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

[T.R. / 2012-2023]

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-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 mutipattern-multiphase cases. These instructions act as VARY but assigning common codewords to a series of variables. The syntax is

PEQU_pat keyword -> Affect all section patterns of a particular phase

PEQU_pha keyword -> Affect 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 COMMANDS block is defined.

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.

VARY / FIX

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 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
uu	refine Caglioti U, Gaussian strain
xx	parameter X for constant wavelength: Lorentzian strain
yy	parameter Y for constant wavelength: Lorentzian isotropic size
gsz	parameter Y for constant wavelength: Gaussian isotropic size

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
  VARY scale uu bov
  VARY cell yy
  VARY occ_Fe2
  FIX xx
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
```

EQUAL

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

```
EQUAL  name_parent_parameter   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 between parameters of different phases or different patterns. In principle the name of the parameters are those appearing in the output files below the title: **SYMBOLIC NAMES AND INITIAL VALUES OF PARAMETERS TO BE VARIED**.
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

```
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 tells to the program that the
                                    U,V,W Caglioti parameters are the same for
                                    all phases

VARY yy gsz                   <---> This makes to refine the Lorentzian and
                                    Gaussian size parameters for the current
                                    phase

EQUAL occ_Si1_ph1             <---> Constraints of occupation factors in
occ_Si2_ph1 -1.0                    phase 1
occ_Al1_ph1 -1.0
occ_Al2_ph1 1.0

EQUAL Biso_Si1_ph1            <---> Atoms Si1 and Si of phases 1 and 2
Biso_Si_ph2 1.0                     respectively have the same Biso

EQUAL Biso_Al3_ph1
Biso_Al1_ph2 1.0

EQUAL Asym1_ph1_pat1          <---> Asymmetry parameter 1 of phase 1 and 2
Asym1_ph2_pat1 1.0                  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

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

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=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).

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.

reference_cell

Using in **FullProf** amplitudes of magnetic modes in Bohr magnetons, the instruction REFERENCE_CELL followed by the reference cell parameters (that used in generating the PCR file from **ISODISTORT**) is needed. The program internally changes the basis vector to unitary vectors in the unitary reference frame {a/|a|, b/|b|, c/|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  13.166700  10.310600   11.113500  90.000000  90.000000  90.000000
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
. . . . . . . . . . . . . . . .
```

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.

sigma2
sigma1
sigma0
sigmaQ
isoGstr
isoGsz
gam2
gam1
gam0
isoLstr
isoLsz
alfa0
alfa1
alfaQ
beta0
beta1
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, wich 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:   2.7425
!------------------------------------------------------------------------------
NAC     FIX xyz b
!
COMMANDS
Generate_new_IRF
END COMMANDS
!Nat Dis Ang Jbt Isy Str Furth        ATZ     Nvk More
. . . . . .
```