

# Magnetic Space Group refinement in FullProf of the commensurate magnetic structure in $\text{Ho}_2\text{BaNiO}_5$ data

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MagStr 2022, ORNL

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U.S. DEPARTMENT OF  
**ENERGY**

- This example has files in the folder “Ho2Ba2NiO5\_MagSpaceGroup”
- In the folder “Ho2Ba2NiO5\_RepAnalysis” There are other example slides that use the alternative representational analysis approach that will be introduced later in the week.
- These can be worked through to see how the different approaches are applied to give the SAME magnetic structure.

Name	Date modified	Type	Size
 Ho2Ba2NiO5_MagSpaceGroup	10/1/2022 2:19 PM	File folder	
 Ho2Ba2NiO5_RepAnalysis	10/1/2022 12:55 PM	File folder	

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

- This example will use the magnetic space group approach to combine Fullprof with results from the Bilbao Crystallographic Server.

Ho2Ba2NiO5\_MagSpaceGroup  
Ho2Ba2NiO5\_RepAnalysis

- There is a Ho<sub>2</sub>BaNiO<sub>5</sub> example using representation analysis (SARAh and Basirep) we will do too to show the different approaches.
- Data and notes are included for you to try both!**

## Magnetic structure determination of Ho<sub>2</sub>BaNiO<sub>5</sub> using FullProf Suite and SARAh



Orthorhombic ( Space group: *Immm*)  
 $a=3.764 \text{ \AA}$ ,  $b=5.761 \text{ \AA}$ ,  $c=11.336 \text{ \AA}$

NiO<sub>6</sub> octahedra form chains along the a-axis.

3D Antiferromagnetic ordering at  $T_N \sim 53 \text{ K}$

Eur. Phys. J. B 24, 59-70 (2001)

THE EUROPEAN  
PHYSICAL JOURNAL B  
EDP Sciences  
© Società Italiana di Fisica  
Springer-Verlag 2001

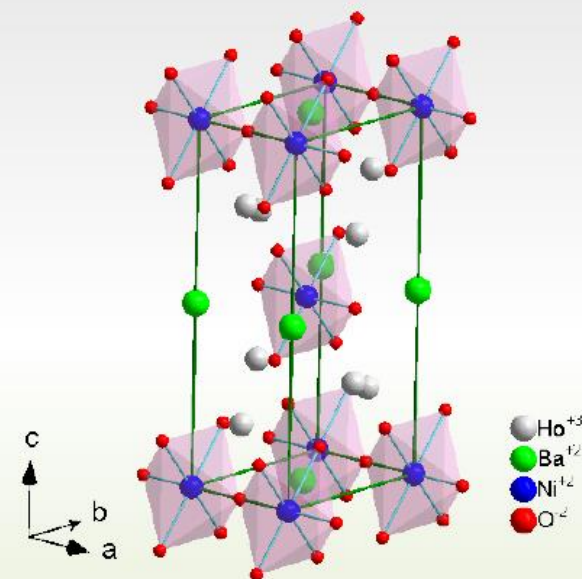
### Neutron diffraction study of the magnetic ordering in the series R<sub>2</sub>BaNiO<sub>5</sub> (R = Rare Earth)

E. García-Matres<sup>1,a</sup>, J.L. Martínez<sup>2</sup>, and J. Rodríguez-Carvajal<sup>3,b</sup>

<sup>1</sup> Institut Laue-Langevin, BP 156, 38042, Grenoble Cedex, France

<sup>2</sup> Instituto de Ciencia de Materiales (CSIC), Fac. Ciencias (C-4), Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>3</sup> Laboratoire Léon Brillouin (CEA-CNRS), Centre d'Études de Saclay, 91191 Gif-sur-Yvette Cedex, France



Atom	Wyck.	Site	x/a	y/b	z/c
Ho	4j	mm2	1/2	0	0.2025(4)
Ni	2a	mmm	0	0	0

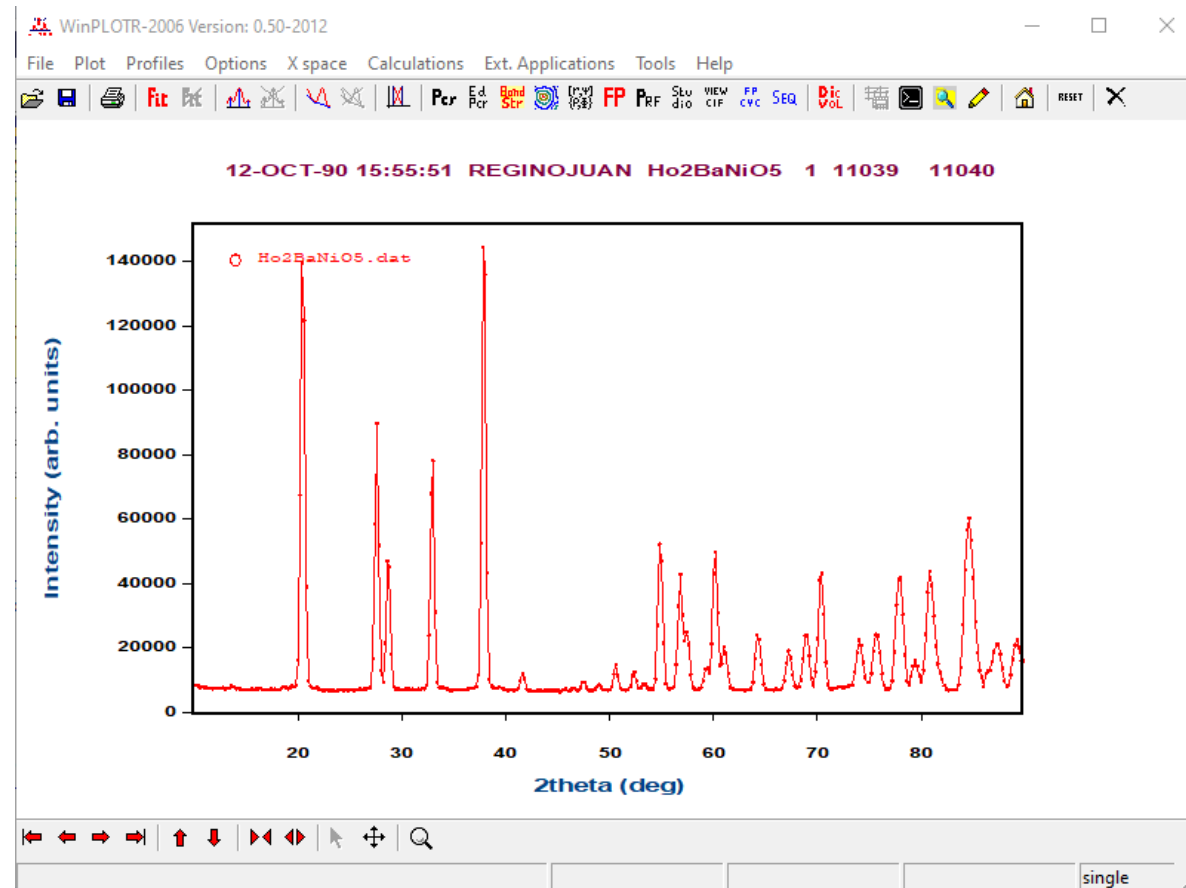


MAGSTR Workshop, Knoxville, TN 2014



# Details of this $\text{Ho}_2\text{BaNiO}_5$ example

- Neutron powder diffraction data collected on D1B at the ILL at 1.5 K using  $\lambda = 2.524 \text{ \AA}$
- Files included in example:
  - Datafile: **Ho2BaNiO5.dat**
  - Instrument resolution file: **d1b\_ill.irf**
  - Crystallographic Information File: **Ho2BaNiO5.cif**



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

- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - Step 3: Create test magnetic space groups using MAXMAGN on the Bilbao Crystallographic Server. mcif file created.
  - Step 4: Convert the mcif file into a .pcr file using mCIF2PCR.
  - Step 5: Use the created .pcr file to fit the nuclear and magnetic neutron data using Fullprof to determined the magnetic structure.

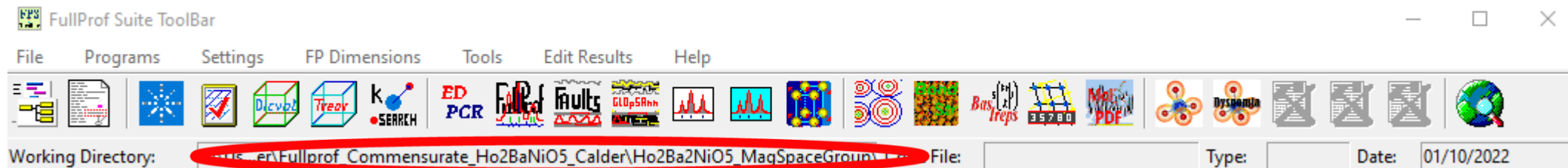
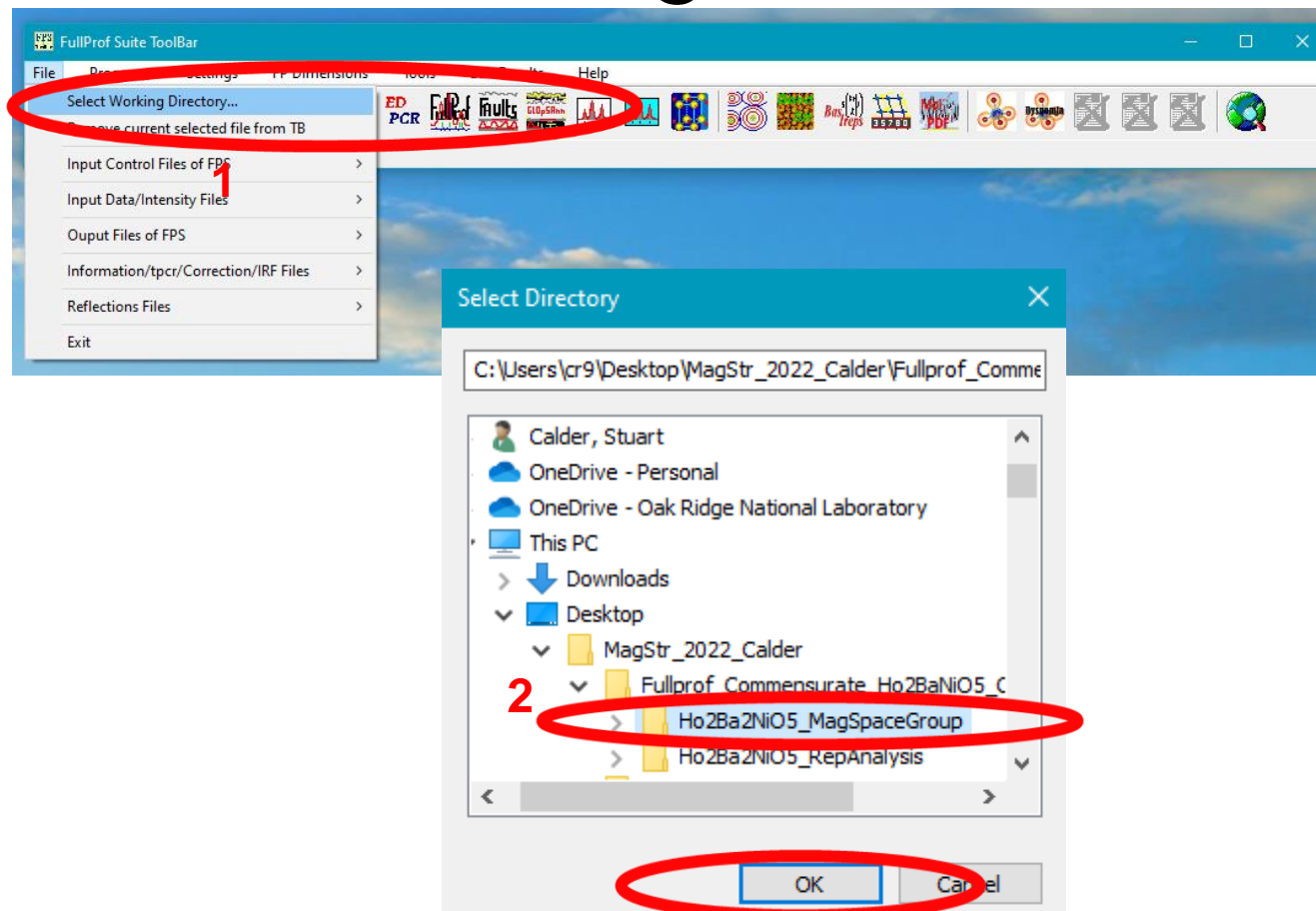
# Ho<sub>2</sub>BaNiO<sub>5</sub>

- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
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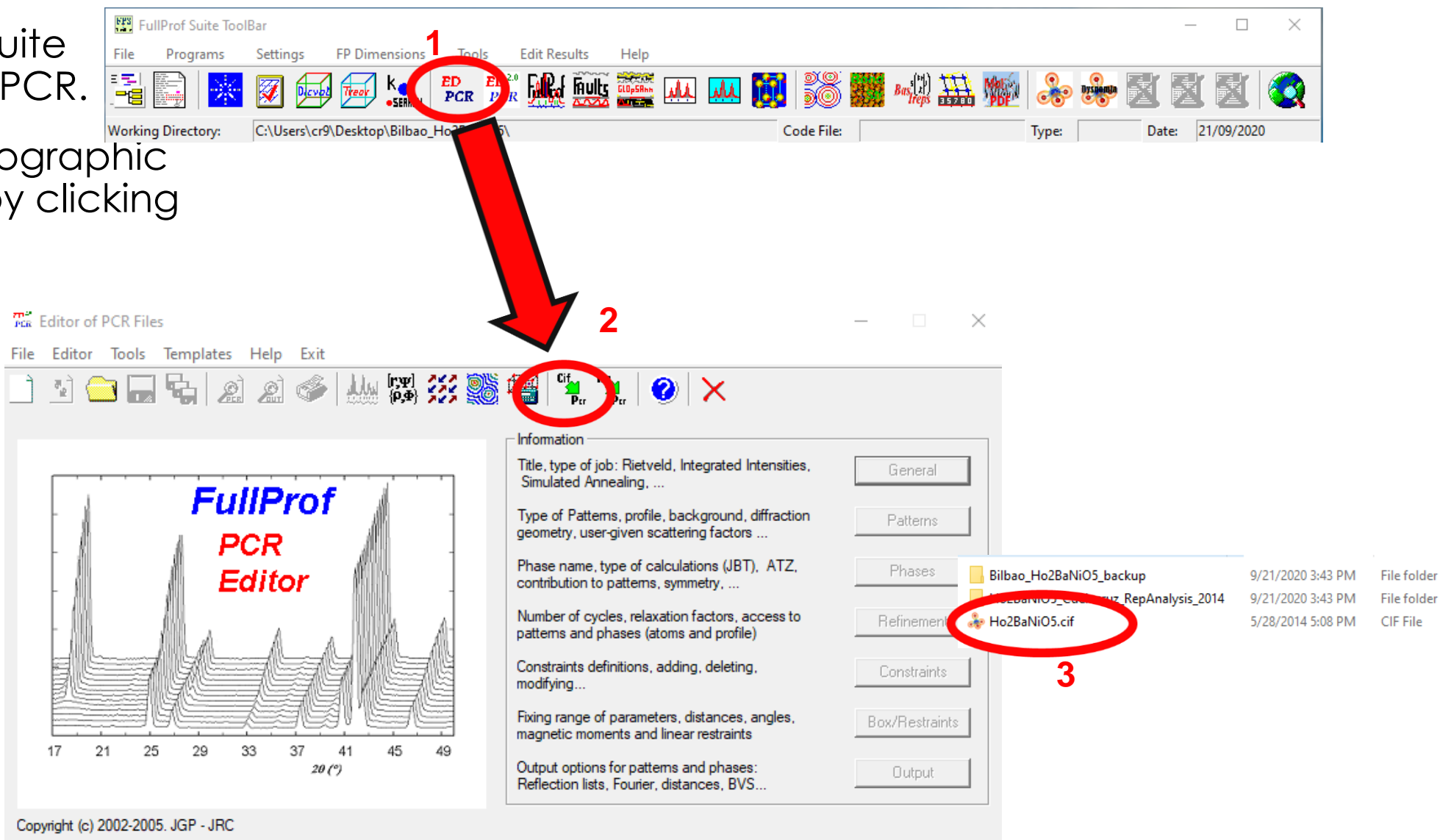
# Step 1: Refine the crystal structure using FullProf

- Open Fullprof Suite toolbar.
  - **1.** Select working directory with data  
“File>Select Working directory...”
  - **2.** Browse to wherever your folder  
“Ho2Ba2NiO5\_MagSpaceGroup” is located on your computer and select “ok”
  - **3.** Path on FP studio toolbar should now be updated. This helps with interacting with other features of Fullprof



# Step 1: Refine the crystal structure using FullProf

- 1. From FullProf Suite Toolbar open EdPCR.
- 2. Import crystallographic information file by clicking on “CIF→PCR”
- 3. Select the file “Ho2BaNiO5.cif”

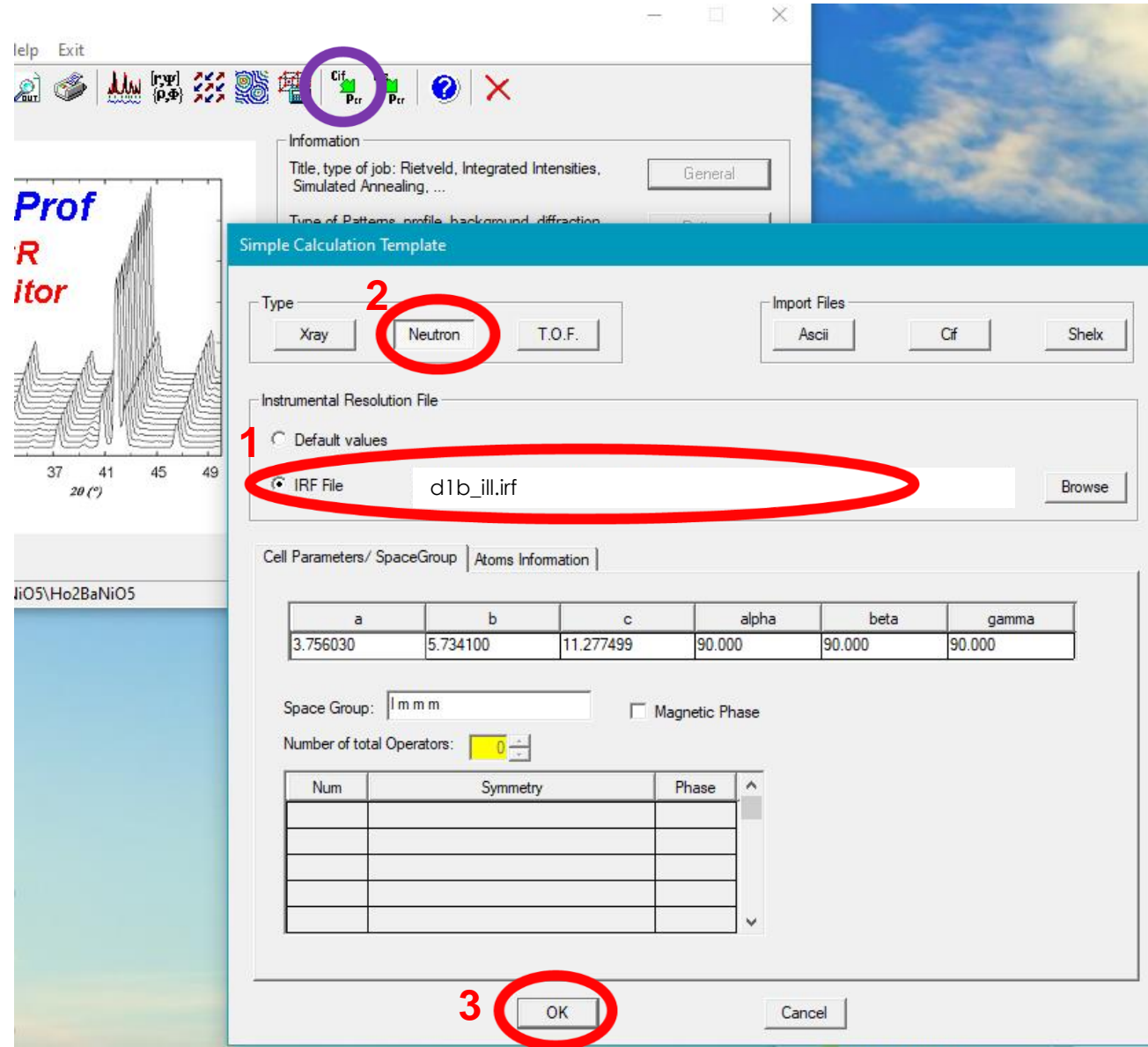




# Step 1: Refine the crystal structure using FullProf

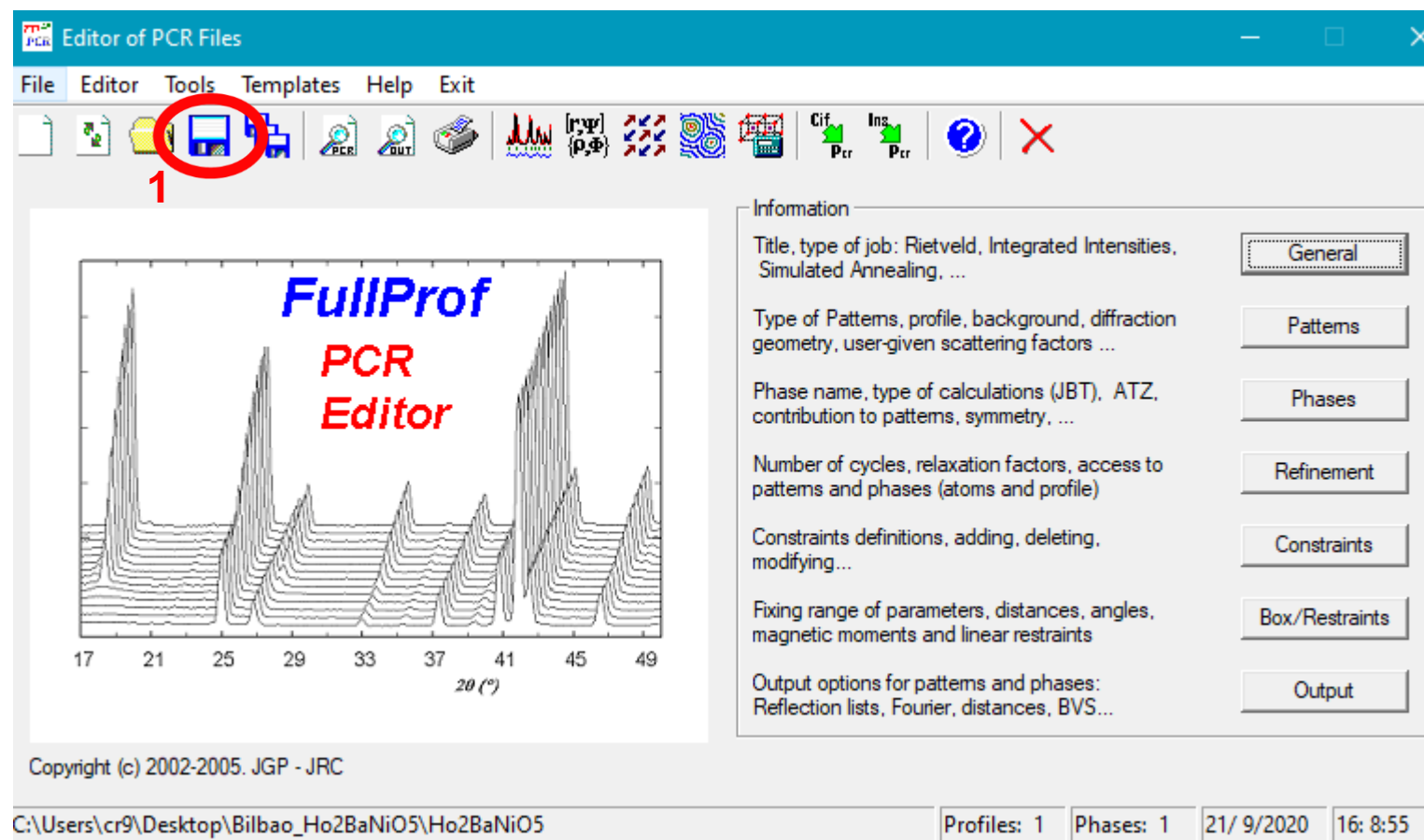
Cif→PCR open a window to input instrument and shows structural info.

- 1. Load the instrument resolution file “d1b\_ill.irf”. *NOTE: remove the full path to just keep “dib\_ill.irf”. If you don’t and move the pcr file to a different directory (or share the pcr with someone else) it will create problems*
- 2. Change “Type” to “Neutron” for constant wavelength
- Starting **Cell Parameters**, **Space Group** and **Atoms Information** are now loaded.
- Note: occ = site multip./general multip. Always check this has been correctly calculated after importing the .cif file.
- 3. Hit “OK”



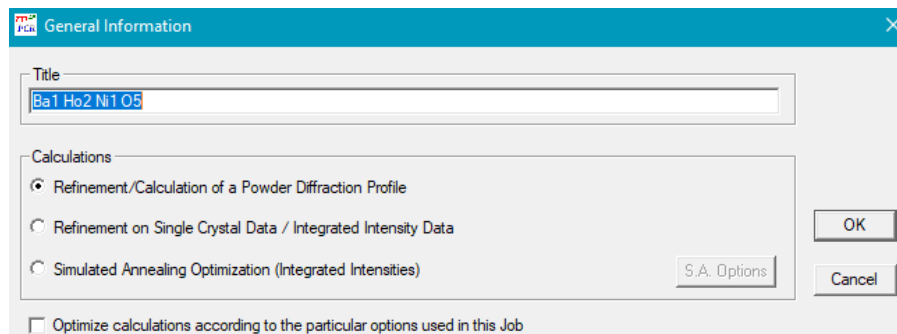
# Step 1: Refine the crystal structure using FullProf

- **1.** Save the changes.
- This should be done whenever changes are made in the GUI.



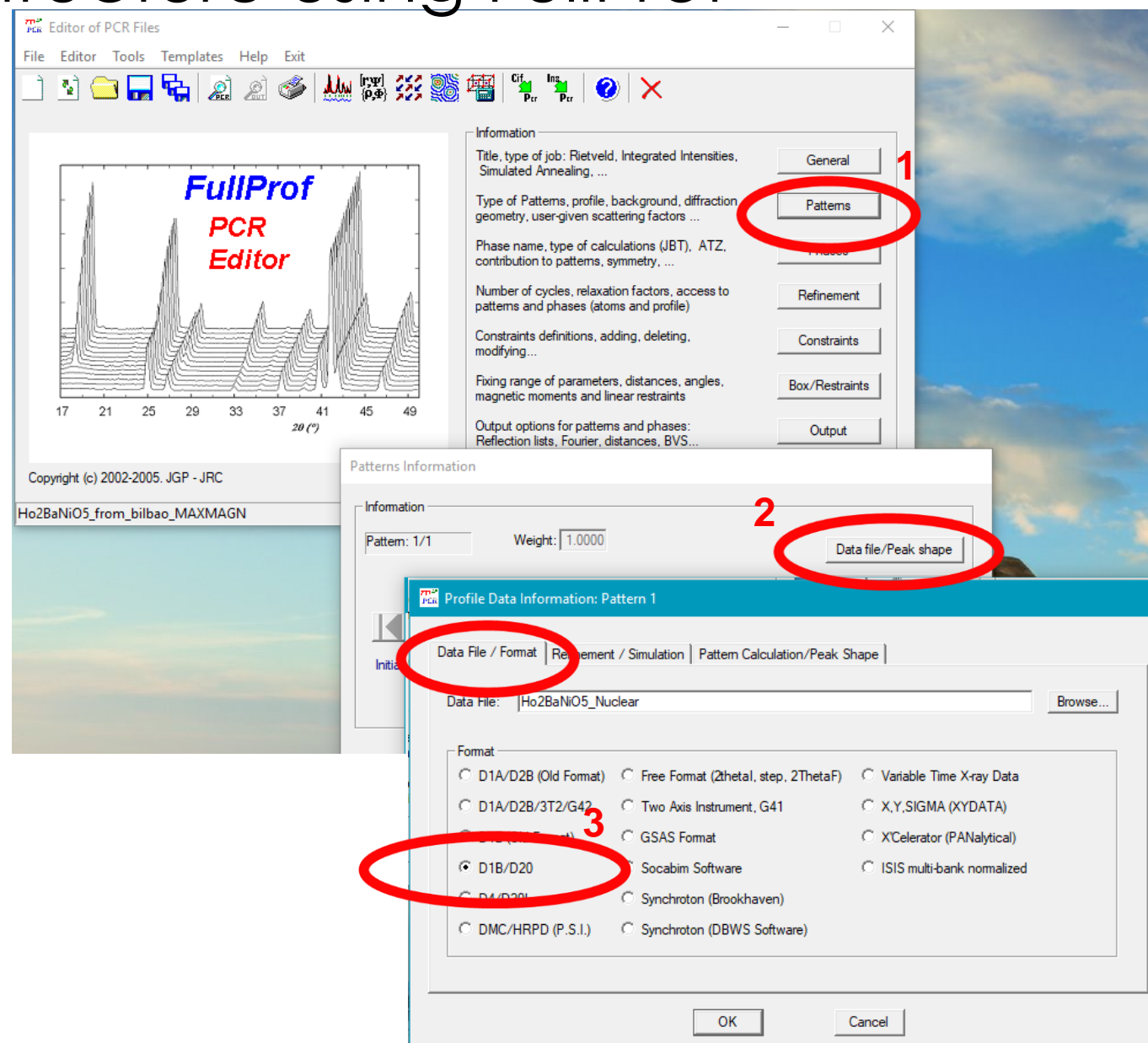
# Step 1: Refine the crystal structure using FullProf

“General” tab has refinement of powder data as default. Can edit title as wanted.



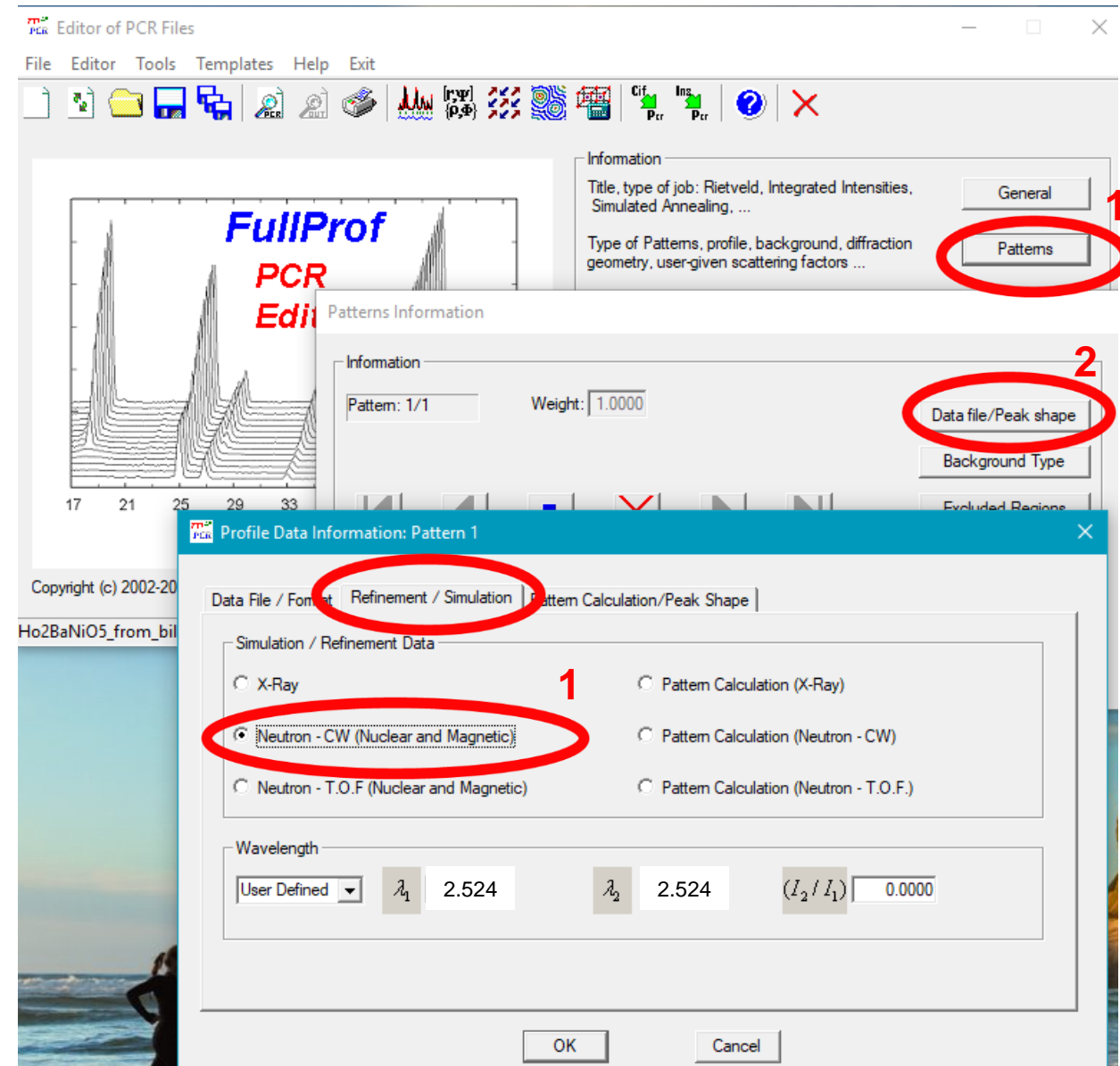
## 1. “Patterns” tab

- 2. Select the format of the data file Fullprof should refine.
- 3. Patterns → Data file/Peak Shape → D1B/D20



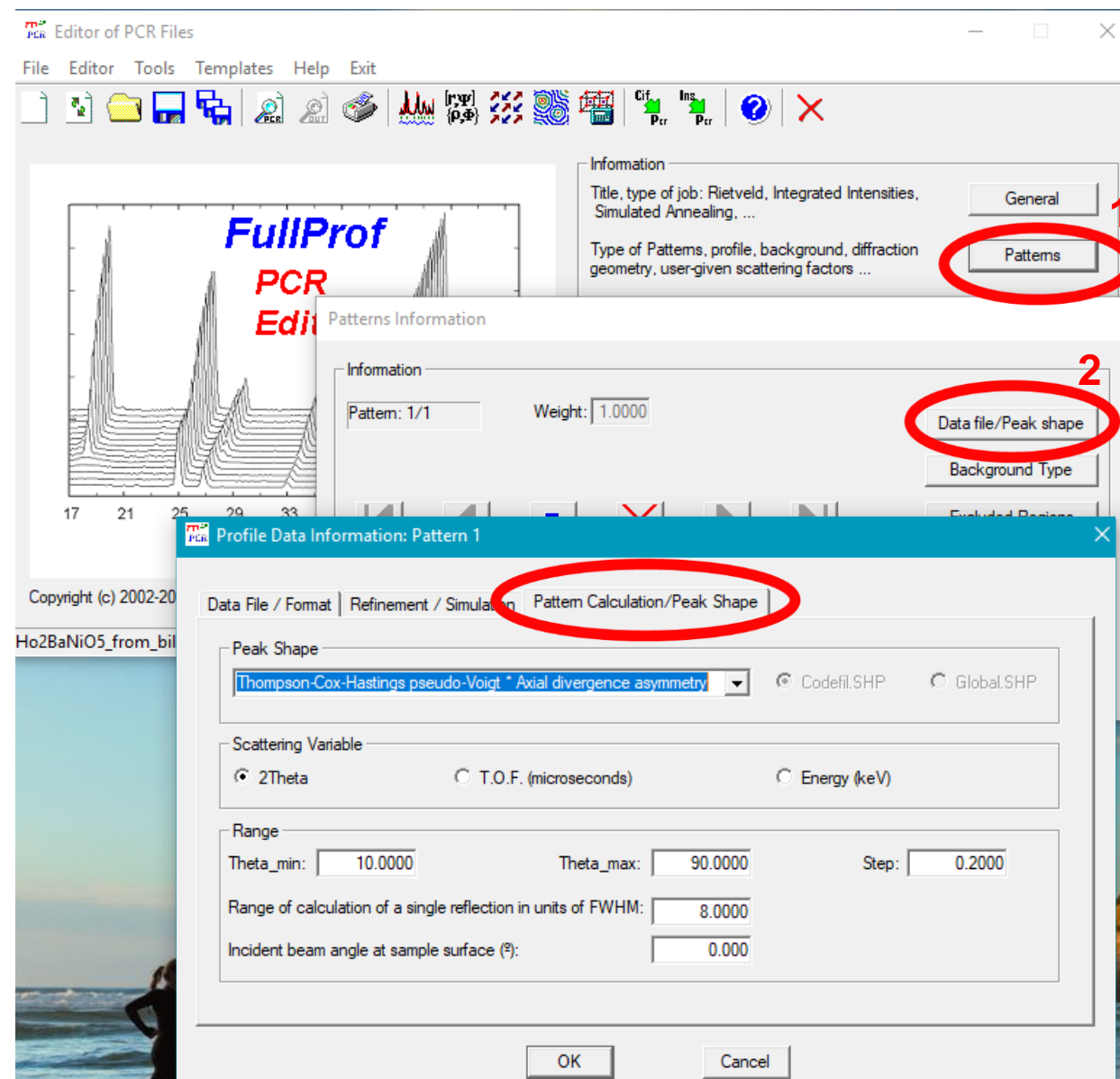
# Step 1: Refine the crystal structure using FullProf

- Patterns → Data file/Peak Shape → Refinement/Simulation
- **[1]** Select Neutron – CW
- Wavelength is already set by irf file, 2.524 in this example.



# Step 1: Refine the crystal structure using FullProf

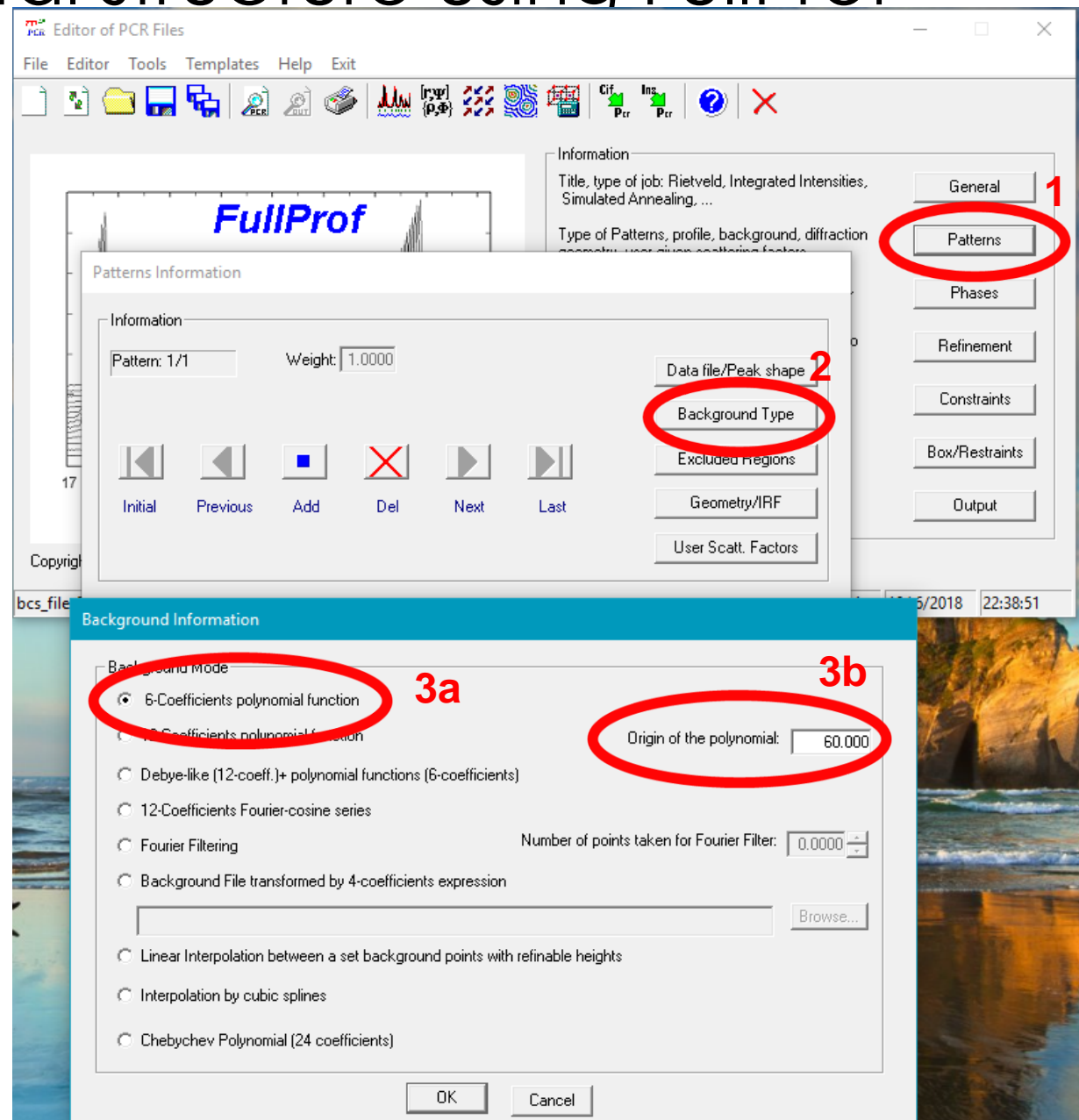
- Check final tab:
- Patterns → Data file/Peak Shape → Pattern Calculation/Peak Shape
- Peak shape is already loaded from irf file.





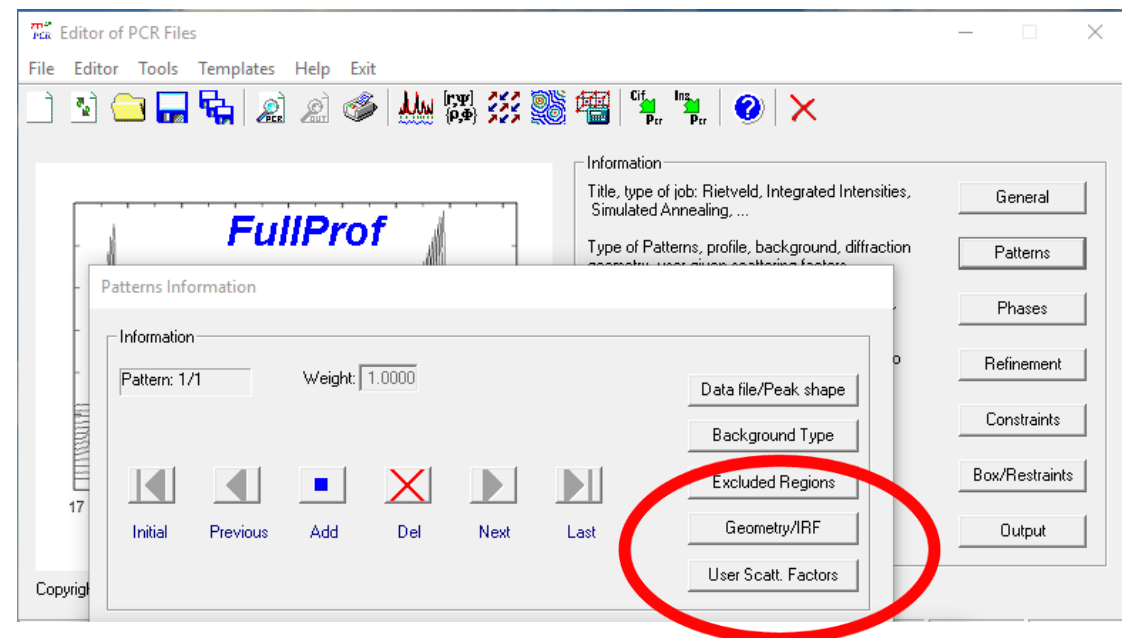
# Step 1: Refine the crystal structure using FullProf

- Move to next tab down to select background type
- Patterns → Background Type  
Check “6-coefficient”
- Put origin of polynomial at 60 for this example.

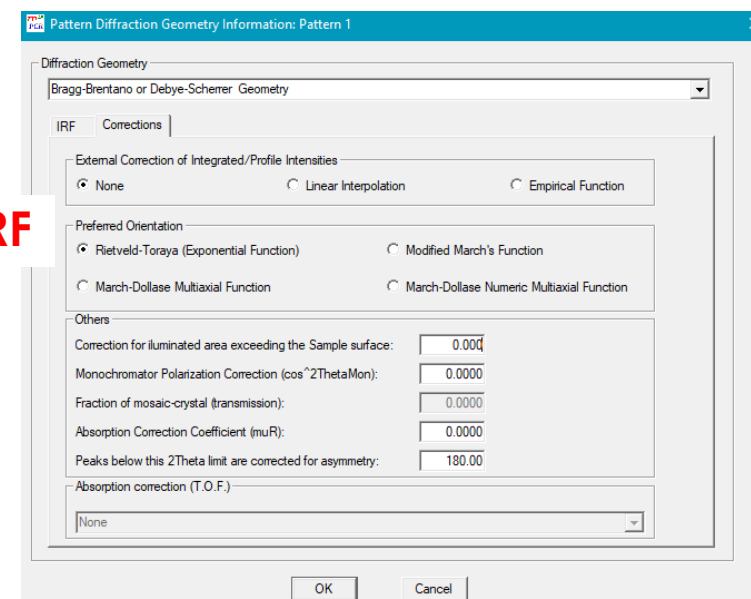


# Step 1: Refine the crystal structure using FullProf

- No further editing should be needed of the remaining “Patterns” tabs:
  - Excluded Region  
Use with care, but can cut out background.
  - Geometry/IRF  
*Populated by irf file.*  
Can add absorption if needed. Check <https://www.ncnr.nist.gov/resources/activation/>  
*Note: if refining asymmetry then go to “Corrections” tab and change “Peaks below this 2Theta limit are corrected for asymmetry” to 180. This is not needed for this example.*
  - User Scatt. Factors  
This can be used to add e.g. a form factor that isn't tabulated



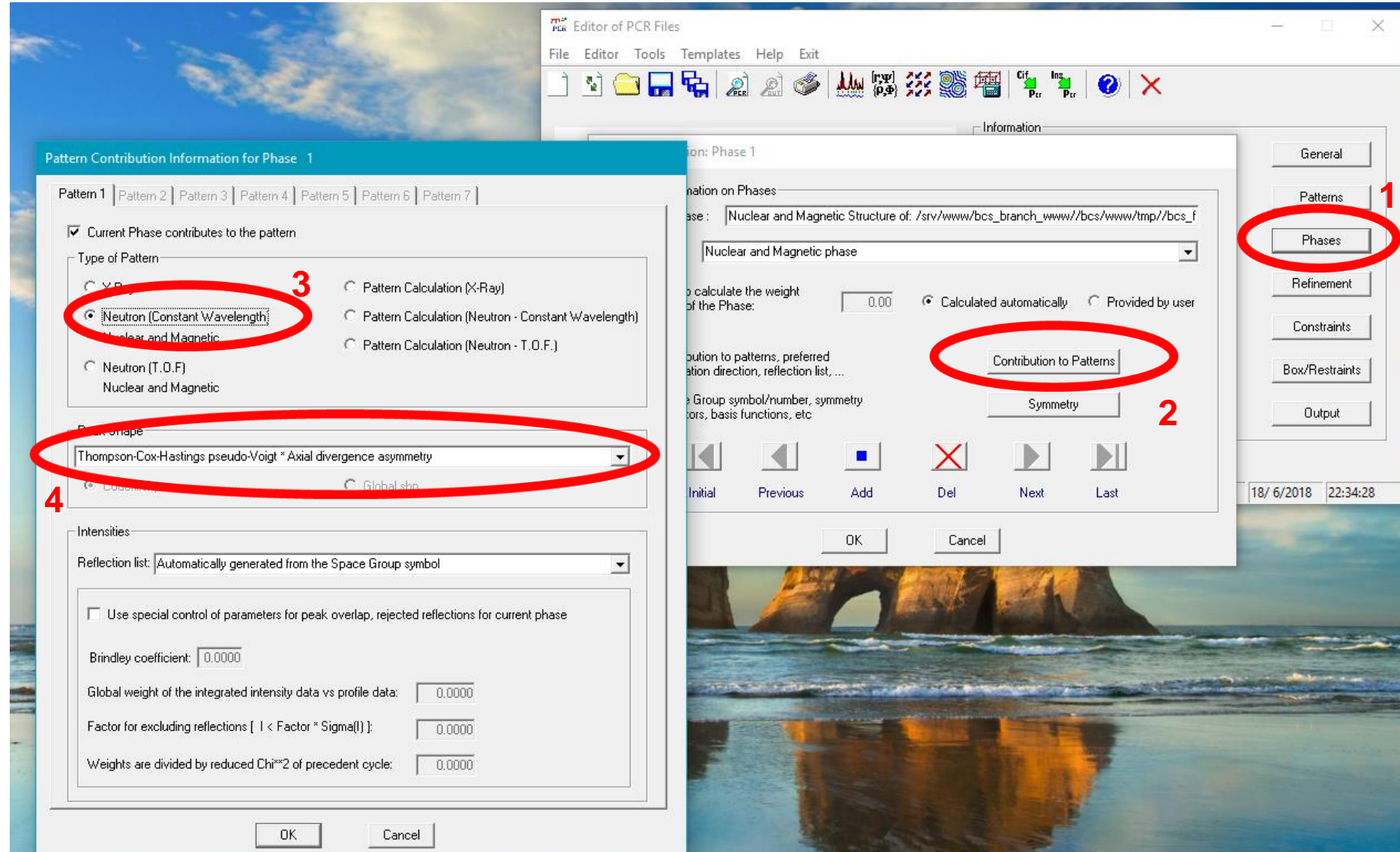
**Geometry/IRF**



# Step 1: Refine the crystal structure using FullProf

## PHASES tab

- Make phase contribute to refinement.
- **[1]** Phases → **[2]** Contribution to Patterns → **[3]** Neutron (constant wavelength)
- Set peak shape to “**Thompson-Cox-Hastings pseudo-Voigt**”



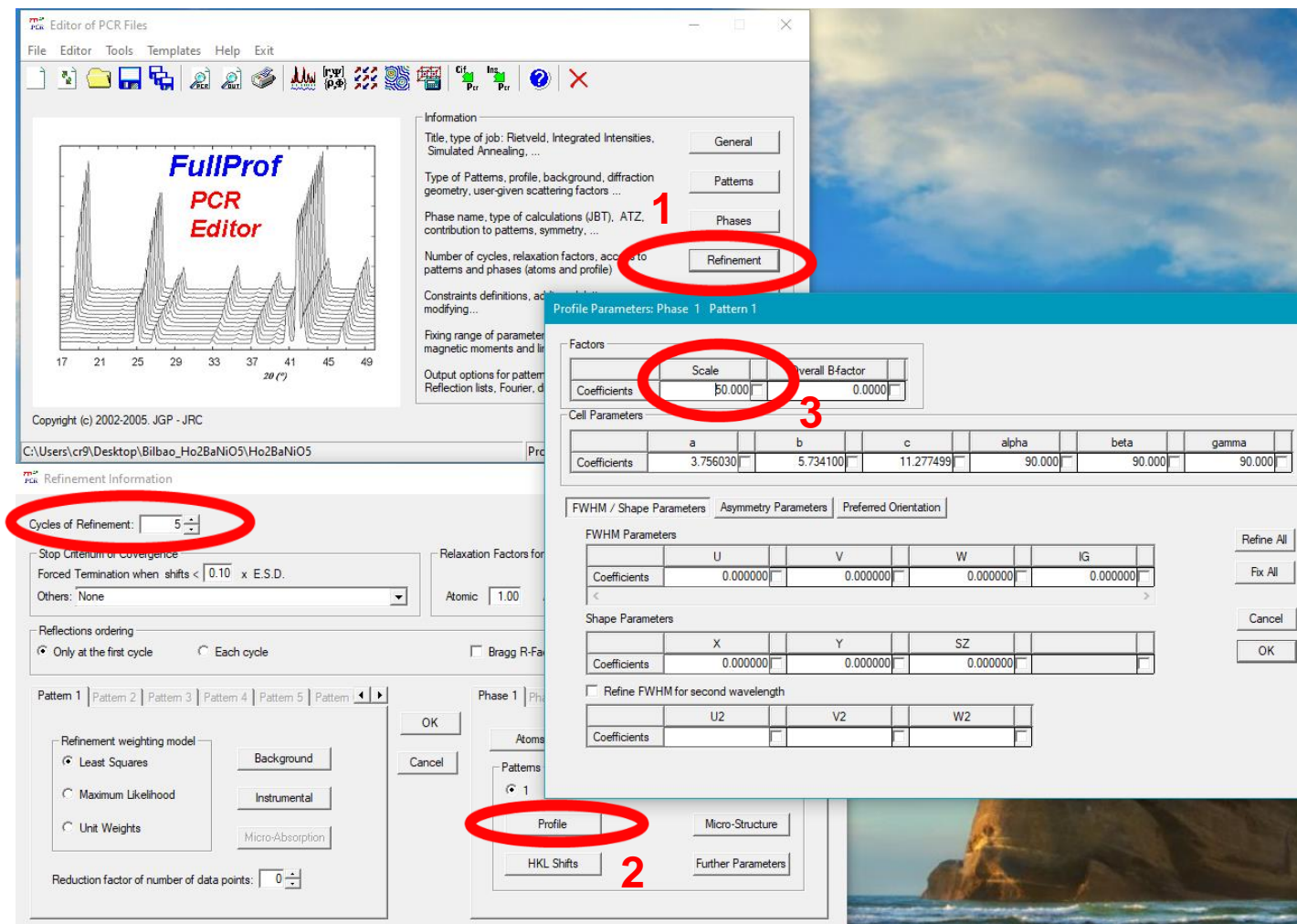
## REFINEMENT tab:

- 
- The screenshot shows the Jmol 14.1.105 Refinement Information dialog box. The 'Refinement' button is circled in red (1). The 'Background' button is circled in red (2). The '6 Coefficients Polynomial Background: Pattern 1' dialog box is open, showing a table of coefficients with 'd\_0' set to 7000. The 'Background' button is circled in red (3). A plot of the diffraction pattern is visible in the bottom left corner.



# Step 1: Refine the crystal structure using FullProf

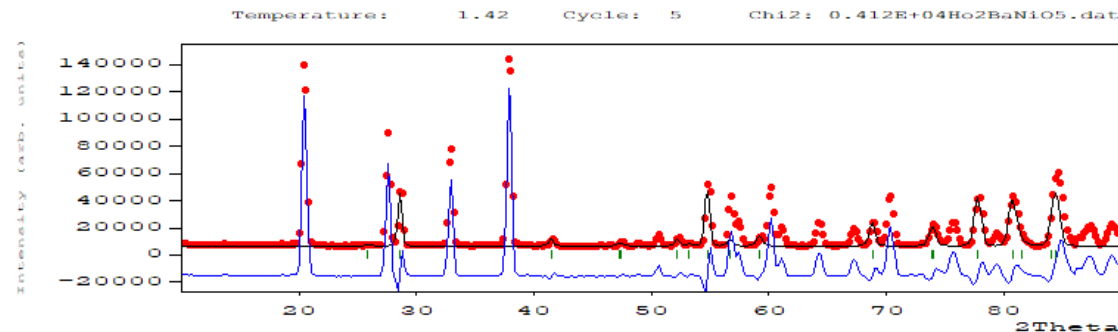
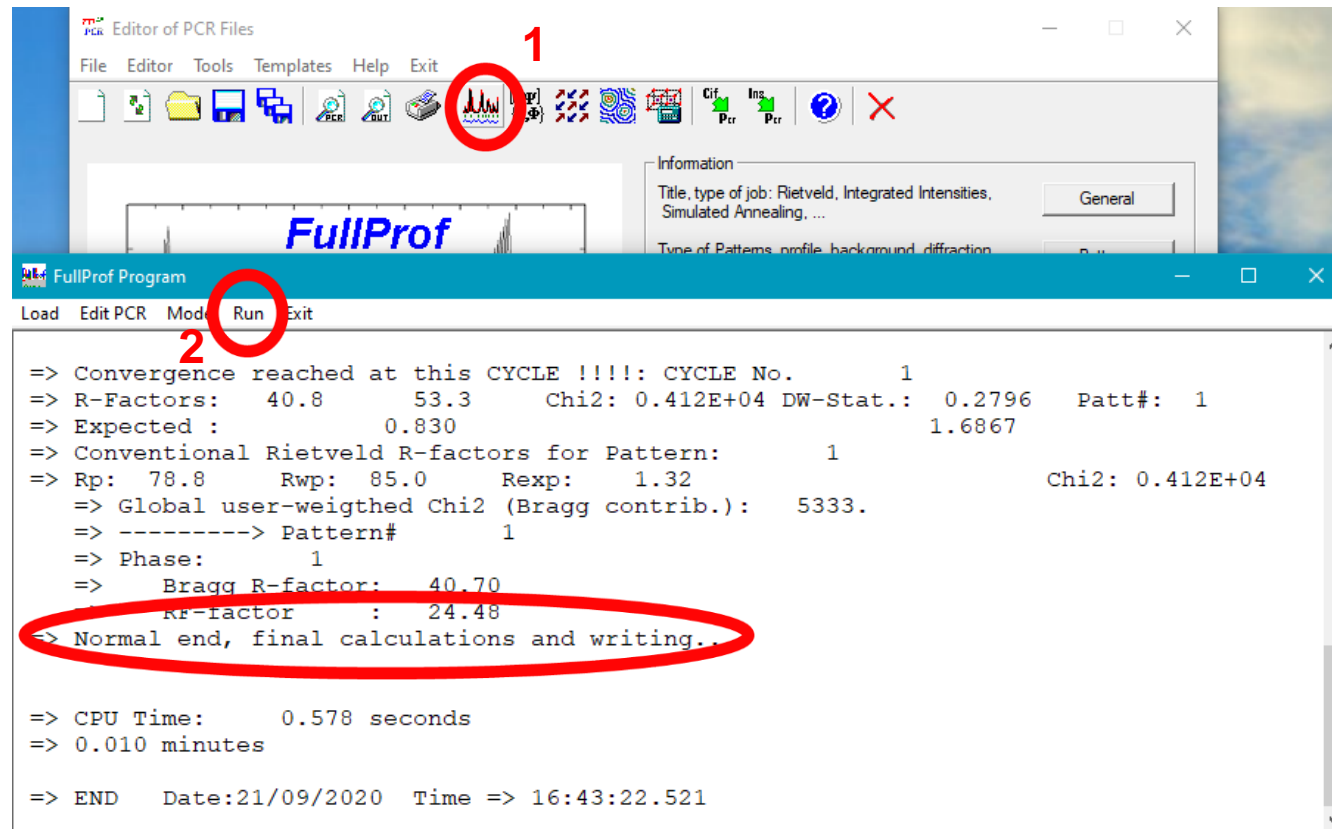
- Select “Refinement” tab again. Update “Cycle of Refinement” to 5
- From “Refinement” tab select: Refinement>Profile
- Change scale to 50.





# Step 1: Refine the crystal structure using FullProf

- 1. Can now run the refinement  
Select the “*Ho2BaNiO5.dat*” data
  - Note: we have not set anything to refine yet. It is good to check your model is close to the data and makes sense before refining.
- 2. Refinement runs for the number of cycles (in this case 5). You can repeat this by pushing run until “Normal end, final calculation and writing...” shows rather than “Convergence not reached”



# Step 1: Refine the crystal structure using FullProf

- Now allow the following to refine to fit the nuclear crystal:
  - Scale factor (*Refinement>Profile*)
  - Lattice parameters (*Refinement>Profile*)
  - Background (*Refinement>Background*)
  - 2theta zero. (*Refinement>Instrumental*)
- Can also try to refine atomic parameters (but in this case data may not have enough reflections to be stable):  
Refinement → Phase tab → Atoms

Checking the box turns the number **blue** to show they are set to refine. If they are **red** then they are constrained to refine with another parameter. Looking in the text of the pcr file shows refined parameters by codes ending in 1.

Those constrained have the same code e.g. 11 and 11 or 511 and 511.

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	52.856 ✓	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	3.751848 ✓	5.733387 ✓	11.270996 ✓	90.000	90.000	90.000

FWHM / Shape Parameters Asymmetry Parameters Preferred Orientation

FWHM Parameters

	U	V	W	IG
Coefficients	0.000000	0.000000	0.000000	0.000000

Refine All Fix All

6 Coefficients Polynomial Background: Pattern 1

	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients	7000.0 ✓	0.0000 ✓	0.0000 ✓	0.0000	0.0000	0.0000

	d_6	d_7	d_8	d_9	d_10	d_11
Coefficients						

Refine All Fix All

Instrumental Parameters Refinement: Pattern 1

2\_Theta

	Zero	Displacement	Transparency	Wavelength
Coefficients	0.000000 ✓	0.000000	0.000000	0.000000

Refine All Fix All Cancel OK

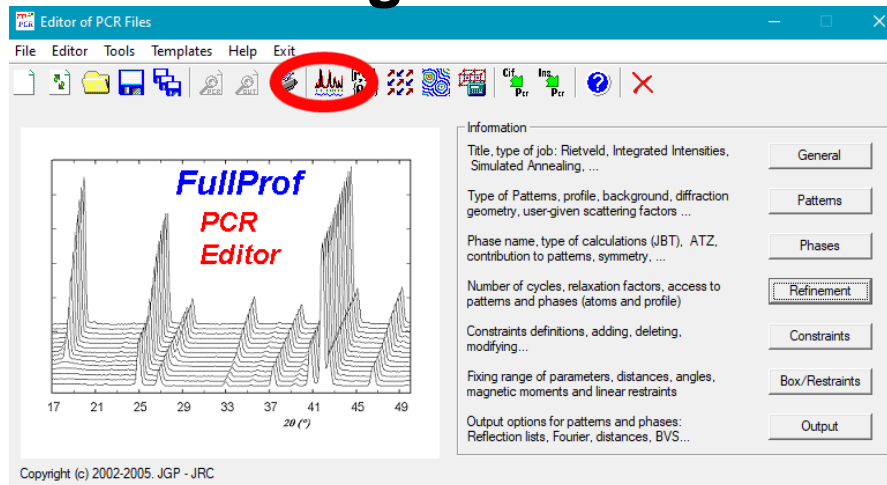
List of Atoms

Number of Atoms: 5

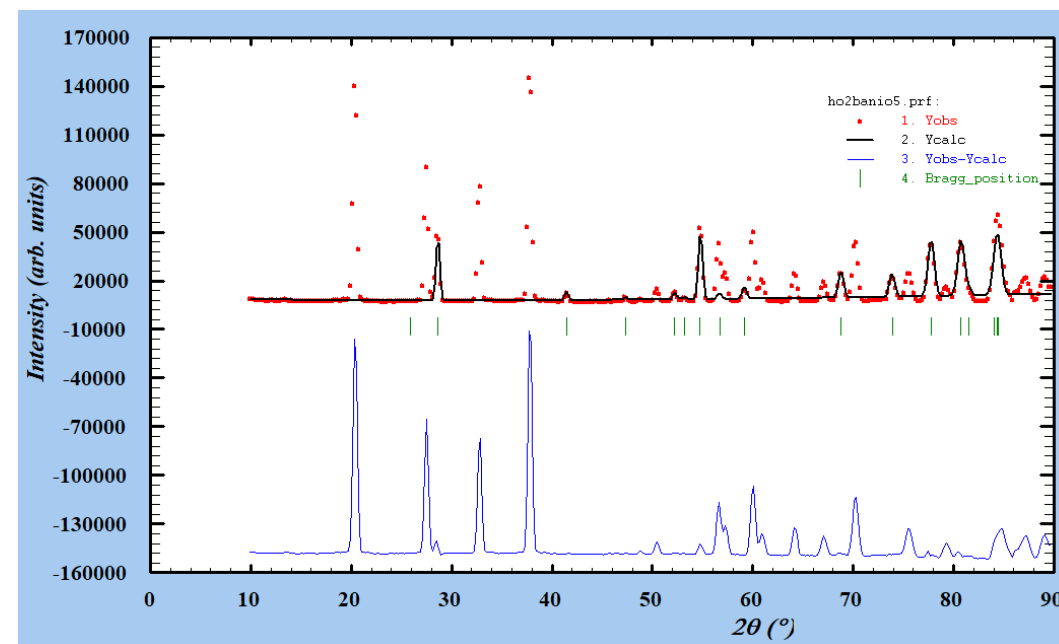
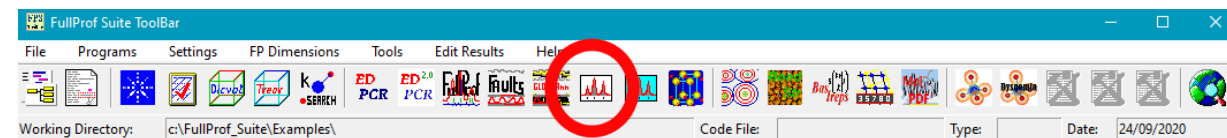
	Label	Ntyp	X	Y	Z	B	Occ	Them. Fact.
Atom # 1	Ho1	Ho	0.50000	0.00000	0.20250 ✓	0.00000	0.25000	Isotropic
Atom # 2	Ba1	Ba	0.50000	0.50000	0.00000	0.00000	0.12500	Isotropic
Atom # 3	Ni1	Ni	0.00000	0.00000	0.00000	0.00000	0.12500	Isotropic
Atom # 4	O1	O	0.00000	0.24140 ✓	0.14950 ✓	0.00000	0.50000	Isotropic

# Step 1: Refine the crystal structure using FullProf

## Run refinement again



- Check refinement in WinPlotr
- Several unindexed reflections (green tick marks) that are magnetic.
  - Ho in particular has a very large magnetic moment.
  - In an experiment would perform temperature dependence to check nature of peaks.

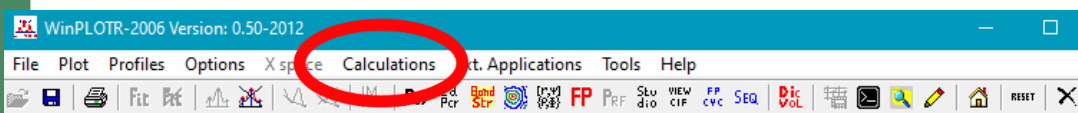


# Ho<sub>2</sub>BaNiO<sub>5</sub>

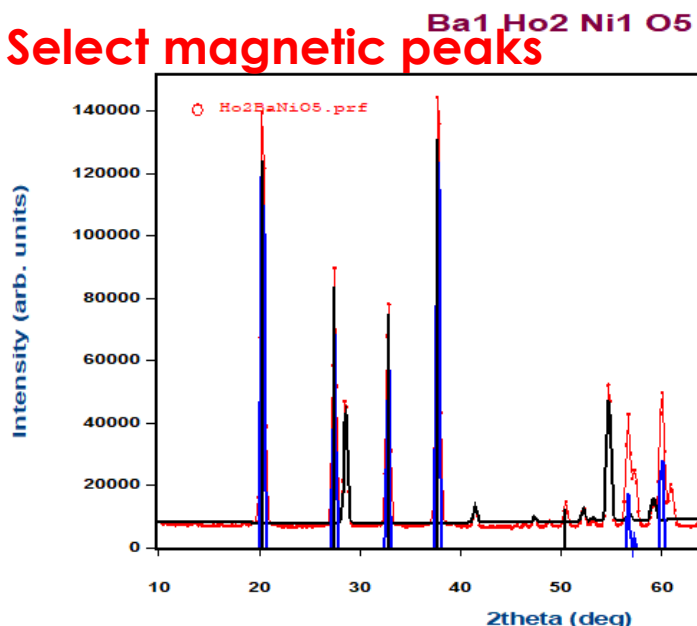
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# Determine the k-vector

- Now the magnetic peaks need to be indexed to find the propagation vector that defines the magnetic unit cell.
- Open the refinement .prf file using **WinPlotr-2006 > File > Open Rietveld/Profile (\*.prf)**
- Select “Calculations”> “peak detection”>”enable” . After enabling, go again to “Calculations”> “peak detection” > “insert peak”. After clicking on magnetic peaks, go to “save peaks” to save them as “K-search format”. Run k-search.



## Select magnetic peaks



## Input structural information

Input parameters for K\_SEARCH

Title: Ba1 Ho2 Ni1 O5

Lattice Type: 1 m m m

Cell Parameters: 3.756030 5.734099 11.277499 90.000000 90.000000 90.000000

Tolerance (TOF/2theta): 0.300

K range (kxmin,kxmax, ...): 0.0 0.5 0.0 0.5 0.0 0.5

Number of Points (Na\* Nb\* Nc): 100 100 100

Wavelength (CW) / Dtt1(TOF): 2.52400

☒ Short Output ☐ Long Output ☐ No output of intermediate calculations

☒ Search only special k-vectors

OK Cancel

```
C:\WINDOWS\SYSTEM32\cmd.exe
*****
*          PROGRAM K_SEARCH          *
*****
(J.R.C. ILL-January 2009)

=> The expected maximum R-factor for a solution is:      5.1522

=> Writing partial results ...

=> Testing 90 internal k-vectors
  Solution:      1 k =( 0.5000 0.0000 0.5000)  R-F:   0.7871
=> Special k-vector solutions found!

=> List of the best 10 solutions for 6 satellites

      Kx          Ky          Kz          R-factor
      0.500000    0.000000    0.500000    0.787100

=> A probable solution is the special kvector ks =( 0.5000 0.0000 0.5000)
    the corresponding R-factor is:      0.7871

Total CPU-Time

CPU-seconds:      0.02
CPU-minutes:      0.00
CPU-hours   :      0.00

=> Press <enter> to finish
```

**k=(0.5,0,0.5)**



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

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## Step 3: Creating mCIF file

- Now the crystal structure and k-vector have been determined the magnetic structure can be found by testing model magnetic space groups.
- This can be done in FullProf by creating a .mcif file from the Bilbao Crystallographic Server.

# Step 3: Creating mCIF file

- Go to Bilbao Crystallographic 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 tools and services, with 'Magnetic Symmetry and Applications' highlighted by a red oval. To the right of the main list is a 'Quick access to some tables' section. On the left, there is a section for 'ECM31-Oviedo Satellite' and a 'News' section with several updates.

**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 3: Creating mCIF file

- Then select “MAXMAGN”

## bilbao crystallographic server

[Contact us](#)[About us](#)[Publications](#)[How to cite the server](#)

### Space-group symmetry

#### Magnetic Symmetry and Applications

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

# Step 3: Creating mCIF file

- **[1]** Need to have a propagation vector. This was determined using k-search in fullprof (to be (0.5,0,0.5)).
- **[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.

Bilbao Crystallographic Server → MAXMAGN Help

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

**3** ☒ Structure data of the paramagnetic phase will be included

**2** ☐ Non-conventional setting

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

Please, enter the propagation vector k:

**4**  **1**

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 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. Elcoro, 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.



# Step 3: Creating mCIF file

- Choose .cif file (crystal structure only).  
The one for this example is “Ho2BaNiO5.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

Ho2BaNiO5.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 3: 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: *Immm* (No. 71)

Lattice parameters (Angstroms and degrees): a=3.75603, b=5.73410, c=11.27750, alpha=90., beta=90., gamma=90.

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	Ho1	Ho	4j	0.50000 0.00000 0.20250	<input checked="" type="checkbox"/>
2	Ba1	Ba	2c	0.50000 0.50000 0.00000	<input type="checkbox"/>
3	Ni1	Ni	2a	0.00000 0.00000 0.00000	<input checked="" type="checkbox"/>
4	O1	O	8l	0.00000 0.24140 0.14950	<input type="checkbox"/>
5	O2	O	2b	0.50000 0.00000 0.00000	<input type="checkbox"/>

Submit

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# Step 3: Creating mCIF file

Maximal magnetic space groups for the parent space group *Immm* (No. 71) and the propagation vector  $k = (1/2, 0, 1/2)$

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>C<sub>c</sub>2/c</i> (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	<i>C<sub>c</sub>2/c</i> (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	<i>C<sub>c</sub>2/m</i> (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	<i>C<sub>c</sub>2/m</i> (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

- The possible magnetic space groups are displayed in grey
- To view magnetic structure and export mcif file click on “Show” in last column.

# Step 3: Creating mCIF file: **Check #1**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$C_2/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$C_2/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$C_2/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$C_2/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show



Selected magnetic space group: 1-  $C_2/c$  (#15.90)  
 Setting parent-like (2a, b, 2c ; 0, 0, 0)  
 Parent space group  $Immm$  (No. 71)  
 Lattice parameters: a=7.51210, b=5.73410, c=22.55500, alpha=90.00, beta=90.00, gamma=90.00  
 [Go to setting standard (a-c, b, 2a ; 0, 0, 1/2)]  
 [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	Ho1 Ho 0.25000 0.00000 0.10125	(1/4, 0, z   $m_x, 0, m_z$ ) (1/4, 0, -z   $m_x, 0, m_z$ ) (0, 1/2, z+1/4   $m_x, 0, m_z$ ) (0, 1/2, -z+1/4   $m_x, 0, m_z$ ) (1/4, 0, z+1/2   $-m_x, 0, -m_z$ ) (1/4, 0, -z+1/2   $-m_x, 0, -m_z$ ) (0, 1/2, z+3/4   $-m_x, 0, -m_z$ ) (0, 1/2, -z+3/4   $-m_x, 0, -m_z$ ) (3/4, 0, z   $-m_x, 0, -m_z$ ) (3/4, 0, -z   $-m_x, 0, -m_z$ ) (1/2, 1/2, z+1/4   $-m_x, 0, -m_z$ ) (1/2, 1/2, -z+1/4   $-m_x, 0, -m_z$ ) (3/4, 0, z+1/2   $m_x, 0, m_z$ ) (3/4, 0, -z+1/2   $m_x, 0, m_z$ ) (1/2, 1/2, z+3/4   $m_x, 0, m_z$ ) (1/2, 1/2, -z+3/4   $m_x, 0, m_z$ )	16	( $M_x, 0, M_z$ )	$M_x = 0.00000$ $M_z = 0.00000$
2	Ba1 Ba 0.25000 0.50000 0.00000	(1/4, 1/2, 0   $m_x, 0, m_z$ ) (0, 0, 1/4   $m_x, 0, m_z$ ) (1/4, 1/2, 1/2   $-m_x, 0, -m_z$ ) (0, 0, 3/4   $-m_x, 0, -m_z$ ) (3/4, 1/2, 0   $-m_x, 0, -m_z$ ) (1/2, 0, 1/4   $-m_x, 0, -m_z$ ) (3/4, 1/2, 1/2   $m_x, 0, m_z$ ) (1/2, 0, 3/4   $m_x, 0, m_z$ )	8	-	-
3	Ni1 Ni 0.00000 0.00000 0.00000	(0, 0, 0   0, 0, 0) (1/4, 1/2, 1/4   0, 0, 0) (0, 0, 1/2   0, 0, 0) (1/4, 1/2, 3/4   0, 0, 0) (1/2, 0, 0   0, 0, 0) (3/4, 1/2, 1/4   0, 0, 0) (1/2, 0, 1/2   0, 0, 0) (3/4, 1/2, 3/4   0, 0, 0)	8	(0, 0, 0)	-
4	O1 O 0.00000 0.24140 0.07475	(0, y, z   $m_x, m_y, m_z$ ) (0, -y, z   $m_x, -m_y, m_z$ ) (0, y, -z   $-m_x, m_y, -m_z$ ) (0, -y, -z   $-m_x, -m_y, -m_z$ ) (1/4, y+1/2, z+1/4   $-m_x, -m_y, -m_z$ ) (1/4, -y+1/2, z+1/4   $-m_x, m_y, -m_z$ ) (1/4, y+1/2, -z+1/4   $m_x, -m_y, m_z$ ) (1/4, -y+1/2, -z+1/4   $m_x, m_y, m_z$ ) (0, y, z+1/2   $-m_x, -m_y, -m_z$ ) (0, -y, z+1/2   $-m_x, m_y, -m_z$ ) (0, y, -z+1/2   $m_x, -m_y, m_z$ ) (0, -y, -z+1/2   $m_x, m_y, m_z$ ) (1/4, y+1/2, z+3/4   $m_x, m_y, m_z$ ) (1/4, -y+1/2, z+3/4   $m_x, -m_y, m_z$ ) (1/4, y+1/2, -z+3/4   $-m_x, m_y, -m_z$ ) (1/4, -y+1/2, -z+3/4   $-m_x, -m_y, -m_z$ ) (1/2, y, z   $-m_x, -m_y, -m_z$ ) (1/2, -y, z   $-m_x, m_y, -m_z$ ) (1/2, y, -z   $m_x, -m_y, m_z$ ) (1/2, -y, -z   $m_x, m_y, m_z$ ) (3/4, y+1/2, z+1/4   $m_x, m_y, m_z$ ) (3/4, -y+1/2, z+1/4   $m_x, -m_y, m_z$ ) (3/4, y+1/2, -z+1/4   $-m_x, m_y, -m_z$ ) (3/4, -y+1/2, -z+1/4   $-m_x, -m_y, -m_z$ ) (1/2, y, z+1/2   $m_x, m_y, m_z$ ) (1/2, -y, z+1/2   $m_x, -m_y, m_z$ ) (1/2, y, -z+1/2   $-m_x, m_y, -m_z$ ) (1/2, -y, -z+1/2   $-m_x, -m_y, -m_z$ ) (3/4, y+1/2, z+3/4   $-m_x, -m_y, -m_z$ ) (3/4, -y+1/2, z+3/4   $-m_x, m_y, -m_z$ ) (3/4, y+1/2, -z+3/4   $m_x, -m_y, m_z$ ) (3/4, -y+1/2, -z+3/4   $m_x, m_y, m_z$ )	32	-	-
5	O2 O 0.00000 0.50000 0.25000	(0, 1/2, 1/4   $m_x, 0, m_z$ ) (1/4, 0, 0   $m_x, 0, m_z$ ) (0, 1/2, 3/4   $-m_x, 0, -m_z$ ) (1/4, 0, 1/2   $-m_x, 0, -m_z$ ) (1/2, 1/2, 1/4   $-m_x, 0, -m_z$ ) (3/4, 0, 0   $-m_x, 0, -m_z$ ) (1/2, 1/2, 3/4   $m_x, 0, m_z$ ) (3/4, 0, 1/2   $m_x, 0, m_z$ )	8	-	-

- Only Ho can contribute to magnetic structure.
- Spins only allowed along x and z (a-axis and c-axis)

# Step 3: Creating mCIF file: **Check #2**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$C_{2c}/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$C_{2c}/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$C_{2c}/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$C_{2c}/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

- Both Ho and Ni can contribute to magnetic structure.
- Spins only allowed along x and z (a-axis and c-axis)

Selected magnetic space group: 2-  $C_{2c}/c$  (#15.90)  
 Setting parent-like (2a, b, 2c ; 0, 0, 0)  
 Parent space group  $Immm$  (No. 71)  
 Lattice parameters: a=7.51210, b=5.73410, c=22.55500, alpha=90.00, beta=90.00, gamma=90.00  
 [Go to setting standard (a-c, b, 2a ; 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	Ho1 Ho 0.25000 0.00000 0.10125	(1/4,0,z   $m_x, 0, m_z$ ) (1/4,0,-z   $-m_x, 0, -m_z$ ) (0,1/2,z+1/4   $m_x, 0, m_z$ ) (0,1/2,-z+1/4   $-m_x, 0, -m_z$ ) (1/4,0,z+1/2   $-m_x, 0, -m_z$ ) (1/4,0,-z+1/2   $m_x, 0, m_z$ ) (0,1/2,z+3/4   $-m_x, 0, -m_z$ ) (0,1/2,-z+3/4   $m_x, 0, m_z$ ) (3/4,0,z   $-m_x, 0, -m_z$ ) (3/4,0,-z   $m_x, 0, m_z$ ) (1/2,1/2,z+1/4   $-m_x, 0, -m_z$ ) (1/2,1/2,-z+1/4   $m_x, 0, m_z$ ) (3/4,0,z+1/2   $m_x, 0, m_z$ ) (3/4,0,-z+1/2   $-m_x, 0, -m_z$ ) (1/2,1/2,z+3/4   $m_x, 0, m_z$ ) (1/2,1/2,-z+3/4   $-m_x, 0, -m_z$ )	16	$(M_x, 0, M_z)$	$M_x = 0.00000$ $M_z = 0.00000$
2	Ba1 Ba 0.25000 0.50000 0.00000	(1/4,1/2,0   0,0,0) (0,0,1/4   0,0,0) (1/4,1/2,1/2   0,0,0) (0,0,3/4   0,0,0) (3/4,1/2,0   0,0,0) (1/2,0,1/4   0,0,0) (3/4,1/2,1/2   0,0,0) (1/2,0,3/4   0,0,0)	8	-	-
3	Ni1 Ni 0.00000 0.00000 0.00000	(0,0,0   $m_x, 0, m_z$ ) (1/4,1/2,1/4   $-m_x, 0, -m_z$ ) (0,0,1/2   $-m_x, 0, -m_z$ ) (1/4,1/2,3/4   $m_x, 0, m_z$ ) (1/2,0,0   $-m_x, 0, -m_z$ ) (3/4,1/2,1/4   $m_x, 0, m_z$ ) (1/2,0,1/2   $m_x, 0, m_z$ ) (3/4,1/2,3/4   $-m_x, 0, -m_z$ )	8	$(M_x, 0, M_z)$	$M_x = 0.00000$ $M_z = 0.00000$
4	O1 O 0.00000 0.24140 0.07475	(0,y,z   $m_x, m_y, m_z$ ) (0,-y,z   $m_x, -m_y, m_z$ ) (0,y,-z   $m_x, -m_y, -m_z$ ) (0,-y,-z   $m_x, m_y, -m_z$ ) (1/4,y+1/2,z+1/4   $-m_x, -m_y, -m_z$ ) (1/4,-y+1/2,z+1/4   $-m_x, m_y, -m_z$ ) (1/4,y+1/2,-z+1/4   $-m_x, m_y, -m_z$ ) (1/4,-y+1/2,-z+1/4   $-m_x, -m_y, -m_z$ ) (0,y,z+1/2   $-m_x, -m_y, -m_z$ ) (0,-y,z+1/2   $-m_x, m_y, -m_z$ ) (0,y,-z+1/2   $-m_x, m_y, -m_z$ ) (0,-y,-z+1/2   $-m_x, -m_y, -m_z$ ) (1/4,y+1/2,z+3/4   $m_x, m_y, m_z$ ) (1/4,-y+1/2,z+3/4   $m_x, -m_y, m_z$ ) (1/4,y+1/2,-z+3/4   $m_x, -m_y, m_z$ ) (1/4,-y+1/2,-z+3/4   $m_x, m_y, m_z$ ) (1/2,y,z   $-m_x, -m_y, -m_z$ ) (1/2,-y,z   $-m_x, m_y, -m_z$ ) (1/2,y,-z   $-m_x, m_y, -m_z$ ) (1/2,-y,-z   $-m_x, -m_y, -m_z$ ) (3/4,y+1/2,z+1/4   $m_x, m_y, m_z$ ) (3/4,-y+1/2,z+1/4   $m_x, -m_y, m_z$ ) (3/4,y+1/2,-z+1/4   $m_x, -m_y, m_z$ ) (3/4,-y+1/2,-z+1/4   $m_x, m_y, m_z$ ) (1/2,y,z+1/2   $m_x, m_y, m_z$ ) (1/2,-y,z+1/2   $m_x, -m_y, m_z$ ) (1/2,y,-z+1/2   $m_x, -m_y, m_z$ ) (1/2,-y,-z+1/2   $m_x, m_y, m_z$ ) (3/4,y+1/2,z+3/4   $-m_x, -m_y, -m_z$ ) (3/4,-y+1/2,z+3/4   $-m_x, m_y, -m_z$ ) (3/4,y+1/2,-z+3/4   $-m_x, m_y, -m_z$ ) (3/4,-y+1/2,-z+3/4   $-m_x, -m_y, -m_z$ )	32	-	-
5	O2 O 0.00000 0.50000 0.25000	(0,1/2,1/4   0,0,0) (1/4,0,0   0,0,0) (0,1/2,3/4   0,0,0) (1/4,0,1/2   0,0,0) (1/2,1/2,1/4   0,0,0) (3/4,0,0   0,0,0) (1/2,1/2,3/4   0,0,0) (3/4,0,1/2   0,0,0)	8	-	-



# Step 3: Creating mCIF file: **Check #3**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$C_2/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$C_2/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$C_2/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$C_2/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Selected magnetic space group: 3-  $C_2/m$  (#12.63)

Setting parent-like (2a, b, 2c ; 0, 0, 0)

Parent space group  $Immm$  (No. 71)

Lattice parameters: a=7.51210, b=5.73410, c=22.55500, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (a-c, b, 2a ; 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	Ho1 Ho 0.25000 0.00000 0.10125	(1/4,0,z   0, $m_y$ ,0) (1/4,0,-z   0,- $m_y$ ,0) (0,1/2,z+1/4   0, $m_y$ ,0) (0,1/2,-z+1/4   0,- $m_y$ ,0) (1/4,0,z+1/2   0,- $m_y$ ,0) (1/4,0,-z+1/2   0, $m_y$ ,0) (0,1/2,z+3/4   0,- $m_y$ ,0) (0,1/2,-z+3/4   0, $m_y$ ,0) (3/4,0,z   0,- $m_y$ ,0) (3/4,0,-z   0, $m_y$ ,0) (1/2,1/2,z+1/4   0,- $m_y$ ,0) (1/2,1/2,-z+1/4   0, $m_y$ ,0) (3/4,0,z+1/2   0, $m_y$ ,0) (3/4,0,-z+1/2   0,- $m_y$ ,0) (1/2,1/2,z+3/4   0, $m_y$ ,0) (1/2,1/2,-z+3/4   0,- $m_y$ ,0)	16	(0, $M_y$ ,0)	$M_y = 0.00000$
2	Ba1 Ba 0.25000 0.50000 0.00000	(1/4,1/2,0   0,0,0) (0,0,1/4   0,0,0) (1/4,1/2,1/2   0,0,0) (0,0,3/4   0,0,0) (3/4,1/2,0   0,0,0) (1/2,0,1/4   0,0,0) (3/4,1/2,1/2   0,0,0) (1/2,0,3/4   0,0,0)	8	-	-
3	Ni1 Ni 0.00000 0.00000 0.00000	(0,0,0   0, $m_y$ ,0) (1/4,1/2,1/4   0,- $m_y$ ,0) (0,0,1/2   0,- $m_y$ ,0) (1/4,1/2,3/4   0, $m_y$ ,0) (1/2,0,0   0,- $m_y$ ,0) (3/4,1/2,1/4   0, $m_y$ ,0) (1/2,0,1/2   0, $m_y$ ,0) (3/4,1/2,3/4   0,- $m_y$ ,0)	8	(0, $M_y$ ,0)	$M_y = 0.00000$
4	O1 O 0.00000 0.24140 0.07475	(0,y,z   $m_x, m_y, m_z$ ) (0,-y,z   - $m_x, m_y, -m_z$ ) (0,y,-z   - $m_x, m_y, -m_z$ ) (0,-y,-z   $m_x, m_y, m_z$ ) (1/4,y+1/2,z+1/4   - $m_x, -m_y, -m_z$ ) (1/4,-y+1/2,z+1/4   $m_x, -m_y, m_z$ ) (1/4,y+1/2,-z+1/4   $m_x, -m_y, m_z$ ) (1/4,-y+1/2,-z+1/4   - $m_x, -m_y, -m_z$ ) (0,y,z+1/2   - $m_x, -m_y, -m_z$ ) (0,-y,z+1/2   $m_x, -m_y, m_z$ ) (0,y,-z+1/2   $m_x, -m_y, m_z$ ) (0,-y,-z+1/2   - $m_x, -m_y, -m_z$ ) (1/4,y+1/2,z+3/4   $m_x, m_y, m_z$ ) (1/4,-y+1/2,z+3/4   - $m_x, m_y, -m_z$ ) (1/4,y+1/2,-z+3/4   - $m_x, m_y, -m_z$ ) (1/4,-y+1/2,-z+3/4   $m_x, m_y, m_z$ ) (1/2,y,z   - $m_x, -m_y, -m_z$ ) (1/2,-y,z   $m_x, -m_y, m_z$ ) (1/2,y,-z   $m_x, -m_y, m_z$ ) (1/2,-y,-z   - $m_x, -m_y, -m_z$ ) (3/4,y+1/2,z+1/4   $m_x, m_y, m_z$ ) (3/4,-y+1/2,z+1/4   - $m_x, m_y, -m_z$ ) (3/4,y+1/2,-z+1/4   - $m_x, m_y, -m_z$ ) (3/4,-y+1/2,-z+1/4   $m_x, m_y, m_z$ ) (1/2,y,z+1/2   $m_x, m_y, m_z$ ) (1/2,-y,z+1/2   - $m_x, m_y, -m_z$ ) (1/2,y,-z+1/2   - $m_x, m_y, -m_z$ ) (1/2,-y,-z+1/2   $m_x, m_y, m_z$ ) (3/4,y+1/2,z+3/4   - $m_x, -m_y, -m_z$ ) (3/4,-y+1/2,z+3/4   $m_x, -m_y, m_z$ ) (3/4,y+1/2,-z+3/4   $m_x, -m_y, m_z$ ) (3/4,-y+1/2,-z+3/4   - $m_x, -m_y, -m_z$ )	32	-	-
5	O2 O 0.00000 0.50000 0.25000	(0,1/2,1/4   0,0,0) (1/4,0,0   0,0,0) (0,1/2,3/4   0,0,0) (1/4,0,1/2   0,0,0) (1/2,1/2,1/4   0,0,0) (3/4,0,0   0,0,0) (1/2,1/2,3/4   0,0,0) (3/4,0,1/2   0,0,0)	8	-	-

- Both Ho and Ni can contribute to magnetic structure.
- Spins only allowed along y (b-axis)

# Step 3: Creating mCIF file: **Check #4**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$C_{2c}/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$C_{2c}/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$C_{2/m}$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$C_{2/m}$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

- Only Ho can contribute to magnetic structure.
- Spins only allowed along y (b-axis)

Selected magnetic space group: 4-  $C_{2/m}$  (#12.63)

Setting parent-like (2a, b, 2c ; 0, 0, 0)

Parent space group  $Immm$  (No. 71)

Lattice parameters: a=7.51210, b=5.73410, c=22.55500, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (a-c, b, 2a ; 0, 0, 1/2)]

[Go to an alternative setting]

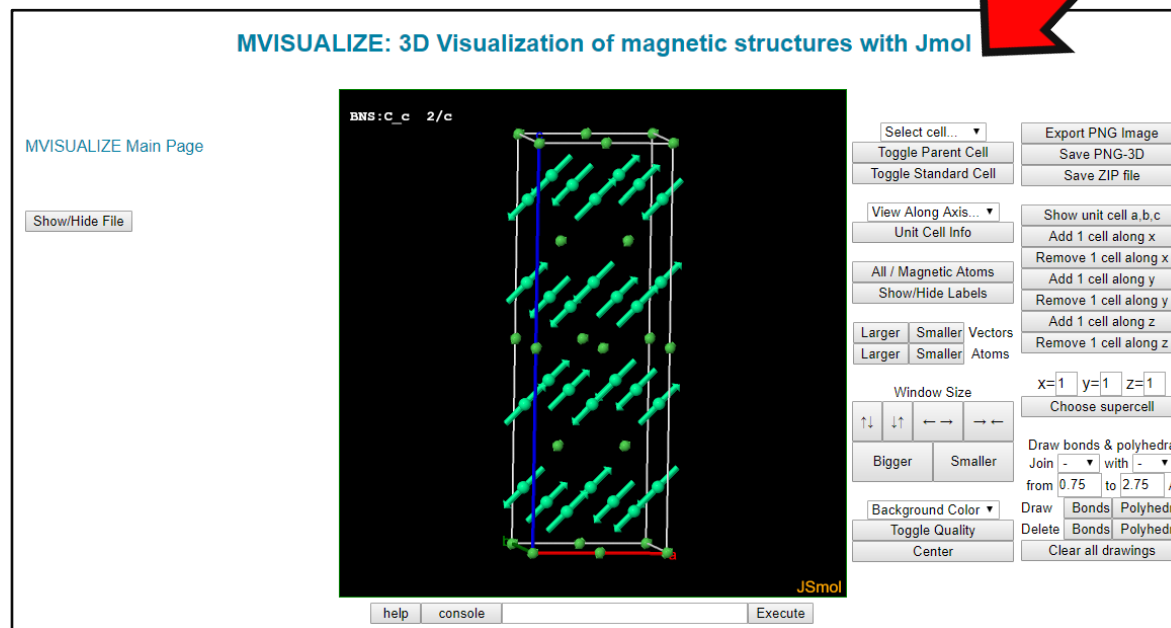
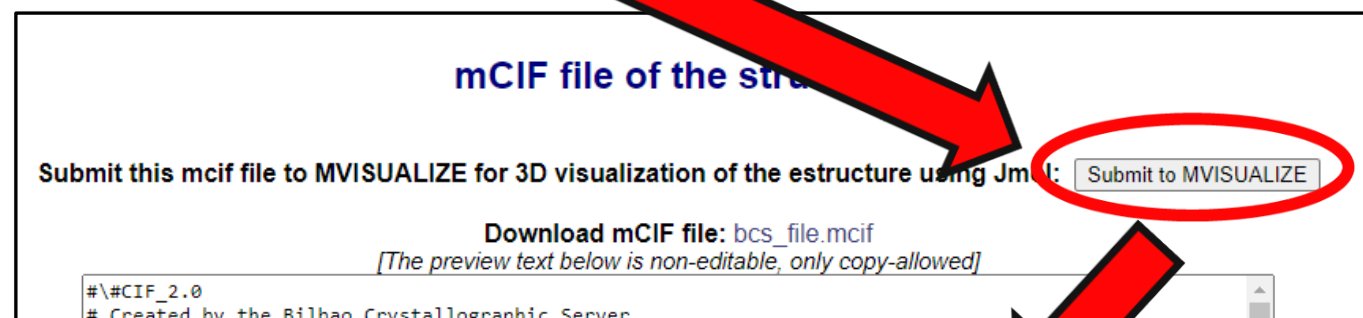
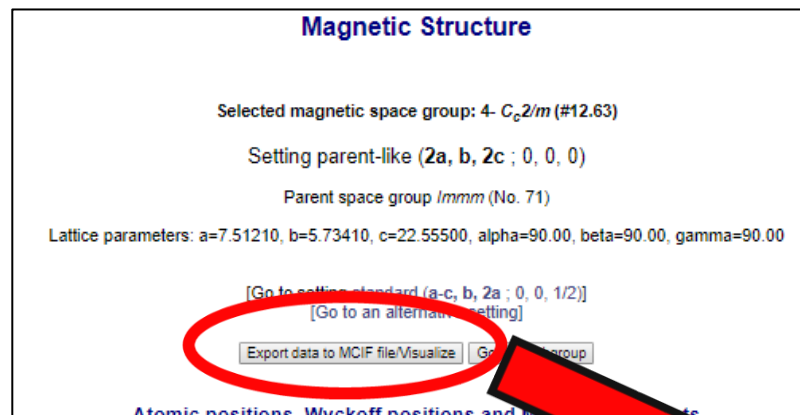
Export data to MCIF file/Visualize Go to a subgroup

## Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of $M_x$ , $M_y$ , $M_z$
1	Ho1 Ho 0.25000 0.00000 0.10125	(1/4,0,z   0, $m_y$ ,0) (1/4,0,-z   0, $m_y$ ,0) (0,1/2,z+1/4   0, $m_y$ ,0) (0,1/2,-z+1/4   0, $m_y$ ,0) (1/4,0,z+1/2   0,- $m_y$ ,0) (1/4,0,-z+1/2   0,- $m_y$ ,0) (0,1/2,z+3/4   0,- $m_y$ ,0) (0,1/2,-z+3/4   0,- $m_y$ ,0) (3/4,0,z   0,- $m_y$ ,0) (3/4,0,-z   0,- $m_y$ ,0) (1/2,1/2,z+1/4   0,- $m_y$ ,0) (1/2,1/2,-z+1/4   0,- $m_y$ ,0) (3/4,0,z+1/2   0, $m_y$ ,0) (3/4,0,-z+1/2   0, $m_y$ ,0) (1/2,1/2,z+3/4   0, $m_y$ ,0) (1/2,1/2,-z+3/4   0, $m_y$ ,0)	16	(0, $M_y$ ,0)	$M_y = 0.00000$
2	Ba1 Ba 0.25000 0.50000 0.00000	(1/4,1/2,0   0, $m_y$ ,0) (0,0,1/4   0, $m_y$ ,0) (1/4,1/2,1/2   0,- $m_y$ ,0) (0,0,3/4   0,- $m_y$ ,0) (3/4,1/2,0   0,- $m_y$ ,0) (1/2,0,1/4   0,- $m_y$ ,0) (3/4,1/2,1/2   0, $m_y$ ,0) (1/2,0,3/4   0, $m_y$ ,0)	8	-	-
3	Ni1 Ni 0.00000 0.00000 0.00000	(0,0,0   0,0,0) (1/4,1/2,1/4   0,0,0) (0,0,1/2   0,0,0) (1/4,1/2,3/4   0,0,0) (1/2,0,0   0,0,0) (3/4,1/2,1/4   0,0,0) (1/2,0,1/2   0,0,0) (3/4,1/2,3/4   0,0,0)	8	(0,0,0)	-
4	O1 O 0.00000 0.24140 0.07475	(0,y,z   $m_x$ , $m_y$ , $m_z$ ) (0,-y,z   - $m_x$ , $m_y$ , $m_z$ ) (0,y,-z   $m_x$ ,- $m_y$ , $m_z$ ) (0,-y,-z   - $m_x$ ,- $m_y$ , $m_z$ ) (1/4,y+1/2,z+1/4   - $m_x$ ,- $m_y$ , $m_z$ ) (1/4,-y+1/2,z+1/4   $m_x$ ,- $m_y$ , $m_z$ ) (1/4,y+1/2,-z+1/4   - $m_x$ , $m_y$ , $m_z$ ) (1/4,-y+1/2,-z+1/4   $m_x$ , $m_y$ , $m_z$ ) (0,y,z+1/2   - $m_x$ ,- $m_y$ , $m_z$ ) (0,-y,z+1/2   $m_x$ ,- $m_y$ , $m_z$ ) (0,y,-z+1/2   - $m_x$ , $m_y$ , $m_z$ ) (0,-y,-z+1/2   $m_x$ , $m_y$ , $m_z$ ) (1/4,y+1/2,z+3/4   $m_x$ , $m_y$ , $m_z$ ) (1/4,-y+1/2,z+3/4   - $m_x$ ,- $m_y$ , $m_z$ ) (1/4,y+1/2,-z+3/4   $m_x$ ,- $m_y$ , $m_z$ ) (1/4,-y+1/2,-z+3/4   - $m_x$ ,- $m_y$ , $m_z$ ) (1/2,y,z   - $m_x$ ,- $m_y$ , $m_z$ ) (1/2,-y,z   $m_x$ ,- $m_y$ , $m_z$ ) (1/2,y,-z   - $m_x$ , $m_y$ , $m_z$ ) (1/2,-y,-z   $m_x$ , $m_y$ , $m_z$ ) (3/4,y+1/2,z+1/4   $m_x$ , $m_y$ , $m_z$ ) (3/4,-y+1/2,z+1/4   - $m_x$ ,- $m_y$ , $m_z$ ) (3/4,y+1/2,-z+1/4   $m_x$ ,- $m_y$ , $m_z$ ) (3/4,-y+1/2,-z+1/4   - $m_x$ ,- $m_y$ , $m_z$ ) (1/2,y,z+1/2   $m_x$ , $m_y$ , $m_z$ ) (1/2,-y,z+1/2   - $m_x$ , $m_y$ , $m_z$ ) (1/2,y,-z+1/2   $m_x$ ,- $m_y$ , $m_z$ ) (1/2,-y,-z+1/2   - $m_x$ ,- $m_y$ , $m_z$ ) (3/4,y+1/2,z+3/4   - $m_x$ ,- $m_y$ , $m_z$ ) (3/4,-y+1/2,z+3/4   $m_x$ ,- $m_y$ , $m_z$ ) (3/4,y+1/2,-z+3/4   - $m_x$ , $m_y$ , $m_z$ ) (3/4,-y+1/2,-z+3/4   $m_x$ , $m_y$ , $m_z$ )	32	-	-
5	O2 O 0.00000 0.50000 0.25000	(0,1/2,1/4   0, $m_y$ ,0) (1/4,0,0   0, $m_y$ ,0) (0,1/2,3/4   0,- $m_y$ ,0) (1/4,0,1/2   0,- $m_y$ ,0) (1/2,1/2,1/4   0,- $m_y$ ,0) (3/4,0,0   0,- $m_y$ ,0) (1/2,1/2,3/4   0, $m_y$ ,0) (3/4,0,1/2   0, $m_y$ ,0)	8	-	-

# Step 3: Creating mCIF file

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



## Step 3: Creating mCIF file:

- We will choose the allowed magnetic structure 2 ( $C_c2/c$  (#15.90)) 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 3: Creating mCIF file

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$C_{2c}/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$C_{2c}/c$ (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$C_{2c}/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$C_{2c}/m$ (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

- We will choose the allowed magnetic structure 2 ( $C_{2c}/c$  (#15.90)) 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

NOTE: In this case if  $M_x=M_z$ , when we run Fullprof it may constrain them to remain the same, but here there is no symmetry requirement that  $M_x=M_z$ . It is given as  $(M_x,0,M_z)$  rather than  $(M_x,0,M_x)$ .

## Magnetic Structure

Selected magnetic space group:  $2-C_{2c}/c$  (#15.90)

Setting parent-like  $(2a, b, 2c; 0, 0, 0)$

Parent space group  $Immm$  (No. 71)

$a=7.51210, b=5.73410, c=22.55500, \alpha=90.00, \beta=90.00, \gamma=90.00$

[Go to setting standard ( $a, b, 2a; 0, 0, 0$ )]

[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	New WP	Multiplicity	Magnetic moment	Values of $M_x, M_y, M_z$
1	Ho1 Ho 0.25000 0.00000 0.10125	$(1/4, 0, z   m_x, 0, m_z) (1/4, 0, -z   -m_x, 0, -m_z)$ $(0, 1/2, z+1/4   m_x, 0, m_z) (0, 1/2, -z+1/4   -m_x, 0, -m_z)$ $(1/4, 0, z+1/2   -m_x, 0, -m_z) (1/4, 0, -z+1/2   m_x, 0, m_z)$ $(0, 1/2, z+3/4   -m_x, 0, -m_z) (0, 1/2, -z+3/4   m_x, 0, m_z)$ $(3/4, 0, z   -m_x, 0, -m_z)$ $(1/2, 1/2, z+1/4   -m_x, 0, -m_z)$ $(3/4, 0, z+1/2   m_x, 0, m_z)$ $(1/2, 1/2, z+3/4   m_x, 0, m_z)$		$(M_x, 0, M_z)$	$M_x = 4$ $M_z = 5$
2	Ba1 Ba 0.25000 0.50000 0.00000	$(1/4, 1/2, 0   0, 0, 0)$ $(1/4, 1/2, 1/2   0, 0, 0)$ $(3/4, 1/2, 0   0, 0, 0)$ $(3/4, 1/2, 1/2   0, 0, 0)$		-	-
3	Ni1 Ni 0.00000 0.00000 0.00000	$(0, 0, 0   m_x, 0, m_z) (1/2, 0, 0   -m_x, 0, -m_z)$ $(0, 0, 1/2   -m_x, 0, -m_z) (0, 0, 1/2   m_x, 0, m_z)$ $(1/2, 0, 0   -m_x, 0, -m_z) (3/4, 1/2, 1/4   m_x, 0, m_z)$ $(1/2, 0, 1/2   m_x, 0, m_z) (3/4, 1/2, 3/4   -m_x, 0, -m_z)$	8	$(M_x, 0, M_z)$	$M_x = 1$ $M_z = 2$
4	O1 O 0.00000 0.24140 0.07475	$(0, y, z   m_x, m_y, m_z) (0, -y, z   m_x, -m_y, -m_z)$ $(0, y, -z   m_x, -m_y, m_z) (0, -y, -z   m_x, m_y, -m_z)$ $(1/4, y+1/2, z+1/4   -m_x, -m_y, -m_z) (1/4, -y+1/2, z+1/4   -m_x, m_y, -m_z)$ $(1/4, y+1/2, -z+1/4   -m_x, m_y, -m_z) (1/4, -y+1/2, -z+1/4   -m_x, -m_y, -m_z)$ $(0, y, z+1/2   -m_x, -m_y, -m_z) (0, -y, z+1/2   -m_x, m_y, -m_z)$ $(0, y, -z+1/2   -m_x, m_y, -m_z) (0, -y, -z+1/2   -m_x, -m_y, -m_z)$ $(1/4, y+1/2, z+3/4   m_x, m_y, m_z) (1/4, -y+1/2, z+3/4   m_x, -m_y, m_z)$ $(1/4, y+1/2, -z+3/4   m_x, -m_y, m_z) (1/4, -y+1/2, -z+3/4   m_x, m_y, m_z)$ $(1/2, y, z   -m_x, -m_y, -m_z) (1/2, -y, z   -m_x, m_y, -m_z)$ $(1/2, y, -z   -m_x, m_y, -m_z) (1/2, -y, -z   -m_x, -m_y, -m_z)$ $(3/4, y+1/2, z+1/4   m_x, m_y, m_z) (3/4, -y+1/2, z+1/4   m_x, -m_y, m_z)$ $(3/4, y+1/2, -z+1/4   m_x, -m_y, m_z) (3/4, -y+1/2, -z+1/4   m_x, m_y, m_z)$ $(1/2, y, z+1/2   m_x, m_y, m_z) (1/2, -y, z+1/2   m_x, -m_y, m_z)$ $(1/2, y, -z+1/2   m_x, -m_y, m_z) (1/2, -y, -z+1/2   m_x, m_y, m_z)$ $(3/4, y+1/2, z+3/4   -m_x, -m_y, -m_z) (3/4, -y+1/2, z+3/4   -m_x, m_y, -m_z)$ $(3/4, y+1/2, -z+3/4   -m_x, m_y, -m_z) (3/4, -y+1/2, -z+3/4   -m_x, -m_y, -m_z)$	32	-	-
5	O2 O 0.00000 0.50000 0.25000	$(0, 1/2, 1/4   0, 0, 0) (1/4, 0, 0   0, 0, 0)$ $(0, 1/2, 3/4   0, 0, 0) (1/4, 0, 1/2   0, 0, 0)$ $(1/2, 1/2, 1/4   0, 0, 0) (3/4, 0, 0   0, 0, 0)$ $(1/2, 1/2, 3/4   0, 0, 0) (3/4, 0, 1/2   0, 0, 0)$	8	-	-

1. Input values for magnetic moment



# Step 3: Creating mCIF file

mCIF file of the structure

2

- 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 MVSUALIZE”

We now need to go to Step 4

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

Download mCIF file: bcs\_file.mcif

```
#\mCIF_2.0
# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
# Date: 09/10/2019 18:17:20
# Ho2BaNiO5.cif

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_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      ?
?

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_atomic_positions_source_other ?

_transition_temperature ?
_experiment_temperature ?

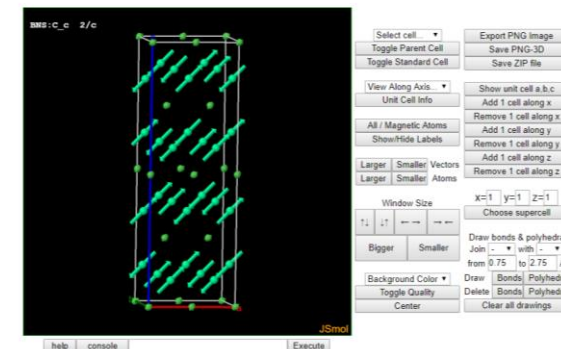
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_irrep_id
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_irrep_small_dimension
_irrep_direction_type
_irrep_action
_irrep_modes_number
_irrep_presence
? ? ? ? ? ? ?

_exptl_crystal_magnetic_properties_details
;
;

_active_magnetic_irreps_details
;
k-maximal magnetic symmetry
;

_parent_space_group.name_H-M_alt 'N o . 71'
_parent_space_group.IT_number 71
_parent_space_group.transform_Pp_abc 'a,b,c;0,0,0'
```

MVSUALIZE: 3D Visualization of magnetic structures with Jmol



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

- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - Step 3: Create test magnetic space groups using MAXMAGN on the Bilbao Crystallographic Server. mcif file created.
  - **Step 4: Convert the mcif file into a .pcr file using mCIF2PCR.**
  - Step 5: Use the created .pcr file to fit the nuclear and magnetic neutron data using Fullprof to determined the magnetic structure.

# Step 4: Creating a pcr from an mcif file

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

## bilbao crystallographic server

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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="#">MAGMODELIZE</a>	Magnetic structure models for any given magnetic symmetry
<a href="#">STRCONVERT</a>	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
<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 portable 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
<a href="#">MAGNETIC REP.</a>	Decomposition of the magnetic representation into irreps
<a href="#">Get_mirreps</a>	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

## Step 4: 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

Ho2BaNiO5\_...MAGN.mcif

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 “Ho2BaNiO5.dat”

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

- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - Step 3: Create test magnetic space groups using MAXMAGN on the Bilbao Crystallographic Server. mcif file created.
  - Step 4: Convert the mcif file into a .pcr file using mCIF2PCR.
  - **Step 5: Use the created .pcr file to fit the nuclear and magnetic neutron data using Fullprof to determined the magnetic structure.**



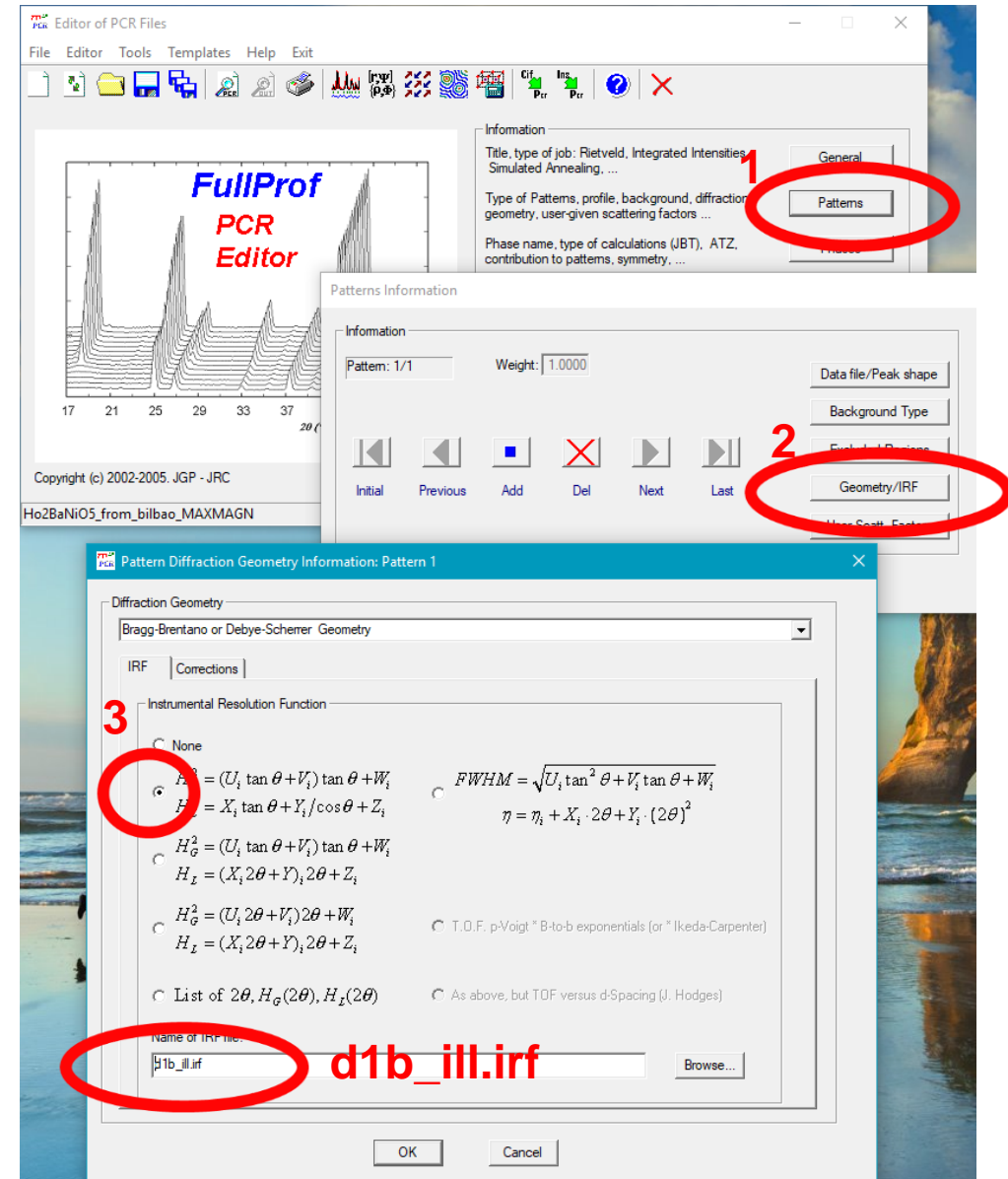
# Step 5: Refining the magnetic structure with Fullprof

- 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.
  - This case is for D1b at ILL. The irf file (dib\_ill.irf) contains the required instrument parameters.

**NOTE: MOST OF THE PARAMATERS CAN BE COPIED DIRECTLY FROM THE CRYSTAL STRUCTURE REFINEMENT DONE IN STEP 1. EITHER DO THAT, OR REPEAT THE STEPS AS DETAILED IN THE FOLLOWING SLIDES**

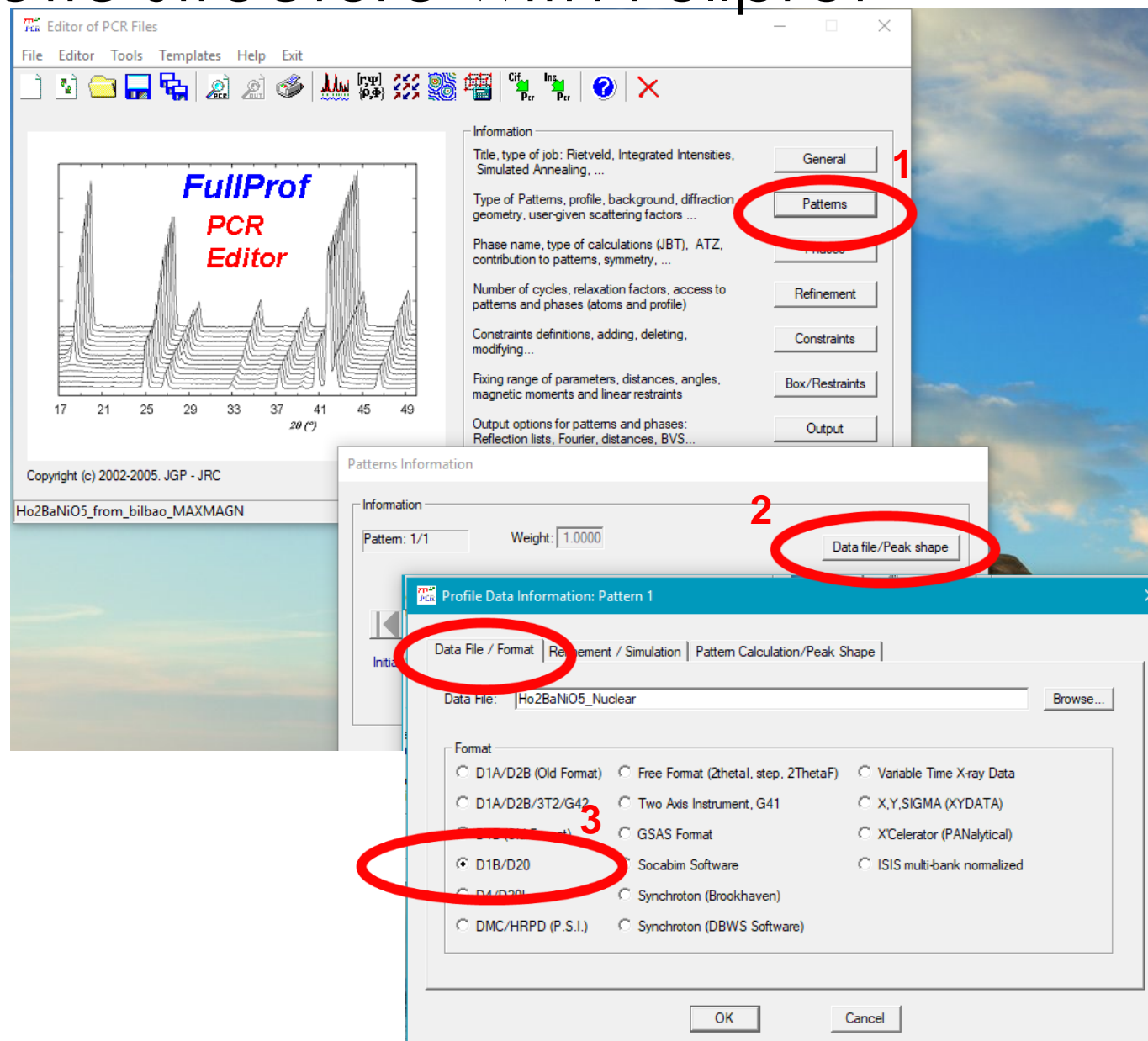
# Step 5: Refining the magnetic structure with Fullprof

- Open pcr file
- Load instrument parameters (irf file)
- Patterns → Geometry/irf → d1b\_ill.irf



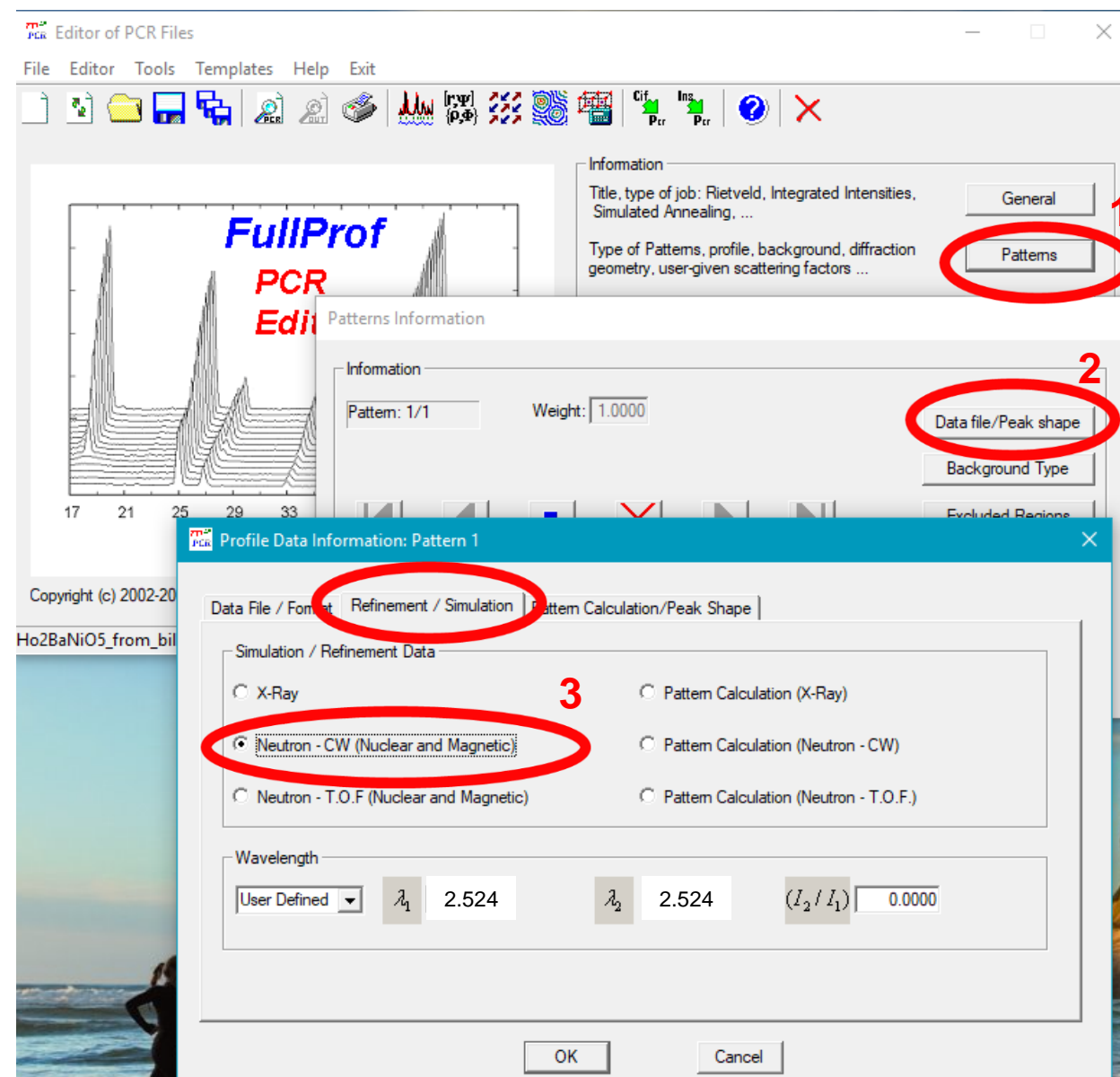
# Step 5: Refining the magnetic structure with Fullprof

- Open pcr file
- Select the format of the data file Fullprof should refine.
- Patterns → Data file/Peak Shape → D1B/D20



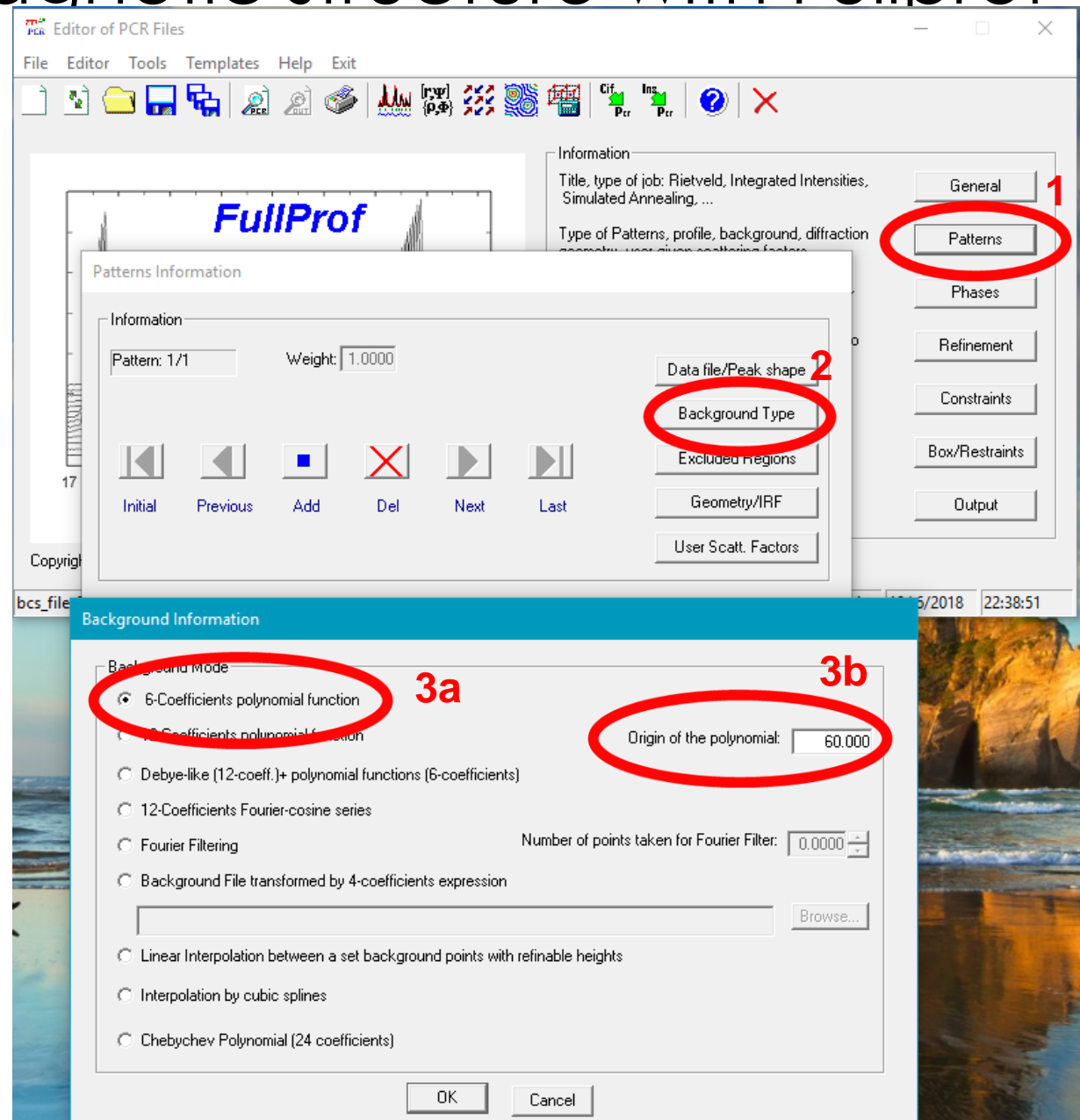
# Step 5: Refining the magnetic structure with Fullprof

- Patterns → Data file/Peak Shape → Refinement/Simulation
- **[3]** Select Neutron – CW
- Wavelength will be set by irf file



# Step 5: Refining the magnetic structure with Fullprof

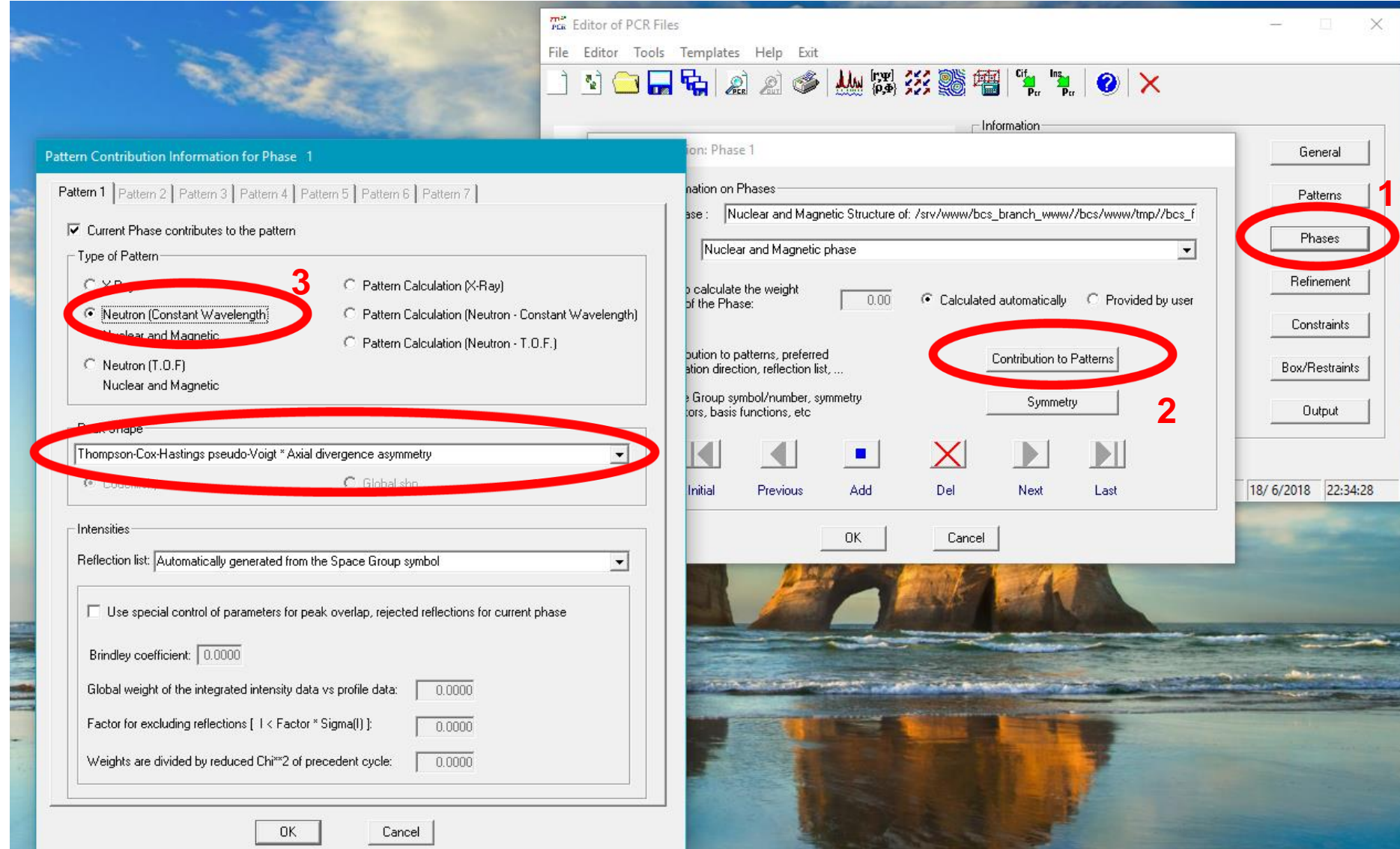
- Patterns → Background Type → 6-coefficient
- Select background type





# Step 5: Refining the magnetic structure with Fullprof

- Make phase contribute to refinement.
- **[1]** Phases → **[2]** Contribution to Patterns → **[3]** Neutron (constant wavelength)
- Peak shape will be set by irf



# Step 5: Refining the magnetic structure with Fullprof

- Setting starting values for refinements
- Starting background values (these can be found from nuclear phase, note mcif2pcr puts 100 in all fields.)

**NOTE: CAN COPY THE VALUES FROM STEP 1 CRYSTAL STRUCTURE REFINEMENT**

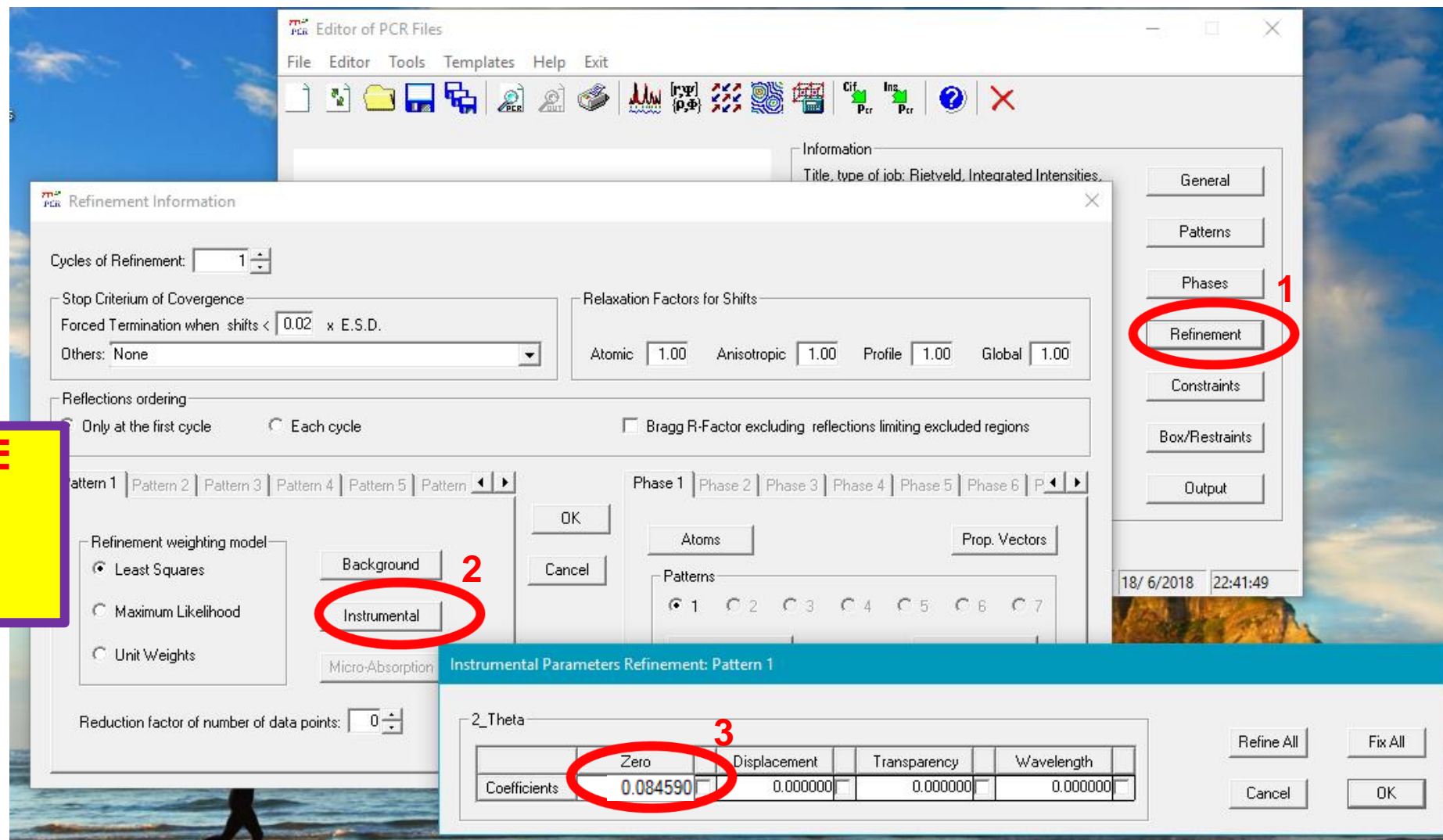
The screenshot shows the Fullprof software interface. The 'Refinement Information' dialog box is open, showing various refinement parameters. The 'Refinement' button in the right-hand pane is circled in red and labeled with a red '1'. The 'Background' button in the 'Refinement weighting model' section is circled in red and labeled with a red '2'. The '6 Coefficients Polynomial Background: Pattern 1' dialog box is also open, showing a table of coefficients. The first row of coefficients is circled in red and labeled with a red '3'. The value '7000' is entered in the 'd\_0' field.

	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients	7000	0.0000	0.0000	0.0000	0.0000	0.0000
	d_6	d_7	d_8	d_9	d_10	d_11
Coefficients						
	d_12	d_13	d_14	d_15	d_16	d_17
Coefficients						
	d_18	d_19	d_20	d_21	d_22	d_23
Coefficients						

# Step 5: Refining the magnetic structure with Fullprof

- Instrumental zero value  
(See nuclear refinement: 0.085)

**NOTE: CAN COPY THE VALUES FROM STEP 1 CRYSTAL STRUCTURE REFINEMENT**

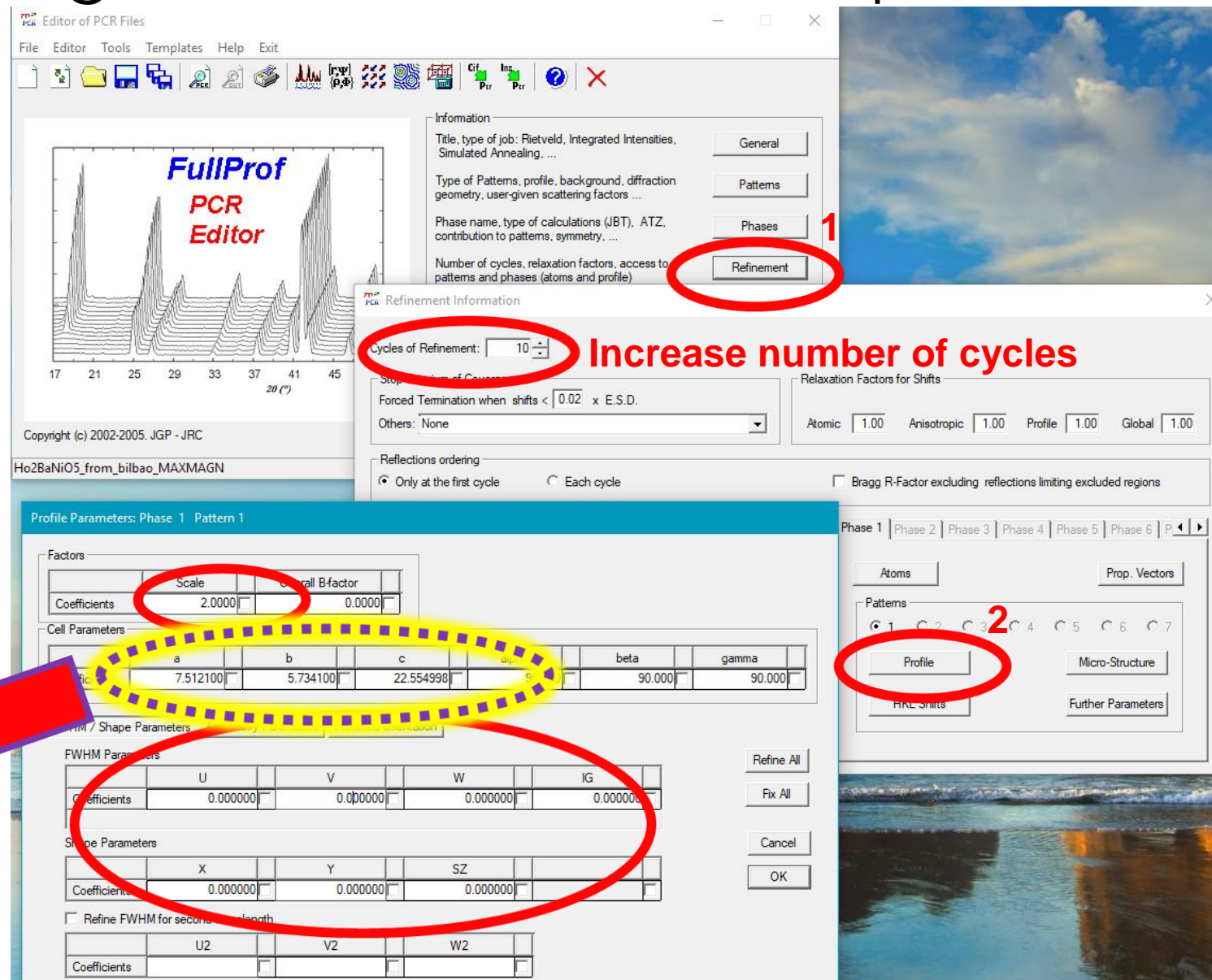




# Step 5: Refining the magnetic structure with Fullprof

- Update “Scale” and “Profile” parameters.
- Set U,V,W,X to 0  
The irf file has values. NOTE: in this data set the magnetic peaks dominate and with a limited Q range the refinement is not stable when profile parameters refine. Keep fixed.

**NOTE:** Magnetic space groups do not use a propagation vector. Instead the unit cell changes. For  $k = (\frac{1}{2} \ 0 \ \frac{1}{2})$  the a and c-unit cell values are doubled.



# Step 5: Refining the magnetic structure with Fullprof

- In "Refinement" → "atoms" input thermal parameters (0.3). **[1,2,3]**
- Note that  $\text{Re}(x)$  and  $\text{Re}(z)$  are set to refine.
- This is a default in files from mcif to pcr that we will turn off in next slide.

The screenshot shows the FullProf PCR Editor interface. The main window displays a plot of intensity versus  $2\theta$  (°) with the text "FullProf PCR Editor" overlaid. The "Refinement" button is circled in red. The "Refinement Information" panel shows "Cycles of Refinement" set to 10 and "Stop Criterion of Coverage" set to "Forced Termination when shifts < 0.02 x E.S.D.". The "Atoms Information: Phase 1" panel shows a list of atoms with their thermal parameters (B) circled in red. The "Atoms" button is also circled in red.

**Atoms Information: Phase 1**

Atom #	Label	Ntype	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Ho1	JHO3	1	0	0.25000	0.00000	0.10125	0.30000	0.50000
Atom # 2	Ba1	Ba	1	0	0.25000	0.50000	0.00000	0.30000	0.25000
Atom # 3	Ni1	MNI2	1	0	0.00000	0.00000	0.00000	0.30000	0.25000
Atom # 4	O1	O	1	0	0.00000	0.24140	0.07475	0.30000	1.00000

**Refinement Information**

Cycles of Refinement: 10

Stop Criterion of Coverage: Forced Termination when shifts < 0.02 x E.S.D.

Others: None

Reflections ordering: ☒ Only at the first cycle ☐ Each cycle

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

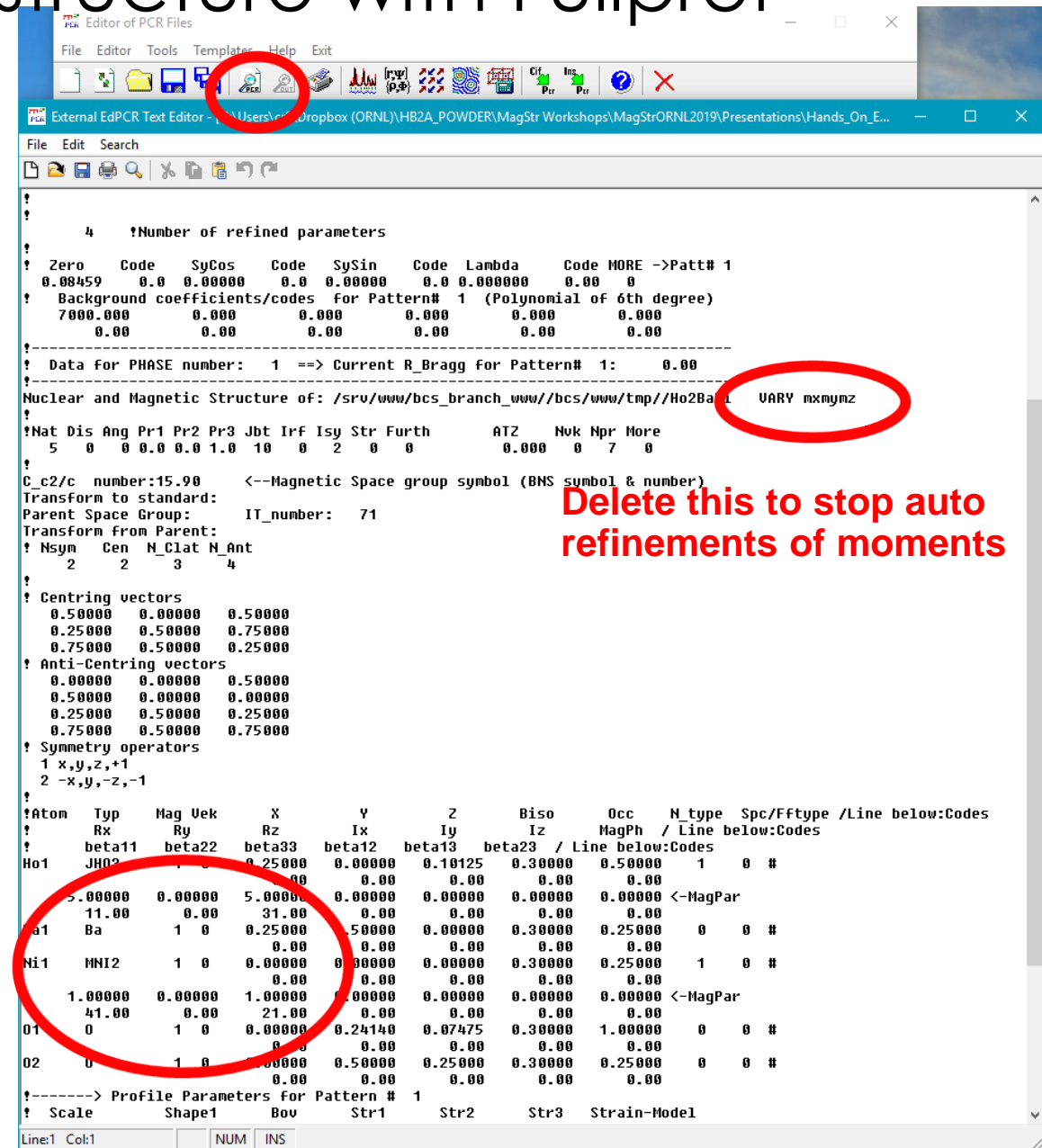
☐ Bragg R-Factor excluding reflections limiting excluded regions

**Atoms Information: Phase 1**

Atom #	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom #1	5.00000	0.00000	5.00000	0.00000	0.00000	0.00000	0.00000
Atom #3	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00000

# Step 5: Refining the magnetic structure with Fullprof

- Open pcr text file.
- Delete “VARY mxmymz” to turn off automatically refining moments.
- Turn off the refinement labels 11.0, 21.0, 31.0 and 41.0



Editor of PCR Files

File Edit Search

4 ?Number of refined parameters

? Zero Code SyCos Code SySin Code Lambda Code MORE ->Patt# 1  
0.08459 0.0 0.00000 0.0 0.00000 0.0 0.00000 0.00 0

? Background coefficients/codes for Pattern# 1 (Polynomial of 6th degree)  
7000.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000  
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

-----  
? 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/Ho2Ba1 VARY mxmymz

? Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More  
5 0 0 0.0 0.0 1.0 10 0 2 0 0 0.000 0 7 0

? C2/c number:15.90 <--Magnetic Space group symbol (BNS symbol & number)  
Transform to standard:  
Parent Space Group: IT\_number: 71  
Transform from Parent:  
? Nsym Cen N\_Clat N\_Ant  
2 2 3 4

? Centring vectors  
0.50000 0.00000 0.50000  
0.25000 0.50000 0.75000  
0.75000 0.50000 0.25000

? Anti-Centring vectors  
0.00000 0.00000 0.50000  
0.50000 0.00000 0.00000  
0.25000 0.50000 0.25000  
0.75000 0.50000 0.75000

? Symmetry operators  
1 x,y,z,+1  
2 -x,y,-z,-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  
Ho1 JH02 1 0 0.25000 0.00000 0.10125 0.30000 0.50000 1 0 #  
0.00 0.00 0.00 0.00 0.00  
5.00000 0.00000 5.00000 0.00000 0.00000 0.00000 0.00000 <--MagPar  
11.00 0.00 31.00 0.00 0.00 0.00 0.00  
a1 Ba 1 0 0.25000 0.00000 0.30000 0.25000 0 0 #  
0.00 0.00 0.00 0.00 0.00  
Ni1 MN12 1 0 0.00000 0.00000 0.00000 0.30000 0.25000 1 0 #  
0.00 0.00 0.00 0.00 0.00  
1.00000 0.00000 1.00000 0.00000 0.00000 0.00000 <--MagPar  
41.00 0.00 21.00 0.00 0.00 0.00 0.00  
01 0 1 0 0.00000 0.24140 0.07475 0.30000 1.00000 0 0 #  
0.00 0.00 0.00 0.00 0.00  
02 0 1 0 0.00000 0.50000 0.25000 0.30000 0.25000 0 0 #  
0.00 0.00 0.00 0.00 0.00

-----> Profile Parameters for Pattern # 1  
? Scale Shape1 Bov Str1 Str2 Str3 Strain-Model

Line:1 Col:1 NUM INS

Delete this to stop auto refinements of moments



# Step 5: Refining the magnetic structure with Fullprof

**Refine background**

FullProf  
PCR  
Editor

File Editor Tools Templates Help Exit

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

General  
Patterns  
Phases  
**Refinement**

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  
Bragg R-Factor excluding reflections limiting excluded regions

Pattern 1 Pattern 2 Pattern 3 Pattern 4 Pattern 5 Pattern 6

Refinement weighting model  
Least Squares **Background**

6 Coefficients Polynomial Background: Pattern 1

Coefficients	d_1	d_2	d_3	d_4	d_5
7000.0	0.0000	0.0000	0.0000	0.0000	0.0000

**Refine scale and lattice constants**

FullProf  
CR  
ditor

File Editor Tools Templates Help Exit

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

General  
Patterns  
Phases  
**Refinement**

Refinement Information

Profile Parameters: Phase 1 Pattern 1

Factors  
Scale 2.0000 Overall B-factor 0.0000

Parameters  
a 7.512101 b 5.734099 c 22.554998 alpha 90.000 beta 90.000 gamma 90.000

FWHM / Shape Parameters  
U 0.000000 V 0.000000 W 0.000000 IG 0.000000

Shape Parameters  
X 0.000000 Y 0.000000 SZ 0.000000

Refine FWHM for second wavelength  
U2 V2 W2

Refine All  
Fix All  
Cancel  
OK

Atoms  
Profile  
HKL Shifts  
Micro-Structure  
Further Parameters

**Refine moments**

FullProf

File Editor Tools Templates Help Exit

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

General  
Patterns  
Phases  
**Refinement**

Refinement Information

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

Bragg R-Factor excluding reflections limiting excluded regions

Refinement weighting model

Phase 1 Phase 2 Phase 3 Phase 4 Phase 5 Phase 6

OK  
Atoms  
Prop. Vectors

Atoms Information: Phase 1

List of Atoms  
Number of Atoms: 5

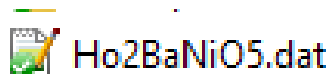
Atom #	Label	Ntype	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Ho1	JHO3	1	0	0.25000	0.00000	0.10125	0.30000	0.50000
Atom # 2	Ba1	Ba	1	0	0.25000	0.50000	0.00000	0.30000	0.25000
Atom # 3	Ni1	MIN2	1	0	0.00000	0.00000	0.00000	0.30000	0.25000
Atom # 4	O1	O	1	0	0.00000	0.24140	0.07475	0.30000	1.00000

Atom #	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom #1	5.00000	0.00000	5.00000	0.00000	0.00000	0.00000	0.00000
Atom #2	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00000

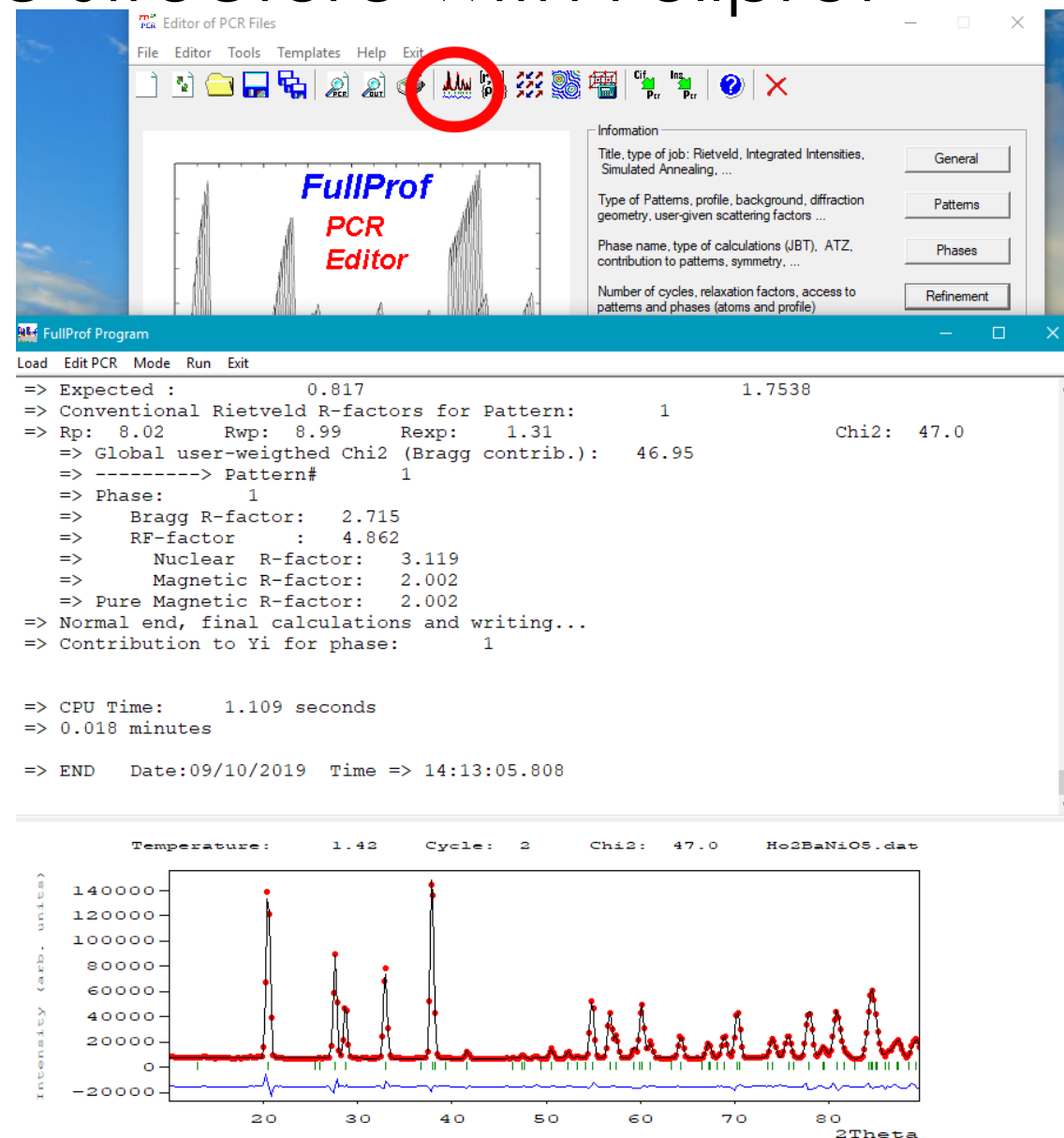
Refine Positions  
Refine B\_iso  
Refine B\_aniso  
Fix All  
Cancel  
OK

# Step 5: Refining the magnetic structure with Fullprof

- Run the refinement.
- Select the “Ho2BaNiO5.dat” neutron data file.



- Refinement models most of the data well.
- Notice high chi2 (due to instrument and background)
- But R-factor and Rf-factor low.



# Step 5: Refining the magnetic structure with Fullprof

- List of files output

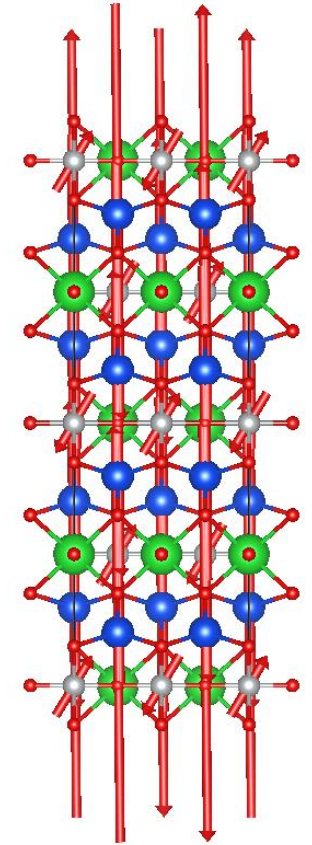
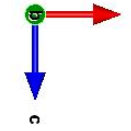
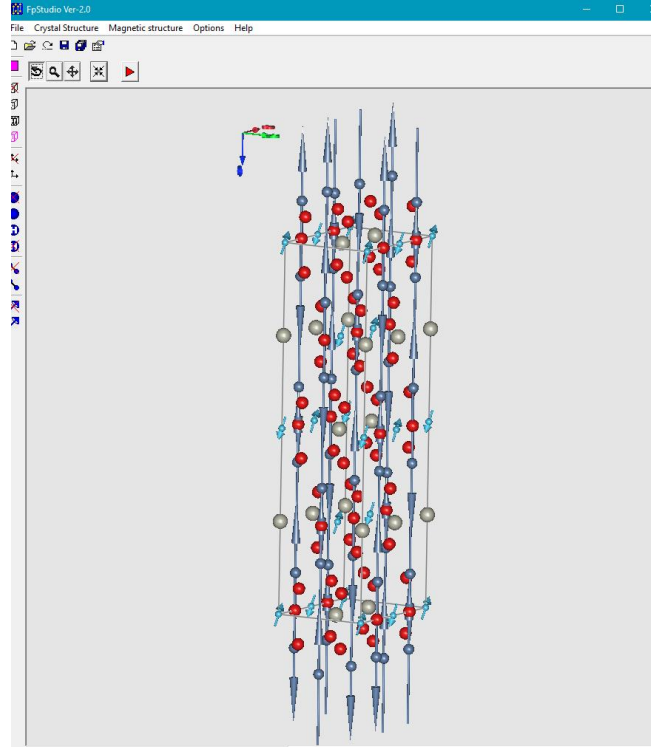
Name

Ho2BaNiO5\_from\_bilbao\_MAXMAGN.pcr  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN.out  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN.prf  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN.sum  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN1.fst  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN1.mcif  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN1.mic  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN1.sub  
Ho2BaNiO5\_from\_bilbao\_MAXMAGN1.VESTA



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

$$\text{Ho: } M_x = 0.11(6) \mu_B; M_z = 9.02(5) \mu_B$$

$$\text{Ni: } M_x = 0.7(1) \mu_B; M_z = -1.30(5) \mu_B$$



- In the folder “Ho2Ba2NiO5\_RepAnalysis” There are other example slides that use the alternative representational analysis approach that will be introduced later in the week.
- These can be worked through to see how the different approaches are applied to give the SAME magnetic structure.

Name	Date modified	Type	Size
 Ho2Ba2NiO5_MagSpaceGroup	10/1/2022 2:19 PM	File folder	
 Ho2Ba2NiO5_RepAnalysis	10/1/2022 12:55 PM	File folder	