Command FPOSITION

PURPOSE Define values and attributes of peak positions.

PARAMETERS

PEAKS List of peak numbers. Each list element may have the syntax "a TO z

BY s" with optional parameters z and s; default step size is s = 1.

/FIX The specified peak positions are **fixed**. They are held constant during

iterations.

/DIFF(p) The specified peak positions are **relatively fixed**. The differences of the

positions of corresponding peaks and reference peak number p are held

constant during iterations.

/SUM(p) The specified peak positions are **relatively fixed**. The sums of the

positions of corresponding peaks and reference peak number p are held

constant during iterations.

/PRODUCT(p) The specified peak positions are **relatively fixed**. The products of the

positions of corresponding peaks and reference peak number p are held

constant during iterations.

/QUOTIENT(p) The specified peak positions are **relatively fixed**. The quotients of the

positions of corresponding peaks and reference peak number p are held

constant during iterations.

/VARY Concerned peak positions are to **vary** again.

/EON A special error analysis is demanded.

/EOFF Reset error analysis flag.

/GUESS(g) Guess values for the peak positions.

General values are assigned to the denoted parameters in the order of appearance (arrays with the rightmost subscripts varying most rapidly.) However, if the list consists of a single one-dimensional array (or array cross section) with asterisk notation (one subscript substituted by '*'), array elements corresponding to the specified peak numbers are

selected and assigned accordingly.

If only a single value is given, it is assigned to each specified

parameter.

/RELATIVE This keyword specifies the interpretation of the guess values. For

relatively fixed fit parameters the guess values are expected to represent a difference, sum or quotient with respect to the

corresponding reference parameters; for others the keyword is ignored

and the guess values are taken absolute.

/MIN(m) List of lower limits which must not exceed the current values of the

peak positions. For details see keyword "/GUESS"

/MAX(m) List of upper limits which must not exceed the current values of the

peak positions. For details see keyword "/GUESS"

/NOLIM Limits of the specified parameters are set to infinity unless nominated

by MIN or MAX.

/LIST List the current guess values and limits of the specified peak positions..

REMARKS

Together with "FAREA" and "FWIDTH" this command provides a more comfortable way of specifying attributes of (Gaussian and Lorentzian) peak parameters than the command "FPAR" does, since parameters are addressed by peak numbers instead of internal serials.

The fit function is evaluated with the current guess values and may be displayed by "<u>FDISP</u>" or listed by "<u>FLIS</u>T" and "<u>FRESULT</u>".

EXAMPLE

FPOS 1..2 / D(3) G(-16.2, -14.6) R

Fix the differences of the positions of peaks no. 1 and 2 relative to peak no. 3. Assign guess values to the positions of peaks 1 and 2 which are smaller than that of peak no. 3 by an amount of 26.1 and 14.6, respectively.

For further examples see command "FPAR".