities)

3. To obtain accurate error estimates by GFIT it is necessary to supply correct one-standard deviation uncertainties in the input data. (If you e.g. were to multiply all input uncertainties by 10 the resulting error estimates would also be 10 times higher.) Thus, if the default weights derived by GFit in some input formats are not correct (e.g. due to a substantial background correction) you must calculate the correct values outside GFit, and use input format 5.

INPUT FORMATS:

Note. If the export parameter in the .ini file is set to "yes" only format 5 below will appear (in addition to -1 and 0).

In most cases (except option 3,5,8) weights are calculated assuming Poisson statistics, hence only "X and I" values are read See comment 3 above!

(-1) "INITIATE READING OF CONSECUTIVE FILES"

This option allows you to read the same section of a number of files automatically without resetting the fit parameters. For example to analyze a lifetime measurement where the spectra at each foil position is stored in a separate file. Only input option 2 (JET), 5 (Free format) and 8 (MAPS) is possible. It is necessary to have files with names of the type NAME-NUMBER.EXT where number is increasing by one from a start value. Selecting this option will append the "Get Next Input File" and "Continue with Automatic Fits" items in the "File" menu.

(0) "INITIATE MULTIPLE INPUT DATA"

This option allows you to work with multiple data sets. All sets will be displayed simultaneously, in the input order, from the bottom up. Fits, scales, cursor-position, smoothing etc. apply only to the active set. Any calibration of the X-scale apply to all sets. After initializing this option you will loop through the input section to read the requested number of sets. The sets may thus contain input data in different formats. Note, the data set with the largest number of points must be read first. Selecting this option will create a new menu "Active Set".

1. "OLD CARATE".

Line 1: Title, format(A80)
Line 2: a and b in X = a + b*(channel number-1), Free format

These constants are used to calculate the input X-values
Rest of file: Intensities only in format(1x,10F8.1)

2. "JET"
Line 1: Title, format(A80)
Rest of file: (dummy, intensity), read in free format, i.e. two columns of data where only the second column is read. "X-value" is set to index of point

3. "BFS"
Both old (alpha-LSI) and new (VME) data sets can be read automatically. If a background subtraction is made, weights are calculated using the unsubtracted intensities. No further documentation given here

4. "BOCHUM"
Line 1: Title, format(A60)
Rest of file: (X, I), in free format (2 columns of data)
X-values are calculated as either xstart+(i-1)*step, (x read from file is not used) or X-values are interpreted as "length-gauge" values converting to chordal position through X=XZST+(x(1)-x(i))/25400.

5. "FREE FORMAT"
(X,I,(ΔI)) read in free format, i.e. three columns of data
If ΔI is present - not necessary - it is interpreted as an uncertainty (one standard deviation) in the intensity value, and used to calculate the weight of this point in the fit according to w = 1/ max((ΔI)^2,1)

6. "GREMLIN"
Line 1: Title, format(A80)
Line 2 and 3: a and b in x = a + b*(channel number-1), "format(12X,*)"
i.e. skip 12 positions, read remaining line in free format
Line 4: Number of data points "format(7x,*)"
Line 5: ignored
Rest of file: Only intensities in format(10f8.1)

7. "LASER 1"
(I), in free format, i.e. one column of intensities
X-value is position on plate in mm calculated as x = 0.002*(index-1), i.e. assuming a step size of 0.002 mm

8. "MAPS FORMAT"
Binary input file of CCD data.
If the measurements have been done in the "exposure only" mode, you will be asked if you want to make a bias subtraction. If the measurements have been done using any other exposure mode this question will not appear. On line 11 in GFIT.path you may give a file name, or a path, leading to an ASCII file to be used for the bias subtraction. No further documentation of the MAPS format will be given here.

Sample of a GFIT.ini file:

```
%                    GFit.ini
%
% This file must be stored in c:\Leforprog\GFit\ or in C:\Program Files\GFit\.
%
% This initialization file allows you to set default values of some parameters
% used by GFit. All comment lines must start with "%", you may have any number of
% comment lines but the information-carrying lines must appear in the given order.
%
% For maintenance reasons there is only one version of GFit. The variable "Export" below
% controls the selection of input formats presented. Export=No results in the complete
% list of 8 different formats, applicable the situation in Lund. Export=Yes limits the
% selection to only the free format input of (x,I,(dI)). See GFit.doc
%
% Export:
NO
%
% Once GFit starts you may select 11 different plot types using the dialog in menu
% Main/Plot Type. Below you may set the default type by giving a number between 1 and 11
% corresponding to the order of the options in this dialog. E.g. Plottype=1 results in
% a default histogram plot, Plottype=2 gives a line plot a.s.o.
%
% Plottype:
1
%
% GFit contains an option to perform an automatic peak-finding to obtain start values
% for the fits. The operation of this option is controlled by 4 parameters, set in a
% dialog under menu Fit Control/Set Parameters Auto Start Values, and documented
% in GFit.doc. Below you may give the default values of these 4 parameters. All must
% be on a single line, which is read in free format, in the same order as in the dialog.
%
% Peak finding
1,100,0.1,4
%
% For the very first fit in each GFit session the start value of the FWHM of the peaks
% is given by a NUMBER of channels times the actual value of the difference between
% the first 2 points read, in the input units. Subsequent fits uses the previous values
% as initial guesses. Below you may give the typical number of points within the FWHM
% used the first time. This is usually not very critical, unless the guess is totally
% wrong.
%
% IFWHM default
4
%
% end of current .ini file
```

Sample of a GFIT.path file:

```
%                    GFit.path
%
% This file must be named c:\Leforprog\GFit\GFit.path or c:\Program Files\GFit\GFit.path
%
% This file is used by GFit to obtain the full or partial names of input/output files.
%
% All comment lines must start with "%". You may have any number of comment lines
% but the information-carrying lines must appear in this order.
%
% Below is the full name, including directory structure, of a file containing
% the full output of the fit results. Normally, this output is disabled by default,
% and can be enabled using the option "Enable Saving To Log File" in menue "File".
% Note that unless you change the name given here new results will overwrite
% the old ones. Thus, rename valuable result files!
% However, if you start multiple GFit sessions the filename will automatically be made
% unique by concatenating a number to the end
% If this line is left blank a normal Windows open dialog will appear the
% first time the program attempts to write.
%
% Log file name:
c:\Leforprog\GFit\GFit.log
%
% Below is the full name, including directory structure, of a file containing
% a more limited output of the fit results in a format to fit the input of the program
% LSQR. Before writing to the file the output may be edited to add comments to the fit
% Saving to this file is selected by the option "Save Fit in LSQR Format" under the
% "File" menu, or the single item menu "Lsqr". Note,  unless you change the name
% given here new results will overwrite the old ones. Thus, rename valuable result files!
% However, if you start multiple GFit sessions the filename will automatically be made
% unique by concatenating a number to the end.
% If this line is left blank a normal Windows open dialog will appear the
% first time the program attempts to write.
%
% LSQR file name:
c:\Leforprog\GFit\GFit.lsqr
%
% Below is the default full or partial name of the input data file. This name may be
% completed or edited during execution using "BS" and the direction arrows.
% Furthermore, if the suggested name is completely deleted during execution you will
% force a Windows open dialog.
% If the line below is left blank a normal Windows open dialog will appear.
%
% Input file name:
c:\Spectra\n\ccd\6.5mev\1200grating\sp2080-17.mps
%
% The final line is the full or partial name of a possible "bias file", used only for
% MAPS input (input format 8). Just as for the input file name this name may be
% completed or edited during execution. Furthermore, if the suggested name is
% completely deleted during execution you will force a Windows open dialog.
% If the line below is left blank a normal Windows open dialog will appear.
%
% Bias file name:
c:\Spectra\n\ccd\6.5mev\1200grating\bias1.stat
%
% end of .path file
```