# FullProf list of commands to be included
## in the `COMMANDS/END_COMMANDS` section

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. The number of these commands is limited to 20 per phase.

## Structural refinement (AUT=1)

**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 a 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-spcing 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).

**VARY**

| | |
|---|---|
| `x_A` | refine the x coordinate of atom labelled as A |
| `y_A` | refine the y coordinate of atom labelled as A |
| `z_A` | refine the z coordinate of atom labelled as A |
| `xyz_A` | refine the x, y and z coordinates of atom labelled as A |
| `b_A` | refine the thermal parameter of atom labelled as A |
| `xyz` | allows to refine 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 at the moment of the run.

| | |
|---|---|
| `cell` | refine cell parameters of the current phase |

**FIX**

| | |
|---|---|
| `x_A` | fix the x coordinate of atom labelled as A |
| `y_A` | fix the y coordinate of atom labelled as A |
| `z_A` | fix the z coordinate of atom labelled as A |

| | |
|---|---|
| `xyz_A` | fix the x, y and z coordinates of atom labelled as A |
| `b_A` | fix the thermal parameter of atom labelled as A |
| `xyz` | fix x, y and z coordinates for all atoms |
| `cell` | fix cell parameters of the current phase |

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_Al
  FIX   b_Mn1 x_C23
END COMMANDS
```

tells to the program that it should 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 Al. If Al 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.

## FIX_SPC spc1 spc2

`spc"i"` is the symbol used for the scattering power of the atom (normaly 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
```

## SAME_BISO spc1 val1 spc2 val2 ... spcN valN

`spc"i"` is the symbol used for the scattering power of the atom (normaly 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
```

## LAYER_A, LAYER_B, LAYER_C

Tell 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*cs, being cs the c-parameter of the subcell. This is needed to conserve the (0,0,l=L/15) reflections that are treated separately. This option is still at a testing stage. A complete account will be given as soon as possible.

## For Xlens

## CONTENT

Create a proper CDR file for Xlens

Format of the command:
```
CONTENT  El1 n1  El2 n2  El3 n3  ....
```

where ni (integer) is the number of atoms of the chemical species Eli (Chemical  symbol of the element).   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 wich 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      .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
  31.00000   41.00000   21.00000   0.00000   0.00000   0.00000
........
```

# For magnetic structures

**EFF_MOMENT**

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

        ex:
```
 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(qh,qk,ql) = Sum(d) { I( q.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.

## MAGDOMT

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 representants) and the rotational part to the Fourier  coefficient of the previous atoms.

ex:

```
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.