

**FullProf keywords to be included
in the global section of a PCR file
(june 2011 – updated oct. 2017)**

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>)
Scale_Factors	produces the refinement of all scale factors
Cells	produces the refinement of all cell parameters (only for automatic mode)
Boverall	produces the refinement of all overall temperature factors <code>Bov</code>
Ysize	produces the refinement of Y (isotropic Lorentzian size) for all phases
Gsize	produces the refinement of G (isotropic Gaussian size) for all phases
Xstrain	produces the refinement of X (isotropic Lorentzian strain) for all phases
Ustrain	produces the refinement of U (isotropic Gaussian strain) for all phases

CW

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

TOF

zero
dtt1
dtt2
Zt
dtt1t
dtt2r
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  
.....
```