

Bilbao Crystallographic Server and Fullprof refinement of LaMnO_3 data

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LaMnO₃

- There is a LaMnO₃ 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 LaMnO₃.

Step 1:

We provide two powder diffraction patterns of LaMnO₃ (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 $\lambda=2.59$ Å. The space group is $G=Pbnm$, the cell parameters are $a \approx 5.53$ Å, $b \approx 5.75$ Å and $c \approx 7.68$ Å 150K (paramagnetic phase, $T_N \approx 140$ K). The format of the data corresponds to $Ins=6$ in FULLPROF. The pattern

para lectione of the magnetic structure determination (analysis) of the powder diffraction data (PDF) is: Once the powder diffraction data is collected, the first step is to determine the unit cell parameters and the space group.

the first step is to determine the unit cell parameters and the space group. This is done by using the program FULLPROF, which performs a least squares refinement of the unit cell parameters and the space group.

150K) the pattern of the data corresponds to $Ins=6$ in FULLPROF. The pattern is shown in the figure. The pattern is a powder diffraction pattern, which is a sum of many single crystal patterns. The pattern is a function of the scattering angle 2θ and the intensity I . The pattern is a function of the scattering angle 2θ and the intensity I .

LaMnO₃: data format and magnetic peaks

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

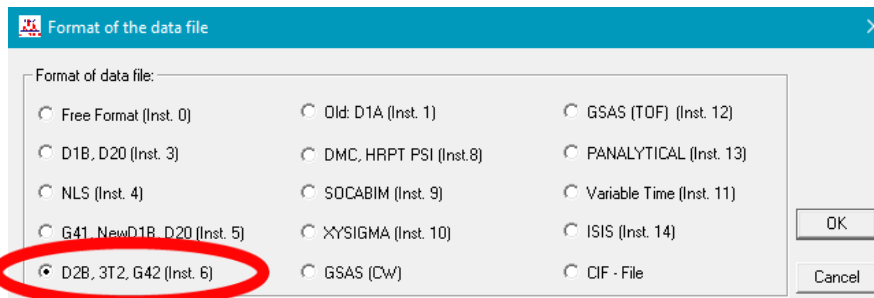
- Nuclear refinement and data for 150 K (no magnetic Bragg peaks):
LaMn150K_nuclear_only.pcr
LaMn150K.dat
- Nuclear refinement and data for 150 K (no magnetic Bragg peaks):
LaMn50K_nuclear_only.pcr
LaMn50K.dat

Spin waves in the antiferromagnet perovskite LaMnO₃: A neutron-scattering study

F. Moussa, M. Hennen, 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 LaMnO₃. 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 MnO₂ planes along **c**. [S0163-1829(96)08545-1]

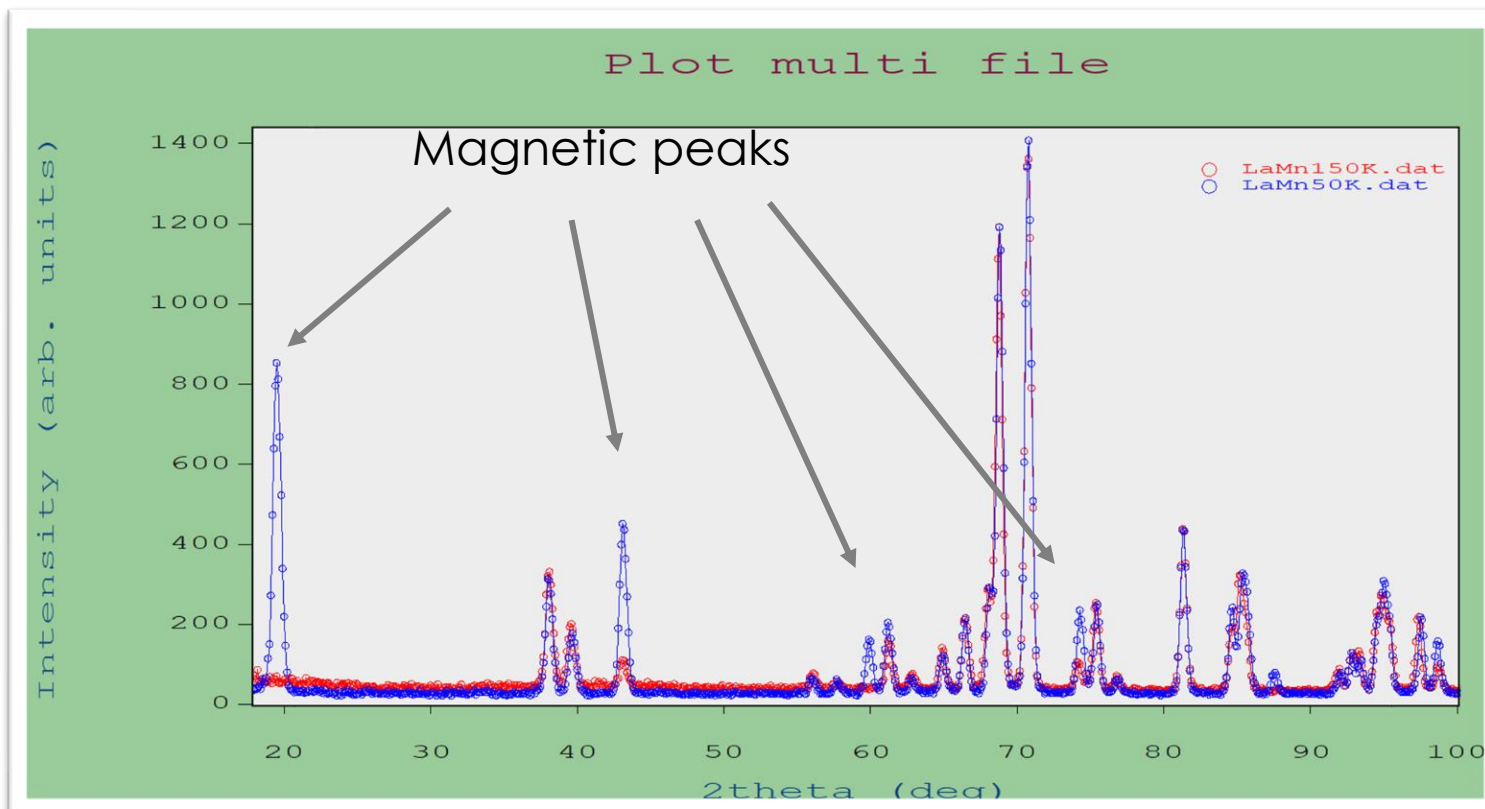


Data taken at G4.2 at LLB ($\lambda=2.59$ Å)

$a=5.53$ 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



LaMnO₃

- 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.

Ho₂BaNiO₅

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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

The screenshot shows the Bilbao Crystallographic Server homepage. The main navigation bar includes links for Contact us, About us, Publications, and How to cite the server. Below this is a list of menu items, with 'Magnetic Symmetry and Applications' highlighted by a red oval. To the right of the menu items is a 'Quick access to some tables' section with links to Space Groups, Plane Groups, Layer Groups, Rod Groups, Frieze Groups, 2D Point Groups, 3D Point Groups, and Magnetic Space Groups. On the left side, there is a section for 'ECM31-Oviedo Satellite' and a 'News' section with several articles.

bilbao crystallographic server

UPV EHU

Contact us About us Publications How to cite the server

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”

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
MAGMODELER	Magnetic structure models for any given magnetic symmetry
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

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_3). 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

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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 constraints 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 MVSUALIZE, 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. Elorrio, 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.

3

2

4

1

☒ Structure data of the paramagnetic phase will be included

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

Please, enter the propagation vector k:

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

- 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.

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

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

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) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	<i>Pn'ma'</i> (#62.448) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
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8	<i>Pnma</i> (#62.441) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show



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 _y ,0) (-x+1/2,3/4,z+1/2 0,m _y ,0) (-x,3/4,-z 0,m _y ,0) (x+1/2,1/4,-z+1/2 0,m _y ,0)	4	-	-
2	Mn1 Mn 0.00000 0.00000 0.50000	(0,0,1/2 m _x ,m _y ,m _z) (1/2,0,0 m _x ,m _y ,m _z) (0,1/2,1/2 -m _x ,m _y ,m _z) (1/2,1/2,0 -m _x ,m _y ,m _z)	4	(M _x ,M _y ,M _z)	M _x = 0.00000 M _y = 0.00000 M _z = 0.00000
3	O1 O 0.48850 0.25000 0.07250	(x,1/4,z 0,m _y ,0) (-x+1/2,3/4,z+1/2 0,m _y ,0) (-x,3/4,-z 0,m _y ,0) (x+1/2,1/4,-z+1/2 0,m _y ,0)	4	-	-
4	O2 O 0.30380 0.03780 0.72570	(x,y,z m _x ,m _y ,m _z) (-x+1/2,-y,z+1/2 m _x ,m _y ,m _z) (-x,y+1/2,-z -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,-z+1/2 m _x ,m _y ,m _z) (x,-y+1/2,z -m _x ,m _y ,m _z) (-x+1/2,y+1/2,z+1/2 -m _x ,m _y ,m _z)	8	-	-

- All magnetic space groups allow spins along either a,b or c.
- Put values for M_x, M_y, M_z.
- 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) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	<i>Pn'ma'</i> (#62.448) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	<i>Pnm'a'</i> (#62.447) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
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8	<i>Pnma</i> (#62.441) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show



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) (-x, 3/4, -z 0, m _x)		
2	Mn1 Mn 0.00000 0.00000 0.50000	(0, 0, 1/2 m _y) (0, 1/2, 1/2 -m _y)		
3	O1 O 0.48850 0.25000 0.07250	(x, 1/4, z 0, m _x) (-x, 3/4, -z 0, m _x)		
4	O2 O 0.30380 0.03780 0.72570	(x, y, z m _x , m _y , m _z) (-x+1/2, -y, z+1/2 m _x , m _y , -m _z) (-x, y+1/2, -z -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, -z+1/2 m _x , m _y , -m _z) (x, -y+1/2, z -m _x , m _y , -m _z) (-x+1/2, y+1/2, z+1/2 -m _x , m _y , m _z)	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 structure 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

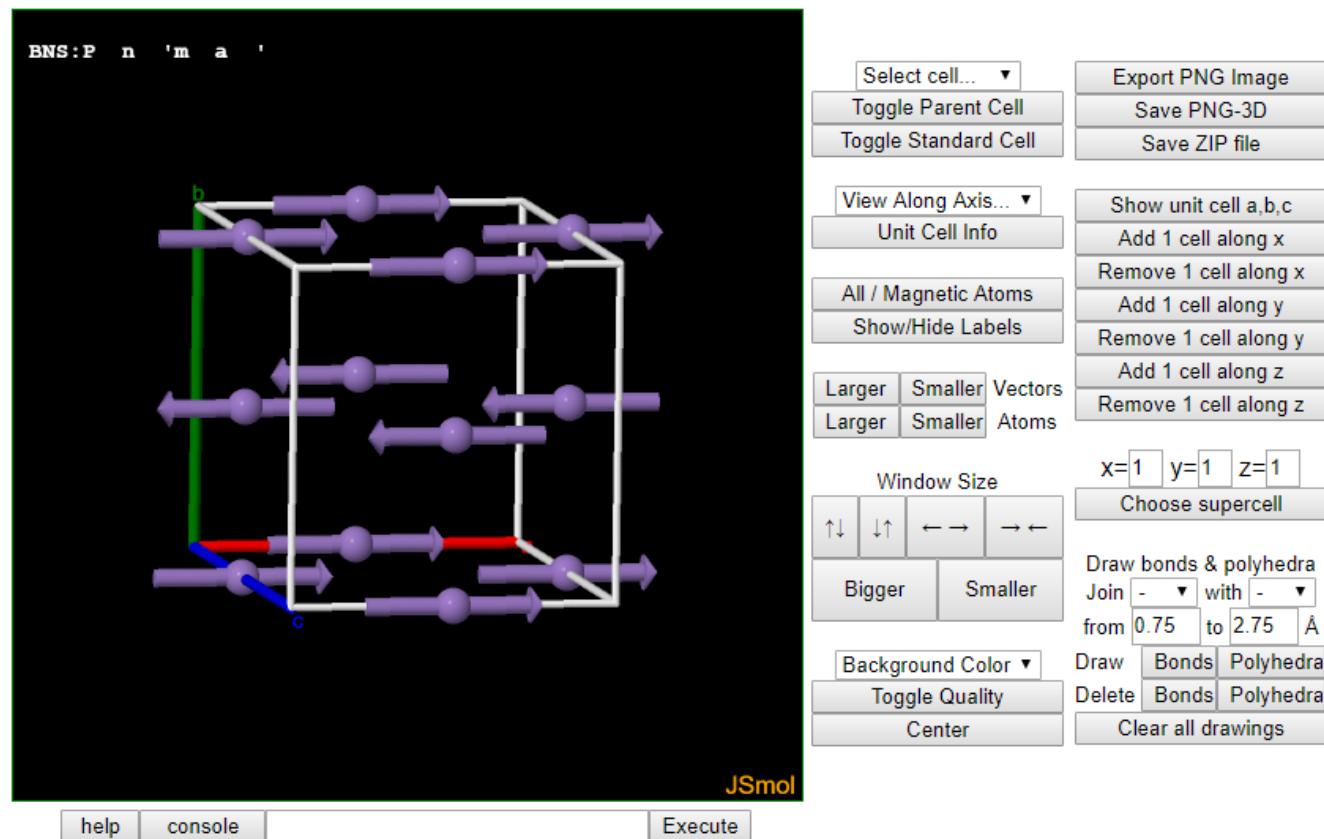
- MVISUALIZE lets you quickly check magnetic structure.
- But we will use the downloaded mcif to fit data using fullprof.

We now need to go to Step 2

MVISUALIZE Main Page

Show/Hide File

MVISUALIZE: 3D Visualization of magnetic structures with Jmol



LaMnO₃

- 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

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
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

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):

Choose File

LaMnO3_cre...MAGN.m

Convert

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”

LaMnO₃

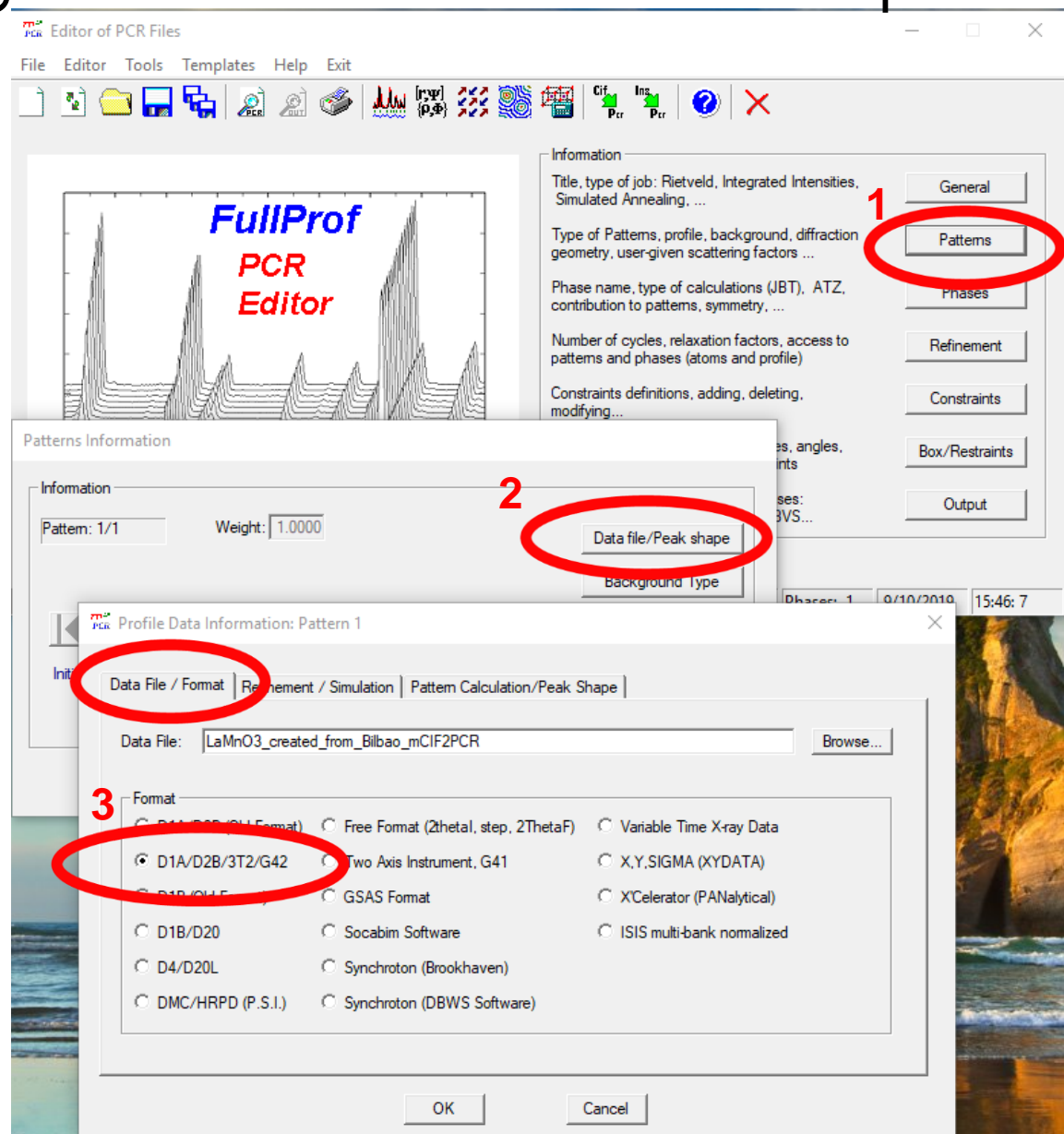
- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
 - Step 1: create an mcif file with MAXMAGN on the Bilbao Crystallographic Server.
 - Step 2: convert that mcif file into a .pcr file using mCIF2PCR.
 - Step 3: use the created .pcr file to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

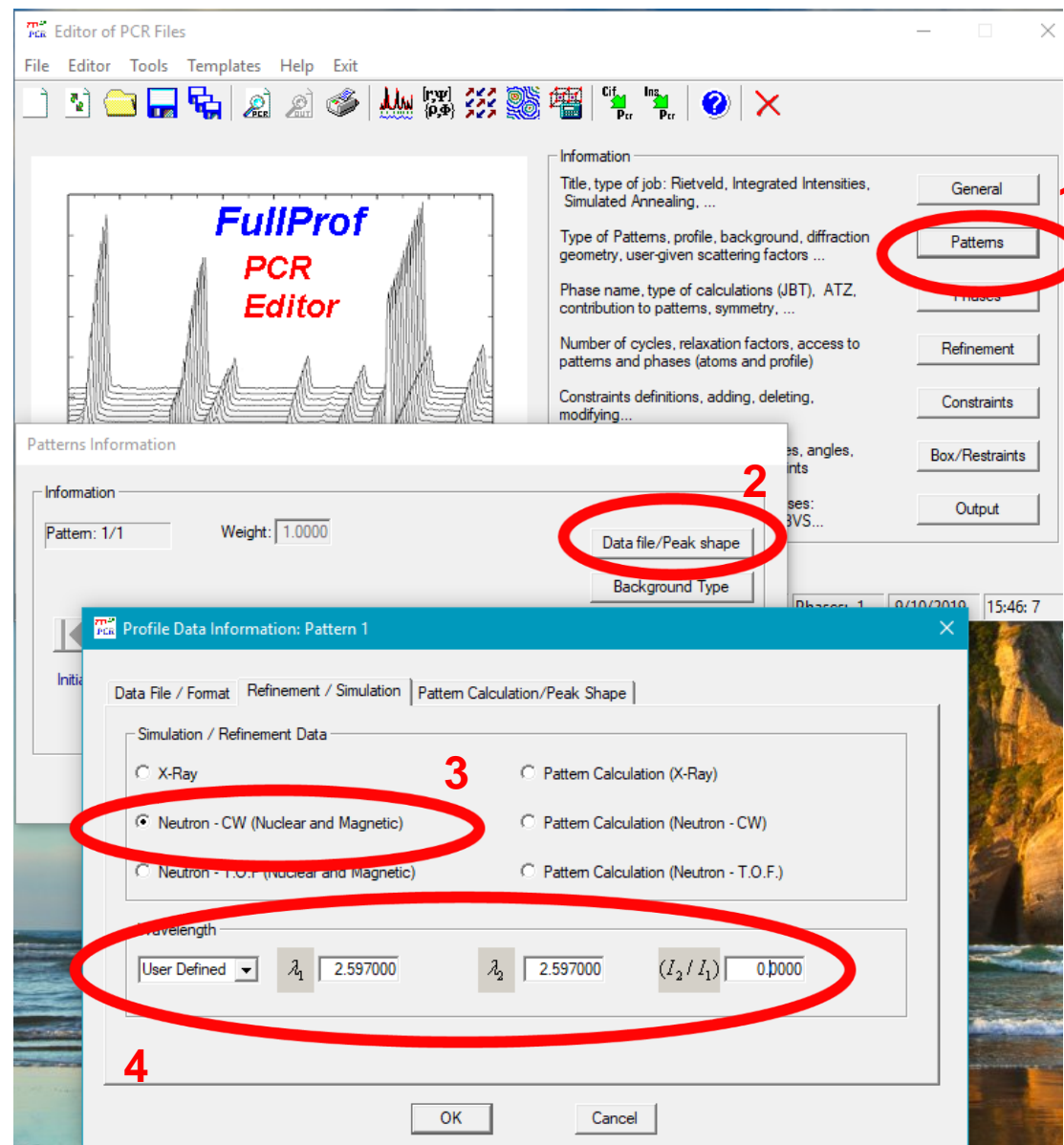
Step 3: Refining the magnetic structure with Fullprof

- 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

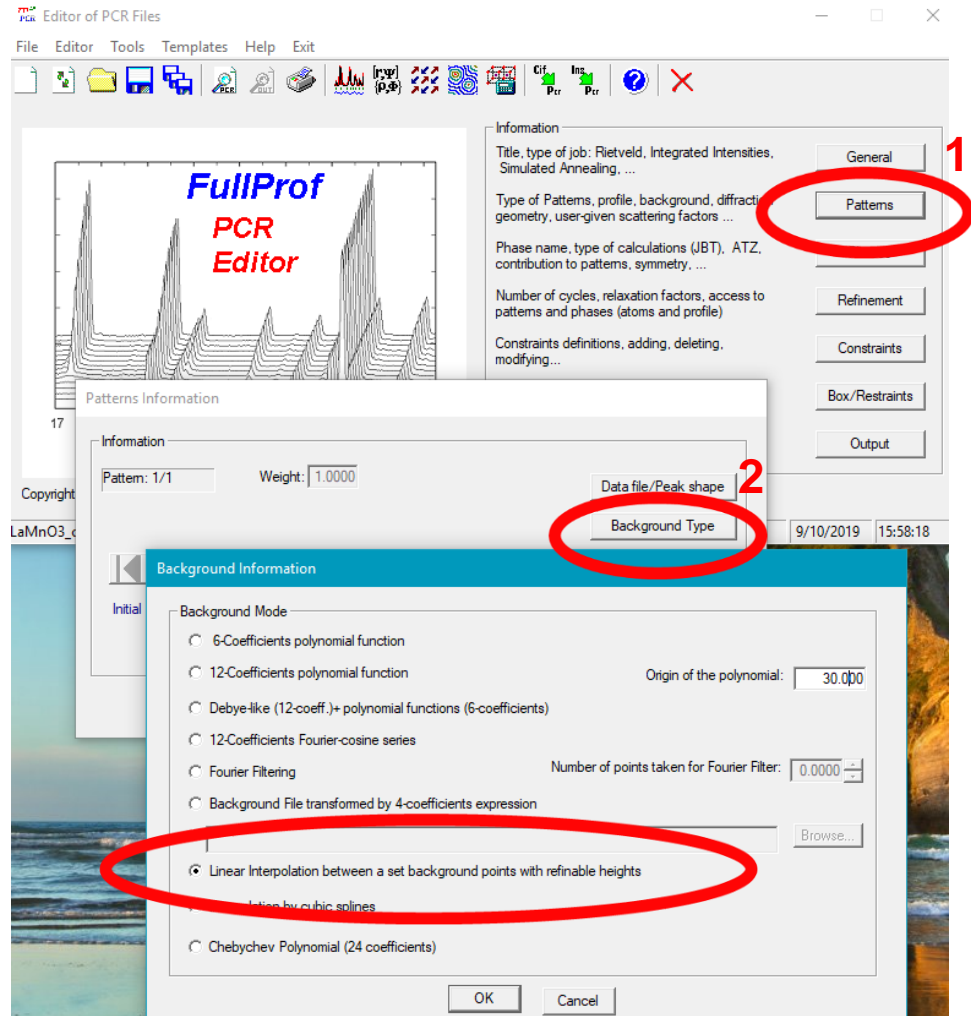
- Patterns → Data file/Peak Shape → Refinement/Simulation
- **[3]** Select Neutron – CW
- **[4]** Wavelength is 2.597 Å



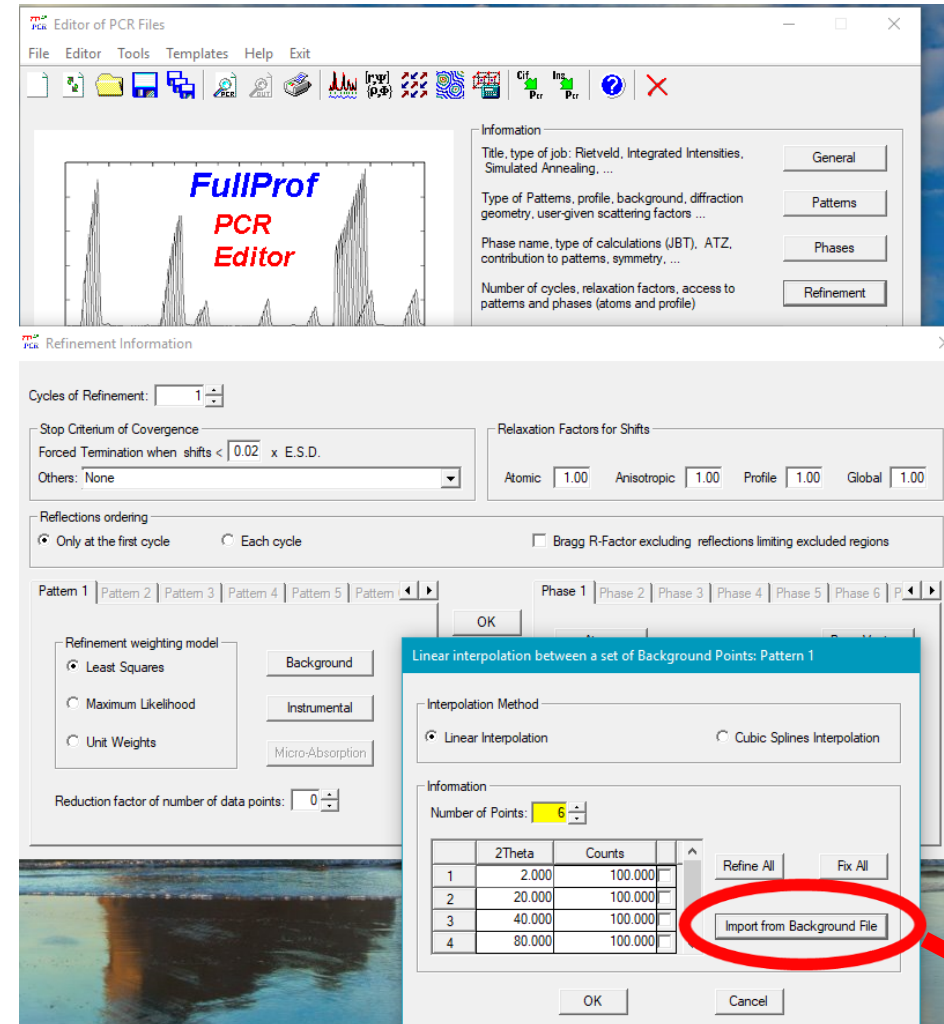
Step 3: Refining the magnetic structure with Fullprof

- 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

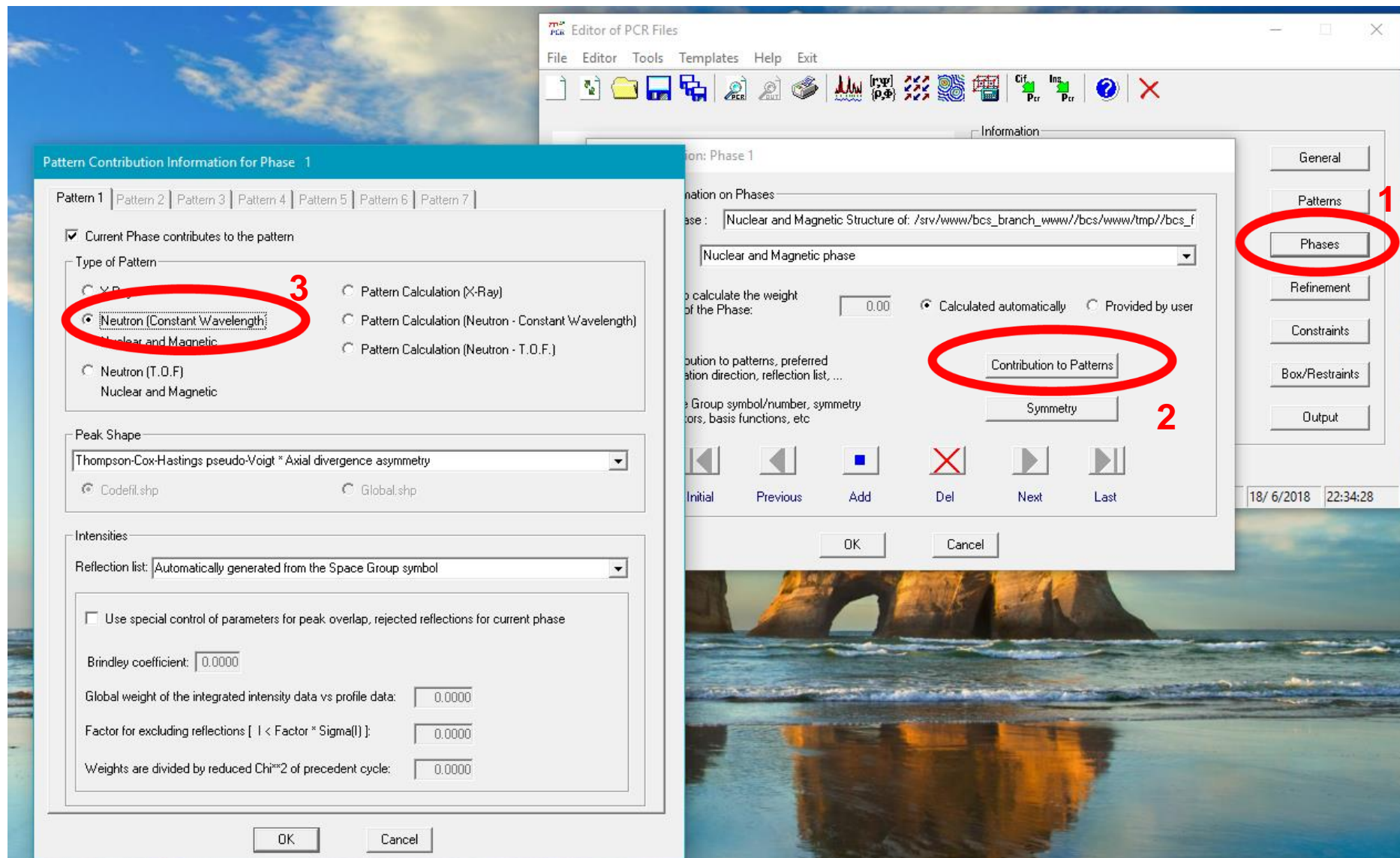
- Add excluded regions (see nuclear pcr)

The screenshot displays the FullProf PCR Editor software interface. The main window shows a plot of diffraction patterns with the text "FullProf PCR Editor" overlaid. On the right, the "Information" panel is open to the "Patterns" tab, which is circled in red and labeled with a red "1". Below this, the "Patterns Information" dialog box is open, showing the "Exclude Regions" button circled in red and labeled with a red "2". The "Exclude Regions: Pattern 1" dialog box is also open, showing the "Number of Excluded Regions" set to 3, circled in red and labeled with a red "3". The dialog box contains a table with the following data:

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

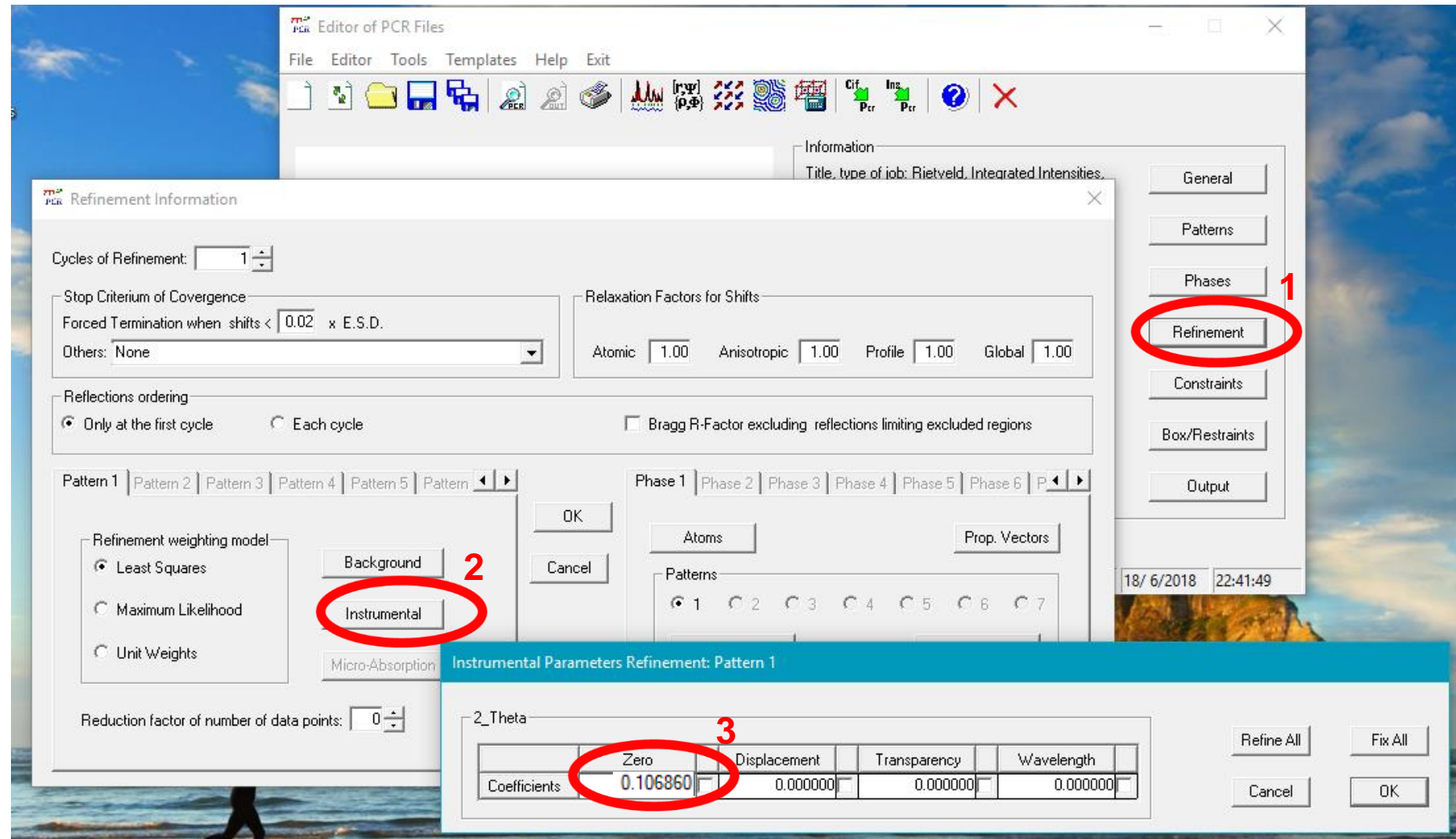
Step 3: Refining the magnetic structure with Fullprof

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



Step 3: Refining the magnetic structure with Fullprof

- Instrumental zero value
(See nuclear refinement:
0.10686)



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
[Icons]
! 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/bcs/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
!
!Atm 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 MMH2 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 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 B0w 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
5.00 152.900 1
```


Step 3: Refining the magnetic structure with Fullprof

- In “Refinement”
→ “atoms” input
thermal
parameters (0.3).
[1,2,3]

- $\text{Re}(x)$, $\text{Re}(y)$,
 $\text{Re}(z)$ can all
contribute, so
should all be
checked.

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

	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

Refine scale and lattice constants
Set number refinement cycles

FullProf PCR Editor

Information
Title, type of job: Rietveld, Integrated Simulated Annealing, ...
Type of Patterns, profile, background geometry, user-given scattering factors
Phase name, type of calculations contribution to patterns, symmetry
Number of cycles, relaxation factors, patterns and phases (atoms and profile)

Refinement Information
Cycles of Refinement: 10
Stop Criterion of Convergence
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

Profile Parameters: Phase 1 Pattern 1

Factors
Scale 0.0617
Overall B-factor 0.0000

Unit Parameters
a 5.749641
b 7.669311
c 5.537108
alpha 90.000
beta 90.000
gamma 90.000

FWHM / Shape Parameters
FWHM Parameters
U 0.076778
V -0.277888
W 0.398159
IG 0.000000
Shape Parameters
X 0.048260
Y 0.000000
SZ 0.000000
Refine FWHM for second wavelength
U2 V2 W2

Phase 1 Phase 2 Phase 3 Phase 4 Phase 5 Phase 6
Atoms Prop. Vectors
Patterns
1 2 3 4 5 6 7
Profile Micro-Structure
HKL Shifts Further Parameters

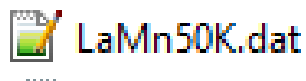
Refine All
Fix All
Cancel
OK

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.

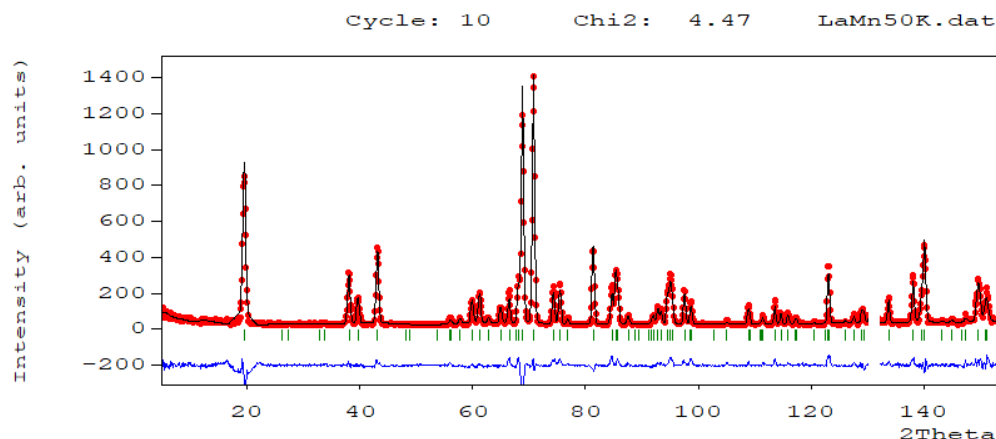
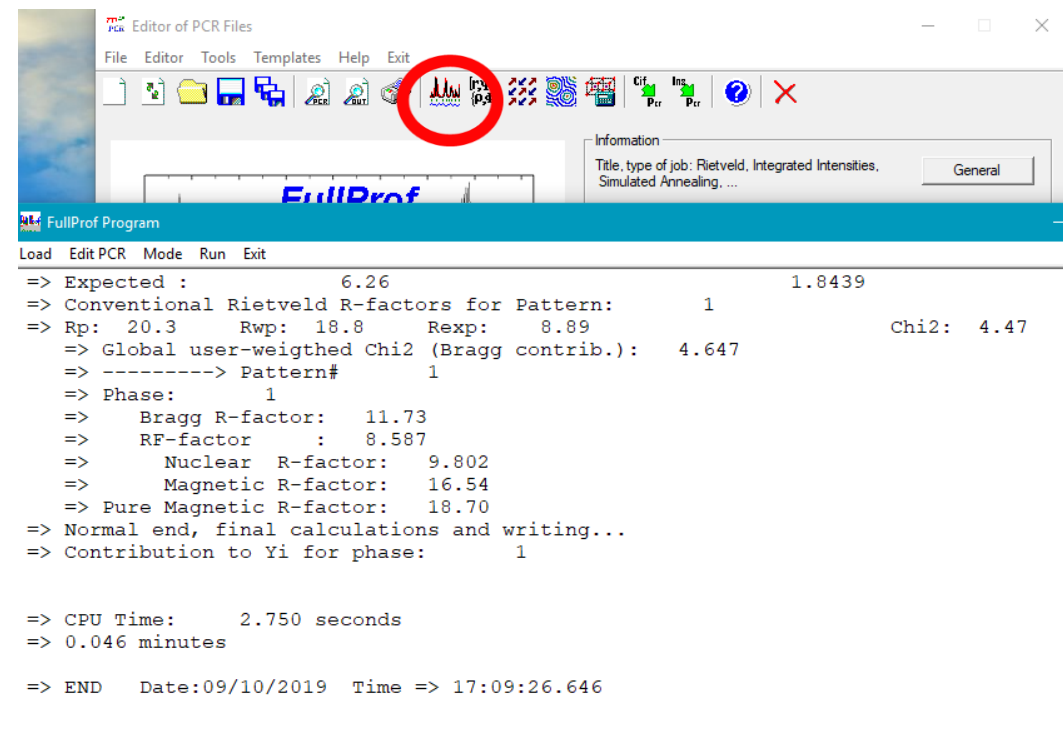
The orthorhombic space group has $b > a > c$ (converted from Pbnm of nuclear example)

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.

