

FullProf keywords to be included in the global section of a PCR file

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The possibility of using two lines starting with `VARY` and `FIX` for controlling the refinement of global parameters of each pattern has been implemented. Moreover using this method one can refine the ratio of the intensity of the two wavelength components in a constant wavelength (CW) pattern.

The lines must be provided in the PCR file just after the place in which appear the following items: `Lambda1, Lambda2, ... (CW)` or `Bkpos, Wdt, Iabscor (TOF)`.

The first line should be the `VARY` line and the second one the `FIX` line. After this two master keywords, other keywords may be give for refining or fixing different parameters.

The presently available keywords are the following (notice that they are case sensitive) :

Global keywords

backgd	all linear interpolation background parameters outside excluded regions.
add_back	all additional parameters of the linear combinations of external profiles
back_nn	background parameters from 1 to n are varied or fixed
Microabs	microabsorption parameters (<code>P0, CP, Tau</code> --> only with <code>FIX</code>)

CW

zero	
sycos	
sysin	
P0	
CP	
Tau	
ratio	ratio of the intensity of the two wavelengths components

TOF

zero
dt1
dt2
Zt
dt1t
dt2r
xcross

width

All these keywords can be combined with the traditional method of putting manually the codes (or just a 1.0) for refining parameters.

Example

```
.....
!
! Lambda1  Lambda2  Ratio  Bkpos  Wdt  Cthm  muR  AsyLim  Rpolarz  ->Patt# 1
1.540560  1.544330  0.45002  25.000  15.0000  0.9100  0.0000  30.00  0.0000
!
VARY ratio  back_4
FIX  Tau
!
!NCY  Eps  R_at  R_an  R_pr  R_gl  Thmin  Step  Thmax  PSD  Sent0
6  0.10  1.00  1.00  1.00  1.00  25.0000  0.025000  143.0000  0.000  0.000
!
!
20  !Number of refined parameters
!
! Zero  Code  SyCos  Code  SySin  Code  Lambda  Code MORE  ->Patt# 1
0.02702  11.0  0.00000  0.0  0.00000  0.0  0.000000  0.00  1
!
! Microabsorption coefficients for Pattern# 1
! P0  Cod_P0  Cp  Cod_Cp  Tau  Cod_Tau
0.0000  0.00  1.1972  141.00  0.1324  0.00
! Background coefficients/codes for Pattern# 1
2.0000  -17.493  6.2242  -0.59210  0.0000  0.0000
151.000  181.000  191.000  201.000  0.000  0.000
.....
```