

Tutorial: LaMnO₃

Magnetic Structure Determination using FullProf: Exploring the different alternatives to refine a magnetic structure using FullProf.

LaMnO₃

Powder data collected at LLB on the diffractometer G4.2 with $\lambda=2.59$ Å.

The space group is S.G.= *Pbnm*, the cell parameters are $a\approx 5.53$ Å, $b\approx 5.75$ Å and $c\approx 7.68$ Å at 150K (paramagnetic phase, $T_N\approx 140$ K).

The structural parameters could be obtained from the input CIF file.

This compound contains a single Mn site and it is an example of the simplest case of a propagation vector $\mathbf{k} = 0$ and only real 1D irreps.

A detailed explanation of symmetry and magnetic structures including this example can be consulted on <https://doi.org/10.1051/epjconf/20122200010>

Input files:

LaMn150K.dat

LaMn50K.dat.

The format of the data corresponds to $\text{Ins} = 6$ in FullProf.

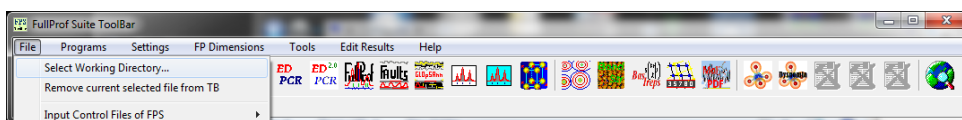
LaMn150K.cif

The standard magnetic structures determination using powder data follows these points:

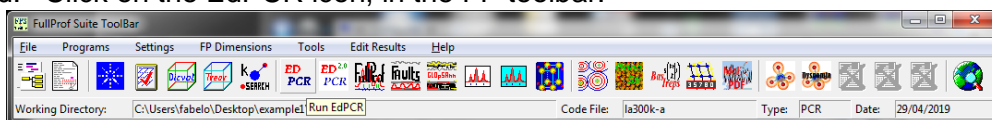
- 1) Plot the NDP above and below order temperature.
 - 2) Refine the crystal structure using the collected data and get all the relevant structural and profile parameters.
 - 3) Normally additional magnetic peaks appear in the low temperature diffraction pattern (below order temperature). Index the new reflection to determine the propagation vector. K-SEARCH program included in the FullProf suite could be used.
 - 4) Determine the possible irreducible representations of the propagation vector group. The program BasIreps could be used to get the basis vectors of the irreducible representations (irreps) of the propagation vector group (G_k). The Shubnikov group and the appropriate magnetic symmetry operators, or, alternatively, the basis vectors of the irreps could be used to refine the experimental data.
 - 5) Alternatively simulated annealing refinement can also be done (no information about the magnetic symmetry is needed)
 - 6) Refine against the data the different models and check the output files to discard incompatibilities or inconsistencies.
- 1) **Create a working directory; do not use space or special characters in the path.**
 - a. Copy in this folder all the input files.

2) **Create an initial PCR file.**

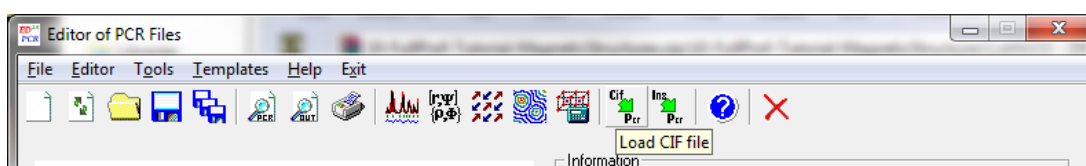
- Open the FullProf toolbar (clicking on the desktop icon)
- Select the working directory. “file > Select working directory...”



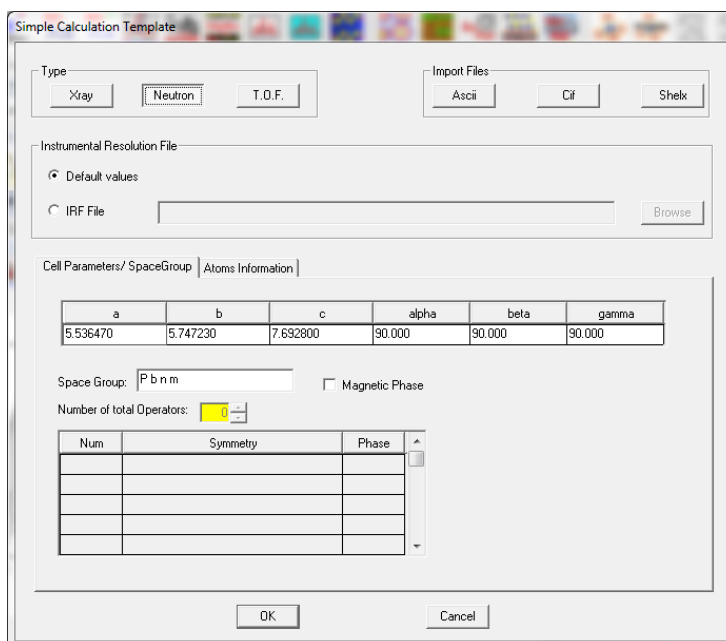
- Locate the working directory and click on OK.
- Click on the EdPCR icon, in the FP toolbar.



- Click on the cif_to_pcr icon in the EdPCR.



- Select Neutron as source type, check that the unit cell and the space group correspond with the provided at the beginning of this file. Check in the “atoms information” windows that all is consistent with the provide CIF file. Click on OK to exit.



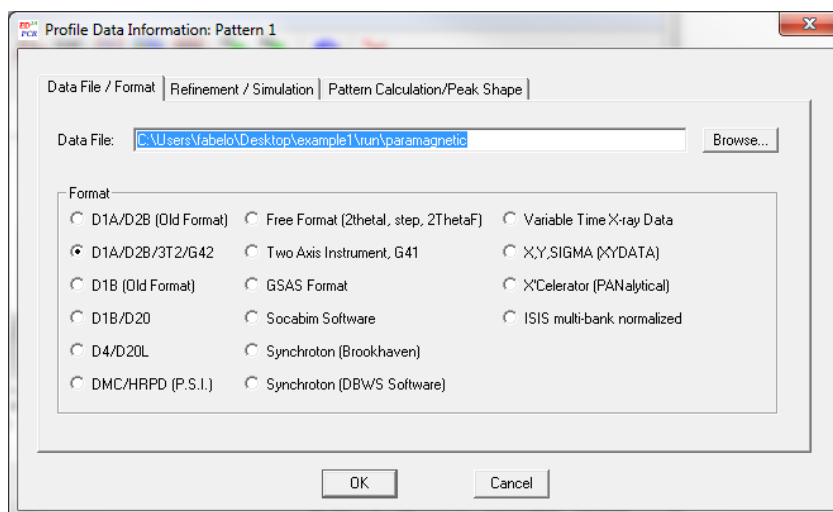
- Save the PCR file clicking on save as icon. Rename the file with an intuitive name in our case will be “paramagnetic.pcr”.

With these simple clicks, you have already created an initial PCR file that will be modified to fit the experimental data. The current PCR file correspond to a calculation with a generic wavelength

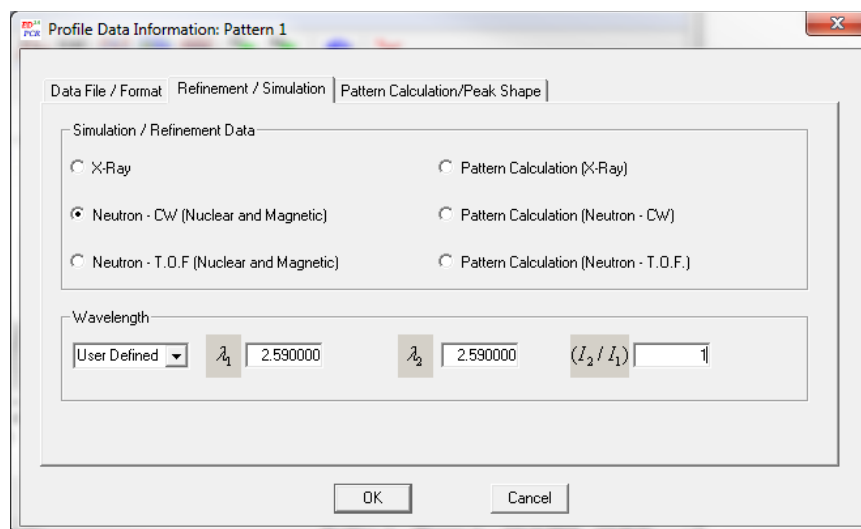
and instrument resolution parameters. In the next step we are going to modify all these parameters using the program EdPCR. Advanced users can modify these parameters directly editing the PCR file. A powerful text editor is highly recommended, we are going to use Notepad++, which is freely distributed (<https://notepad-plus-plus.org/download/>).

3) **Modify the PCR file according to the current example.**

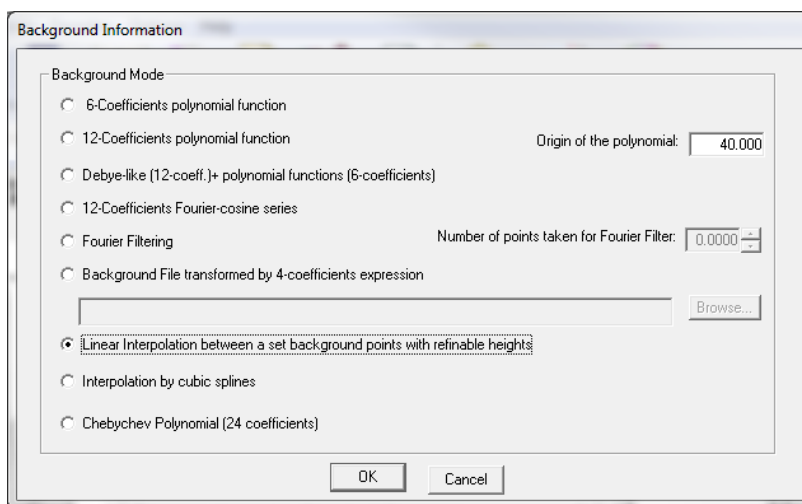
- a. Click on General and modify the name “LaMnO₃ paramagnetic”.
- b. In calculation, the item “Refinement/Calculation of a Powder Diffraction Profile” should be selected.
- c. Click on OK.
- d. Click on “patterns”
- e. Click on Data file/Peak shape > in format select D1A/D2B/3T2/G42 which correspond with $\text{Ins} = 6$.



- f. In “Refinement/simulation” select “Neutron-CW” (CW = constant wavelength).
- g. In wavelength, roll out the menu and select “user defined” and write the correct wavelength and fix the ratio I_2/I_1 to 1 (or zero, assuming a pure monochromatic neutron beam).



- h. Click on OK.
- i. Click on Background type and select “Linear Interpolation...” this option allows the user to define a background by clicking on the experimental pattern. We will do it in a further step. Of course other background functions can be used, in particular Chebychev Polynomials give quite stable refinements.



- j. Other parameters Excluded Regions will be changed later after exploring the experimental pattern.
- k. Click on OK.
- l. Click on “Phase”, and modify the phase name and check that the calculation is “structural model (Rietveld Method)”.

Phase Information: Phase 1

General Information on Phases

Name of Phase :

Calculation:

Coefficient to calculate the weight percentage of the Phase: ☒ Calculated automatically ☐ Provided by user

Contribution to patterns, preferred orientation direction, reflection list, ...

Space Group symbol/number, symmetry operators, basis functions, etc

Initial Previous Add Del Next Last

OK Cancel

m. Click on contribution to patterns and select the next options:

Pattern Contribution Information for Phase 1

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

☒ Current Phase contributes to the pattern

Type of Pattern

☐ X-Ray ☐ Pattern Calculation (X-Ray)

☒ Neutron (Constant Wavelength) ☐ Pattern Calculation (Neutron - Constant Wavelength)

Nuclear and Magnetic ☐ Pattern Calculation (Neutron - T.O.F.)

☐ Neutron (T.O.F.)

Nuclear and Magnetic

Peak Shape

☒ Codefil.shp ☐ Global.shp

Intensities

Reflection list:

☐ Use special control of parameters for peak overlap, rejected reflections for current phase

Brindley coefficient:

Global weight of the integrated intensity data vs profile data:

Factor for excluding reflections [$1 < \text{Factor} * \text{Sigma}(I)$]:

Weights are divided by reduced χ^2 of precedent cycle:

OK Cancel

- n. Click on OK.
- o. Click on symmetry and check that the selected space group is right.
- p. Click on OK and save the file from the EdPCR windows.
- q. Click on Refinement

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
 Forced Termination when shifts < x E.S.D.
 Others:

Relaxation Factors for Shifts
 Atomic Anisotropic Profile Global

Reflections ordering
☒ Only at the first cycle ☐ Each cycle ☐ Bragg R-Factor excluding reflections limiting excluded regions

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7 | Pattern 8 | Pattern 9 | Pattern 10

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Reduction factor of number of data points:

OK Cancel

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5 | Phase 6 | Phase 7 | Phase 8 | Phase 9 | Phase 10

Atoms Prop. Vectors

Patterns
☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7

- r. Change the number of cycles. Other parameters as Background or Instrumental will be modified later.
- s. The instrumental resolution parameters can be modified clicking on Profile. Initial values for the G4.2 diffractometer can be consulted within the FullProf IRF database (C:\FullProf_Suite\IRF_Files\LLB\ g42-nacalf.irf). Editing this file we can obtain this initial values that can be copied into the PCR file.

```
! S_L D_L
ASYM 0.03 0.02
! Uins Vins Wins Xins Yins Zins
0.11313 -0.21987 0.22756 0.00000 0.00177 0.000
```

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	0.10000E-02	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	5.536470	5.747230	7.692800	90.000	90.000	90.000

FWHM / Shape Parameters Asymmetry Parameters Preferred Orientation

FWHM Parameters

	U	V	W	IG
Coefficients	0.113130	-0.219870	0.227560	0.000000

Shape Parameters

	X	Y	SZ
Coefficients	0.000000	0.001770	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Refine All Fix All Cancel OK

Profile Parameters: Phase 1 Pattern 1

Factors	
Scale	Overall B-factor
Coefficients	0.10000E-02 0.0000

Cell Parameters						
a	b	c	alpha	beta	gamma	
Coefficients	5.536470	5.747230	7.692800	90.000	90.000	90.000

FWHM / Shape Parameters Asymmetry Parameters Preferred Orientation

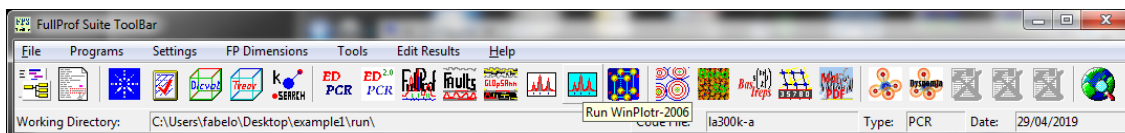
S_L		D_L	
Coefficients	0.030000	0.020000	

Asym1		Asym2		Asym3		Asym4	
Coefficients	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

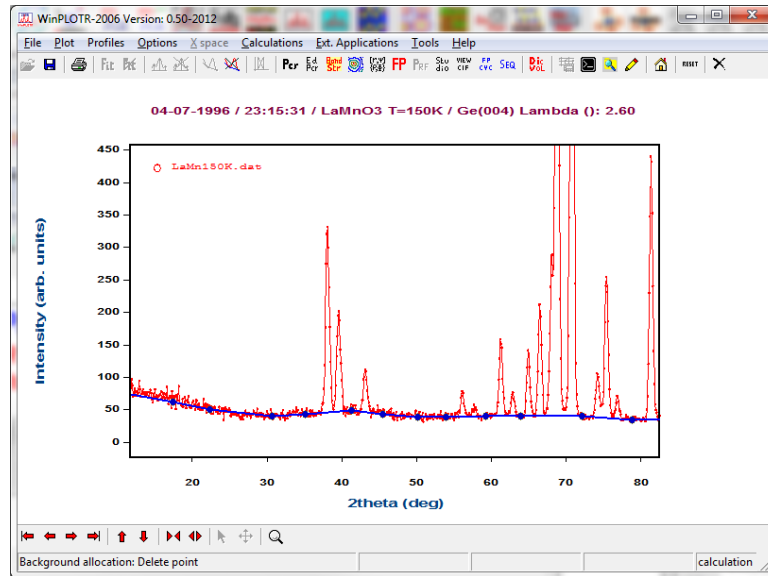
P5		P6		P7		P8	
Coefficients							

Refine All
Fix All
Cancel
OK

- t. Save the file and click on Editor > Input control file (PCR) to see the current PCR file.
- u. Before running this PCR file, we should include a realistic background. To do that we are going to open the experimental data on WinPLOTR-2006.



- v. Click on open icon or in File > open pattern file (.dat) and select LaMn150K.dat. The data are in format lns = 6.
- w. Click on Calculation > Background > enable and Calculation > Background > Insert point. This allow us define a series of points that could be included into the PCR file. Each background point is included clicking on the left button your mouse. If a wrong point is included, in the same menu you can find "Delete point" which is used in the same way than "Insert point".
In order to increase the accuracy, you can zoom in by clicking on the left button of your mouse and dragging simultaneously. A simple click on the right button reverse the zoom.



- x. The created list of points can be saved clicking on Calculations > Background > save background leave the proposed name “background.bgr” and save.
- y. Now we can include this information in to the PCR file, we can edit the PCR file with a text editor or using the program EdPCR. We are going to use the latter. Click on Refinements > Background > import from background file.
After importing the background click on OK and save in the main window of EdPCR.

Linear interpolation between a set of Background Points: Pattern 1

Interpolation Method

☒ Linear Interpolation ☐ Cubic Splines Interpolation

Information

Number of Points:

	2Theta	Counts	
1	0.000	0.000	<input type="checkbox"/>
2	0.000	0.000	<input type="checkbox"/>
3	0.000	0.000	<input type="checkbox"/>
4	0.000	0.000	<input type="checkbox"/>

Refine All Fix All

Import from Background File

OK Cancel

Linear interpolation between a set of Background Points: Pattern 1

Interpolation Method

☒ Linear Interpolation ☐ Cubic Splines Interpolation

Information

Number of Points:

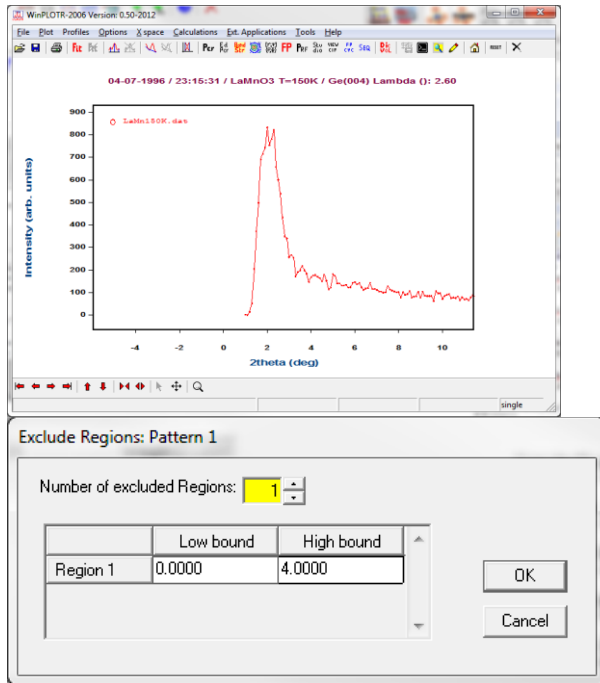
	2Theta	Counts	
1	1.450	229.447	<input type="checkbox"/>
2	1.958	748.628	<input type="checkbox"/>
3	2.365	792.580	<input type="checkbox"/>
4	2.569	550.845	<input type="checkbox"/>

Refine All Fix All

Import from Background File

OK Cancel

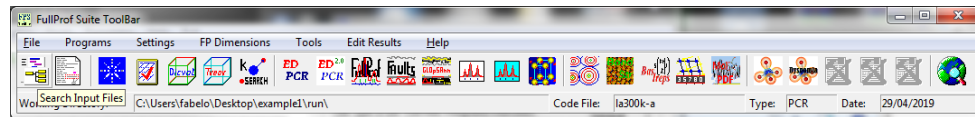
After the data exploration in the previous step, we can observe an important contribution of the direct beam. This contribution can be masked using excluded regions. Click on Patterns > Excluded Regions and in number of excluded regions increase the number up to 1. Now you can define the lower limit and the higher limit. In this case, you can set the limits between 0 and 4 degrees in 2theta. Click on OK and save in the main window of EdPCR.



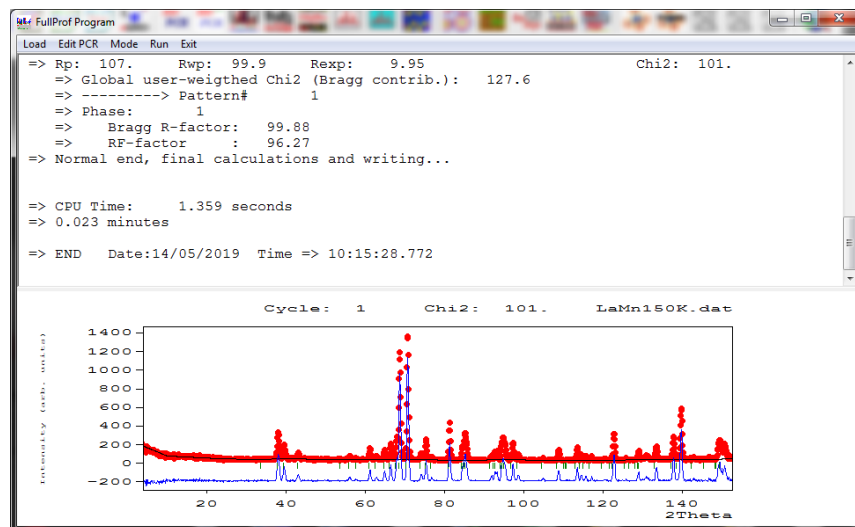
z. The PCR file for refining the nuclear structure is done. We can check the PCR file clicking on Editor > Input control file or opening the file with our favourite text editor.

4) Run FP to refine the 150K data.

a. Load into the FP tool bar the “paramagnetic.pcr” file. That can be done clicking on Search Input files icon. Be sure that the PCR file and the data file are in the same folder.



b. Now you can click on the FullProf icon and run. But the result is clearly non-satisfactory. It deserve to be noted that for the moment all the parameters are fixed.



- c. Let us start refining first the Scale factor (refinement > Profile), the second parameter the zero (refinement > instrumental) and finally the unit cell (refinement > Profile). Refining only these parameters, we obtain a good initial fit.
- d. The sample is slightly absorbing, an effective absorption coefficient ($\mu_R=0.65$) should be included in the PCR file, in the same way an asymmetry correction is applied everywhere ($AsyLim=180.0$). For neutron diffraction the Cthm (square of $\cos(2\theta)$ for polarization correction) should be fixed to 0. The easy way to change these parameters is modifying directly the PCR file as is shown in the next figure.

```

COMM LaMnO3 paramagnetic
! Current global Chi2 (Bragg contrib.) = 14.71
! Files => DAT-file: LaMn150K.dat, PCR-file: paramagnetic
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
  1   7   1  36   1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   1
!
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
  0   0   1   0   1   0   4   0   0   1   6   0   0   0   0   0   0   0   0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolaz 2nd-muR -> Pat
  2.590000 2.590000 1.00000 40.000 8.0000 0.000 0.6500 180.00 0.0000 0.0000
!
!NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
  10 0.10 1.00 1.00 1.00 1.00 1.0000 0.100000 152.9000 0.000 0.000
!
!2Theta/TOF/E(Kev) Background for Pattern# 1
  1.4498 229.4474 0.00
  1.9584 748.6284 0.00
  2.3653 792.5802 0.00
  2.5687 550.8452 0.00
  3.4842 193.7366 0.00
 10.0453 78.3631 0.00
 17.4201 61.8811 0.00
 22.4044 50.8832 0.00

```

- e. Finally we can refine the shape parameters (refinement > Profile)

Profile Parameters: Phase 1 Pattern 1

Factors	
Scale	2.9262
Overall B-factor	0.0000

Cell Parameters						
a	b	c	alpha	beta	gamma	
5.518893	5.736761	7.659899	90.000	90.000	90.000	

FWHM / Shape Parameters Asymmetry Parameters Preferred Orientation

FWHM Parameters			
U	V	W	IG
0.080949	0.273868	0.387430	0.000000

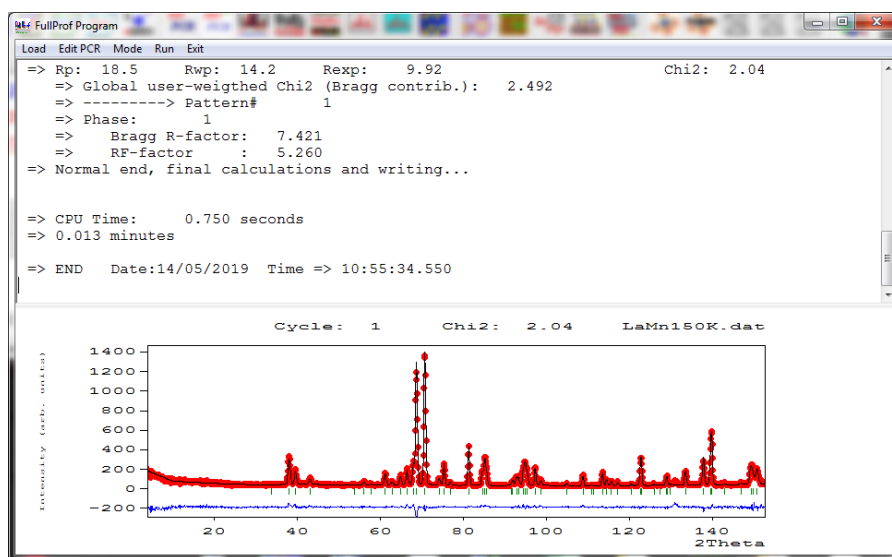
Shape Parameters		
X	Y	SZ
0.000000	0.032893	0.000000

☐ Refine FWHM for second wavelength

U2	V2	W2

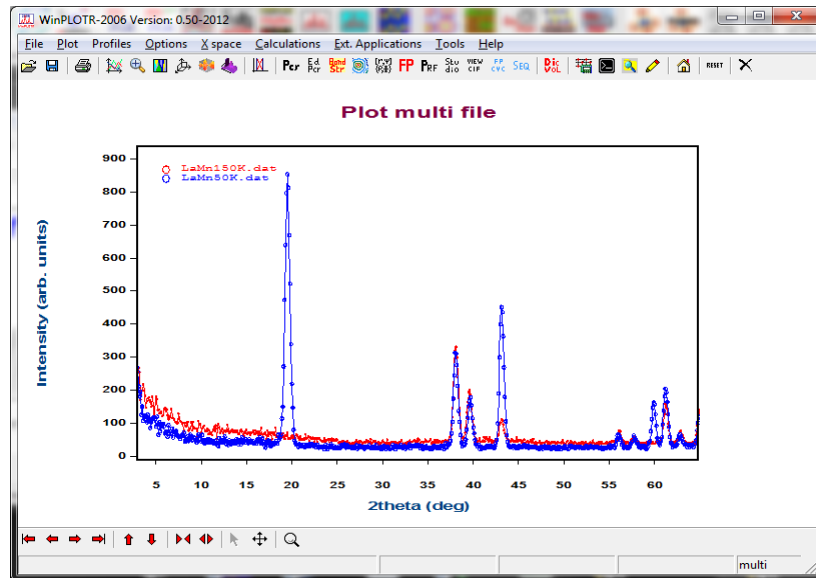
Buttons: Refine All, Fix All, Cancel, OK

- f. The data were collected on a medium resolution instrument, so we have not enough resolution to refine all the structural parameters. Here below we show the final refinement.

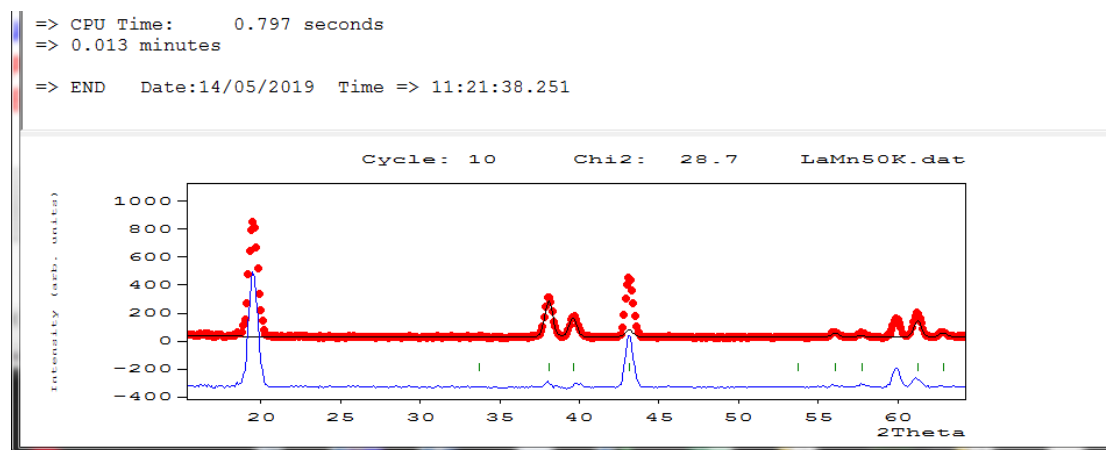


5) Refinement of the low temperature phase.

- Change the name of the final PCR file for a new one. We are going to use `nucl_mag1.pcr`.
Select on the FP tool bar the new PCR file. This PCR file will be refined against the data collected at 50K, so be sure that both files are in the same folder.
- Comparing the 150 K and 50 K data sets on WinPLOT, we can see that there are new reflections as well as the increase of intensity on the top of some nuclear reflections. Other feature is the decreasing of background in the low temperature pattern, due to the occurrence of magnetic reflections.



- c. To refine the low temperature data using the high temperature PCR file we should include in this file a new background. So repeat the steps from 3 (v) to 3 (y) with the 50K data.
- d. After including the new background into the PCR file, we should fix all the parameters. We can do it unclicking all the boxes within the EdPCR or changing into the PCR file the code AUT from 1 (automatic) to 0 (manual) and changing the number of "Number of refined parameters" to 0.
We run FP using as data the low temperature pattern. The blue line correspond to the difference between calculated (paramagnetic) and the observed (magnetic + nuclear), therefore, the blue line is mainly the magnetic contribution.



- e. This fit can be used by index the magnetic propagation vector, however in this example we know that the propagation vector correspond with the $\mathbf{k}=0$. In order to check it, we are going to add a second phase into our PCR file using the same unit cell and the P1 space group. If all magnetic reflections are fitted this will be a confirmation of the $\mathbf{k}=0$ propagation vector.

6) **Adding a second phase to fit the magnetic reflections.**

- a. We are going to use the EdPCR, open nucl_mag1.pcr file and click on Phases > add change the Name of phase to “magnetic contribution, without model” in calculation select “Profile Matching with constant scale factor”.

Click on “Contribution to Patterns” and select the options showed here below and click on OK.

The “Satellite reflections are generated automatically from Space group symbol” is particular useful for those magnetic structures with **k** different of 0.

Pattern Contribution Information for Phase 2

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

☒ Current Phase contributes to the pattern

Type of Pattern

☐ X-Ray

☒ Neutron (Constant Wavelength) Nuclear and Magnetic

☐ Neutron (T.O.F.) Nuclear and Magnetic

☐ Pattern Calculation (X-Ray)

☐ Pattern Calculation (Neutron - Constant Wavelength)

☐ Pattern Calculation (Neutron - T.O.F.)

Peak Shape

Thompson-Cox-Hastings pseudo-Voigt * Axial divergence asymmetry

☒ Codefit.shp

☐ Global.shp

Intensities

Reflection list: Satellite reflections are generated automatically from Space group symbol

☐ Use special control of parameters for peak overlap, rejected reflections for current phase

Brindley coefficient: 0.0000

Global weight of the integrated intensity data vs profile data: 0.0000

Factor for excluding reflections [1 < Factor * Sigma()]: 0.0000

Weights are divided by reduced Chi² of precedent cycle: 0.0000

OK Cancel

Click on symmetry and add P-1 space group. NB: the space group in FP should be written with a space between elements (P -1, in this particular case). Click on “Symm. Op. Automatic” and on OK and save in the main window of EdPCR.

Symmetry Information

Space Group Properties

Symmetry Operators: Generated automatically from the symbol

Spacegroup: P -1

Symm.Op. Automatic

Symmetry operators

Magnetic/Displacement Operators

Irreducible representations

Laue Class: -1

Centrosymmetric Case

Number of Symmetry Operators: 1

Num	Symmetry	TR	Num	Symmetry	TR
1	x,y,z				

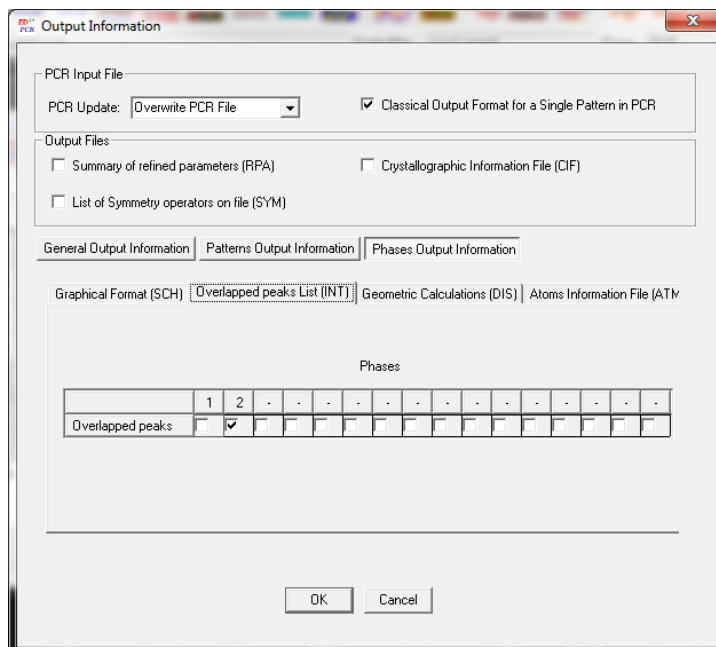
TR=Time reversal associated to symmetry operator

☐ Time Reversal for Inversion operator

OK Cancel

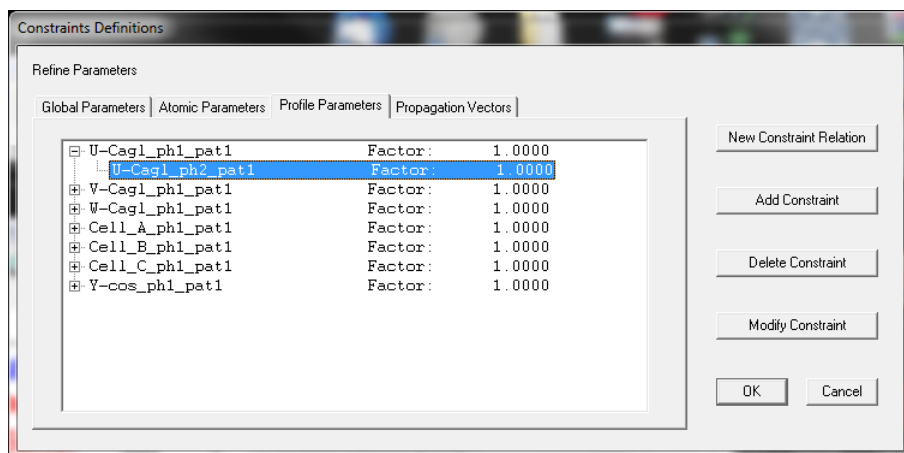
- b. Now we need to fill for the phase 2, the unit cell the scale, U, V, W, X, Y, SL and DL. You can use the EdPCR or edit the “nucl_mag1.pcr” file with a text editor and copy from phase 1 to phase 2.

Finally if we want that the “magnetic contribution” to be saved in a special file to run a simulated annealing refinement we need to click on Output > Phases Output Information > Overlapped peaks List (INT) and select phase 2. Click on OK and save in the main window of EdPCR.



- c. Now we can run FP and start to refine parameters. Change AUT from 0 to 1 and be sure that those parameter from phase 1 and phase 2 that should be the same have the same refine code.

To add constrains you can use the same code into the PCR file (see the next figure as an example) or you can use the program EdPCR by clicking on Constrains > Profiles Parameters (U, V, W, a, b, c, X, Y...). In a first step create a new constraint relation and secondly add a second parameter to constrain. In that case, factor 1 means that if U in phase 1 increase one unit, U in phase 2 increase the same unit. Negative values means that one parameter increase while the second decrease.

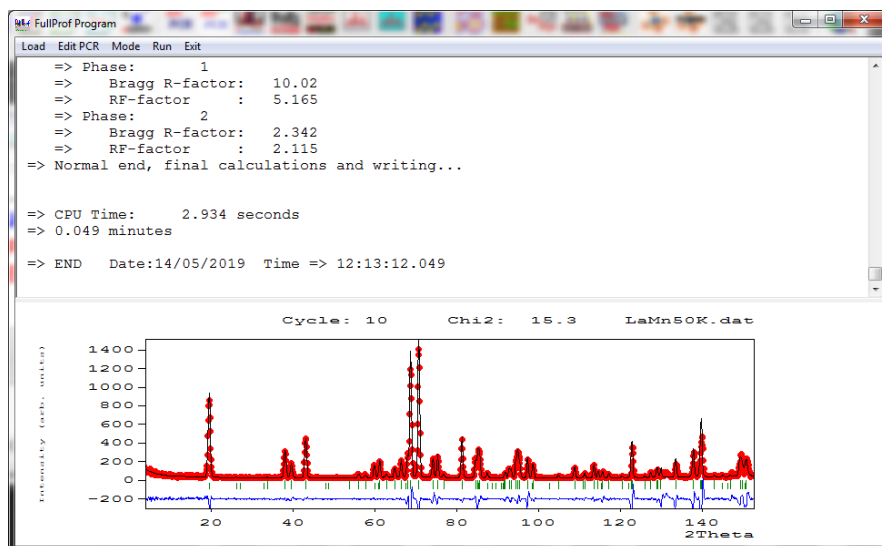


```

!-----> Profile Parameters for Pattern # 1
!  Scale      Shape1      Box      Str1      Str2      Str3      Strain-Model
    2.9261      0.00000      0.00000      0.00000      0.00000      0.00000      0
    | 0.00000      0.000      0.000      0.000      0.000      0.000
!      U      V      W      X      Y      GauSiz      LorSiz Size-Model
    0.081051 -0.272037 0.378889 0.000000 0.044660 0.000000 0.000000 0
    | 61.000      71.000      81.000      0.000      11.000      0.000      0.000
!      a      b      c      alpha      beta      gamma      #Cell Info
    5.521249 5.733683 7.647707 90.000000 90.000000 90.000000
    | 31.00000 41.00000 51.00000 0.00000 0.00000 0.00000
!  Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D L
    0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03000 0.02000
    | 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
!-----
!  Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 0.77
!-----
magnetic contribution, without model
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
    0 0 0 0.0 0.0 1.0 2 2 0 0 0 0.000 1 7 1
!
!Jvi Jdi Hel Sol Mom Ter Brind RMua RMub RMuc Jtyp Nsp_Ref Ph_Shift N_Domains
    11 0 0 0 0 0 1.0000 0.0000 0.0000 0.0000 1 0 0 0
!
!
P -1 <--Space group symbol
!-----> Profile Parameters for Pattern # 1
!  Scale      Shape1      Box      Str1      Str2      Str3      Strain-Model
    2.9261      0.00000      0.00000      0.00000      0.00000      0.00000      0
    | 0.00000      0.000      0.000      0.000      0.000      0.000
!      U      V      W      X      Y      GauSiz      LorSiz Size-Model
    0.081051 -0.272037 0.378889 0.000000 0.044660 0.000000 0.000000 0
    | 61.000      71.000      81.000      0.000      11.000      0.000      0.000
!      a      b      c      alpha      beta      gamma      #Cell Info
    5.521249 5.733683 7.647707 90.000000 90.000000 90.000000
    | 31.00000 41.00000 51.00000 0.00000 0.00000 0.00000
!  Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D L
    0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03000 0.02000
    | 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

```

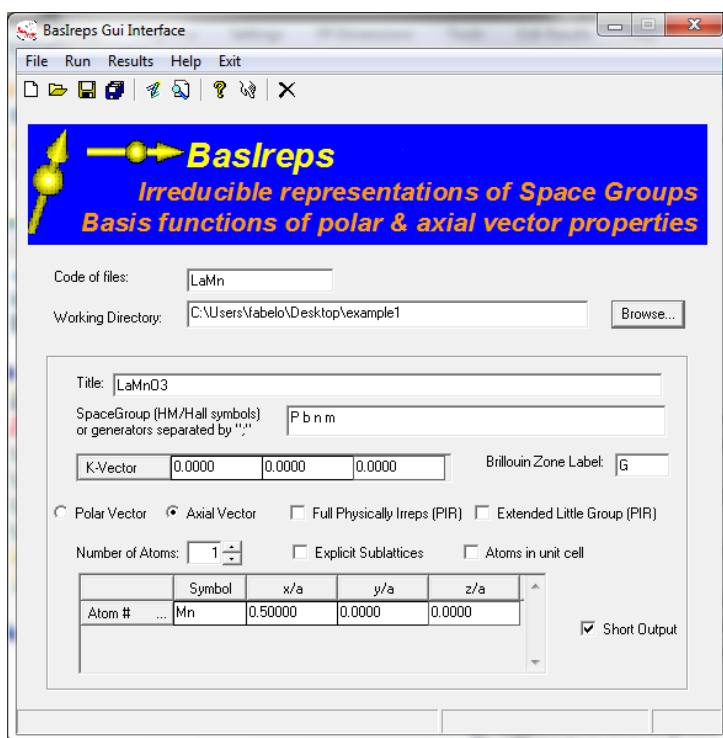
d. After refining, here we show the final result:



- e. The program has produced several file containing intensities, in particular the file called "nucl_mag12_cltr.int" containing exclusively the magnetic contribution with reflections re-grouped when forming part of a cluster. The file may be used for doing a S.A. job for determining the magnetic structure.

7) Calculation of Irreducible representations.

- a. For the Irreps calculation, we are going to use Baslreps program. Click on the Baslreps icon on the FP tool bar. Fill the information, code of file, the working directory the nuclear space group, the propagation vector (in this case $\mathbf{k}=0$), remember than magnetic moments are axial vectors. The number of atoms within the unit cell can be provided explicitly or the program can calculate the different orbit using the space group symmetry. In this case with *Pbnm* space group at the Mn atom on the (0.500, 0.000, 0.000) position (4b Wyckoff position). Fill all the boxes and click on Run. NB: check carefully the output information!!



- b. The list of the irreducible representations (all of them of dimension 1) can be consulted on the output of Basreps. Here below you have the same table slightly modified for a clear visualization and including the magnetic Shubnikov S.G. (The character -1 of a symmetry operator means that it is combined with time reversal so that it is a *primed* symmetry operator).

Irreps	$\{1\}$	$\{2_z 00p\}$	$\{2_x pp0\}$	$\{2_y ppp\}$	$\{-1\}$	$m=\{m_z 00p\}$	$b=\{m_x pp0\}$	$n=\{m_y ppp\}$	SG
Γ_1 :	1	1	1	1	1	1	1	1	Pbr
Γ_2 :	1	1	1	1	-1	-1	-1	-1	Pb'
Γ_3 :	1	1	-1	-1	1	1	-1	-1	Pb'
Γ_4 :	1	1	-1	-1	-1	-1	1	1	Pbr
Γ_5 :	1	-1	1	-1	1	-1	1	-1	Pbr
Γ_6 :	1	-1	1	-1	-1	1	-1	1	Pb'
Γ_7 :	1	-1	-1	1	1	-1	-1	1	Pb'
Γ_8 :	1	-1	-1	1	-1	1	1	-1	Pbr

- c. Basreps program gives an output (filename.fp) with a block for each IR, ready to be copied and pasted into the PCR file.

```

Baslreps Text Editor - [C:\Users\fabelo\Desktop\example1\LaMn.fp]
File Edit Search
-----
Output of BasIREPS for FullProf
-----
The group of lines starting with the symbol of space groups and
finishing with the last keyword BASI, may be pasted into the PCR file

      X      Y      Z      For site: 1
-> Mn_1   :   0.5000  0.0000  0.0000  : (x,y,z)
-> Mn_2   :  -0.5000  0.0000  0.5000  : (-x,-y,z+1/2)
-> Mn_3   :   1.0000  0.5000  0.0000  : (x+1/2,-y+1/2,-z)
-> Mn_4   :   0.0000  0.5000  0.5000  : (-x+1/2,y+1/2,-z+1/2)

=> Basis functions of Representation IRrep( 1) of dimension 1 contained 3 times in GAMMA
Representation number : 1 For Site: 1
Number of basis functions: 3

----- Block-of-lines for PCR start just below this line
P -1                                     <--Space group symbol for hkl generation
! Nsym   Cen   Laue Ireps N_Bas
   4       1       1      -1      3
! Real(0)-Imaginary(1) indicator for Ci
   0   0   0
SYMM x,y,z
BASR   1   0   0   0   1   0   0   0   1
BASI   0   0   0   0   0   0   0   0   0
SYMM -x,-y,z+1/2
BASR  -1   0   0   0  -1   0   0   0   1
BASI   0   0   0   0   0   0   0   0   0
SYMM x+1/2,-y+1/2,-z
BASR   1   0   0   0  -1   0   0   0  -1
BASI   0   0   0   0   0   0   0   0   0
SYMM -x+1/2,y+1/2,-z+1/2
BASR  -1   0   0   0   1   0   0   0  -1
BASI   0   0   0   0   0   0   0   0   0
----- End-of-block of lines for PCR

```

8) Including the IR into the PCR file.

- Rename the previous PCR file, in our case nucl_mag_bv.pcr (BV corresponding to basic vectors).
- Open the new PCR with the EdPCR and click on phases and click NEXT to move to the phase 2. Here you can change the type of calculation from "Profile Matching with constant scale factor" to "Magnetic Phase (Rietveld Method)" or "Magnetic Phase with magnetic moments in spherical mode (Rietveld Method)". In our case, we are going to use the first one.
- Click on symmetry and select "Basis functions of the irreducible representations of the propagation vector group". Here you can add the "magnetic/displacement" and the "irreducible representation" using the boxes. However, the easy way is to copy this information from the .FP file (Baslreps).

In order to create the lines into the PCR file we can add only one basic function and one IR. Click on OK and save from the main window of EdPCR.

Symmetry Information

Space Group Properties

Symmetry Operators: Basis functions of the irreducible representations of the propagation vector group

Spacegroup: P-1

Symm.Op. Automatic

Symmetry operators | Magnetic/Displacement Operators | Irreducible representations

Number of Atomic basis functions: 1

Number of Irreducible Representations: 1

Complex basis functions

Num	Coefficient	CI Type
Real		

Num	Expression
Real	0
Imag	0

OK Cancel

- d. Edit the PCR file and replace the blue area for the block obtained from Basreps. Save the file and reopen it file with EdPCR.

```

External EdPCR Text Editor - [C:\Users\fabelo\Desktop\example1\run\nucl_mag_bv.pcr]
File Edit Search
[Icons]
-----
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03000 0.02000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
-----
! Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 0.00
-----
magnetic contribution, without model
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
0 0 0 0.0 0.0 1.0 2 2 -2 0 0 0.000 1 7 1
!
!Jui Jdi Hel Sol Mon Ter Brind RMua RMub RMuc Jtyp Nsp_Ref Ph_Shift N_Domains
11 0 0 0 0 0 0 1.0000 0.0000 0.0000 0.0000 1 0 0 0 0
!
! -1
! Nsym Cen Laue Irep5 N_Bas
1 2 1 1 1
! Real(0)-Imaginary(1) indicator for Ci
0 0
!
!-----> Profile Parameters for Pattern # 1
! Scale Shape1 Bou Str1 Str2 Str3 Strain-Model
2.9261 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00000 0.000 0.000 0.000 0.000 0.000
!
! U U W X Y GauSiz LorSiz Size-Model
0.081051 -0.272837 0.378889 0.000000 0.044660 0.000000 0.000000 0
61.000 71.000 81.000 0.000 11.000 0.000 0.000
!
! a b c alpha beta gamma NCell Info
5.521249 5.733683 7.647707 90.000000 90.000000 90.000000
31.00000 41.00000 51.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03000 0.02000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
0.000000 0.000000 0.000000
0.000000 0.000000 0.000000
Propagation Vector 1
Line102 Col2 NUM INS

```

```

External EdPCR Text Editor - [C:\Users\fabelo\Desktop\example1\run\nucl_mag_bv.pcr]
File Edit Search
[Icons]
-----
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03000 0.02000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
-----
! Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 0.00
-----
magnetic contribution, without model
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
0 0 0 0.0 0.0 1.0 2 2 -2 0 0 0.000 1 7 1
!
!Jui Jdi Hel Sol Mon Ter Brind RMua RMub RMuc Jtyp Nsp_Ref Ph_Shift N_Domains
11 0 0 0 0 0 0 1.0000 0.0000 0.0000 0.0000 1 0 0 0 0
!
! -1
! Nsym Cen Laue Irep5 N_Bas
1 2 1 1 1
! Real(0)-Imaginary(1) indicator for Ci
0 0 0
!
!-----> Profile Parameters for Pattern # 1
! Scale Shape1 Bou Str1 Str2 Str3 Strain-Model
2.9261 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00000 0.000 0.000 0.000 0.000 0.000
!
! U U W X Y GauSiz LorSiz Size-Model
0.081051 -0.272837 0.378889 0.000000 0.044660 0.000000 0.000000 0
61.000 71.000 81.000 0.000 11.000 0.000 0.000
!
! a b c alpha beta gamma NCell Info
5.521249 5.733683 7.647707 90.000000 90.000000 90.000000
31.00000 41.00000 51.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03000 0.02000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
0.000000 0.000000 0.000000
0.000000 0.000000 0.000000
Propagation Vector 1
Line112 Col35 NUM INS

```

- e. Using EdPCR we need to include the magnetic atoms into the PCR file. Click on "refinements > phase 2 > atoms" add a new atom. Click on OK and save the PCR.

Atoms Information: Phase 2

List of Atoms

Number of Atoms: 1

	Label	Ntyp	Mag Rot	Prog Vec.	X	Y	Z	B	Occ
Atom # 1	Mn1	MMN3	1	1	0.50000	0.0000	0.0000	0.50000	1.0000

Magnetic Parameters

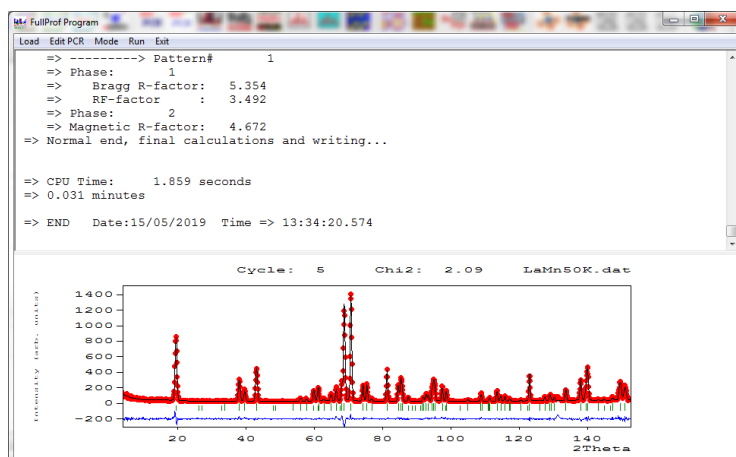
	Rx	Ry	Rz	Ix	Iy	Iz	MPhase
Atom #1							
Atom #2							
Atom #3							
Atom #4							

Other Parameters

	C1	C2	C3	C4	C5	C6	C7
Atom # 1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Buttons: Refine Positions, Refine B_iso, Fix All, Cancel, OK

- f. Now you can run the PCR file. If you want to refine the magnetic structure you can refine from C1 to C3. If you are using “Magnetic Phase with magnetic moments in spherical mode (Rietveld Method)” the refined parameters are R_m , R_{ϕ} and R_{θ} . Refine all possible magnetic models, modifying the PCR file, and determine which is the correct. NB: is a good idea rename the PCR file to know which IR you are using.



- g. The previous example was done using basis vectors, but it can easily transformed to a Fourier coefficient formalism. Here below we are going to change the Gamma1 from basis vector to Fourier coefficient as example.

Open the .BSR file from BASIREP and look for IRrep(1) section.

The Sk(1) line “Sk(1): (u,v,w)” should be transformed to “MSYM u,v,w,0.0” where MSYM is the magnetic symmetry label, u,v,w is the same vector and the 0.0 is the phase (this phase is only useful for incommensurate structures).

Initial block:

```

SYMM x,y,z
Sk(1): (u,v,w)
SYMM -x,-y,z+1/2
Sk(2): (-u,-v,w)
SYMM x+1/2,-y+1/2,-z
Sk(3): (u,-v,-w)

```

SYMM $-x+1/2, y+1/2, -z+1/2$
 Sk (4) : $(-u, v, -w)$

final block:

SYMM x, y, z
 MSYM $u, v, w, 0.0$
 SYMM $-x, -y, z+1/2$
 MSYM $-u, -v, w, 0.0$
 SYMM $x+1/2, -y+1/2, -z$
 MSYM $u, -v, -w, 0.0$
 SYMM $-x+1/2, y+1/2, -z+1/2$
 MSYM $-u, v, -w, 0.0$

- h. Rename your previous PCR file to nucl_mag_fc.pcr, open this file with the EdPCR and click on “Phase>Next (phase 2)>symmetry” change symmetry operator to “User defined”. In symmetry operators, we can write the four SYMM from the previous step and in Magnetic/Displacement Operators the four MSYM. Alternatively, you can add the number of symmetry operators (4) and the number of magnetic matrices (1) and fill the box with generic information, save the PCR and copy and paste the previous block into the new PCR file.

Symmetry Information

Space Group Properties
 Symmetry Operators: User defined
 Spacegroup: $P-1$ Symm.Op. Automatic

Symmetry operators | Magnetic/Displacement Operators | Irreducible representations

Laue Class: -1 ☐ Centrosymmetric Case
 Number of Symmetry Operators: 4

Num	Symmetry	TR
1	x, y, z	<input type="checkbox"/>
2	$-x, -y, z+1/2$	<input type="checkbox"/>
3	$x+1/2, y+1/2, -z$	<input type="checkbox"/>
4	$-x+1/2, y+1/2, -z+1/2$	<input type="checkbox"/>

TR=Time reversal associated to symmetry operator
☐ Time Reversal for Inversion operator

OK Cancel

Symmetry Information

Space Group Properties
 Symmetry Operators: User defined
 Spacegroup: $P-1$ Symm.Op. Automatic

Symmetry operators | Magnetic/Displacement Operators | Irreducible representations

Number of Magnetic Rotation Matrices for each symmetry operator: 1
 Number of Atomic Displacement rotation matrices for each symmetry operator: 0

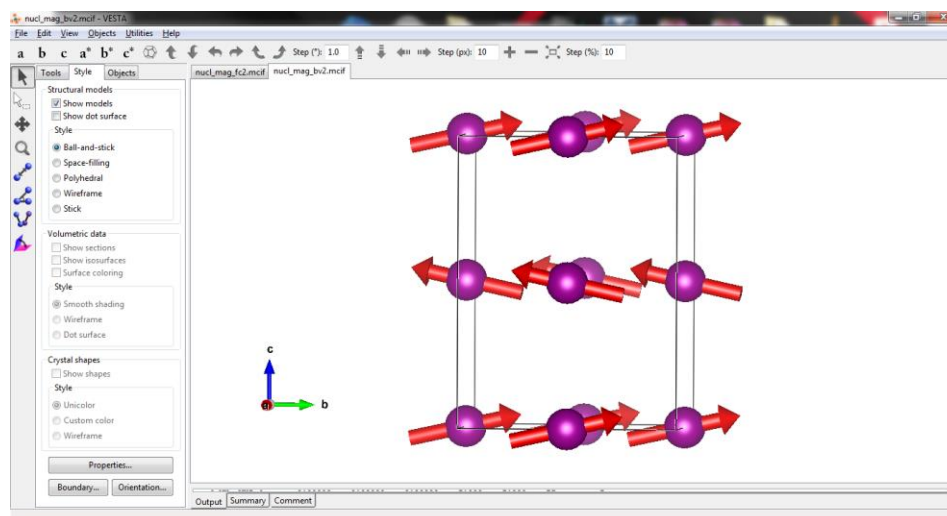
Num	Rotation	Phase
1	u, v, w	0.000
2	$-u, -v, w$	0.000
3	$u, -v, -w$	0.000

Num	Displacement	Phase

OK Cancel

- i. After running FullProf, a mCIF (magnetic CIF) will be automatically created with the magnetic structure. You can use VESTA (or FullProf Studio) program to plot the different magnetic models.

NB: Check always the output file from FullProf, there is plenty of useful information that can help you to understand the results.



9) **PCR file using the Shubnikov magnetic space group.**

- a. In order to determine the possible Shubnikov space group compatible with our system we can use the program Baslreps as was shown in the previous sections. However, using the Bilbao Crystallographic Server we can create a list of mCIF files (one for each Shubnikov S.G.), that can be transformed into a PCR file with a single click.

Open a web browser and write <http://www.cryst.ehu.es/>

Click on Magnetic Symmetry and Applications

bilbao crystallographic server

Contact us	About us	Publications	How to cite the server
Space-group symmetry			
Magnetic Symmetry and Applications			
MGENPOS	General Positions of Magnetic Space Groups		
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups		
MNORMALIZER	Normalizers of Magnetic Space Groups		
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting		
BNS2OG	Transformation of symmetry operations between BNS and OG settings		
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).		
MPOINT	Magnetic Point Group Tables		
MAGNEXT	Extinction Rules of Magnetic Space Groups		
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector		
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry		
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)		
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell		
MAGNDATA	A collection of magnetic structures with transportable cif-type files		
MVISUALIZE	3D Visualization of magnetic structures with Jmol		
MTENSOR	Symmetry-adapted form of crystal tensors in magnetic phases		
MAGNETIC REP.	Decomposition of the magnetic representation into irreps		
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition		

Click on MAXMAGN, fill the boxes and click on submit.

☒ Structure data of the paramagnetic phase will be included

☒ Non-conventional setting

Please, enter the label of the space group of the paramagnetic phase (parent group)

choose it

Please, enter the propagation vector k:

k_x

0

k_y

0

k_z

0

Submit

Upload a structural model (CIF file). You can use the provide CIF file (la300k-a.cif). If there is not errors in your CIF file, the program will ask for the magnetic atoms. Select the Mn atom and click on submit.

Parent phase structure data: Magnetic A

Parent space group: *Pnma* (No. 62)

***Parent space group in non-conventional setting (-b, c, -a; 0, 0, 0)**

Lattice parameters (Angstroms and degrees): a=5.53647, b=5.74723, c=7.69280, alpha=90.000000, beta=90.000000, gamma=90.000000

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	La	La	4c	-0.00811 0.04928 0.25000	<input type="checkbox"/>
2	Mn	Mn	4b	0.50000 0.00000 0.00000	<input checked="" type="checkbox"/>
3	O1	O	4c	0.07440 0.48700 0.25000	<input type="checkbox"/>
4	O2	O	8d	0.72572 0.30656 0.03848	<input type="checkbox"/>

Submit

The program gives a list of maximal magnetic space groups compatible with the propagation vector. In addition, the transformation to the standard setting is provided.

Maximal magnetic space groups for the parent space group $Pnma$ (No. 62) and the propagation vector $\mathbf{k} = (0, 0, 0)$

Parent space group in non-standard setting $(-b, c, -a; 0, 0, 0)$

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$Pn'm'a'$ (#62.449) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$Pn'm'a'$ (#62.448) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$Pnm'a'$ (#62.447) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$Pn'm'a'$ (#62.446) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
5	$Pnma'$ (#62.445) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
6	$Pnm'a'$ (#62.444) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
7	$Pn'm'a'$ (#62.443) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
8	$Pnma$ (#62.441) Go to a subgroup	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

In this example we are going to select the $Pn'm'a'$ (#62.448) magnetic space group which corresponds with Gamma2 in the previous table. Click on Show (magnetic structure), and as we do not know the magnetic components, we can fix all of them to $0.5 \mu_B$.

Magnetic Structure

Selected magnetic space group: 2- *Pn'ma'* (#62.448)

Setting of the parent group

Parent space group *Pnma* (No. 62), in non-standard setting (-b, c, -a; 0, 0, 0)

Lattice parameters: a=5.53647, b=5.74723, c=7.69280, alpha=90.000000, beta=90.000000, gamma=90.000000

[Go to setting standard (-b, c, -a; 0, 0, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x , M_y , M_z
1	La La 0.99189 0.04928 0.25000	(x,y,1/4 0,0,m _z) (x+1/2,-y+1/2,3/4 0,0,m _z) (-x,-y,3/4 0,0,m _z) (-x+1/2,y+1/2,1/4 0,0,m _z)	4	-	-
2	Mn Mn 0.50000 0.00000 0.00000	(1/2,0,0 m _x ,m _y ,m _z) (0,1/2,0 -m _x ,m _y ,m _z) (1/2,0,1/2 -m _x ,m _y ,m _z) (0,1/2,1/2 m _x ,m _y ,m _z)	4	(M_x, M_y, M_z)	$M_x = 0.5000$ $M_y = 0.5000$ $M_z = 0.5000$
3	O1 O 0.07440 0.48700 0.25000	(x,y,1/4 0,0,m _z) (x+1/2,-y+1/2,3/4 0,0,m _z) (-x,-y,3/4 0,0,m _z) (-x+1/2,y+1/2,1/4 0,0,m _z)	4	-	-
4	O2 O 0.72572 0.30656 0.03848	(x,y,z m _x ,m _y ,m _z) (x+1/2,-y+1/2,-z -m _x ,m _y ,m _z) (-x,-y,z+1/2 -m _x ,m _y ,m _z) (-x+1/2,y+1/2,-z+1/2 m _x ,m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (-x+1/2,y+1/2,z -m _x ,m _y ,m _z) (x,y,-z+1/2 -m _x ,m _y ,m _z) (x+1/2,-y+1/2,z+1/2 m _x ,m _y ,m _z)	8	-	-

Click on Export data to MCIF/Visualize.

Click on Download mCIF.

Rename the file with an intuitive name "P_np_m_ap.mcif"

Go to FullProf tool bar and click on "file>select working directory" and select the directory of your .mcif.

Click on "file>Information/tpcr/corrections/lrf files>mcif" and select the mcif.

Go to tools and select mCIF_to_PCR. (A similar tool is also included in the BCS <http://www.cryst.ehu.es/cgi-bin/cryst/programs/mCIF2PCR.pl>).

```

=> Crystal system:
=> Lattice type:
=> Lattice type Symbol:
=> Number of centring vectors: 0
=> Number of anti-translations: 0
=> Number of reduced set of S.O.: 4
=> General Multiplicity: 8
=> Centred: 2
=> Centrosymmetry: Centric (-1 at origin)
=> Generators (exc. -1&L): 0

=> List of all Symmetry Operators and Symmetry Symbols

=> SYMM< 1>: x,y,z mx,my,mz +1 Symbol: 1
=> SYMM< 2>: x,y,-z+1/2 -mx,-my,mz +1 Symbol: n x,y,1/4
=> SYMM< 3>: x+1/2,-y+1/2,-z -mx,my,mz -1 Symbol: 2' <1/2,0,0> x,1/4,0
=> SYMM< 4>: -x+1/2,y+1/2,-z+1/2 mx,-my,mz -1 Symbol: 2' <0,1/2,0> 1/4,y,1/4
=> SYMM< 5>: -x,-y,-z mx,my,mz +1 Symbol: -1 0,0,0
=> SYMM< 6>: -x,-y,z+1/2 -mx,-my,mz +1 Symbol: 2 <0,0,1/2> 0,0,z
=> SYMM< 7>: -x+1/2,y+1/2,z -mx,my,mz -1 Symbol: b' 1/4,y,z
=> SYMM< 8>: x+1/2,-y+1/2,z+1/2 mx,-my,mz -1 Symbol: n' <1/2,0,1/2> x,1/4,z

=> Press <enter> to finish

```

In the same directory, the program has created a PCR file that can be used as a template. This PCR is ready to be used, but in calculation mode. We should replace the JOB = 3 to JOB = 1 in order to do a fit.

Replace into the PCR file all the information related with your instrument and with the measurements. Lambda, background, muR, zero, U, V, W, unit cell and Scale. All this information can be obtained from the previous PCR file.

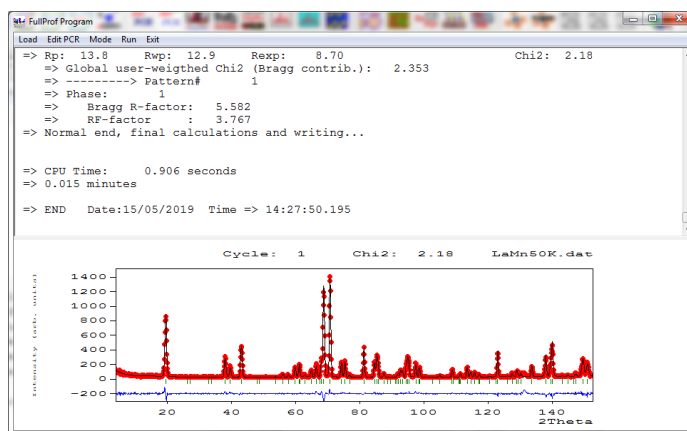
- b. Here below you have a picture with a block defining a magnetic space group in FullProf using the Shubnikov formalism. It deserves to be noted that nuclear and magnetic part are in the same phase (JBT = 10), so only one phase is needed.

```

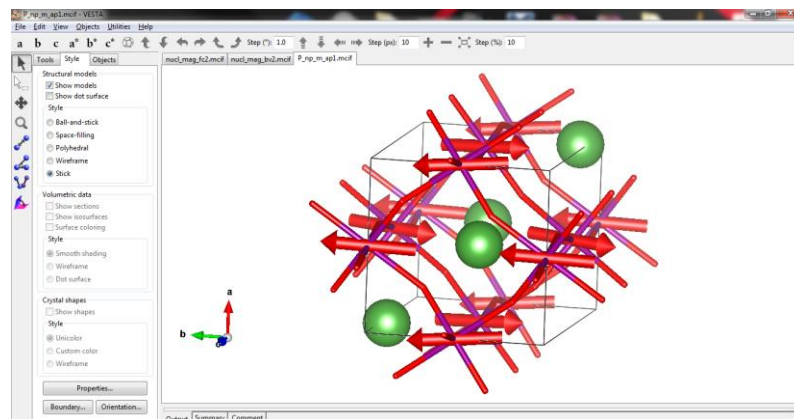
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 5.74
!-----
Nuclear and Magnetic Structure of: P_np_m_ap VARY mxmymz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
4 0 0 0.0 0.0 1.0 10 0 2 0 0 967.367 0 7 0
!
Pn'ma' number:62.448 <--Magnetic Space group symbol (BNS symbol & number)
Transform to standard: -b,c,-a;0,0,0
Parent Space Group: No.62 IT_number: 62
Transform from Parent: a,b,c;0,0,0
! Nsym Cen N_Clat N_Ant
4 2 0 0
!
! Symmetry operators
1 x,y,z,+1
2 x,y,-z+1/2,+1
3 x+1/2,-y+1/2,-z,-1
4 -x+1/2,y+1/2,-z+1/2,-1
!
!Atom Typ Mag Vek X Y Z Biso Occ N_type Spc/Eftype /Line below:Codes
! Rx Ry Rz Ix Iy Iz Iz MagPh / Line below:Codes
! beta11 beta22 beta33 beta12 beta13 beta23 / Line below:Codes
La La 1 0 0.99189 0.04928 0.25000 0.00000 0.50000 0 0 #
0.00 0.00 0.00 0.00 0.00
Mn MMN2 1 0 0.50000 0.00000 0.00000 0.00000 0.50000 1 0 #
0.00 0.00 0.00 0.00 0.00
0.23542 3.95797 0.82959 0.00000 0.00000 0.00000 0.00000 <--MagPar
111.00 101.00 91.00 0.00 0.00
O1 O 1 0 0.07440 0.48700 0.25000 0.00000 0.50000 0 0 #
0.00 0.00 0.00 0.00
O2 O 1 0 0.72572 0.30656 0.03848 0.00000 1.00000 0 0 #
0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1

```

- c. The instruction VARY mxmymz, activates automatically the refinement of the magnetic moment components, which are compatible with the symmetry. If the user wants to fix one component this instruction should be removed.
- d. In the FullProf tool bar select the PCR file and refine.



- e. Plot the mCIF into VESTA, in this case as nuclear and magnetic structures were refined in the same phase both are included into the mCIF.



- f. Repeat the procedure using the full list of Shubnikov space group.