

FullProf list of commands to handle refinement codes and constraints

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For instructing the program **FullProf** to perform some actions, there are two places in the **PCR** file for setting up a series of commands (mostly using **VARY** and **FIX** instructions). There are local commands (for each phase) and global commands affecting the whole set of parameters. These commands work only when the automatic mode is activated (**Aut=1**). In the case of pure magnetic phase, described in terms of basis functions of irreducible representations or in terms of Fourier coefficients of magnetic moments, most of the commands described below are not operative. In such cases, the user should control the refinement codes by hand or use other commands like **MVARY** or **MFIX** in which the keywords referred to atoms use the exact name given in **FullProf**. In general the commands and keywords are case sensitive.

Global **VARY/FIX** commands

For refining or fixing parameters in the whole scope of the PCR file the user can provide one **VARY** and/or one **FIX** instructions per pattern, followed by keywords representing variables. These keywords are case sensitive. They have to be placed below the line containing the wavelengths for CW case, or below the line containing the values of “!Bkpos Wdt ...” for TOF.

Global keywords (case sensitive) to be used in **VARY/FIX** commands:

Scale_Factors	→ refinement of all scale factors
Cells	→ refinement of all cell parameters
Boverallls	→ refinement of all overall temperature factors Bov
Ysize	→ refinement of Y (isotropic Lorentzian size) for all phases
Gsize	→ refinement of G (isotropic Gaussian size) for all phases
Xstrain	→ refinement of X (isotropic Lorentzian strain) for all phases
Ustrain	→ refinement of U (isotropic Gaussian strain) for all phases
backgd	→ all linear interpolation background points outside excluded regions
add_back	→ all parameters of the linear combinations of external profiles
back_nn	→ Background parameters from 1 to nn are varied or fixed
Microabs	→ Micro-absorption parameters (P0, Cp, Tau)

CW:

zero, sycos, sysin, P0, Cp, Tau

ratio → Ratio of the intensity of the two wavelength components

TOF:

zero, dtt1, dtt2, Zt, dtt1t, dtt2t, xcross, width, dtt_loverd

Example (CW):

```
...  
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolarz 2nd-muR -> Patt# 1
```

```

1.540600 1.544300 0.49192 40.000 15.000 0.7998 0.0000 60.00 0.0000 0.0000
!
VARY Scale_Factors ratio back_4 zero Cells
FIX Boveralls
!
!NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
...

```

Example (TOF):

```

. . .
! Bkpos Wdt Iabscor for Pattern# 1
7000.000 8.20 2
VARY Scale_Factors zero back_4
FIX Cells dtt2
. . .

```

Phase-Dependent commands

Particular keywords can be included in the **COMMANDS/END_COMMANDS** section of a **PCR** file, after the line given the name of the current phase. When the commands are simple, they may be included in the same line as the title of the phase. The number of these commands is limited to 20 per phase.

This kind of section appear in the line just below the title of the phase, as shown below:

```

!-----
My phase name
COMMANDS
. . .
END_COMMANDS
!Nat Dis ....

```

Keyword commands:

DLIM

Modify the behaviour of the program in relation with the generation of reflections.

Format of the command:

DLIM pat d_min

Where **pat** is the number of the pattern and **d_min** the value of the lowest d spacing. Only the reflections having a d spacing greater than the provided **d_min** value are used in the refinement of the data.

Example:

```

!-----
My phase name DLIM 2 2.14 DLIM 3 1.5
!Nat Dis ....

```

The reflections of pattern number 2 are limited to d spacing greater than d=2.14 angstroms and those of pattern number 3 to d spacing greater than 1.5 angstroms. This may be useful for

magnetic structure refinement when using a diffraction pattern going far in Q (for instance in TOF case). In case of multiple patterns the **VARY/FIX** keywords affect to all the pattern sections of the particular phase, in which the **COMMANDS** block is defined, providing independent codewords. For varying or fixing parameters for an individual pattern, the suffix "_n" is appended to the keyword with "n" being the number of the pattern. Instructions have been introduced to make constraints between profile parameters in multi-pattern multiphase cases. These instructions act as **VARY** but assigning common codewords to a series of variables. The syntax is

PEQU_pat keyword → affects all section patterns of a particular phase
PEQU pha keyword → affects all phases and patterns

Examples:

PEQU_pat cell → the cell parameters of a particular phase are equal for all patterns to which the phase, where the **COMMANDS** block is defined, contributes.

PEQU pha sigma2 → the **sigma2** parameters for the different phases and different patterns are attributed the same codeword, irrespective of the phase in which the **COMMANDS** block is defined.

Keywords for **VARY/FIX** commands

scale	→ refine/fix scale factor
x_A	→ refine/fix the x coordinate of atom labelled as A
y_A	→ refine/fix the y coordinate of atom labelled as A
z_A	→ refine/fix the z coordinate of atom labelled as A
xyz_A	→ refine/fix the x, y and z coordinates of atom labelled as A
b_A	→ refine/fix the thermal parameter of atom labelled as A
bov	→ refine/fix overall b-factor
occ_A	→ refine/fix occupation number for atom A
xyz	→ allows to refine/fix x, y and z coordinates of all atoms
xyz 0.1	→ same as before but a multiplier 0.1 will be used to limit the shift of parameters during refinement. This affect only the parameters that have no codeword when running the program.
cell	→ refine/fix cell parameters of the current phase
uu	→ refine/fix Caglioti U , Gaussian strain
vv	→ refine/fix Caglioti V $H_G^2 = W + V \tan \theta + U \tan^2 \theta + GauSiz(\cos \theta)^{-2}$
ww	→ refine/fix Caglioti W $H_L = X \tan \theta + Y(\cos \theta)^{-1}$
xx	→ refine/fix parameter X for constant wavelength: Lorentzian strain
yy	→ refine/fix parameter Y for constant wavelength: Lorentzian size
gsz	→ refine/fix parameter GauSiz for constant wavelength: Gaussian size
mxmymz	→ refine/fix magnetic moments of all magnetic atoms
McosMsin	→ refine/fix modulation functions of all magnetic atoms

The program takes care of symmetry constraints automatically. Be careful with disordered structures. If two atoms of different species occupy the same position, the user should give an explicit code, using the usual explicit constraints, to positions and displacement parameters. Note that the instructions are applied as they appear. For instance a **FIX** instruction after a **VARY** may suppress a refinement code.

Example:

COMMANDS

```
VARY xyz_Fe xyz_O1
VARY x_Mn1 z_O27 y_Ho1 b_A1
FIX b_Mn1 x_C23
VARY scale uu bov
VARY cell yy
VARY occ_Fe2
FIX xx
```

END_COMMANDS

This set of commands instruct the program to refine all positional parameters of atoms Fe and O1, the "x" coordinate of Mn1, the "z" coordinate of O27, the "y" coordinate of Ho1 and the temperature factor(s) of atom A1. If A1 is anisotropic, all beta-parameters compatible with the site symmetry are refined. The instruction **FIX** avoid the refinement of the thermal parameters of Mn1 and the "x" coordinate of atom C23.

We

FIX_SPC spc1 spc2

spc"i" is the symbol used for the scattering power of the atom (normally the chemical element symbol). The command **FIX_SPC** means that all free parameters of a particular chemical species are fixed. For instance, if one wants to fix all hydrogen atoms of a structure the command **FIX_SPC H** will fix all coordinates, occupation and displacement parameters of H atoms.

Example:

COMMANDS

```
...
FIX O H
...
```

END_COMMANDS

EQUAL

Make constraints between parameters belonging to different phases or patterns. The format of the instruction **EQUAL** is the following:

```
EQUAL name_parent_par name1 mult1 name2 mult2 ... nameN multN
```

The name of the parent parameter informs the program that this parameter will be refined (implicit **VARY**) and the other parameters are simultaneously refined using the same code but with other multipliers. An example is given below:

```
EQUAL occ_Fe2_ph1 occ_Mg2_ph1 -1.0 occ_Fe3_ph1 -1.0 occ_Mg3_ph1 1.0
```

This means that we are refining the distribution of Fe and Mg between two sites maintaining full occupation of both sites and fixing the composition. Remember that the **EQUAL** instruction means that the variations of the initial parameters are constrained and not the values themselves. For structural parameters it is not needed to explicit the number of the pattern, however, for some parameters it is needed to explicit this.

It is possible to make constraints, using the keyword **EQUAL**, between parameters of different phases or different patterns. In principle, the name of the parameters are those appearing in the output file of **FullProf** below the line:

SYMBOLIC NAMES AND INITIAL VALUES OF PARAMETERS TO BE VARIED.

These names are also those used in instructions like **MVARY** and **MFIX**. Not everything has been tested and may be some bugs. This is an alternative to manually writing the explicit codewords numbers.

An example of command block is given below

Example:

COMMANDS

```
VARY xyz b → this is for refining all positions and thermal parameter  
FIX z_Ba1 → this is for fixing an atom coordinate because the space group is non-  
centrosymmetric  
PEQU pha uu vv ww → this instructs the program that the U, V, W Caglioti parameters  
are the same for all phases  
VARY yy gsz → this refines the Lorentzian and Gaussian size parameters for the current phase  
EQUAL occ_Si1_ph1 occ_Si2_ph1 -1 occ_Al1_ph1 -1 occ_Al2_ph1 1  
↓→ Constraints of occupation factors in phase 1  
EQUAL Biso_Si1_ph1 Biso_Si_ph2 1.0  
↓→ Atoms Si1 and Si of phases 1 and 2 have the same Biso  
EQUAL Biso_Al3_ph1 Biso_Al1_ph2 1.0  
EQUAL Asym1_ph1_pat1 Asym1_ph2_pat1 1.0  
↓→ Asymmetry parameter 1 of phase 1 and 2 are the same for pattern 1.  
EQUAL Asym2_ph1_pat1  
Asym2_ph2_pat1 1.0  
VARY uu_1 vv_1  
VARY uu_2 vv_2  
MVARY Ry_Cu1_ph2 1.0 Rx_Cu2_ph2 1.0  
MFIX Rz_Cu1_ph2  
END_COMMANDS
```

Note that in the above **COMMANDS** block we use in the **EQUAL** instruction with the explicit symbolic names of the refined parameters. For instance instead of setting **b_A13_ph1** we should use **Biso_A13_ph1**. This is to avoid ambiguities with the b-cell parameter. As a rule of thumb in **EQUAL** instructions, we should always use the complete symbolic name of the parameter to be constrained. One can use also **MVARY**, **MFIX** together with the explicit symbolic names instead of the simplified names used with **VARY** and **FIX** instructions. This is compulsory for magnetic cases treated using representational analysis or the Fourier coefficients formalisms. In the above **COMMANDS** block, the **MVARY** instruction is followed by the explicit name of the variable followed by the selected multiplier that should be always provided.

Another important keyword is:

```
SAME_Biso spc1 val1 spc2 val2 ... spcN valN
```

spc"i" is the symbol used for the scattering power of the atom (normally the chemical element symbol). The values **val"i"** correspond to the value of the isotropic temperature factor to be assigned commonly to all atoms of species **spc"i"**. This value should be initially be given as negative. The program will change that to positive and only when the negative value appears in the PCR file the **Biso** already existing in the file are replaced by those given in the **SAME_Biso** instruction.

Example:
COMMANDS

```
...  
SAME_Biso O -0.93 F -0.98  
...  
END COMMANDS
```

Instructions changing the interpretation and description of the provided “phase”:

```
LAYER_A, LAYER_B, LAYER_C
```

The above keywords instruct the program that the current phase will be treated as a single layer, so the reflections (H00), (0K0) or (00L), respectively, will be suppressed and the atom coordinates will be given in angstroms along the corresponding direction. Considering an artificial (quasi-empty) supercell with a very long axis in the perpendicular direction to the layer, the 3D diffraction pattern approach to that of the single layer diffraction pattern without need of integrating the rods in reciprocal space. To eliminate the ripples a long axis together with a special broadening is enough. The method is based in the idea developed by K. Ufer *et al.* Z. Kristallogr. **219**, 519 (2004), making the method perfectly compatible with the Rietveld method.

The keywords **LAYER_A**, **LAYER_B** and **LAYER_C** must be followed by the order of the supercell used, as in:

```
COMMANDS
  LAYER_C 15
  . . . . .
END_COMMANDS
```

This means that corresponding supercell parameter (as given in the unit cell line) is $c=15 \cdot c_s$, being c_s the c-parameter of the subcell. This is needed to conserve the (0, 0, $l=L/15$) reflections that are treated separately.

For Xlens

CONTENT

Create a proper CDR file for Xlens

Format of the command:

```
CONTENT E11 n1 E12 n2 E13 n3....
```

Where **ni** (integer) is the number of atoms of the chemical species **E1i** (Chemical symbol of the element **i**). CONTENT is only useful when doing a Le Bail fit in order to generate the POW and CDR files for XLENS.

For quantitative analysis

FILE_HKL

It is now possible to create a database using **FullProf** for quantitative phase analysis. One can calculate the structure factors of a particular crystalline phase and store them in a file using **HKL=5** (see note of 3 July 2003). A new line containing the space group and the cell parameters has been included. The created file can be renamed arbitrarily and the file can be read back by a job with **NAT=0**, **JBT=-3** and **IRF=2**.

Format of the command:

```
FILE_HKL n_pat my_hkl_file_name
```

Where n_{pat} is the number of the pattern for which the structure factors file named **my_hkl_file_name** is given. If the space group and the cell parameters do not coincide with what is written in the file **my_hkl_file_name** the stored values are re-copied to the PCR file. The cell parameters are re-copied only in the case the sum of the absolute differences is greater than 4.

Otherwise the parameters of the PCR file are kept. In the following example the space group and cell parameters are imported from the file "**quant.hkl**"

```
!-----
! Data for PHASE number:1 ==> Current R_Bragg for Pattern#1:0.23
```

```

!-----
My Phase name
!
COMMANDS
..... (Other commands)
      file_hkl 1 quant.hkl
..... (Other commands)
END COMMANDS
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
  0    0    0 0.0 0.0 1.0 -3    2    0    0    0 2147.799 0    7    0
!
P 1    <--Space group symbol
!-----> Profile Parameters for Pattern # 1
! Scale   Shape1   Bov   Str1   Str2   Str3 Strain-Model
 13.492   0.00000 0.00000 0.00000 0.00000 0.00000 0
 11.00000 0.000   0.000   0.000   0.000   0.000
!      U      V      W      X      Y GauSiz LorSiz Size-Model
0.0161020 -0.00158 0.00291 0.000000 0.000000 0.000000 0.000000 0
      0.000      0.000      0.000      0.000      0.000      0.000      0.000
!      a      b      c      alpha      beta      gamma #Cell Info
0.00000 0.000000 0.000000 90.000000 90.000000 90.000000
 31.00   41.00   21.00      0.00      0.00      0.00
.....

```

For magnetic structures

MDLIM

Calculation of magnetic contribution, distinct from the usual DLIM instruction.

Format of the command:

```
MDLIM n_pat d-spacing
```

Where **n_pat** is the number of the pattern and d-spacing the value of a d-spacing. Only the reflections having a d-spacing greater than the provided d-spacing value are used in the magnetic refinement of the data.

Example:

```

!-----
My phase name
!-----
COMMANDS
MDLIM 1 1.8 MDLIM 2 1.8 MDLIM 3 1.9 MDLIM 4 2.0 MDLIM 5 2.2
save_mag_strf
END_COMMANDS
!Nat Dis ....

```

The reflections of pattern number 2 are limited to d-spacing greater than d=1.8 angstroms and those of pattern number 3 to d-spacing greater than 1.5 angstroms. This may be useful for

magnetic structure refinement when using a diffraction pattern going far in Q (for instance in TOF case).

EFF_MOMENT

Force the program to use "effective moments" that correspond to the values of the magnetic moments in the case of $\mathbf{k}=1/2\mathbf{H}$. In such a case, if the difference $\mathbf{k}-1/2\mathbf{H}$ is greater than 0.00001, one can set **Nvk=-1**, for instance when $k_y=0.49993$, and the values of the components of Fourier coefficients are the same as those obtained when we put $Nvk=1$ and $k_y=0.5$.

Example:

Magnetic phase name

!

COMMANDS

eff_moment

END COMMANDS

!Nat	Dis	Mom	Pr1	Pr2	Pr3	Jbt	Irf	Isy	Str	Furth	ATZ	Nvk	Npr	More
3	0	0	0.0	0.0	1.0	1	-1	-1	0	0	0.000	-1	7	0

...

SAVE_MAG_STRF

A file, named "codefile_phn.mstf", where "n" in "_phn" is the number of the phase, is created, containing the magnetic structure factor and magnetic interaction vector for magnetic phase.

MAGDOM / TWIN

Introduce a set of magnetic domains in the case of single crystal data.

Format of the command:

MAGDOM (including the domain 1 with identity matrix) followed by rotational operators, a real number (as for a magnetic symmetry operators used in MSYM) a colon symbol and the values and refinement codes for the populations.

Example 1:

!-----

My Magnetic phase name

!-----

COMMANDS

magdom u, v, w, 0.0 : 0.650 121.00

magdom -v, u, w, 0.0 : 0.250 131.00

magdom u, -v, w, 0.0 : 0.100 0.00

END COMMANDS

!Nat	Dis	Mom	Pr1	Pr2	Pr3	Jbt	Irf	Isy	Str	Furth	ATZ	Nvk	Npr	More
2	0	0	0.0	0.0	1.0	1	4	-1	0	0	0.000	-1	0	0

.

In this example, there are three domains in total. Notice that the first domain corresponds to that of the magnetic model described in the PCR file. The sum of the populations are always 1.0. The

refinement code of the last domain should always be zero. It is calculated as a function of the previous values in order to ensure that the sum is always 1.

Example 2:

My Magnetic phase name

!

COMMANDS

magdom u, v, w, 0.1 : 0.250 0.250 121.0 131.0

magdom u,-v, w, 0.1 : 0.200 0.300 141.0 0.0

END COMMANDS

```
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
  3   0   0 0.0 0.0 1.0   1   4  -1   0   0 0.000  -1   0   0
. . . . .
```

In this second example, there are two domains and two chirality domains, four domains in total. Notice that the first domain corresponds to that of the magnetic model described in the **PCR** file. A value of the real number following the operator greater than 0.001 means that we have chirality domains (second population value and second refinement code). The sum of all populations should be equal to 1.0 and the last one should not have a refinement code. The rotational operators should be those of the paramagnetic group that are lost in the transition to the ordered state. Be careful with trying to refine all domain populations. There are situations where two domains give exactly the same module of the magnetic interaction vector so that the relative population cannot be determined using non-polarised neutron diffraction. Force the program to interpret the magnetic domain rotation matrices as "twin" matrices. The effect is equivalent to consider that there is a single configuration of magnetic moments but a superposition in the same magnetic observation of several reflections corresponding to different orientations of the unit cell axes. The keyword should appear in the same line as **MAGDOM** after the refinement codes

Example:

magdom u, v,w 0.0 : 0.20000 111.00 twin

magdom u,-v,w 0.0 : 0.80000 0.00 twin

If the keyword appears only in one of the lines, all matrices are applied to the scattering vector. The intensity of an observation is calculated as:

$$I(q_h, q_k, q_l) = \text{Sum}(d) \{ I(q \cdot M(d)) \}$$

If no **TWIN** keyword appear in the list of **MAGDOM** lines, the intensity is considered as the superposition of different magnetic configurations, obtained by applying the matrices to the Fourier coefficients of magnetic moments, for the same reflection indices.

Force the program to interpret the magnetic domain as follows: A magnetic domain is characterised by a complete symmetry operator of the space group that has been lost in the transition. It corresponds to the magnetic structure obtained by applying the symmetry operator to all representative atoms (obtaining then other equivalent representatives) and the rotational part to the Fourier coefficient of the previous atoms.

Example:

```
magdomt x,y,z : 0.80000 111.00
magdomt x+1/2,-y+1/2,-z : 0.20000 0.00
```

When commands like **magdom** or **magdomt** are given, the program generates an FST file per given domain in order to display the magnetic structure of the corresponding domain. The name of these files are constructed as "**filecode_PhN_DomM.fst**", where "**filecode**" is the code of the **PCR** file, N is the number of the phase and M is the ordinal number of the domain. The normal **FST** files are also generated.

reference_cell

To use Bohr magnetons as unit for the amplitudes of magnetic modes in **FullProf**, we need the instruction **REFERENCE_CELL** followed by the reference cell parameters (that used in generating the PCR file from ISODISTORT). The program internally changes the basis vector to unitary vectors in the unitary reference frame $\{\mathbf{a}/|\mathbf{a}|, \mathbf{b}/|\mathbf{b}|, \mathbf{c}/|\mathbf{c}|\}$. The new PCR file maintains the basis vectors with the normalization performed in ISODISTORT but the coefficient (normally =1.0) is changed.

Example:

```
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern#1:3.4267 Magnetic R-Factor: 4.3742
!-----
My Compound (Magnetic modes at HT: T > 15K) : P_a2_1/c (P_b 1 1 2_1/a) Num=14 FIX xyz
!
COMMANDS
  reference_cell 13.1667 10.3106 11.1135 90.0 90.0 90.0
END_COMMANDS
!Nat Dis Ang Jbt Isy Str Furth ATZ Nvk More
  9 0 0 -6 2 0 36 2442.9751 0 0
!Contributions (0/1) of this phase to the 1 patterns
1
. . . . .
.....
```

For Time-of-flight (TOF)

In case of multiple patterns the instruction **VARY** keyword affect to all the pattern sections of the particular phase, in which the **COMMANDS** block is defined, providing independent codewords. For varying or fixing parameters for an individual pattern, the suffix "_n" is appended to the keyword with "n" being the number of the pattern.

Keywords for **VARY/FIX** commands

sigma2	→ Gaussian variance
sigma1	→ $\sigma^2 = \sigma_2 d^4 + \sigma_1 d^2 + \sigma_0 d + \sigma_0$

sigma0	
sigmaQ	
isoGstr	→ Isotropic Gaussian Strain
isoGsz	→ Isotropic Gaussian Size
gam2	→ Lorentzian full width at half maximum
gam1	→ $\gamma = \gamma_2 d^2 + \gamma_1 d + \gamma_0$
gam0	
isoLstr	→ Isotropic Lorentzian Strain
isoLsz	→ Isotropic Lorentzian Size
alfa0	→ Rising exponential
alfa1	→ $\alpha = \alpha_0 + \alpha_1 d^{-1} + \alpha_0 d^{-1/2}$
alfaQ	
beta0	→ Decaying exponential
beta1	→ $\beta = \beta_0 + \beta_1 d^{-4} + \beta_0 d^{-2}$
betaQ	

Generate_new_IRF

For facilitating the creation of an IRF file for Res=5 using the interpolation, we can refine limited ranges of the patterns, which produces *.irf files that can be merged into a single **IRF** file.

FullProf is producing this kind of files after a refinement and its generation can be forced even if we are already reading a raw IRF file. For doing that, one can include in the **COMMANDS** block the keyword **Generate_new_IRF**, as in the following example:

```
. . . . .
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 2.7
!-----
NAC FIX xyz b
!
COMMANDS
  Generate_new_IRF
END COMMANDS
!Nat Dis Ang Jbt Isy Str Furth ATZ Nvk More
. . . . .
```