Command FPTAIL

PURPOSE Specify Gaussian or Lorentzian peaks convoluted with an exponential

function as fit function via automatic search, prompting input or global

fit windows.

PARAMETERS

N Maximum number of peaks to be located; default is n = 30. If n = "*",

peaks are defined by the fit window (see command "FWIN") assuming

each window to contain one peak.

/GAUSS Specify Gaussian peaks convoluted with an exponential as fit function.

/LORENTZ Specify Lorentzian peaks convoluted with an exponential as fit

function.

(The peak mode keyword may be omitted. Initially and after the

command "FINIT" Gaussian peaks convoluted with an exponential are

assumed, otherwise the last specified mode is valid.

/FWHM(c) Expected peak widths (FWHM) in units of channels; a start value is

determined from the peak structure in the spectrum by an automatic

algorithm.

The width parameter is used when peaks are searched automatically or

only the peak centers are given as prompting input.

/AREA(a) Lower limit of net peak areas for automatic peak search; replaceable

default is a = 0.

/SIGNIFICANCE(s) Lower limit of significance of peaks for automatic peak search,

replaceable default is s = 2.

/FULL Automatic peak search in the whole spectrum, not limited to the

displayed range.

/PROMPT Peak locations are given by cursor or by terminal input.

Using the cursor, single points (denoting the peak centers) or separate windows (lower and upper limits) may be specified. The cursor is repeatedly activated until the specified number of peaks is reached or

input is stopped by pressing the right mouse button.

If the number of peaks was omitted, it is replaced by the final number

of specified peaks.

Peak windows may overlap. Peak windows are only used to determine the initial values of the fit parameters, they do not act as fit windows. That means that the region included in the fit is not limited to the peak

window.

/CURSOR Alias of /PROMPT

/TAIL(r1,r2,r3..) Guess parameters for tail slope of each peak. Negative values specify

an exponential tail to the left, positive values an exponential tail to the

right side. Only one tail is supported per peak.

/DELETE Some peaks may be removed from the current fit function by cursor.

/NODISP The located peaks are not displayed.

FUNCTION Parameters of a peak function are

a1 area,

a2 first moment,

- a3 2.35 times the standard deviation (approximately the full width at half maximum.)
- a4 relative skewness,

accordingly parameters of further peaks are denoted by subsequent indices. (See <u>HELP FITGEN</u> for a full documentation.)

Unless an asterisk is given for a peak number or the keyword "/PROMPT" is specified, the automatic peak search routine is invoked using the parameters FWHM and AREA. For details see command AFPEAK.

Area, mean and full width at half maximum of the net data (i.e. with regard to background functions) in the located windows are calculated for initial values of the peak parameters. If only a peak center is given as prompting input, the area is determined by the corresponding channel contents multiplied by the specified FWHM. Lower limits of areas and FWHM are set to zero; minimum and maximum of the peak positions are set equal to the window limits.

REMARKS

Peak parameters may be modified by the command <u>FPAR</u>.

The SATAN fit package supports the following peak functions:

Command FPEAK / GAUSS: Gaussian shape

Command FPEAK / LORENTZ: Lorentzian shape

Command FPTAIL: Convolution of Gaussian (or Lorentzian) and exponential

Command <u>FPBOX</u>: Convolution of Gaussian (or Lorentzian) and rectangle

Command <u>FPVOIGT</u>: Convolution of Gaussian and Lorentzian (Voigt function)

EXAMPLE

FPTAIL / G

Locate up to 30 Gaussian peaks convoluted with an exponential distribution each in the actually displayed spectrum with a FWHM determined from the peak structure in the spectrum; display the resulting peak function.

FPTAIL *

Gaussian peaks convoluted with an exponential are located referring to the fit windows; if no windows have been defined by "FWIN", the displayed data are expected to contain one peak.

FPTAIL 2 / LOR PROM NOD

Two Lorentzian peaks convoluted with an exponential are specified by cursor or terminal input; the function is not displayed.