"LINESHAPE": A COMPUTER PROGRAM
FOR DOPPLER-BROADENED LINESHAPE LIFETIME ANALYSIS

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A set of general-purpose computer programs for analysis of
Doppler-broadened gamma-ray lineshapes for deducing nuclear lifetimes has
been developed at ORNL incorporating several existing programs made
available to us from other sources.

The program DECHIST_OR is based on the program DECHIST, written by
Bacelar [1], using the formalism of Currie [2], which simulates the
velocity history, including direction, of a series of recoiling nuclei
using Monte Carlo techniques. We have combined it with the stopping power
routine STOPO, written by Milner [3], which generates a set of stopping
powers for the recoil nucleus in the target and backing materials using
one of a choice of three options: (1) Ward's effective charge [4] and
Ziegler's proton stopping powers [5], (2) Ziegler's heavy-ion stopping
powers [5], or (3) shell-corrected Northcliffe and Schilling stopping
powers [6].

The program HISTAVER_OR is adapted from the program HISTAVER, also by
Bacelar [1], which converts the velocity histories of the recoil nuclei
into time-dependent velocity profiles as seen by a particular detector.

The program LINESHAPE is a combination of the program DSAMFT, written
by Gascon [7], which has been extensively modified and combined with the
least-squares minimization routine MINUIT, written by James and Roos [8].
MINUIT includes minimization routines MIGRAD, SIMPLEX, and SEEK, and the
error routine MINOS.

SIMPLEX, by Nelder and Mead [9], uses the simplex method for the minimization of a function of N parameters. The method depends on the comparison of the function values at the N+1 vertices of a general simplex followed by the replacement of the vertex with the highest value by another point. A simplex is the smallest N-dimensional geometrical figure with N+1 vertices: a triangle for N=2, a tetrahedron for N=3, etc. New simpleces are formed by reflecting one point in the hyperplane of the other points. The simplex adapts itself to the local landscape of the function, elongating down inclined planes, changing direction upon encountering a valley at an angle, and contracting in the neighborhood of a minimum.

MIGRAD, a gradient search method using Fletcher's switching variation [10] to the Davidon-Fletcher-Powell variable metric algorithm [11], approaches a local minimum closely and generates parabolic error estimates, which would be true errors if the chi-square function were really quadratic with respect to each parameter.

SEEK performs a minimization using a Monte Carlo technique. The parameter values are chosen randomly according to uniform distributions centered at the best previous set of values. If chi-square is lower for these new values, they become the starting point for the next iteration, otherwise the previous set remains the starting point as the process is continued through a series of iterations.

MINOS finds the true positive and negative errors (confidence intervals) of a parameter by examining the behavior of chi square in the vicinity of the best value of the parameter. The value of the parameter of interest is varied in steps, both increasing and decreasing from its best value, and at each step, chi-square is reminimized by varying the N-1 remaining parameters. This process is continued until chi-square increases by one unit.

LINESHAPE incorporates the routines from DSAMFT to calculate lineshapes using the velocity profiles from the Monte Carlo simulation and assumed values for the lifetimes of the observed transitions and also of unobserved feeder transitions. These lifetimes (and other parameters such as normalizations, backgrounds, and impurity peak areas) are varied by the minimization routines to produce the best least-squares fit to the data lineshapes.

The program handles simple cascades and also coupled bands. The side feeding to individual levels can be modeled either by a cascade of up to

5 transitions with independently variable lifetimes, or by a rotational
band with a fixed moment of inertia and a variable quadrupole moment. The
program can handle overlapping transitions, and include impurity peaks in
the calculated spectrum if they overlap the lineshape of interest, and
exclude them if they don't. It allows data for different transitions to
come from different spectra. Any of the variable parameters can be fixed
during the fitting procedure, and upper and lower limits can be imposed to
constrain the parameters to stay in a "physically meaningful" range.

REFERENCES:

[1]   J. C. Bacelar, private communication.
[2]   W. M. Currie, Nucl. Instrum. Methods 73, 173 (1969).
[3]   W. T. Milner, ORNL, private communication.
[4]   D. Ward et al., Stopping Powers for Heavy Ions, AECL-5313, Chalk
        River (1976), and Compilation of Realistic Stopping Powers for Helium
        Ions in Selected Materials, AECL-4914, Chalk River (1975).
[5]   J. F. Ziegler, The Stopping and Ranges of Ions in Matter, Vols. 3 and
        5, Pergamon Press (1980).
[6]   L. C. Northcliffe and R. F. Schilling, Nucl. Data Tables 7, (1970).
[7]   J. Gascon et al.,Nucl. Phys. A513, 344 (1990), and private
        communication.
[8]   F. James and M. Roos, Comput. Phys. Commun. 10, 343 (1975).
[9]   J. A. Nelder and R. Mead, Comput. J. 7, 308, (1965).
[10]   R. Fletcher, comput. J., 13, 317 (1970).
[11]   R. Fletcher and M. J. D. Powell, Comput. J. 6, 163 (1963).
[12]   F. James, Comput. Phys. Commun. 20, 29 (1980).

HOW TO RUN THE PROGRAMS AT ORNL:

Type: /usr/orph24/users/wells/Ddbls/dechist
               /usr/orph24/users/wells/Ddbls/histaver
               /usr/orph24/users/wells/Ddbls/lineshape

HOW TO OBTAIN THE SOURCE CODES:

1. Copy the following files (from /usr/orph24/users/wells/Ddbls/):

dechist.make

dechist_or.f
DECHIST_OR.CMN
stopp.f
stopp.cdi

histaver_or.f
HISTAVER.CMN

x_dbls.make
dbls.f
dbls_setup.f
minuit.f
utilities.f
x_disp.f
xjwlibu.f
xjwlibc.c
tek_dummy.f
PARAM.CMN
DBLS.CMN
MINUIT.CMN

lineshape.doc (this document)

2. Compile and link 'dechist_or.f' and 'stopp.f' using 'dechist.make'.
'DECHIST_OR.CMN' contains the common blocks. 'stopp.cdi' is a data file
of stopping powers read during execution. Edit 'stopp.f' and change the
statement 'OPEN (8,FILE='stopp.cdi'...' to show your path for the file.

3. Compile and link 'histaver_or.f'. 'HISTAVER.CMN' contains the common
blocks.

4. Compile and link the remaining files using 'x_dbls.make'. 'PARAM.CMN'
contains parameters for the dimensioned variables, and 'DBLS.CMN'and
'MINUIT.CMN' contain common blocks.

     The files 'xjwlibu.f' and 'xjwlibc.c' form the graphics package for
X-Windows. 'xjwlibc.c' is written in C as an interface between the
intrinsic X-Windows functions which can only be called from a C program,
and the FORTRAN program which needs to call them.

     A version of the program is available which supports graphics
displays on the old Tektronix 4105 series terminals. Several additional
files are needed for this version. 'tek_dummy.f' contains substitute

subroutines so that the program can link and run without these additional files.

GETTING STARTED:

1.   Run the program 'dechist'. It simulates by Monte Carlo techniques the slowing-down process of the recoils in the target and in the backing. It reads input data from a data file 'filename.dat' and produces a list file 'filename.lis' and a history file 'filename.his' that contains the velocity and direction of the recoils at every time step for each simulated recoil. These two output files are given the same filename as the '.dat' file.

       The following input information is needed: the Z and A of the projectile, target, backing, and recoil nucleus, the densities of the target and backing in g/cm**3, the target thickness in mg/cm**2, the angle between the target and beam in degrees, and the beam energy in MeV. These may be read from a '.dat' file or entered interactively in response to the program's questions (and saved in a '.dat' file). One must also give the time step in ps, an integer seed to start the random number generator, and the number of recoil histories desired. Suggested values: for the time step, 0.01 times the shortest expected life-time; and 5000 or more histories.

       Stopping powers are generated internally from one of several models. Your choice of models can be selected from a menu. A file 'stopp.out' is generated which contains a tabulation of stopping powers as a function of ion energy for (1) recoil in target, (2) recoil in backing, and (3) projectile in target.

       It is possible to simulate reaction products recoiling into a vacuum, rather than into a solid backing, by setting the density of the stopper equal to zero. In this case, it is necessary to specify the maximum number of time steps, which should be large enough that the total time (time-step interval times maximum number of time steps) be several times larger than the largest expected lifetime. The maximum number of time steps is determined internally for a solid backing by the time required to reduce the initial kinetic energy of the recoiling nuclei by a factor of 1000.

       The output '.lis' file is written as a text file and contains

information about the recoil histories such as the time step interval,
maximum recoil velocity, maximum number of time steps, average number of
time steps, average number of collisions, average x and y distances
traveled by the recoils, and some information about the recoils at the
target-stopper boundary.

      The output '.his' file is normally written as a binary file for
saving space and speed in reading and writing. It contains, for each
recoil history, the recoil velocity and three direction cosines for each
time step. It is possible to also write this same information as a text
file if you wish to examine the results directly. This is done by
specifying a negative value for the time step interval, and the text file
is designated 'filename.tst'.

2.   Run the program 'histaver'. It takes the output from the '.lis' file
and '.his' file generated by 'dechist' and produces another '.lis' file
and '.his' file containing, for each time step, the velocity profile as
seen by a detector at a certain angle. You will need to run this program
once for every angle used in the analysis, and for each of these a '.lis'
and '.his' file will be generated. The program requests a filename for
these output files. It should be different from the filename of the
input '.lis' and '.his' files so that these will not be overwritten.

      The following input information is needed: the target-detector
distance, the detector radius, the detector angle theta in degrees, the
number of detectors at that angle, and, for each detector, its relative
efficiency and angle phi.

3.   Select the level scheme which contains the transitions you wish to
analyze. Obtain energies for the transitions between these levels.
Number the levels consecutively starting with the upper level of the
lowest transition. If you are analyzing two coupled bands, number the
levels in order of increasing energy, which means that one band will have
even numbers and the other odd. Determine the spin of the upper level of
the lowest transition and the K value of the band.

      For coupled bands, determine the M1/E2 branching ratios out of each
level. These must be greater than zero and LESS THAN ONE. For a single
band of E2 transitions, set all of the branching ratios EQUAL TO 1.0.
This is how the LINESHAPE tells which case to analyze.

      Determine the intensity of the side-feeding (in relative units) into
each level included in the analysis. This should be obtained, if

possible, from spectroscopic data for the same reaction at the same beam energy. Choose the side-feeding model for each level, either a rotational band or a cascade whose transitions will have independently varied lifetimes. For rotational bands, choose the number of transitions in the bands (from 1 to 6), and the moment of inertia (I/hbar**2 in 1/MeV). A value of 65/MeV is typical. These must be the same for all rotational bands. For independently varied side-feeders, the number of transitions in the cascade (from 1 to 5) and the initial lifetimes (which must all be different) must be specified for each level being fed. The number of transitions in the feeding cascades may be different for different levels being fed. It is possible to use rotational band feeding for some levels and independently varied cascade feeding for others.

 4.   Select the spectra that you will use for the analysis, one per angle. Including the 90 degree angle in the analysis is recommended, as it helps to identify contaminants. If a spectrum contains the sum of events from detectors at different theta angles, the calculated shapes are obtained by summing over these angles. The program 'histaver' must be run for each of the theta angles to be summed. It is also possible to use different spectra for different transitions (see SPECTRA).

        Obtain a linear energy calibration (intercept (in MeV), slope (in MeV/ch) and optionally a quadratic term coefficient (in MeV/ch**2)). All spectra must have the same energy calibration.

        For each data spectrum, construct an error spectrum which contains, for each channel, the SQUARE of the error in the corresponding data channel. If these errors are not accurate, the error results of MINOS analysis will not be valid. For a singles spectrum, the spectrum itself may serve as the error spectrum. This is the default if no error spectrum is provided. For a peak gate spectrum from which a (weighted) background gate spectrum has been subtracted, the error spectrum may be generated by adding the original raw peak gate spectrum to the (weighted) background gate spectrum. Spectra can be read in the (ORNL) '.spk' format and in the (NBI) '.spe' format. A spectrum filename with no extension is assumed to be '.spk'.

        For each gamma-ray transition you wish to analyze, select the low-channel and high-channel limits of a 'window' which contains the Doppler-broadened photopeak and sufficient channels on each side to fit a linear background. Making the window wider than necessary will increase the running time and dilute the normalized chi-square. The program can currently handle window widths of up to 251 channels. Determine the FWHM

(in channels) for stopped (unbroadened) peaks in the window for each angle.

   If two or more Doppler-broadened photopeaks overlap, they must be fitted together in the same window. To do this you must use the SAME low- and high-channel limits for each transition in the window. It is permissible, however, for two different windows to overlap in the background area as long as the peaks being fitted to not overlap.

   If there are any contaminant peaks in the window, determine their centroids accurately, and the program will include them in the fit. It can handle up to eight peaks per window. If any of the contaminant peaks do not overlap the peak whose lineshape is being fitted, they can be eliminated from the fit by specifying regions to be excluded. The FWHM of contaminant peaks may be different from that of the broadened photopeak.

5.   Obtain an efficiency calibration for the detector(s) at each angle. Create a '.eff' file for each angle in the form: A1,B1,C1,A2,B2,C2,EC where

$$LOG(EFF) = A1 + B1*LOG(EGAM) + C1*LOG(EGAM)**2 \quad EGAM(keV)<EC$$
$$LOG(EFF) = A2 + B2*LOG(EGAM) + C2*LOG(EGAM)**2 \quad EGAM(keV)>EC$$

6.   Run the program 'lineshape'. Use the SETUP command to set up the entire level scheme (see SETUP). Supply the information as the program asks for it. Save (DUMP) that setup (see DUMP). Next, use the CAL command (see CALCULATE). It creates shape-versus-time arrays for each of the gamma-rays included in the analysis for which there is data. Save those shapes with DU/S (dump/shape). You can look at those shapes on a graphics terminal with the DS command.

7.   Start the least-squares fit. Start from the top, using the SW (Select Window) command to exclude the lower transitions from the analysis, and then move down the band fitting successive windows in turn. Results are saved after each fit in a '.tmp' file to avoid losing results if there is a computer or program malfunction.

   LINESHAPE contains three minimization routines from the program MINUIT developed at CERN. These are SEEK, SIMPLEX, and MIGRAD. SEEK searches randomly over a region around the starting values of the parameters. SIMPLEX moves in quickly to the region of the minimum, and MIGRAD converges very closely to the minimum when starting not too far away. The recommended fitting procedure is to call SEEK if the starting

values of the parameters are only "wild guesses", then call SIMPLEX and MIGRAD in that order. If the starting values of the parameters are reasonable, then start with SIMPLEX followed by MIGRAD.

    You can observe the quality of the fit on a graphics terminal with the DF command, which displays the data with the fitted curve overlaid. You can also observe the decay curves with the DC command.

    Using ALT (Alter) you can change the values of parameters and observe the effect on the fit, on the decay curves, etc.

8.   At the initial stage of the analysis, you should try to obtain the best values of the peak widths for each window, and also the best positions and peak widths of the contaminant peaks ("best" meaning the values that give the lowest chi-squares). These parameters can be varied with the ALT command.

9.   After obtaining the best fits for each window separately, you should fix the window parameters (NORM, A, B, and PA) and vary Q and TS and/or QS for several adjacent levels; perhaps for the entire level scheme. The command FW or FIX/WIN is useful for fixing all window parameters.

10.   The errors on the parameters after MIGRAD has converged are derived from the covariance matrix, and should be reasonably good if the parameters are not strongly correlated. However, since the Q and TS and/or QS for a given transition are probably correlated (e.g. one could increase and the other decrease without changing chi-square much), one should call the MINOS error analysis routine only after obtaining the best fits to all of the parameters. When running MINOS, all of the Q and TS and/or QS parameters above the state of interest should be free.

11.   Have fun...

OUTPUT:

    A complete record of input data, procedures, and results is written in file 'filename.log', where 'filename' is the parameter listed in your command line (see "How to run the programs"). The default is 'lineshape.log'. In addition, the command PRINT and the /P qualifier with the DISPLAY commands write information to file 'filename.out' (default 'lineshape.out').

PARAMETERS:

Here is a list of the parameters that can be least-squares fitted:

Q i   : Transition quadrupole moment of level i
TS k i   : Lifetime of feeding transition k to level i
QS i   : Transition quadrupole moment of the side-feeding cascade of
           level i
NORM w a   : Normalization of fitted transition for window w at angle a
A w a   : Left intercept of background in window w at angle a
B w a   : Slope of background in window w at angle a
PH k w a   : Height of contaminant peak k in window w at angle a
WID w a   : FWHM of photopeaks (intrinsic resolution) in window w at
           angle a

Here is a list of the parameters that can be changed using the ALT command but not least-square fitted:

BR i   : Total branching ratio of the delta-I = 1 transition out of
           level i (INCLUDING internal conversion)
EG i   : Energy of transition out of level i
INTS i   : Absolute intensity of the side feeding of level i (in
           arbitrary units)
PP k w   : Position of contaminant peak k in window w
PW k w a   : FWHM of contaminant peak k in window w at angle a
Y1 w a   : Left intercept of background in window w at angle a
Y2 w a   : Right intercept of background in window w at angle a

The parameters Y1 and Y2 are functions of A and B: Y1=A and Y2=A+B*(window width). However, altering Y1 leaves Y2 unchanged and changes B, and altering Y2 leaves Y1 unchanged and changes B, whereas altering A leaves B unchanged and changes Y2, and altering B leaves A unchanged and changes Y2.

Here is a list of the parameters that can be changed via the SETUP command, and do NOT require a new CAL (Calculate) command:

The number of levels in side-feeding cascades,
The moment of inertia used to extrapolate the gamma-ray energies in the side-feeding cascade (Default = 65/MeV),
The upper bound of a window, if the new value is smaller,
Regions to be excluded from the fit in a window,

The spin of the first level and K of the band (Default = 100 and 0),
The upper and lower limits for Q, TS, and QS (Default 1.0E8 and 1.0E-8).

Here is a list of the parameters that can be changed via the SETUP command, but DO require a new CAL command (i.e. once they are changed, the calculated shape-versus-time matrices are no longer valid):

The lower bound of a window,
The upper bound of a window, if the new value is larger,
The energy calibration,
The energy of a transition for which a shape is fitted,
The number of levels in the main cascade (unless just deleting levels at the top).

Here is a list of things that you can change using other commands:

The data spectra: command SPEC and SETUP/F,
The windows included in the fit: command EW, DW, and SW,
The angles included in the fit: command SA.

COMMANDS:

All commands and keywords can be abbreviated by the fewest letters needed to uniquely identify them.

AFX (ALTERNATE FIX)

This is an alternate FIX command. After entering AFX, a list of parameters which are currently free is displayed, and instructions are given to select those to fix. This command is useful if you wish to see which parameters are currently free, or to fix a number of parameters quickly.

AFR (ALTERNATE FREE)

This is an alternate FREE command. After entering AFR, a list of parameters which are currently fixed is displayed, and instructions are given to select those to free. This command is useful if you wish to see which parameters are currently fixed, or to free a number of parameters quickly.

AL (ALTER)

Changes the value of a parameter. The program asks for the necessary information, then shows the current value and asks for a new value; RETURN keeps the old value.

BAT (BATCH)

Should be the first command entered when running in batch mode. It suppresses the writing to the batch log file of a lot of information that would normally come to the terminal during interactive mode.

CAL (CALCULATE)

Calculates shapes as a function of time for the gamma-rays listed in the setup. The shapes are calculated from a '.his' file produced by the program 'histaver_or'. The information in that file is used to produce a matrix of shape versus time for each gamma ray defined in the setup. These matrices can be saved in a dump file, by using the DU/S (DUMP/SHAPE) command. The dump files with shapes saved will be much larger than if shapes are not saved, so they only need to be saved in one file.

CEN (CENTROID)

Calculates the centroid of the calculated lineshape, and the F(tau) function, for transitions in thin-target experiments in which the recoiling nucleus recoils out of the target into a vacuum. F(tau) is the velocity corresponding to the centroid over the maximum recoil velocity.

CF (COMMAND_FILE)

Calls a command file. A command file can include any LINESHAPE command, except CTRL_C. However, you cannot "cascade" command files. The default extension is '.cmd'.

CL (CLEBSCH)

Allows the spin I of the upper level of the first transition and K of the band to be altered, and displays the Clebsch-Gordon coefficients for all of the transitions.

CTRL_C (Press C while holding CTRL key down)

This is an interrupt command, which may be used whenever SEEK, SIMPLEX, MIGRAD, or MINOS is executing. After giving this command, a menu will appear. Enter STOP to stop the fit smoothly after the current iteration, LIST to list current values of parameters and continue the fit, or RETURN to continue the fit.

DC (DISPLAY CURVE)

Display the decay curve, corresponding to the I0/(I0+IS) ratio of the Doppler-shift recoil-distance analysis, as a function of time, for a selected level, using the current parameters. The curve is normalized to unity. With the /E qualifier, the emission rate as a function of time is displayed. This emission rate is the derivative of the I0/(I0+IS) ratio with the area under the curve set to one. The last channel regroups all the intensity from the last time step to t = infinity. The time range is specified by /T=it1,it2. If no time range (in time steps) is specified, the entire time range is displayed. If the /P qualifier is present, the displayed values will be printed in the formatted text file 'filename.out' in (x,y) form so they can be used as input for other graphics or plotting programs. If the /X qualifier is present, the display will be with white lines only (no color) for printing on black and white printers.

Syntax: DC[/L=i][/E][/P][/T=it1,it2][/X]

DD (DISPLAY DATA)

Displays the data spectrum alone. The user can either specify which window to be displayed (/W qualifier), or which level (/L qualifier), and then the program will find out the corresponding window. The data for one, several, or all angles can be displayed using the /A qualifier. Once a level, a window and/or a list of angles is specified, it remains the default for all subsequent DD and DF commands until a new one is

specified. If the /P qualifier is present, the displayed values will be printed in the formatted text file 'filename.out' in (x,y) form so they can be used as input for other graphics or plotting programs. If the /X qualifier is present, the display will be with white lines only (no color) for printing on black and white printers.

     Syntax: DD[/L=i][/A=a1,...,an][/P][/X]
             DD[/W=w][/A=a1,...,an][/P][/X]

DF (DISPLAY FIT)

Displays the current fit overlaid on the data spectrum. You do not need to perform a fit before asking to display the fit. If you change a parameter using ALTER, the current fit will be updated before display. You can thus change any parameter by hand and directly see the effect on the fit. If the /D qualifier is present, the difference between the data and calculated values will be displayed below the graph of the fit. The /L, /W, /A, /P, and /X qualifiers are the same as for DD above.

     Syntax: DF[/L=i][/A=a1,...,an][/P][/D][/X]
             DF[/W=w][/A=a1,...,an][/P][/D][/X]

DS (DISPLAY SHAPES)

Displays the shapes contained in the shape-versus-time matrices created by the CAL command. The shape for any level (as long as the gamma-ray is within one of the windows) and for any angle can be displayed, and for any interval of time.   The time range is specified by /T=it1,it2. If no time range (in time steps) is specified, the entire time range is displayed. The time interval must be expressed in integer time steps (type LIST to find the value of each time step). When a range of more than one time interval is specified, the shapes for each step within this interval are added with an equal weight. To sum them weighted by the current fitted decay curve, use the /C modifier. If no time interval is specified, all intervals are summed. If the /P qualifier is present, the displayed values will be printed in the formatted text file 'filename.out' in (x,y) form so they can be used as input for other graphics or plotting programs. If the /X qualifier is present, the display will be with white lines only (no color) for printing on black and white printers.

Syntax: DS[/L=i][/A=a1,...,an][/C][/P][/T=it1,it2][/X]

DU (DUMP)

Dumps (saves) the current level scheme setup and the parameters of
the latest fit in a dump shape file [.dsf]. This file can be read in at
any time (INDUMP command) and the saved setup and parameters become the
current setup and parameters. If the /S qualifier is present, the
shape-versus-time matrices created by the CAL command are also stored in
the dump file. The resulting file is much larger, but these matrices have
only to be saved once in one dump file. If a dump with no shapes is read
in, the current shape matrices are not modified. If the /F qualifier is
present, the .dsf file is a formatted text file which can be transported
to a different computer system, but which takes up considerably more disk
space than the unformatted binary file created if the /F qualifier isw not
present.

Syntax: DU[/S][/F] filename

DW (DISABLE WINDOW)

Disable a window (or group of windows), i.e. exclude its data points
from the fit. The level and window parameters associated with the
window(s) are automatically fixed. This command only affects the number
of data points on which the fit will be based. This way, you can set up
your entire level scheme initially, with all the windows in place, but
still only fit selected data sets. For instance, you could start fitting
at the top, disabling all lower windows (see also the commands EW and SW),
and then go down the cascade, enabling the window corresponding to the
next lower level, and disabling the windows of the top levels that are too
far away from the current level to influence the fit.

If window 'w1' only is specified, it will be disabled. If window
'w2' is specified, all windows between 'w1' and 'w2' will be disabled. If
'w1' is not specified, the status of all windows is displayed and the
window to be disabled can then be selected (RETURN leaves all windows
unchanged). This last option provides a convenient way to quickly see the
status of all windows.

Syntax: DW [w1][,w2]

EW (ENABLE WINDOW)

Enable a window (or group of windows), i.e. include its data points
in the fit. The level and window parameters associated with the window(s)
are automatically freed. This command only affects the number of data
points on which the fit will be based. This way, you can set up your
entire level scheme initially, with all the windows in place, but still
only fit selected data sets. For instance, you could start fitting at the
top, disabling all lower windows (see also the commands DW and SW), and
then go down the cascade, enabling the window corresponding to the next
lower level, and disabling the windows of the top levels that are too far
away from the current level to influence the fit.

If window 'w1' only is specified, it will be enabled. If window 'w2'
is specified, all windows between 'w1' and 'w2' will be enabled. If 'w1'
is not specified, the status of all windows is displayed and the window to
be enabled can then be selected (RETURN leaves all windows unchanged).
This last option provides a convenient way to quickly see the status of
all windows.

Syntax: EW [w1][,w2]

ER (ERASE)

Deletes the graphics screens.

EX (EXIT)

Exits from the program. Deletes the graphics screens if necessary.

FX (FIX)

Fixes one or more of the variable parameters and, optionally, changes
the value of one parameter. The program asks for the necessary
information, then shows the current value and asks for a new value; RETURN
keeps the old value.

If WIN is selected when the program asks which parameter to fix, it

causes all window parameters to be fixed, but leaves all level parameters as they were. After having fitted all windows individually and obtained the best values for the window parameters, it is often desirable to fit only level parameters for a number of levels at a time. See FW.

FW (FIX WINDOW)

The command FW causes all window parameters to be fixed, but leaves all level parameters as they were. After having fitted all windows individually and obtained the best values for the window parameters, it is often desirable to fit only level parameters for a number of levels at a time. To do this, first enable all the desired windows using EW, and then call FW to conveniently fix the window parameters.

FR (FREE)

Frees one or more of the variable parameters. It can only be used with parameters that can be variable.

IN (INDUMP)

Reads level scheme setup and parameters from a dump shape file [.dsf] (see DU). To save the current setup and parameters, use the DUMP command. If a dump with no shapes is read in, the current shapes matrices are not modified. If the file being read was dumped in a formatted text file with the /F qualifier, then the /F qualifier MUST be used to read the file.

Syntax: IN[/F] filename

LIST

Lists the current level scheme setup, parameters and errors on fitted parameters. Only enabled windows are listed (see EW and DW). The /F (FULL) qualifier causes the listing of information on all levels and windows, and more information about where the data comes from. The /P qualifier displays the current values of the parameters currently being varied.

Syntax: LIST[/F][/P]

LIN (LINEAR)

Causes graphs to be displayed with a linear scale on the y axis. This is the default option. This option continues in effect until the LOG command is entered. /LIN can be used as a qualifier with any display command.

LOG (LOGARITHMIC)

Causes graphs to be displayed with a logarithmic scale on the y axis. This option continues in effect until the LIN command is entered. /LOG can be used as a qualifier with any display command.

MG (MIGRAD)

Calls the least-squares fitting routine MIGRAD. This is a gradient search routine which can move in very close to the true chi-square minimum if it doesn't start too far away. It is usually best to use MIGRAD after SIMPLEX has converged.

MN (MINOS)

Calls the MINOS error analysis routine. MINOS finds the true errors (confidence intervals) by examining the behavior of chi-square as one parameter is varied. MINOS varies one parameter in steps in the positive (and negative) directions and, at each step, reminimizes chi-square with respect to all the other parameters. The step at which chi-square increases by one unit above its lowest value gives the positive (or negative) error of the parameter.

In this program, MINOS will determine the positive and negative errors of the quadrupole moment Q for one or more levels, and also the errors of the feeder lifetimes (TS) or the feeder quadrupole moments (QS) if requested

MP (MINOS PLOT)

Calculates and displays graphically on the terminal the values of chi-square for ten equally spaced values of a selected quadrupole moment

on each side of its best value.

OFF

Deletes the graphics screen.

OP (ORDER PEAKS)

Renumbers impurity peaks in a window so that peak 1 is the one with lowest channel number, peak 2 is the next lowest, etc.

PR (PRINT)

Writes the current level scheme setup, parameters, and errors on fitted parameters in the file 'filename.out'. Only enabled windows are listed (see EW and DW). The /F (FULL) qualifier causes information on all levels and windows, and more information about where the data comes from to be written.

Syntax: PR[/F]

QUIT

Exits from the program. Deletes the graphics screens if necessary.

SA (SELECT ANGLE)

This command allows one to fit data from only one angle at a time, even though two or more angles may have been included during SETUP. If an angle number is specified on the command line, then only data for that angle are included in the fits. If it is not specified, then, after calling SA, you will be asked which angle you wish to include in the fit (RETURN = ALL). The angle selected remains the default angle for all subsequent fitting until changed with another SA command, and is also saved in dump files.

Syntax: SA [angle]

SEEK

Calls the least-squares fitting routine SEEK. This is a Monte Carlo search routine which searches randomly throughout a region surrounding the initial parameter values. It is useful at the beginning of a fit when the initial parameter values are only estimates.

SET (SETUP)

Command to set up the level scheme and give values to all parameters. The program asks for the required information, and shows the previous value. A new value can be entered, or RETURN keeps the old value. After completing a setup, it is a good idea to save the values with a DU command.

Part of the setup can be re-done without changing the other parts by using one or more of the following qualifiers: /F (files), /C (energy calibration), /SF (side feeding), /L (level information), /W (window information), /SP (spin of lowest level to calculate Clebsch-Gordon coefficients).

For the /L (level) and /W (window) qualifiers, specifying a level or window number immediately after the qualifier permits setup for that level or window only, and avoids having to step through all the other levels or windows.

For the /SP (spin) qualifier, you only have to give K and the spin value I of the upper level of the lowest transition. One unit of spin is added for each level, unless the branching ratio is set equal to 1.0, in which case two units of spin are added. The minimum spin value is 2.

Syntax: SET[/F][/C][/SF][/L[i]][/W[i]][/SP]

SM (SIMPLEX)

Calls the least-squares fitting routine SIMPLEX. This is a geometrical method which can move in toward a minimum in chi-square rapidly, even move over a relative maximum to find a lower minimum on the other side, but is not as efficient near the true minimum. It is usually

best to follow SIMPLEX with MIGRAD.

SP (SPECTRA)

Reads in a new data spectrum, but only updates the windows which are currently enabled when the command is executed. If you want to change data for ALL windows, then it is better to use the SETUP command.

To change a data spectrum for some, but not all, of the windows, do the following:

1.   Disable all windows other than the one(s) for which you want to read in the new spectrum.
2.   Use the SP command: it will ask for the filenames of the new data spectrum and error spectrum.
3.   Re-enable the windows that were temporarily disabled. These window will have kept the old specfile data.
4.   The LIST and PR commands will show these new spectra, and their names will be stored in the '.dsf' files.
5.   These spectra will be lost, however, upon calling SET, SET/F, or SET/L, and making any CHANGES in the data spectra or error spectra files, in the number of levels, or in the upper or lower channel numbers of any windows. The specfiles specified by SET/F will then be read in for ALL windows.

SW (SELECT WINDOW)

Enables one window, and disables all the other windows. All level and window parameters associated with other windows are fixed. (It is equivalent to the command DW 1,n followed by EW i, where n is the highest window and i is the window to enable.) This way, you can set up your entire level scheme initially, with all the windows in place, and then fit one window at a time to obtain the best values for the parameters associated with only that window (slope and intercept of the background, normalization, and impurity peak areas).

Syntax: SW i   (where i is a window number)

X0 (X ZERO)

Defines the origin of the x axis, in channels.

Syntax: X0 value

XM (X MAX)

Defines the maximum value of the x axis of the display, in channels. If value = 0, the display is autoscaled over the full width of the window (i.e. setting value = 0 resets both XMAX and X0 to the high and low channels of the window).

Syntax: XM value

Y0 (Y ZERO)

Defines the origin of the y axis. Default is value = 0. If value =0, the origin is 0 in linear mode and is autoscaled in logarithmic mode.

Syntax: Y0 value

YM (Y MAX)

Defines the maximum value of the y axis of the display. If value = 0, the maximum value of the displayed function is used with a small upper margin added.

Syntax: YMAX value