Command **FPBOX**

PURPOSE Specify Gaussian or Lorentzian peaks convoluted with a rectangular

function (box) as fit function via automatic search, prompting input or

global fit windows.

PARAMETERS

Maximum number of peaks to be located; default is n = 30. If n = "*", 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. Specify Lorentzian peaks as fit function. /LORENTZ

> (The peak mode keyword may be omitted. Initially and after the command "FINIT" Gaussian peaks are assumed, otherwise the last

specified mode is valid.

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

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.

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

default is a = 0.

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

replaceable default is s = 2.

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.

Alias of /PROMPT /CURSOR

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

The located peaks are not displayed. /NODISP

FUNCTION Parameters of a peak function are

> a1 area,

a2 mean value.

full width at half maximum. a3

box width

accordingly parameters of further peaks are denoted by subsequent indices.

/FULL

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 FPBOX: Convolution of Gaussian (or Lorentzian) and

rectangle

Command **FPVOIGT**: Convolution of Gaussian and Lorentzian (Voigt

function)

EXAMPLE

FPBOX / G

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

FPBOX *

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.

FPBOX 2 / LOR PROM NOD

Two Lorentzian peaks, convoluted with a box, are specified by cursor or terminal input; the function is not displayed.