

# Bilbao Crystallographic Server and Fullprof refinement of $\text{LaMnO}_3$ data

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# LaMnO<sub>3</sub>

- There is a LaMnO<sub>3</sub> example (data/notes) using representation analysis by Juan Rodríguez-Carvajal. See 2014 Magnetic Structure Notes (also in this folder "Tutorial\_Magnetic\_Structures\_LaMnO3\_Juan2014.pdf").
- We will start from the same .cif file used in the other example and use the same neutron data set. The k-vector has been previously found using k-search as  $k = (0,0,0)$ .

**WORK THROUGH PREVIOUS EXAMPLE!!**

## Tutorial on Magnetic Structure Determination and Refinement using Neutron Powder Diffraction and FULLPROF

Juan Rodríguez-Carvajal

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### Introduction

This document is a simple tutorial for using FULLPROF as a tool for determining magnetic structures using neutron powder diffraction (NPD). The user of this document should know the basic facts of magnetism and magnetic structures. It is supposed a good knowledge of crystallography and some practice and basic knowledge of the structure of a PCR file (the input control file needed for running FULLPROF). Magnetic symmetry considerations will not be treated in detail here (it is assumed that the user has some knowledge on that subject); however, the available document: *Symmetry and Magnetic Structures*, by J. Rodríguez-Carvajal and F. Bourée, that will be published in the Editions de Physique, treats largely the subject from the point of view of the representation theory. This document will be referenced hereafter as SMS. Some parts of the SMS text and the examples treated there have been taken for the present tutorial. A summary of the most important parts of SMS for this tutorial is given in the appendix of this document. In FullProf there are many ways of writing PCR files for treating magnetic structures; in this document we describe only the simplest ones.

### Determination of magnetic structures using the programs of the FULLPROF SUITE

The procedure for determining a magnetic structure using powder diffraction is relatively simple. It can be summarised as follows:

1: Collect a NPD of the sample in the paramagnetic state ( $T > T_N$  or  $T_C$ ). Refine the crystal structure using the collected data and get all the relevant structural and profile parameters. Use FULLPROF and WnPLOTR for doing this task.

2: Collect a NPD below the ordering temperature. Normally additional magnetic peaks appear in the diffraction pattern. It is important to make a refinement by fixing all the structural parameters, without putting a magnetic model in the PCR file, in order to see clearly the magnetic contributions to the diffraction pattern. Get the peak positions of the additional peaks using WnPLOTR-2006 and save them in a format adequate to the program K-SEARCH.

3: Determine the propagation vector(s) of the magnetic structure (See appendix for a summary of the formalism of propagation vectors) by using the program K-SEARCH or by trial and error with an additional phase in the PCR file treated in Le Bail Fit (LBF) mode (no magnetic model). If there are no additional peaks and only an additional contribution to the nuclear peaks is observed, the magnetic structure has as propagation vector  $k = (0, 0, 0)$ .

4: Once the propagation vector is determined, use the program BASIREPS in order to get the basis vectors of the irreducible representations (*irreps*) of the propagation vector group ( $G_k$ ;

see SMS or the appendix for more details). With the help of this program one can determine the Shubnikov group and the appropriate magnetic symmetry operators, or, alternatively, use directly the basis vectors of the *irreps*.

5: Solve the magnetic structure by using the symmetry information obtained in step 4 using trial and error methods (5-1) or the simulated annealing (SAnn) procedure (5-2) implemented in FULLPROF.

5-1: In the first case one has to modify the PCR file used in step 2 by adding an additional magnetic phase by putting  $Jbt=1$  (magnetic phase with Fourier coefficients/magnetic moments referred to the unitary basis along the unit cell axes),  $Trf=-1$  (only satellites will be generated). The best way to create such additional magnetic phase is to copy it from an already existing PCR file similar to that of the current case and modify it using the symmetry information obtained in step 4. Run FULLPROF fixing nearly all parameters, except the magnetic moments or the coefficients of the basis functions, and check in the plots if the calculated magnetic peaks have intensities close to the observed ones. If not, change the magnetic model (use another representation or other magnetic symmetry operators) and try again. In some cases this is enough to solve the magnetic structure. In case this does not work use the method described in 5-2.

5-2: In the second case one has to modify the PCR file used in step 2 by adding an additional phase in LBF mode (as for one of the options in step 3). This additional phase has no atoms and we have to put  $Jbt=2$ ,  $Trf=-1$  and  $Jview=11$ . The nuclear phase has to be treated with fixed scale factor and structural parameters. This allows getting the purely magnetic reflections in a separate file that can be used by FULLPROF in SAnn mode. This method will be explained later in detail.

6: Refine the magnetic using the Rietveld method implemented in FULLPROF. Once the magnetic model gives a calculated powder diffraction pattern close enough to the observed one, we start the refinement phase. If we use the trial and error method (5-1) the refinement step is just the continuation of the previous step. If the simulated annealing method (5-2) was used we have to translate the final solution stored in an automatically generated PCR file to the file for treating directly the powder diffraction profile.

The different steps described above and their order may be changed slightly depending on the previous knowledge the user has on the sample. We will illustrate these steps with a very simple case that may be useful for beginners in magnetic structure determination. We provide together with this document the data files of this example as well as other data files and PCR files corresponding to the examples treated in the SMS document.

### Determination of the magnetic structure of LaMnO<sub>3</sub>.

#### Step 1:

We provide two powder diffraction patterns of LaMnO<sub>3</sub> (F. Moussa, M. Hennion, J. Rodríguez-Carvajal, L. Pinsard and A. Revcolevschi, *Physical Review B* 54 (21), 15149 (1996)) taken at the LLB diffractometer G4.2 with  $\lambda=2.59 \text{ \AA}$ . The space group is  $G=Pbnm$ , the cell parameters are  $a \approx 5.53 \text{ \AA}$ ,  $b \approx 5.75 \text{ \AA}$  and  $c \approx 7.68 \text{ \AA}$  150K (paramagnetic phase,  $T_N \approx 140\text{K}$ ). The format of the data corresponds to  $Tns=6$  in FULLPROF. The pattern

presented is the result of the subtraction of the paramagnetic phase (see appendix for details) from the experimental data (see appendix for details).

The magnetic structure is determined by using the simulated annealing method (5-2) and the results are shown in the appendix.

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# LaMnO<sub>3</sub>: data format and magnetic peaks

Starting files to find nuclear refinement, magnetic peaks and k-vector

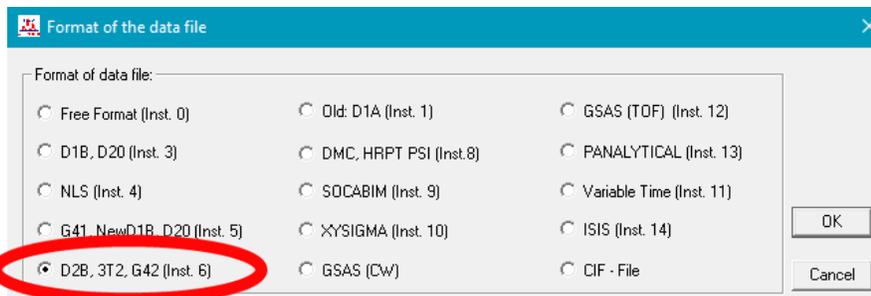
- Nuclear refinement and data for 150 K (no magnetic Bragg peaks):  
LaMn150K\_nuclear\_only.pcr  
LaMn150K.dat
- Nuclear refinement and data for 50 K (no magnetic Bragg peaks):  
LaMn50K\_nuclear\_only.pcr  
LaMn50K.dat

## Spin waves in the antiferromagnet perovskite LaMnO<sub>3</sub>: A neutron-scattering study

F. Moussa, M. Hennon, J. Rodriguez-Carvajal, and H. Moudden  
*Laboratoire Léon Brillouin, Centre d'Etudes de Saclay, 91191 Gif-sur-Yvette Cedex, France*

L. Pinsard and A. Revcolevschi  
*Laboratoire de Chimie des Solides, Université Paris-Sud, 91405 Orsay Cedex, France*  
(Received 17 May 1996)

As part of a general work on doped manganese perovskites, we have carried out detailed neutron-scattering experiments on powder and single crystals of the orthorhombic phase of undoped LaMnO<sub>3</sub>. The temperature dependence of the sublattice magnetization has been determined in the antiferromagnetic phase ( $T_N=139.5$  K), and the critical exponent is  $\beta=0.28$ , well below that corresponding to a pure three-dimensional Heisenberg antiferromagnet. We have measured the dispersion of the spin waves propagating in the highest symmetry directions solving the problems related to twinning. The whole spin wave spectrum is well accounted for with a Heisenberg Hamiltonian and a single ion anisotropy term responsible for the easy magnetization direction (**b** axis). This term induces a gap of 2.7 meV at low temperature in the spin wave dispersion curve. An important result is that the ferromagnetic exchange integral ( $J_1 \approx 0.83$  meV), coupling the spins within the ferromagnetic basal plane (**a,b**), is larger by a factor 1.4 than the antiferromagnetic exchange integral ( $J_2 \approx -0.58$  meV) coupling spins belonging to adjacent MnO<sub>2</sub> planes along **c**. [S0163-1829(96)08545-1]

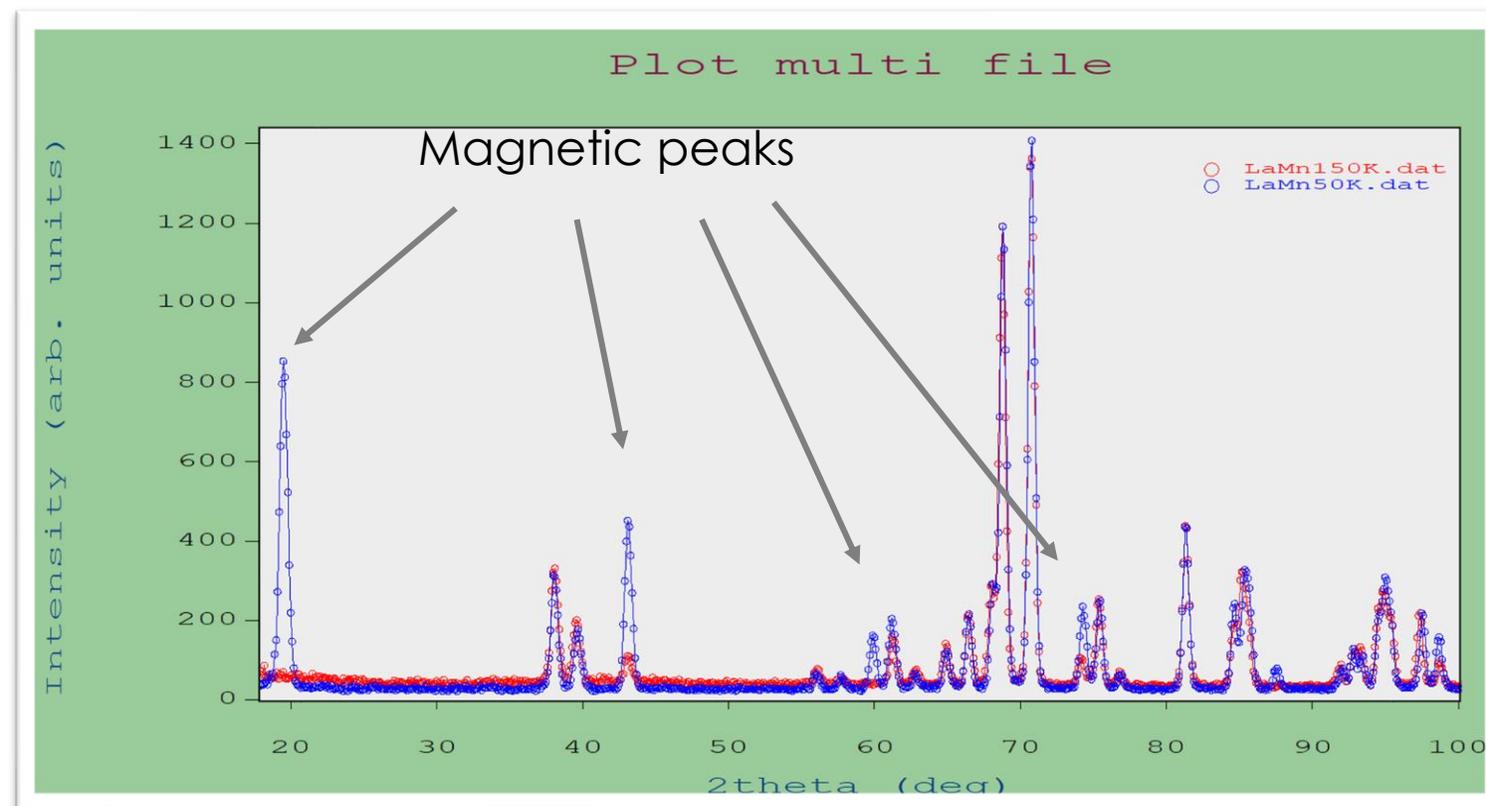


Data taken at G4.2 at LLB ( $\lambda=2.59$  Å)

$a=5.53$  Å,  $b=5.75$  Å and  $c=7.68$  Å.

Pbnm (62)

	x	y	z	Occ.	B	Site
La1	-0.00630	0.04430	0.25000	1.000	0.800	4c
Mn1	0.50000	0.00000	0.00000	1.000	0.460	4b
O1	0.07250	0.48850	0.25000	1.000	1.000	4c
O2	0.72570	0.30380	0.03780	1.000	0.910	8d



# LaMnO<sub>3</sub>

- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
  - Step 1: create an mcif file with MAXMAGN on the Bilbao Crystallographic Server.
  - Step 2: convert that mcif file into a .pcr file using mCIF2PCR.
  - Step 3: use the created .pcr file to fit the neutron data using Fullprof to determined the magnetic structure.

# Ho<sub>2</sub>BaNiO<sub>5</sub>

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# Step 1: Creating mCIF file

- Go to Bilbao server: <http://www.cryst.ehu.es/>
- Select “Magnetic Symmetry and Applications” to open the drop-down menu

**bilbao crystallographic server**

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Space-group symmetry

**Magnetic Symmetry and Applications**

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Double point and space groups

Quick access to some tables

- Space Groups
- Plane Groups
- Layer Groups
- Rod Groups
- Frieze Groups
- 2D Point Groups
- 3D Point Groups
- Magnetic Space Groups

**ECM31-Oviedo Satellite**

Crystallography online: workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

20-21 August 2018

**News:**

- **New Article in Nature**  
07/2017: Bradlyn et al. "Topological quantum chemistry" *Nature* (2017), 547, 298-305.
- **New program: BANDREP**  
04/2017: Band representations and Elementary Band representations of Double Space Groups.
- **New section: Double point and space groups**
  - New program: DGENPOS  
04/2017: General positions of Double Space Groups
  - New program: REPRESENTATIONS DPG  
04/2017: Irreducible representations of the Double Point Groups
  - New program: REPRESENTATIONS DSG  
04/2017: Irreducible representations of the Double Space Groups
  - New program: DSITESYM  
04/2017: Site-symmetry induced representations of Double Space Groups
  - New program: DCOMPREL  
04/2017: Compatibility relations between the irreducible representations of Double Space Groups

# Step 1: Creating mCIF file

- Then select “MAXMAGN”

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## Space-group symmetry

### Magnetic Symmetry and Applications

<a href="#">MGENPOS</a>	General Positions of Magnetic Space Groups
<a href="#">MWYCKPOS</a>	Wyckoff Positions of Magnetic Space Groups
<a href="#">MNORMALIZER</a>	Normalizers of Magnetic Space Groups
<a href="#">IDENTIFY MAGNETIC GROUP</a>	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
<a href="#">BNS2OG</a> 	Transformation of symmetry operations between BNS and OG settings
<a href="#">mCIF2PCR</a> 	Transformation from mCIF to PCR format (FullProf).
<a href="#">MPOINT</a> 	Magnetic Point Group Tables
<a href="#">MAGNEXT</a>	Extinction Rules of magnetic Space Groups
<a href="#">MAXMAGN</a> 	Maximal magnetic space groups for a given space group and a propagation vector
<a href="#">MAGMODELS</a>	Magnetic structure models for any given magnetic symmetry
<a href="#">k-SUBGROUPSMAG</a> 	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
<a href="#">MAGNDATA</a> 	A collection of magnetic structures with transportable cif-type files
<a href="#">MVISUALIZE</a> 	3D Visualization of magnetic structures with Jmol
<a href="#">MTENSOR</a> 	Symmetry-adapted form of crystal tensors in magnetic phases

### Group-Subgroup Relations of Space Groups

### Representations and Applications

### Solid State Theory Applications

# Step 1: Creating mCIF file

- **[1]** Need to have a propagation vector. This can be determined using k-search in fullprof (see other example for LaMnO<sub>3</sub>). It is (0,0,0).
- **[2]** Input the space group number of the crystal structure (or choose from a list of all space groups)- *Note: if you have a cif file this step is not necessary.*
- **[3]** Check the box “Structure data of the paramagnetic phase will be included”. This allows you to input a .cif file.

## MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models

**MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models**

MAXMAGN provides the possible magnetic space groups that can be assigned to a 1-k commensurate magnetic phase assuming that the magnetic symmetry is a maximal one. The space group of the paramagnetic phase (parent group) and the observed propagation vector are required as input. Optionally, the parent paramagnetic structure can be introduced (by hand or by a cif file). In this latter case the program provides the constrains for the different possible symmetries and cif-like files can be produced. These files permit the different alternative models to be analyzed, refined, shown graphically, transported to ab-initio codes etc., with programs as ISODISTORT, JANA2006, StrConvert, VESTA, etc. These cif-like files can also be submitted to the program MVISUALIZE, which allow 3D visualization of magnetic structures with Jmol. A controlled descent to lower symmetries is also possible.

This program provides an alternative to the traditional representation method for the parameterization of magnetic structures.

**MAXMAGN tutorials:**

Abbreviated tutorial: [download](#)  
Extended tutorial: [download](#)  
Last tutorial: [download](#)

Examples and further information can be found in the following paper:

J.M. Perez-Mato, S.V. Gallego, E.S. Tasci, L. Elororo, G. de la Flor, and M.I. Aroyo  
*Annu. Rev. Mater. Res.* (2015), 45:13.1-13.32

which can be used to cite this program.

The screenshot shows the MAXMAGN web interface with several elements highlighted by red circles and numbered 1 through 4:

- 1:** A red circle highlights the "choose it" button next to the space group input field.
- 2:** A red circle highlights the "Non-conventional setting" checkbox.
- 3:** A red circle highlights the checked checkbox "Structure data of the paramagnetic phase will be included".
- 4:** A red circle highlights the "Submit" button.

The input fields are: "Please, enter the label of the space group of the paramagnetic phase (parent group)" with a "choose it" button; "Please, enter the propagation vector k:" with input boxes for k<sub>x</sub> (0), k<sub>y</sub> (0), and k<sub>z</sub> (0); and a "Submit" button.

# Step 1: Creating mCIF file

- Choose .cif file (crystal structure only).  
The one for this example is “LaMnO3.cif”
- Then upload the file.
- If you don't have a cif file then have to fill out the details in “Option 2”

Bilbao Crystallographic Server → MAXMAGN - Maximal magnetic space groups

**Parent paramagnetic structure cif file**

**Option 1: Please submit a structure file (CIF format):**

Choose File LaMnO3.cif

Upload the file

No space group provided. The space group indicated in the cif file will be taken

Bilbao Crystallographic Server  
<http://www.cryst.ehu.es>

# Step 1: Creating mCIF file

- The paramagnetic phase information is displayed.
  - Select the magnetic atom(s). This case is Cr only.
  - Push Submit. This may take a few seconds to run the calculations.....

Bilbao Crystallographic Server → MAXMAGN - Maximal magnetic space groups

## Parent phase structure data: Magnetic Atoms

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

Lattice parameters (Angstroms and degrees): a=5.72690, b=7.73650, c=5.55200, alpha=90.00, beta=90.00, gamma=90.00

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	La1	La	4c	0.04430 0.25000 -0.00630	<input type="checkbox"/>
2	Mn1	Mn	4b	0.00000 0.00000 0.50000	<input checked="" type="checkbox"/>
3	O1	O	4c	0.48850 0.25000 0.07250	<input type="checkbox"/>
4	O2	O	8d	0.30380 0.03780 0.72570	<input type="checkbox"/>

Submit

Bilbao Crystallographic Server  
<http://www.cryst.ehu.es>

# Step 1: Creating mCIF file

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

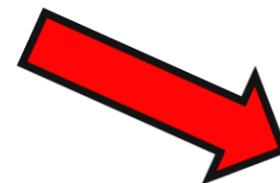
Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

- The possible magnetic space groups are displayed in grey. White have zero ordered moments.
- To view magnetic structure and export mcif file click on "Show" in last column.

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

# Step 1: Creating mCIF file: **Check #2,3,4,8**

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



**Magnetic Structure**

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

Setting of the parent group

Parent space group *Pnma* (No. 62)

Lattice parameters: a=5.72690, b=7.73650, c=5.55200, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (a, b, c ; 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	La1 La 0.04430 0.25000 0.99370	(x, 1/4, z   0, m <sub>y</sub> , 0) (-x+1/2, 3/4, z+1/2   0, m <sub>y</sub> , 0) (-x, 3/4, -z   0, m <sub>y</sub> , 0) (x+1/2, 1/4, -z+1/2   0, m <sub>y</sub> , 0)	4	-	-
2	Mn1 Mn 0.00000 0.00000 0.50000	(0, 0, 1/2   m <sub>x</sub> , m <sub>y</sub> , m <sub>z</sub> ) (1/2, 0, 0   m <sub>x</sub> , m <sub>y</sub> , -m <sub>z</sub> ) (0, 1/2, 1/2   -m <sub>x</sub> , m <sub>y</sub> , -m <sub>z</sub> ) (1/2, 1/2, 0   -m <sub>x</sub> , m <sub>y</sub> , m <sub>z</sub> )	4	(M <sub>x</sub> , M <sub>y</sub> , M <sub>z</sub> )	M <sub>x</sub> = 0.00000 M <sub>y</sub> = 0.00000 M <sub>z</sub> = 0.00000
3	O1 O 0.48850 0.25000 0.07250	(x, 1/4, z   0, m <sub>y</sub> , 0) (-x+1/2, 3/4, z+1/2   0, m <sub>y</sub> , 0) (-x, 3/4, -z   0, m <sub>y</sub> , 0) (x+1/2, 1/4, -z+1/2   0, m <sub>y</sub> , 0)	4	-	-
4	O2 O 0.30380 0.03780 0.72570	(x, y, z   m <sub>x</sub> , m <sub>y</sub> , m <sub>z</sub> ) (-x+1/2, -y, z+1/2   m <sub>x</sub> , m <sub>y</sub> , -m <sub>z</sub> ) (-x, y+1/2, -z   -m <sub>x</sub> , m <sub>y</sub> , -m <sub>z</sub> ) (x+1/2, -y+1/2, -z+1/2   -m <sub>x</sub> , m <sub>y</sub> , m <sub>z</sub> ) (-x, -y, -z   m <sub>x</sub> , m <sub>y</sub> , m <sub>z</sub> ) (x+1/2, y, -z+1/2   m <sub>x</sub> , m <sub>y</sub> , -m <sub>z</sub> ) (x, -y+1/2, z   -m <sub>x</sub> , m <sub>y</sub> , -m <sub>z</sub> ) (-x+1/2, y+1/2, z+1/2   -m <sub>x</sub> , m <sub>y</sub> , m <sub>z</sub> )	8	-	-

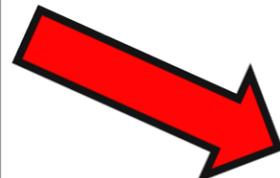
- All magnetic space groups allow spins along either a,b or c.
- Put values for M<sub>x</sub>, M<sub>y</sub>, M<sub>z</sub>.
- All give unique possible magnetic structures. Since k=000 some are AFM and some are FM.

# Step 1: Creating mCIF file: **Check #2**

- We will choose the allowed magnetic structure 2 (*Pn'ma'* (#62.448)) for this example,
- But all should be checked to ensure the solution is uniquely correct or to determine equivalent solutions.
- If none of the shown space groups work → go to a subgroup

# Step 1: Creating mCIF file: **Check #2**

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



**Magnetic Structure**

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

Setting of the parent group  
Parent space group *Pnma* (No. 62)

Lattice parameters: a=5.72690, b=7.73650, c=5.55200, alpha=90.00, beta=90.00, gamma=90.00

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

[Export data to MCIF file/Visualize](#) | [Go to a subgroup](#)

**2. Click export/view**

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	Occupancy	Magnetic moment	Values of $M_x, M_y, M_z$
1	La1 La 0.04430 0.25000 0.99370	(x,1/4,z   0,m (-x,3/4,-z   0,m		
2	Mn1 Mn 0.00000 0.00000 0.50000	(0,0,1/2   m <sub>x</sub> (0,1/2,1/2   -m <sub>x</sub>		
3	O1 O 0.48850 0.25000 0.07250	(x,1/4,z   0,m (-x,3/4,-z   0,m		
4	O2 O 0.30380 0.03780 0.72570	(x,y,z   m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (-x+1/2,-y,z+1/2   m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (-x,y+1/2,-z   -m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (x+1/2,-y+1/2,-z+1/2   -m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (-x,-y,-z   m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (x+1/2,y,-z+1/2   m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (x,-y+1/2,z   -m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> ) (-x+1/2,y+1/2,z+1/2   -m <sub>x</sub> ,m <sub>y</sub> ,m <sub>z</sub> )	8	

**1. Input values for magnetic moment**

$(M_x, M_y, M_z)$

$M_x = 1$   
 $M_y = 0.00000$   
 $M_z = 0.00000$

- We will choose the allowed magnetic structure 2 (*Pn'ma'* (#62.448)) for this example,
- But all should be checked to ensure the solution is uniquely correct or to determine equivalent solutions.
- If none of the shown space groups work → go to a subgroup

# Step 1: Creating mCIF file

- The mcif file is displayed.
- **[1]** This can be downloaded by clicking on “bcs\_file.mcif”
- **[2]** Magnetic structure can also be visualized by clicking “Submit to MVISUALIZE”

mCIF file of the structure

2

Submit this mcif file to MVISUALIZE for 3D visualization of the estructure using Jmol:

1

Download mCIF file: bcs\_file.mcif

```
#\#CIF_2.0
# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
# Date: 09/10/2019 21:39:22
# LaMnO3.cif

data_SyOhtAoR
_audit_creation_date      2019-10-09
_audit_creation_method    "Bilbao Crystallographic Server"

_citation_journal_abbrev  ?
_citation_journal_volume ?
_citation_page_first     ?
_citation_page_last      ?
_citation_article_id     ?
_citation_year           ?
_citation_DOI            ?

loop_
_citation_author_name
?

_atomic_positions_source_database_code_ICSD ?
_atomic_positions_source_other             ?

_transition_temperature ?
_experiment_temperature ?

loop_
_irrep_id
_irrep_dimension
_irrep_small_dimension
_irrep_direction_type
_irrep_action
_irrep_modes_number
_irrep_presence
? ? ? ? ? ? ?

_exptl_crystal_magnetic_properties_details
;
;

_active_magnetic_irreps_details
;
k-maximal magnetic symmetry
;

_parent_space_group.name_H-M_alt 'N o . 62'
_parent_space_group.IT_number    62
_parent_space_group.transform_Pp_abc 'a,b,c;0,0,0'
```

# Step 1: Creating mCIF file

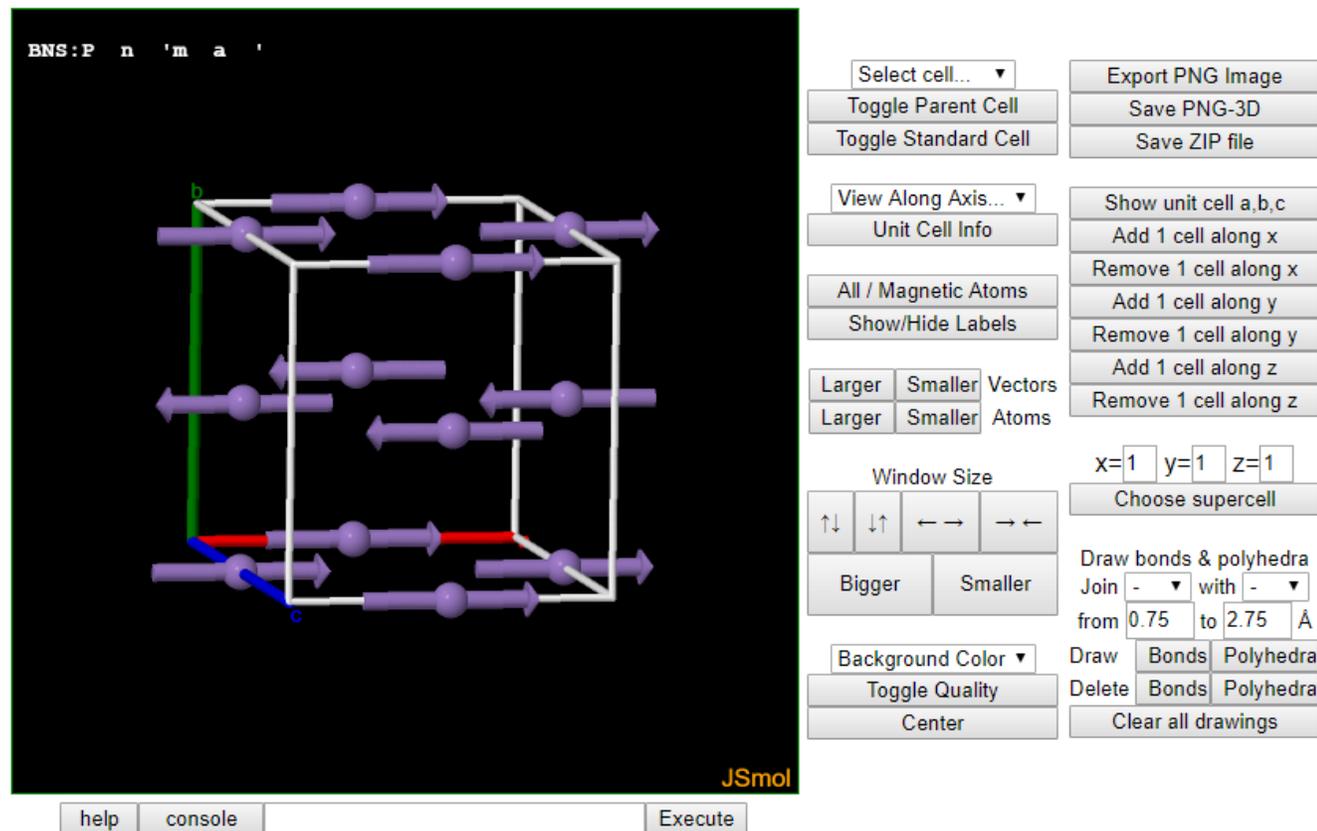
- MVISUALIZE lets you quickly check magnetic structure.
- But we will use the downloaded mcif to fit data using fullprof.

[We now need to go to Step 2](#)

MVISUALIZE Main Page

Show/Hide File

## MVISUALIZE: 3D Visualization of magnetic structures with Jmol



The screenshot displays the MVISUALIZE web interface. The main window shows a 3D visualization of a magnetic structure, likely a perovskite, with purple spheres representing atoms and arrows indicating magnetic moments. The structure is enclosed in a white unit cell box. The interface includes a control panel on the right with various options:

- Select cell... (dropdown)
- Toggle Parent Cell
- Toggle Standard Cell
- Export PNG Image
- Save PNG-3D
- Save ZIP file
- View Along Axis... (dropdown)
- Unit Cell Info
- Show unit cell a,b,c
- Add 1 cell along x
- Remove 1 cell along x
- Add 1 cell along y
- Remove 1 cell along y
- Add 1 cell along z
- Remove 1 cell along z
- All / Magnetic Atoms
- Show/Hide Labels
- Larger Smaller Vectors
- Larger Smaller Atoms
- Window Size (arrows)
- Bigger Smaller
- Background Color (dropdown)
- Toggle Quality
- Center
- x=1 y=1 z=1
- Choose supercell
- Draw bonds & polyhedra
- Join - with -
- from 0.75 to 2.75 Å
- Draw Bonds Polyhedra
- Delete Bonds Polyhedra
- Clear all drawings

At the bottom of the interface, there are buttons for 'help', 'console', and 'Execute'.

# LaMnO<sub>3</sub>

- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
  - Step 1: create an mcif file with MAXMAGN on the Bilbao Crystallographic Server.
  - Step 2: convert that mcif file into a .pcr file using mCIF2PCR.
  - Step 3: use the created .pcr file to fit the neutron data using Fullprof to determined the magnetic structure.

# Step 2: Creating a pcr from an mcif file

- Go back to the main page on server and open mCIF2PCR

Contact us      About us      Publications      How to cite the server

## Space-group symmetry

### Magnetic Symmetry and Applications

<a href="#">MGENPOS</a>	General Positions of Magnetic Space Groups
<a href="#">MWYCKPOS</a>	Wyckoff Positions of Magnetic Space Groups
<a href="#">MNORMALIZER</a>	Normalizers of Magnetic Space Groups
<a href="#">IDENTIFY MAGNETIC GROUP</a>	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
<a href="#">BNS2OG</a>	Transformation of symmetry operations between BNS and OG settings
<a href="#">mCIF2PCR</a>	Transformation from mCIF to PCR format (FullProf).
<a href="#">MPOINT</a>	Magnetic Point Group Tables
<a href="#">MAGNEXT</a>	Extinction Rules of Magnetic Space Groups
<a href="#">MAXMAGN</a>	Maximal magnetic space groups for a given space group and a propagation vector
<a href="#">MAGMODELIZE</a>	Magnetic structure models for any given magnetic symmetry
<a href="#">k-SUBGROUPSMAG</a>	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
<a href="#">MAGNDATA</a>	A collection of magnetic structures with transportable cif-type files
<a href="#">MVISUALIZE</a>	3D Visualization of magnetic structures with Jmol
<a href="#">MTENSOR</a>	Symmetry-adapted form of crystal tensors in magnetic phases

### Group-Subgroup Relations of Space Groups

### Representations and Applications

### Solid State Theory Applications

# Step 2: Creating a pcr from an mcif file

## mCIF2PCR: Transformation from mCIF to PCR format (FullProf).

### mCIF\_to\_PCR

Given a magCIF file, it produces a PCR template that can be used as input for FullProf (the program mCIF\_to\_PCR (FullProf) is used). By default the provided PCR file is intended for a simulation. The file can be then modified by hand for a refinement of the model.

### Choose a structure file (mCIF format):

LaMnO3\_cre... MAGN.m cif

1

2

- **[1]** Choose the mcif we just created through MAXMAGN
- **[2]** Click convert

The file has been successfully converted.

[Click to download it](#)

- This will convert the file and “Click to download it” will download the .pcr file
- We will use this .pcr file in Step 3. Put it in the same folder as the data file “LaMn50K.dat”

# LaMnO<sub>3</sub>

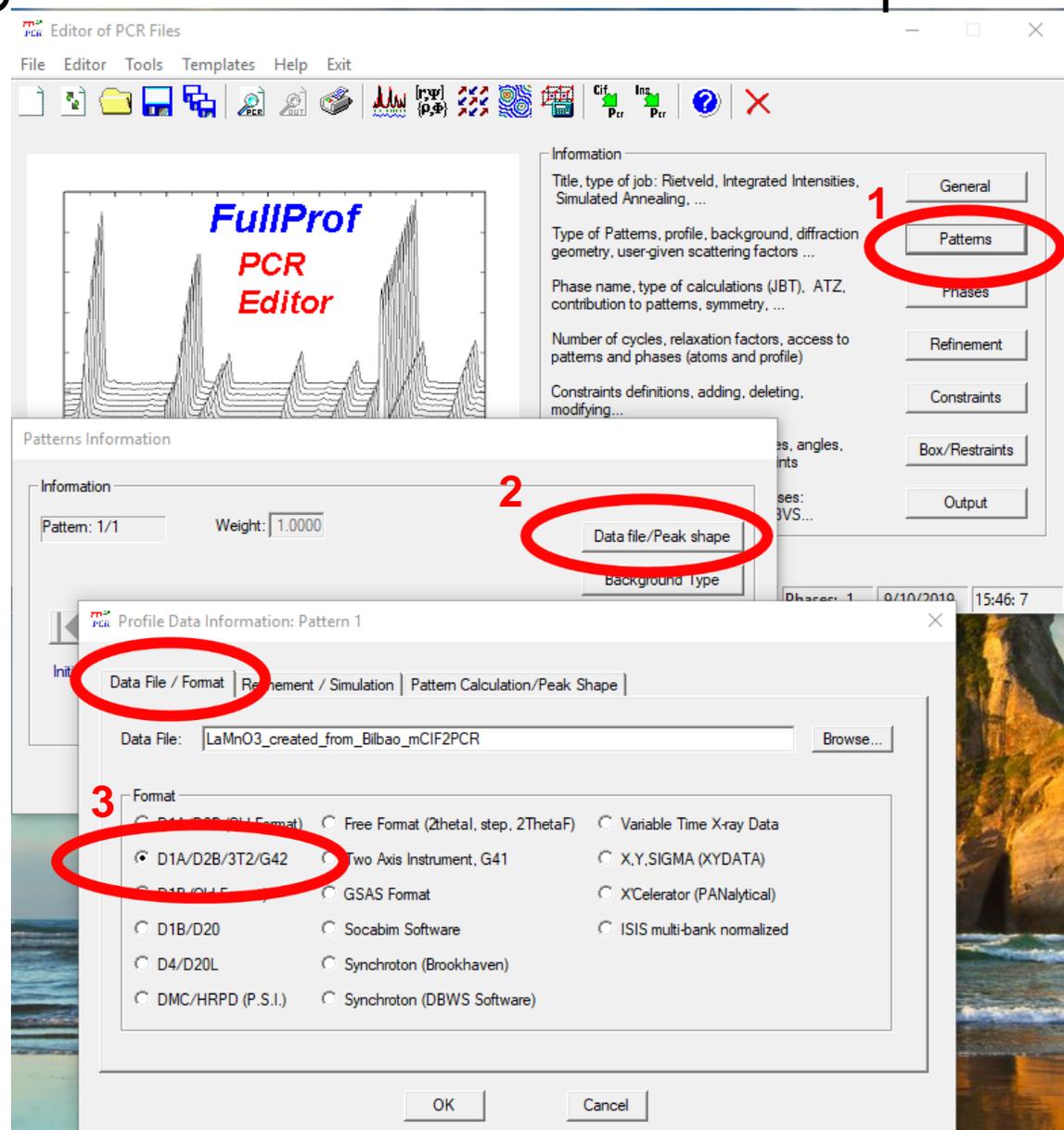
- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
  - Step 1: create an mcif file with MAXMAGN on the Bilbao Crystallographic Server.
  - Step 2: convert that mcif file into a .pcr file using mCIF2PCR.
  - Step 3: use the created .pcr file to fit the neutron data using Fullprof to determined the magnetic structure.

# Step 3: Refining the magnetic structure with Fullprof

- Pcr file created contains a single phase with crystal structure and magnetic ions described by a magnetic space group.
- The initial downloaded pcr file calculates the pattern based on default values.
- We need to change the defaults in the .pcr file in the same way as done for the examples created from a .cif file.
- To do this we work down the Tabs in the GUI (General/Patterns/Phases/Refinement) and/or edit the text file.
- The values will depend on the instrument the data was collected on. For this example use values already refined for the nuclear phase (LaMn50K\_nuclear\_only.pcr)

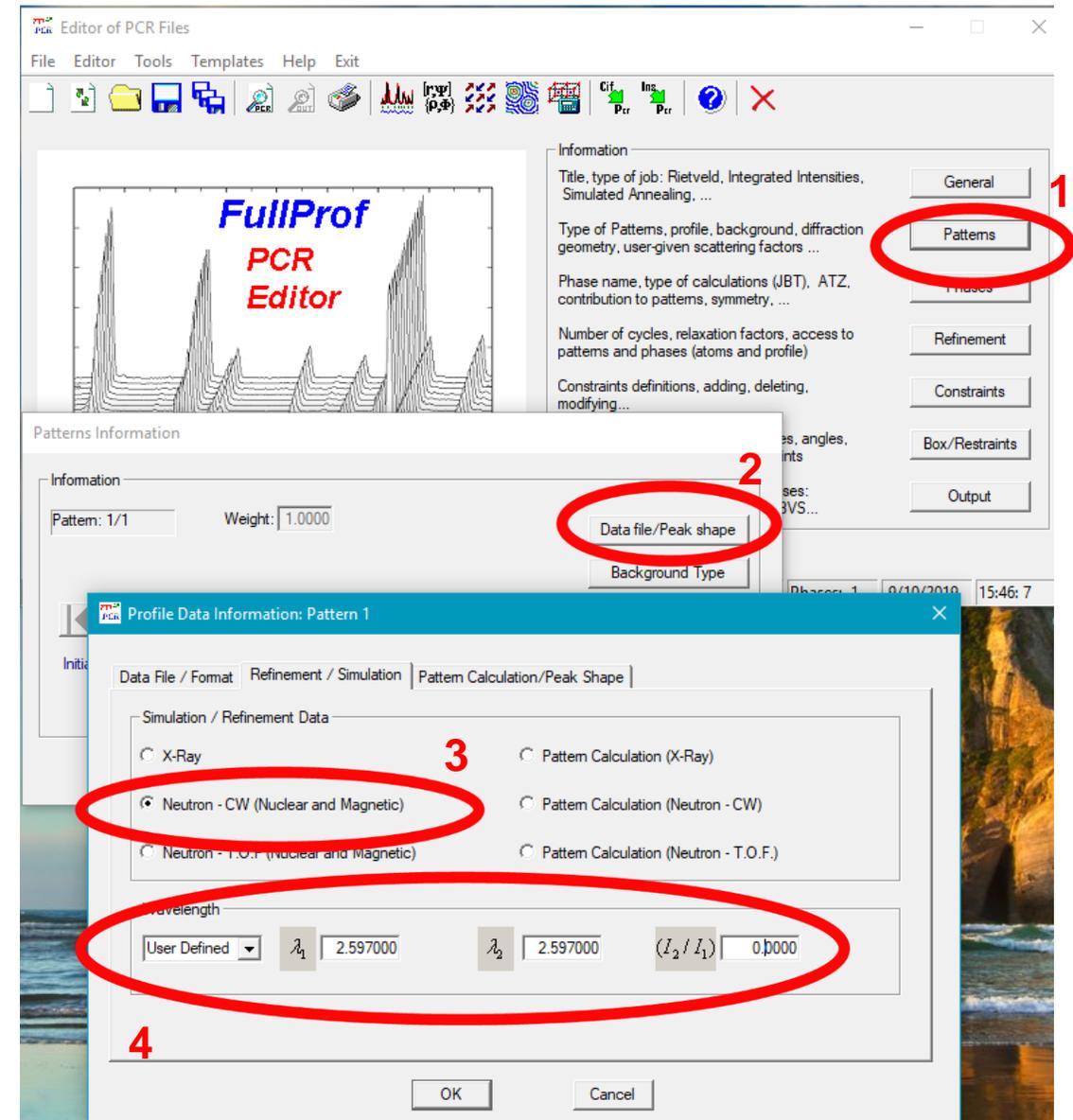
# Step 3: Refining the magnetic structure with Fullprof

- Open pcr file
- Select the format of the data file  
Fullprof should refine.
- Patterns → Data file/Peak Shape  
→ D1A/D2B/3T2/G42



# Step 3: Refining the magnetic structure with Fullprof

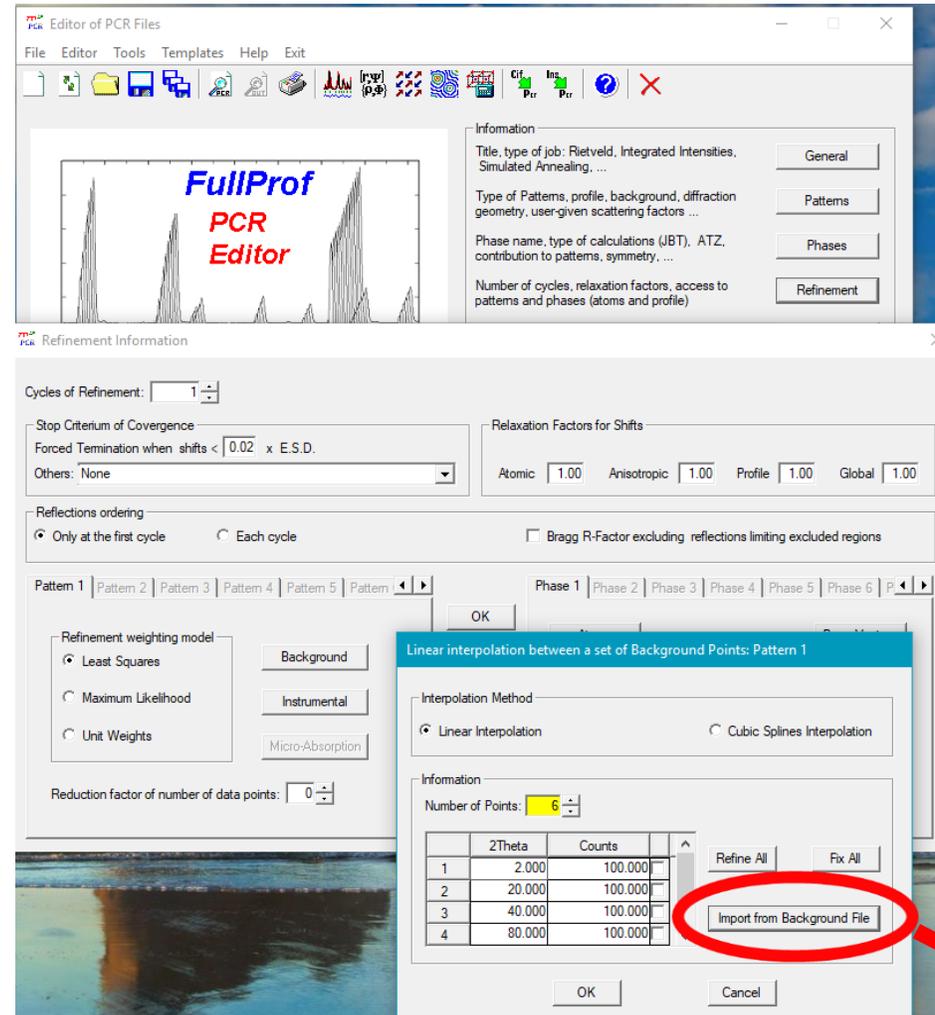
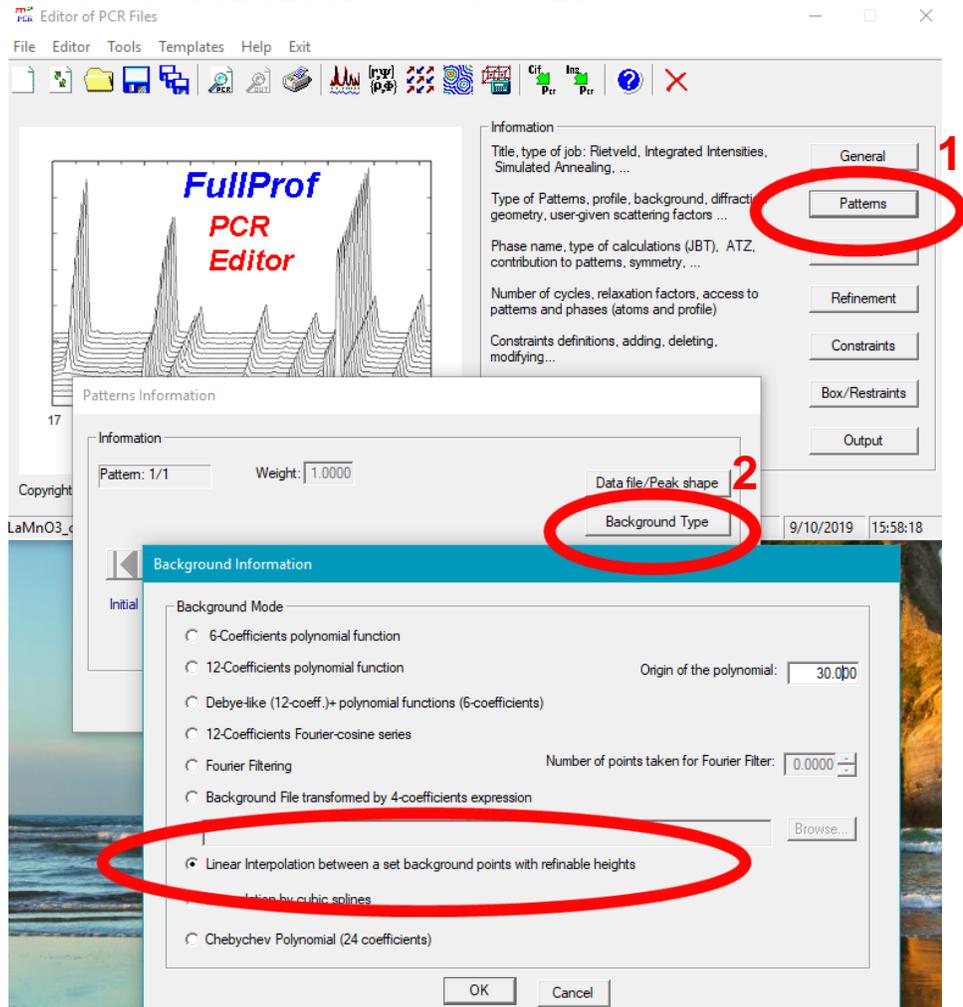
- Patterns → Data file/Peak Shape → Refinement/Simulation
- **[3]** Select Neutron – CW
- **[4]** Wavelength is 2.597 Å



# Step 3: Refining the magnetic structure with Fullprof

- Patterns → Background Type → Linear Interpolation between .....  
**THIS IS ALREADY CHOSEN**

- Unusual instrument background → Need to import background values **Background.bgr**



# Step 3: Refining the magnetic structure with Fullprof

- Add excluded regions (see nuclear pcr)

The screenshot displays the FullProf PCR Editor interface. The main window shows a plot of diffraction patterns with the text "FullProf PCR Editor" overlaid. On the right, the "Information" panel has several tabs: "General", "Patterns", "Phases", "Refinement", "Constraints", "Box/Restrains", and "Output". The "Patterns" tab is selected and circled in red, with a red "1" next to it. Below this, the "Patterns Information" dialog box is open, showing "Pattern: 1/1" and "Weight: 1.0000". It has buttons for "Data file/Peak shape", "Background Type", and "Excluded Regions". The "Excluded Regions" button is circled in red, with a red "2" next to it. A sub-dialog box titled "Exclude Regions: Pattern 1" is also open, showing "Number of Excluded Regions: 3" (circled in red with a red "3") and a table of regions:

	Low bound	High bound
Region 1	0.00	5.00
Region 2	130.30	132.00
Region 3	160.00	180.00

# Step 3: Refining the magnetic structure with Fullprof

- Make phase contribute to refinement.
- **[1]** Phases → **[2]** Contribution to Patterns → **[3]** Neutron (constant wavelength)

The screenshot displays the Fullprof software interface. The main window shows the 'Information' dialog box with the 'Phases' button circled in red (1). The 'Pattern Contribution Information for Phase 1' dialog box is open, showing the 'Type of Pattern' section with the 'Neutron (Constant Wavelength)' option circled in red (3). The 'Contribution to Patterns' button is also circled in red (2). The background shows a scenic view of a beach with waves and a rock formation.

# Step 3: Refining the magnetic structure with Fullprof

- Instrumental zero value (See nuclear refinement: 0.10686)

Refinement Information

Cycles of Refinement: 1

Stop Criterium of Coverage  
Forced Termination when shifts < 0.02 x E.S.D.  
Others: None

Relaxation Factors for Shifts  
Atomic: 1.00 Anisotropic: 1.00 Profile: 1.00 Global: 1.00

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

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

Refinement weighting model  
 Least Squares  Maximum Likelihood  Unit Weights

Background  Instrumental  Micro-Absorption

Reduction factor of number of data points: 0

Instrumental Parameters Refinement: Pattern 1

	Zero	Displacement	Transparency	Wavelength
Coefficients	0.106860	0.000000	0.000000	0.000000

# Step 3: Refining the magnetic structure with Fullprof

- Copy values from nuclear pcr for the instrumental profile parameters.

**NOTE:** Magnetic space groups do not use a propagation vector. Instead the unit cell changes. For  $k = (0\ 0\ 0)$  there is no change in unit cell.

The orthorhombic space group has  $b > a > c$  (converted from Pbnm of nuclear example)

**Delete vary mxmymz  
This stops the moments  
automatically refining.  
But make sure to keep  
track of allowed  
moments.**

```

External EdPCR Text Editor - [C:\Users\cr9\Desktop\LaMnO3\LaMnO3_created_from_Bilbao_mCIF2PCR.pcr]
File Edit Search
Excluded regions (LowT HighT) for Pattern# 1
  0.00 5.00
 130.30 132.00
 160.00 180.00

3 ?Number of refined parameters

? Zero Code SyCos Code SySin Code Lambda Code MORE ->Patt# 1
0.10686 0.0 0.00000 0.0 0.00000 0.0 0.00000 0.00 0

? Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 0.00

Nuclear and Magnetic Structure of: /srv/www/bcs_branch_www/www/tmp//LaMnO3_ VARY mxmymz

?Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
4 0 0 0.0 0.0 1.0 10 0 2 0 0 0.000 0 7 0

Pn'ma' number:62.448 <--Magnetic Space group symbol (BNS symbol & number)
Transform to standard:
Parent Space Group: IT_number: 62
Transform from Parent:
?Nsym Cen N_Clat N_Ant
4 2 0 0

? Symmetry operators
1 x,y,z,+1
2 x,-y+1/2,z,+1
3 -x+1/2,-y,z+1/2,-1
4 x+1/2,-y+1/2,z+1/2,-1

?Atom Typ Mag Ueq X Y Z Biso Occ N_type Spc/FFtype /Line below:Codes;
? beta11 beta22 beta33 beta12 beta13 beta23 / Line below:Codes
La1 La 1 0 0.04430 0.25000 0.99370 0.08078 0.50000 0 0 #
Mn1 MMN2 1 0 0.00000 0.00000 0.50000 0.50114 0.50000 1 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 <-MagPar
01 0 1 0 0.48850 0.25000 0.07250 0.62354 0.00000 0 0 #
0 1 0 0.30380 0.03780 0.72570 0.62354 1.00000 0 0 #

-----> Profile Parameters for Pattern # 1
? Scale Shape1 Bvw Str1 Str2 Str3 Strain-Model
3.0620 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
0.076778 -0.277888 0.398159 0.048260 0.000000 0.000000 0.000000 0
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

? a b c alpha beta gamma #Cell Info
5.749681 7.669302 5.537057 90.000000 90.000000 90.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

? Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.03500 0.02200
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

? 2Th1/TOF1 2Th2/TOF2 Pattern to plot
5.000 152.900 1
  
```

# Step 3: Refining the magnetic structure with Fullprof

- In “Refinement”  
→ “atoms” input thermal parameters (0.3).  
**[1,2,3]**
- $Re(x)$ ,  $Re(y)$ ,  $Re(z)$  can all contribute, so should all be checked.

The screenshot shows the FullProf PCR Editor interface. The main window displays a diffraction pattern plot with the text "FullProf PCR Editor". On the right, the "Information" panel has the "Refinement" button circled in red and labeled with a red "1". Below this, the "Refinement Information" dialog box is open, showing "Cycles of Refinement" set to 1, "Stop Criterion of Convergence" set to "Forced Termination when shifts < 0.02 x E.S.D.", and "Relaxation Factors for Shifts" set to 1.00 for Atomic, Anisotropic, Profile, and Global. The "Atoms" button in the dialog is circled in red and labeled with a red "2". At the bottom, the "List of Atoms" dialog box is open, showing a table of atoms with columns for Label, Ntyp, Mag. Rot., Prog. V..., X, Y, Z, B, and Occ. The "Number of Atoms" is set to 4. The "Re[x]" column for Atom # 2 is circled in red and labeled with a red "3".

**Refine moments**

Atoms Information: Phase 1

Atom #	Label	Ntyp	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	La1	La	1	0	0.04430	0.25000	0.99000	0.30000	0.50000
Atom # 2	Mn1	MMN2	1	0	0.00000	0.00000	0.50000	0.30000	0.50000
Atom # 3	O1	O	1	0	0.48850	0.25000	0.00250	0.30000	0.50000
Atom # 4	O2	O	1	0	0.30380	0.03780	0.72000	0.30000	1.00000

Atom	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom # 2	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

# Step 3: Refining the magnetic structure with Fullprof

The screenshot displays the FullProf PCR Editor interface. A yellow box highlights the text: "Refine scale and lattice constants Set number refinement cycles". A red circle highlights the "Cycles of Refinement" field, which is set to 10. Another red circle highlights the "Scale" field in the "Factors" table, which is set to 3.0617. The "Lattice Parameters" table shows values for a, b, and c. The "FWHM Parameters" table shows values for U, V, W, and IG. The "Shape Parameters" table shows values for X, Y, and SZ. The "Refinement Information" dialog box is open, showing the "Stop Criterion of Convergence" and "Relaxation Factors for Shifts". The "Profile Parameters: Phase 1 Pattern 1" dialog box is also open, showing the "Factors" table and "Lattice Parameters" table.

Factors	Scale	Overall B-factor
Coefficients	3.0617	0.0000

Lattice Parameters	a	b	c	alpha	beta	gamma
Coefficients	5.749641	7.669311	5.537108	90.000	90.000	90.000

FWHM Parameters	U	V	W	IG
Coefficients	0.076778	-0.277888	0.398159	0.000000

Shape Parameters	X	Y	SZ
Coefficients	0.048260	0.000000	0.000000

**NOTE:** Magnetic space groups do not use a propagation vector. Instead the unit cell changes. For  $k = (0\ 0\ 0)$  there is no change in unit cell.

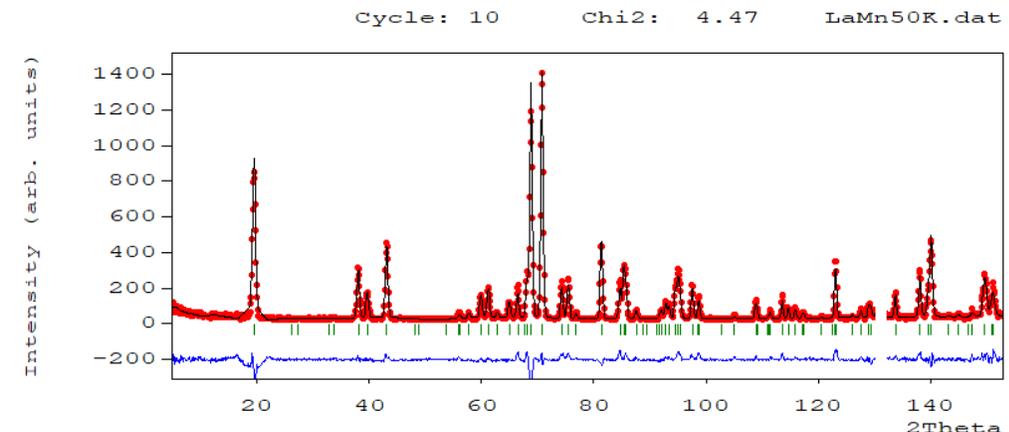
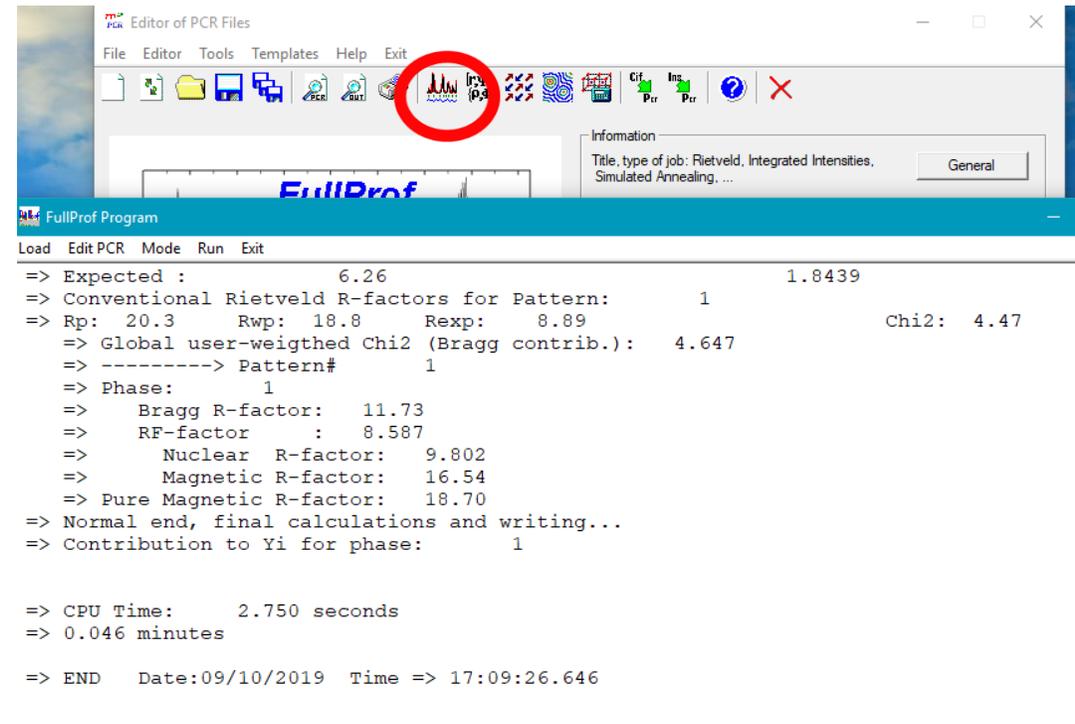
The orthorhombic space group has  $b > a > c$  (converted from Pbnm of nuclear example)

# Step 3: Refining the magnetic structure with Fullprof

- Run the refinement.
- Select the “LaMn50K.dat” neutron data file.



- Refinement models most of the data well.



# Step 3: Refining the magnetic structure with Fullprof

- List of files output

```
LaMnO3_created_from_Bilbao_mCIF2PCR.out
LaMnO3_created_from_Bilbao_mCIF2PCR.pcr
LaMnO3_created_from_Bilbao_mCIF2PCR.prf
LaMnO3_created_from_Bilbao_mCIF2PCR.sum
LaMnO3_created_from_Bilbao_mCIF2PCR1.fst
LaMnO3_created_from_Bilbao_mCIF2PCR1.mcif
LaMnO3_created_from_Bilbao_mCIF2PCR1.sub
LaMnO3_created_from_Bilbao_mCIF2PCR1.vesta
```

- Check magnetic structure with .fst file (Fpstudio) or .vesta or .mcif outputs.
- Values with errors in .sum file

$$\text{Mn: } M_x = 3.72(2) \mu_B$$

Moments along  $M_y$  and  $M_z$  are allowed, but if refined give small values with large errors.

