Command FPEAKS

PURPOSE Specify Gaussian or Lorentzian peaks 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 as fit function.
/LORENTZ	Specify Lorentzian peaks as fit function. (The peak mode keyword may be omitted. Initially and after the command "FINIT" Gaussian peaks 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 when 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
/NOSEARCH	No automatic peak search.
/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 center,
- a3 full width at half maximum.

accordingly parameters of further peaks are denoted by subsequent indices.

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 commands FAREA, FPOS, FWIDTH or FPAR.

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 FPBOX: Convolution of Gaussian (or Lorentzian) and rectangle
Command FPVOIGT: Convolution of Gaussian and Lorentzian (Voigt function)

EXAMPLE

FPEAKS / G
Locate up to 30 Gaussian peaks in the actually displayed spectrum with a FWHM determined from the peak structure in the spectrum; display the resulting peak function.

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

FPEAKS 2 / LOR PROM NOD
Two Lorentzian peaks are specified by cursor or terminal input; the function is not displayed.