Magnetic Space Group refinement in FullProf of the commensurate magnetic structure in Ho_2BaNiO_5 data

Stuart Calder

MagStr 2022, ORNL

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	

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Ho$_2$BaNiO$_5$

- 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$_2$BaNiO$_5$ 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$_2$BaNiO$_5$ using FullProf Suite and SARAh

Ho$_2$BaNiO$_5$

Orthorhombic (Space group: *Immm*)
a=3.764 A, *b*=5.761 A, *c*,=11.336 A)

NiO$_6$ octahedra form chains along the a-axis.

3D Antiferromagnetic ordering at T_N ~ 53 K

Eur. Phys. J. B 24, 59–70 (2001)

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EDP Sciences
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Springer-Verlag 2001

Neutron diffraction study of the magnetic ordering in the series R$_2$BaNiO$_5$ (R = Rare Earth)

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Ho^{+3}
Ba^{+2}
Ni^{+2}
O^{-2}
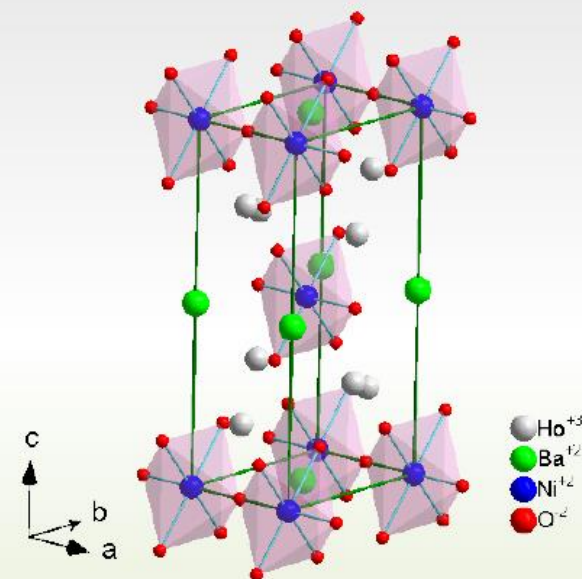
Atom	Wyck.	Site	x/a	y/b	z/c
Ho	4j	mm2	1/2	0	0.2025(4)
Ni	2a	mmm	0	0	0

MAGSTR Workshop, Knoxville, TN 2014

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Details of this Ho_2BaNiO_5 example

- Neutron powder diffraction data collected on D1B at the ILL at 1.5 K using λ= 2.524 Å

- Files included in example:
  - Datafile: **Ho2BaNiO5.dat**
  - Instrument resolution file: **d1b_ill.irf**
  - Crystallographic Information File: **Ho2BaNiO5.cif**

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Ho$_2$BaNiO$_5$

- 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.

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Ho_2BaNiO_5

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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

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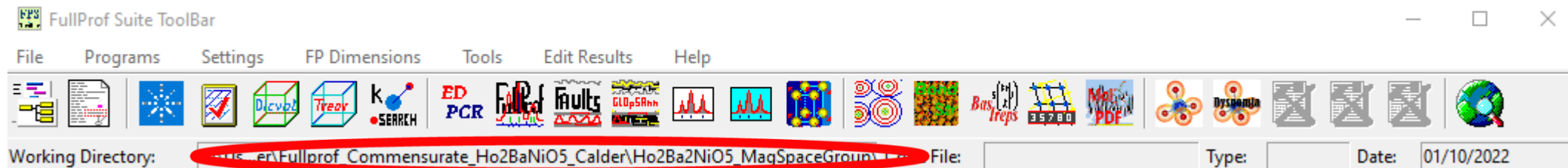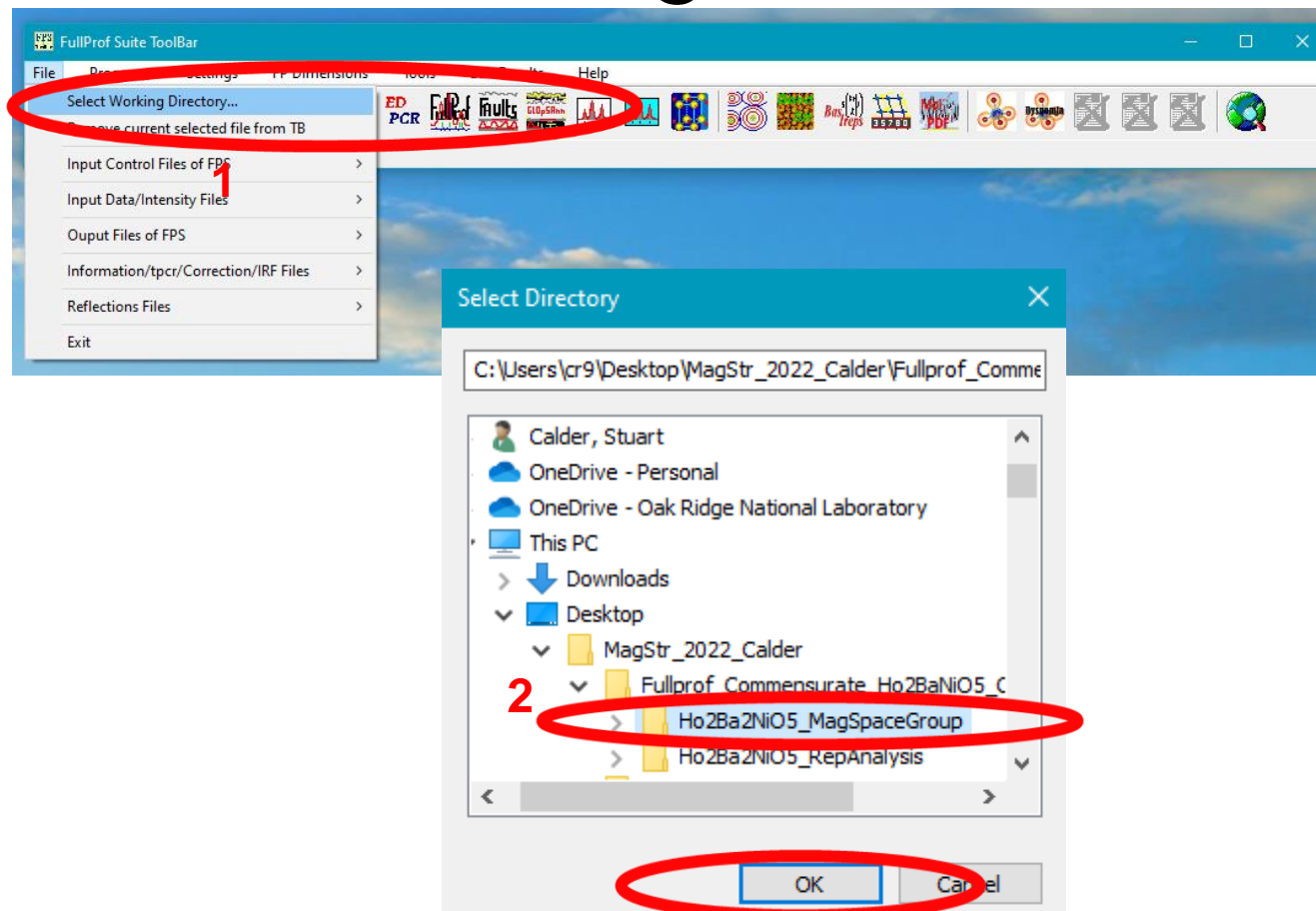
Step 1: Refine the crystal structure using FullProf

- **1.** From FullProf Suite Toolbar open EdPCR.

- **2.** Import crystallographic information file by clicking on "CIF→PCR"

- **3.** Select the file "Ho2BaNiO5.cif"
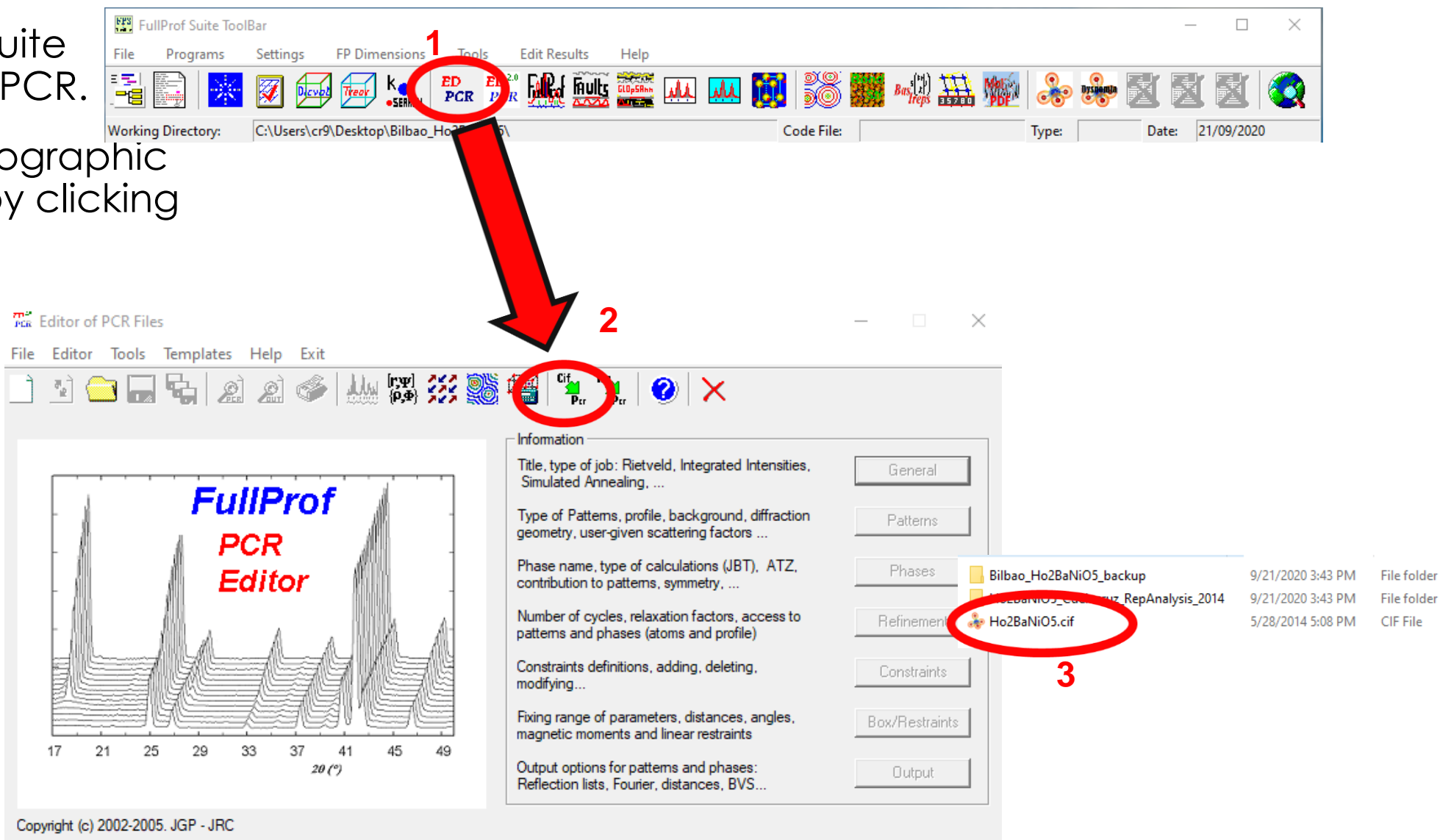
Step 1: Refine the crystal structure using FullProf

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"
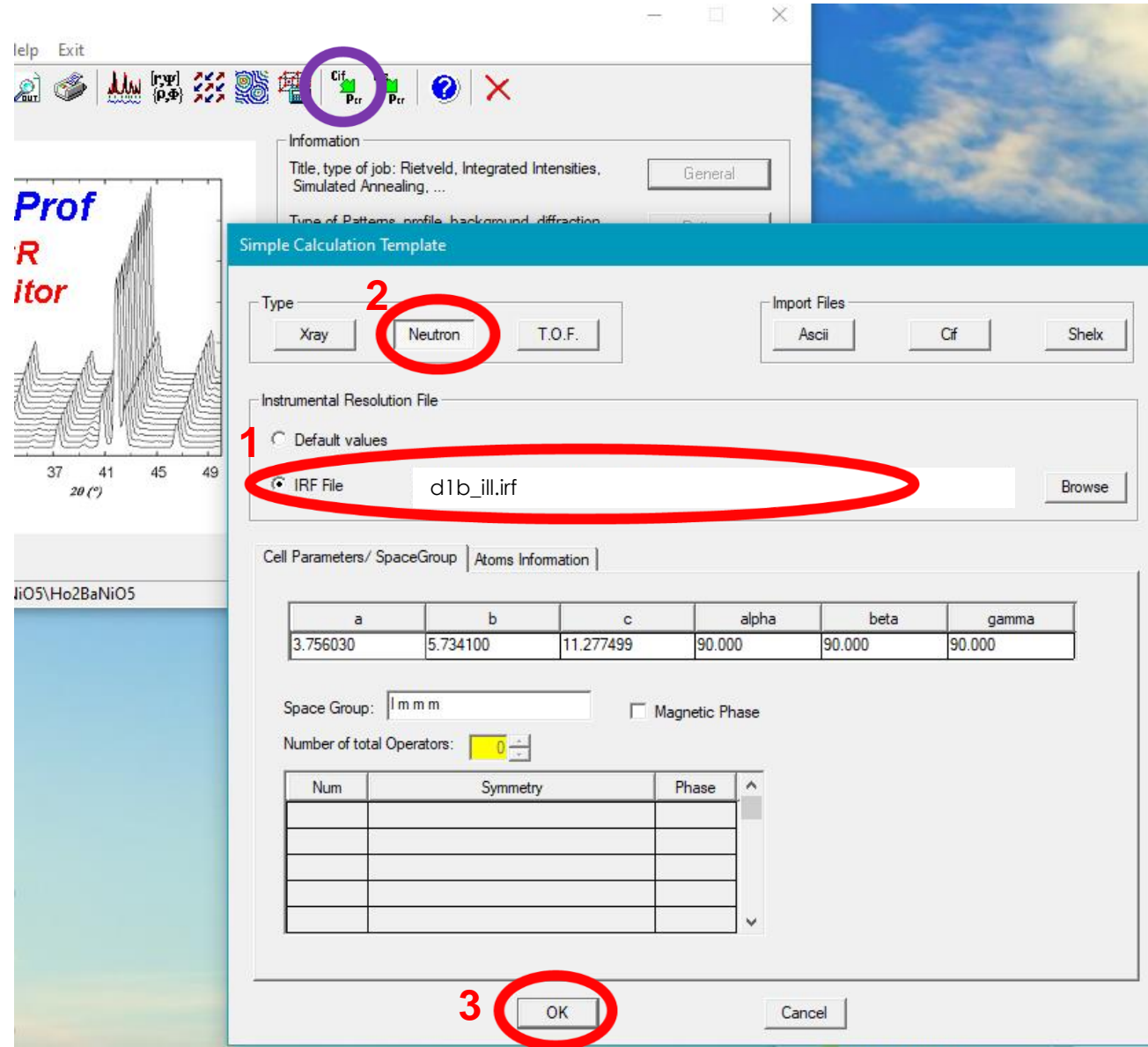
Step 1: Refine the crystal structure using FullProf

- **1.** Save the changes.

- This should be done whenever changes are made in the GUI.
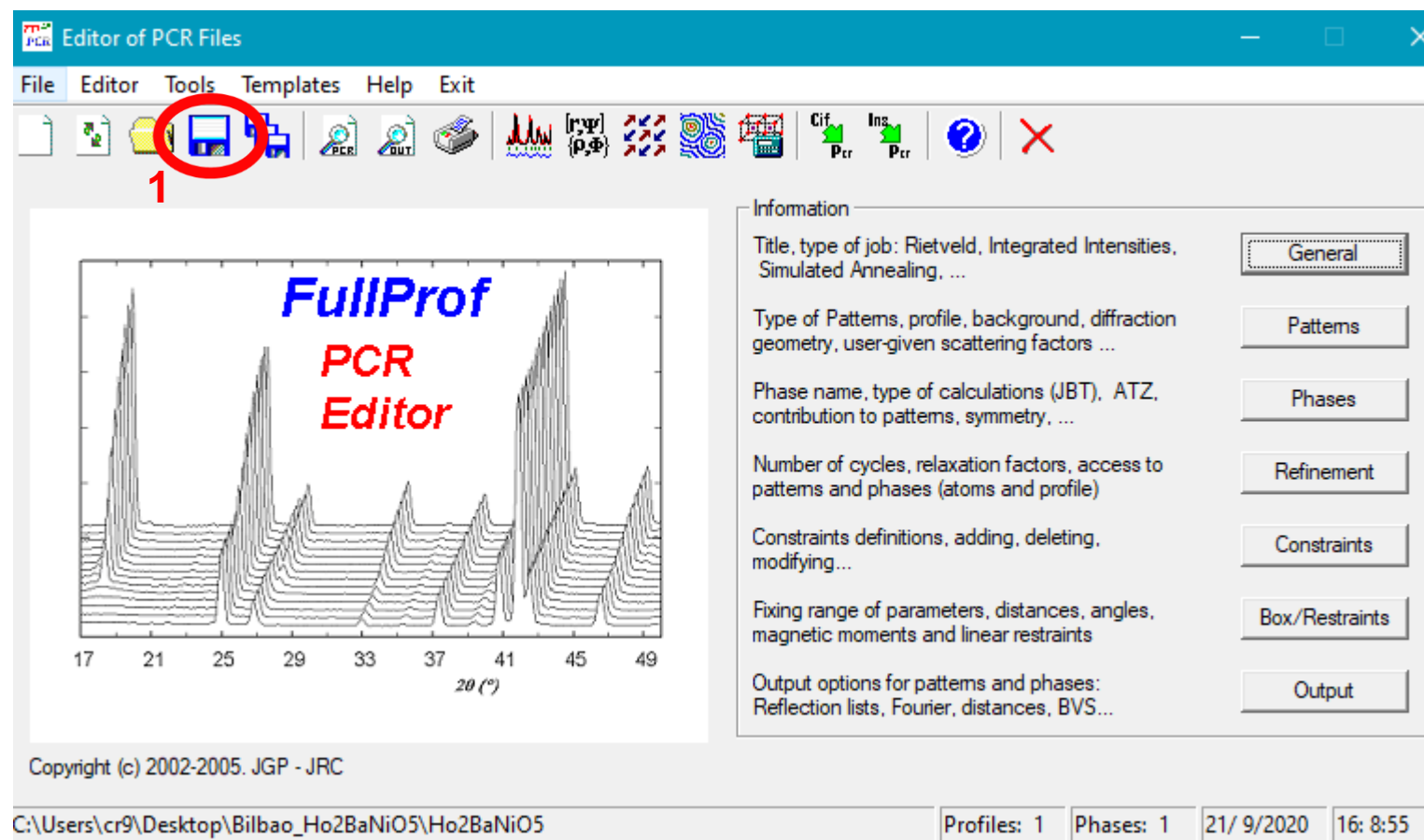
Step 1: Refine the crystal structure using FullProf

"**General**" tab has refinement of powder data as default. Can edit title as wanted.
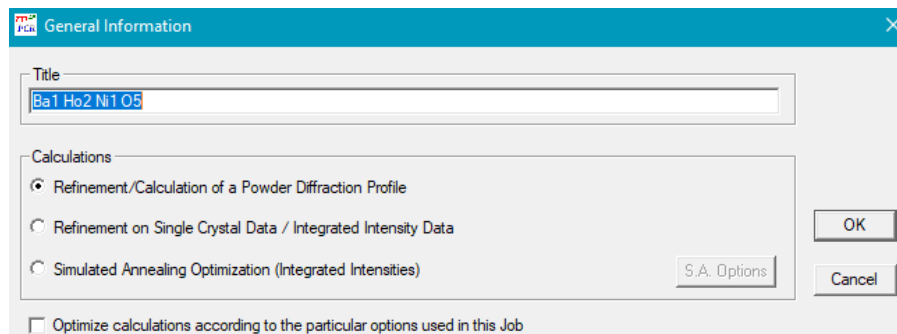
1. "**Patterns**" tab

- **2.** Select the format of the data file Fullprof should refine.

- **3.** Patterns → Data file/Peak Shape → D1B/D20

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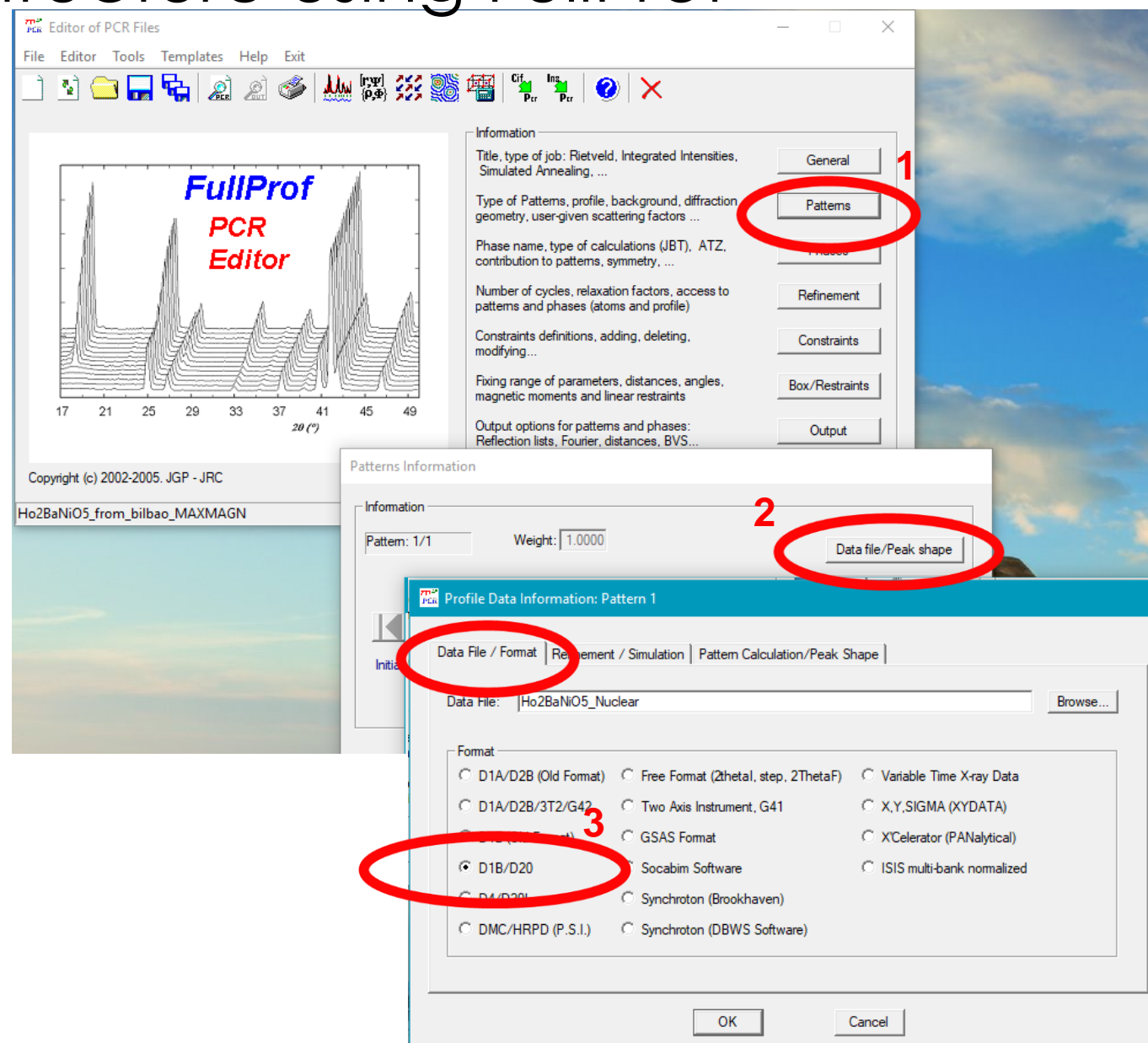
Step 1: Refine the crystal structure using FullProf

- Patterns → Data file/Peak Shape →Refinement/Simulation

- **[1]** Select Neutron – CW

- Wavelength is already set by irf file, 2.524 in this example.
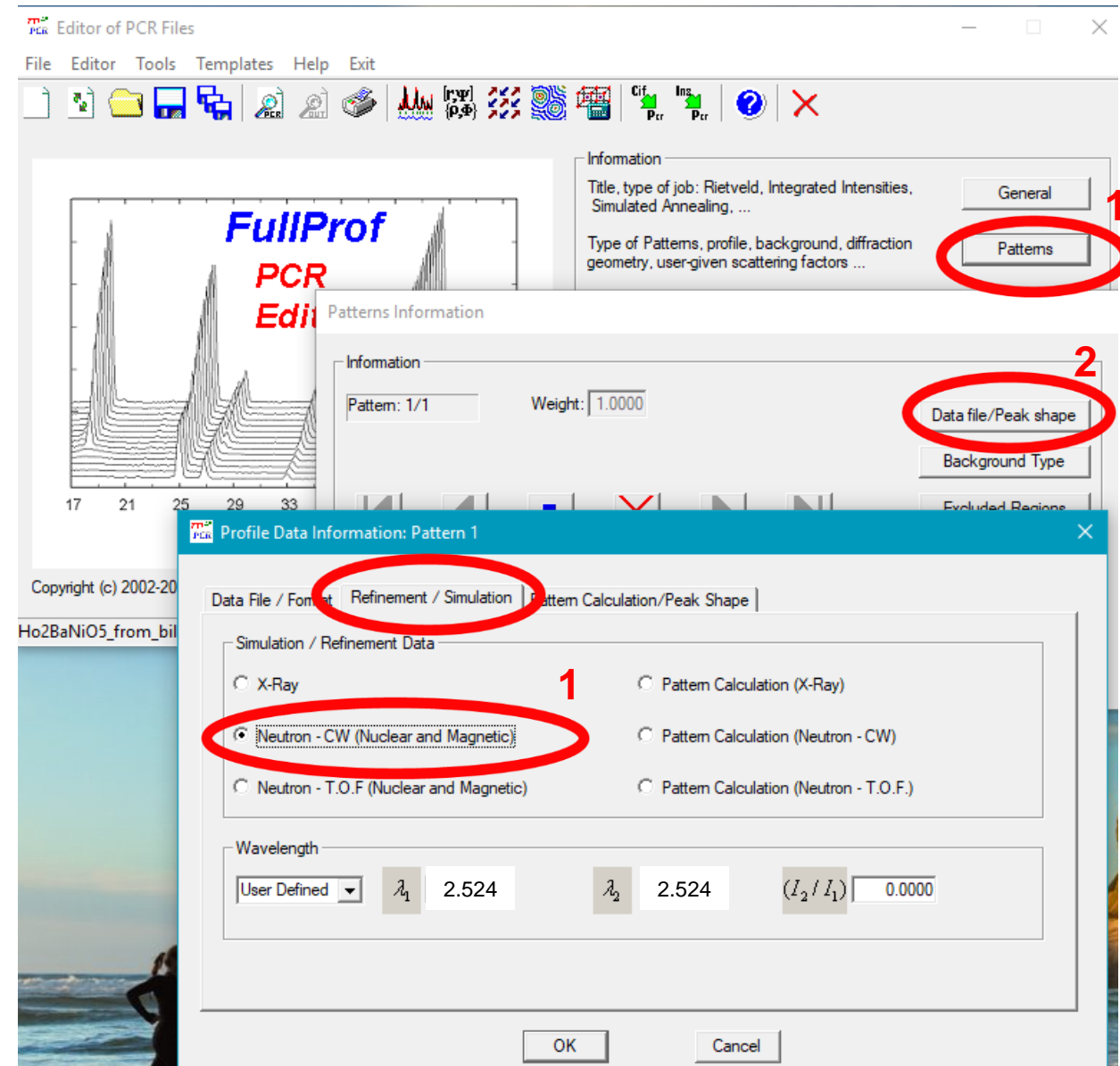
Step 1: Refine the crystal structure using FullProf

- Check final tab:

- Patterns → Data file/Peak Shape →Pattern Calculation/Peak Shape

- Peak shape is already loaded from irf file.
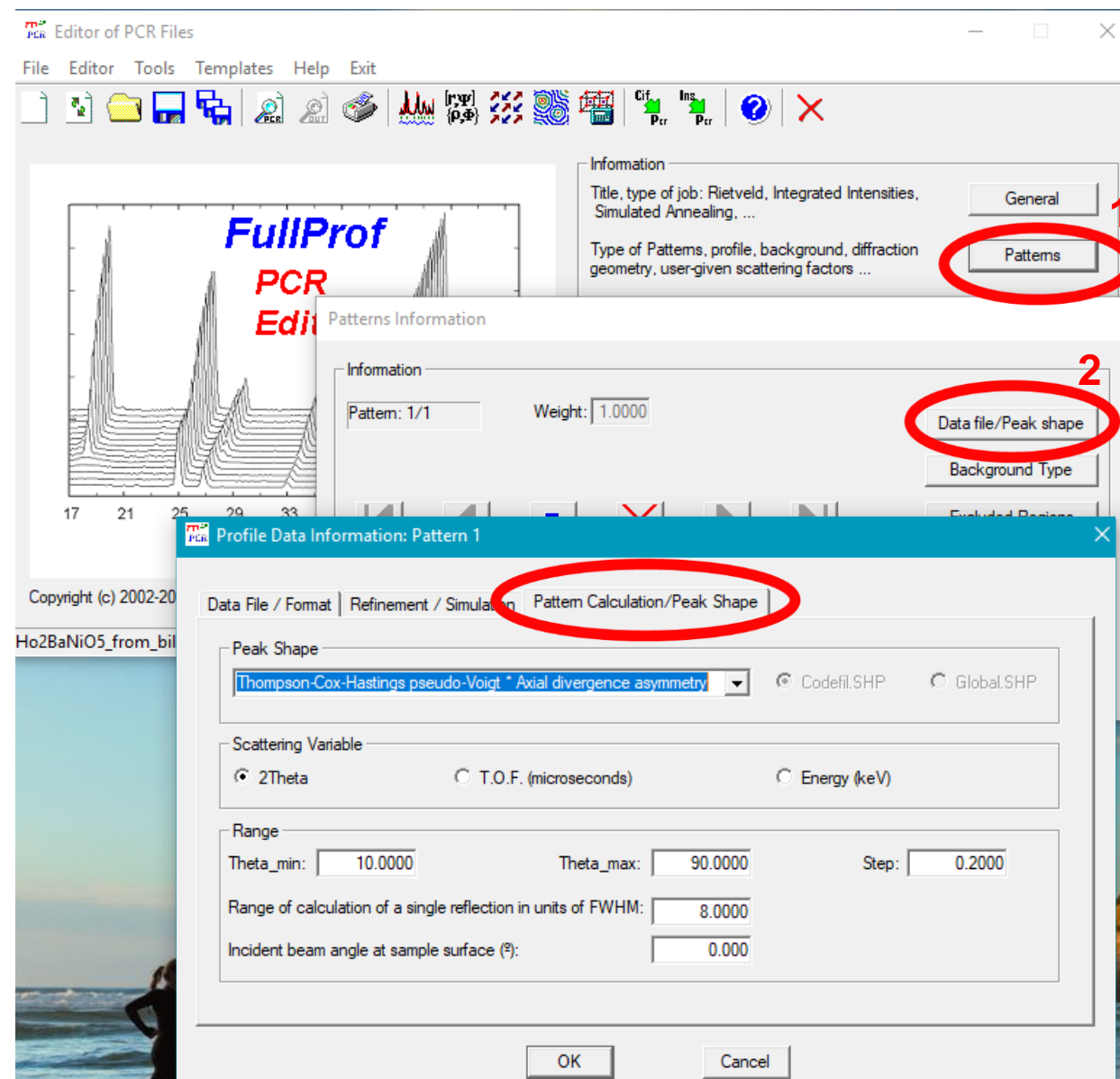
Step 1: Refine the crystal structure using FullProf

- Move to next tab down to select background type

- Patterns→ Background Type Check "6-coefficient"

- Put origin of polynomial at 60 for this example.
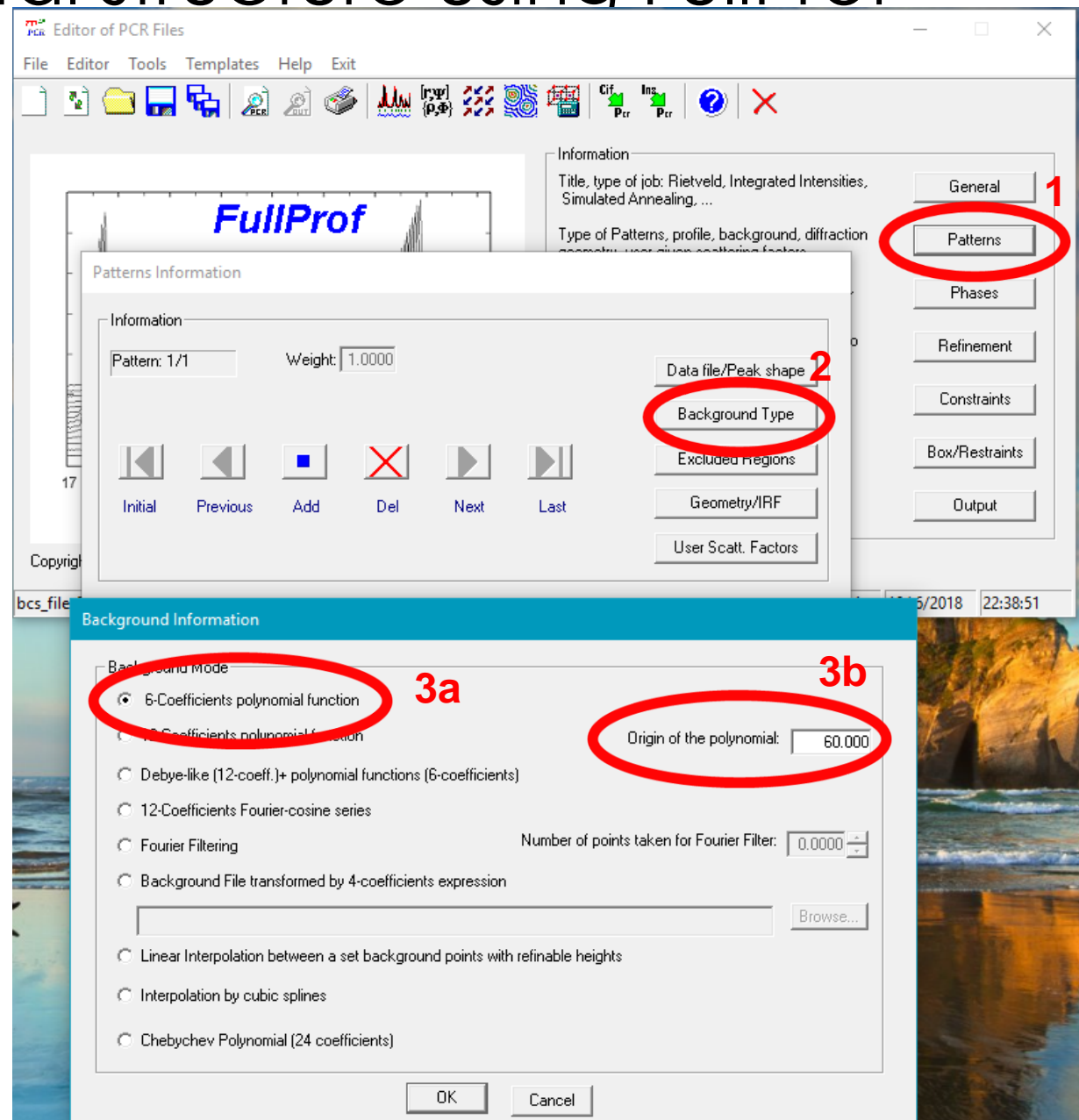
Step 1: Refine the crystal structure using FullProf

- 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

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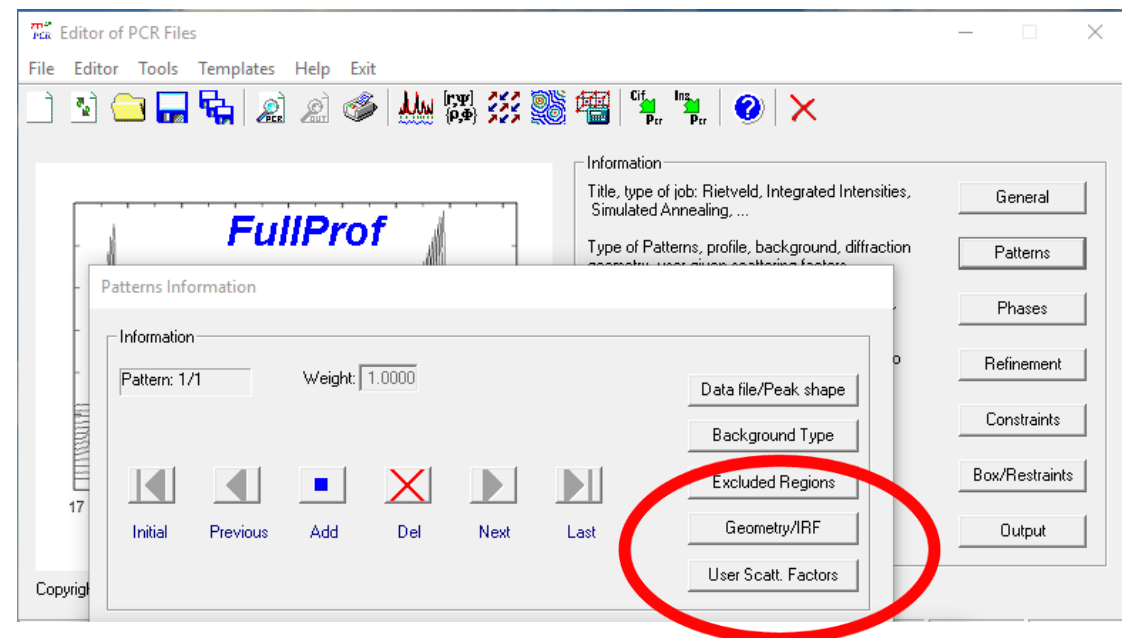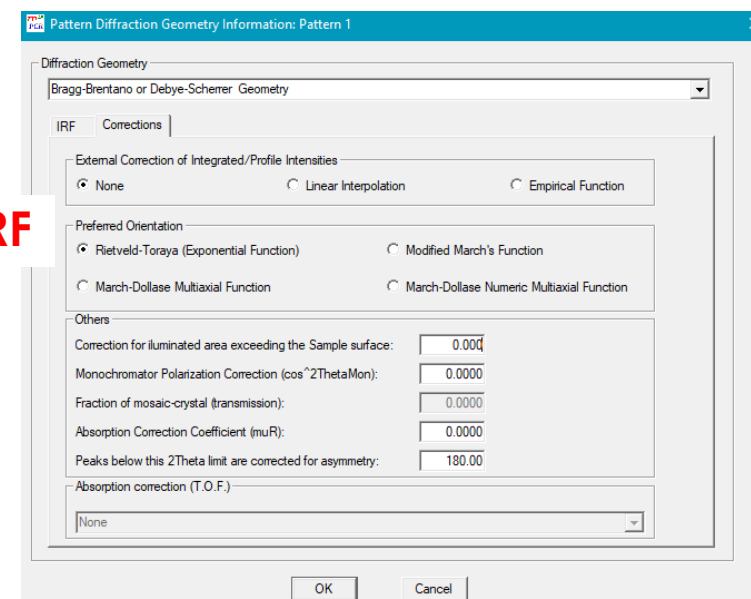
Step 1: Refine the crystal structure using FullProf

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***"
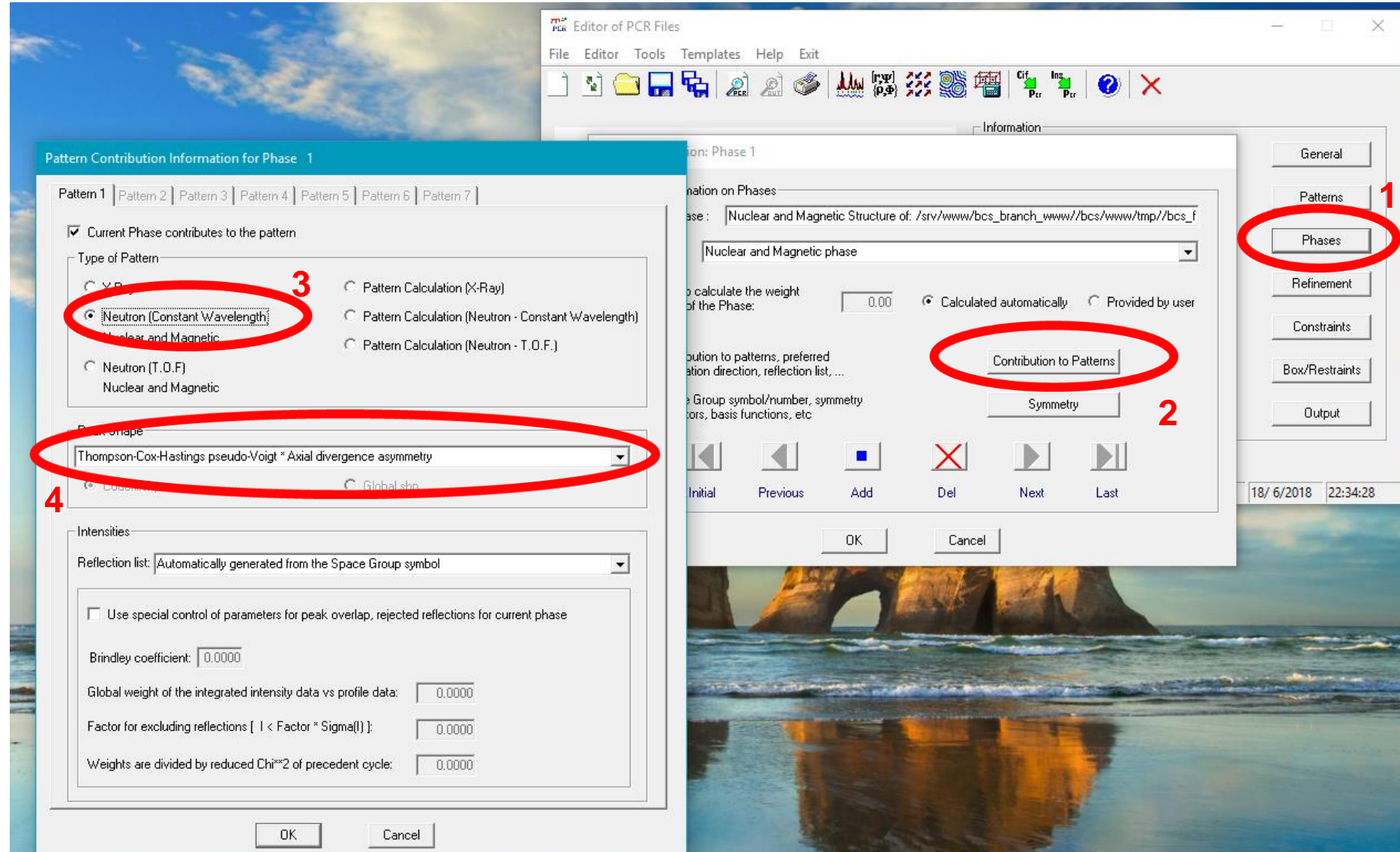
Step 1: Refine the crystal structure using FullProf

REFINEMENT tab:

- Setting starting values for refinements

- Starting background value of 7000 (check data)

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.
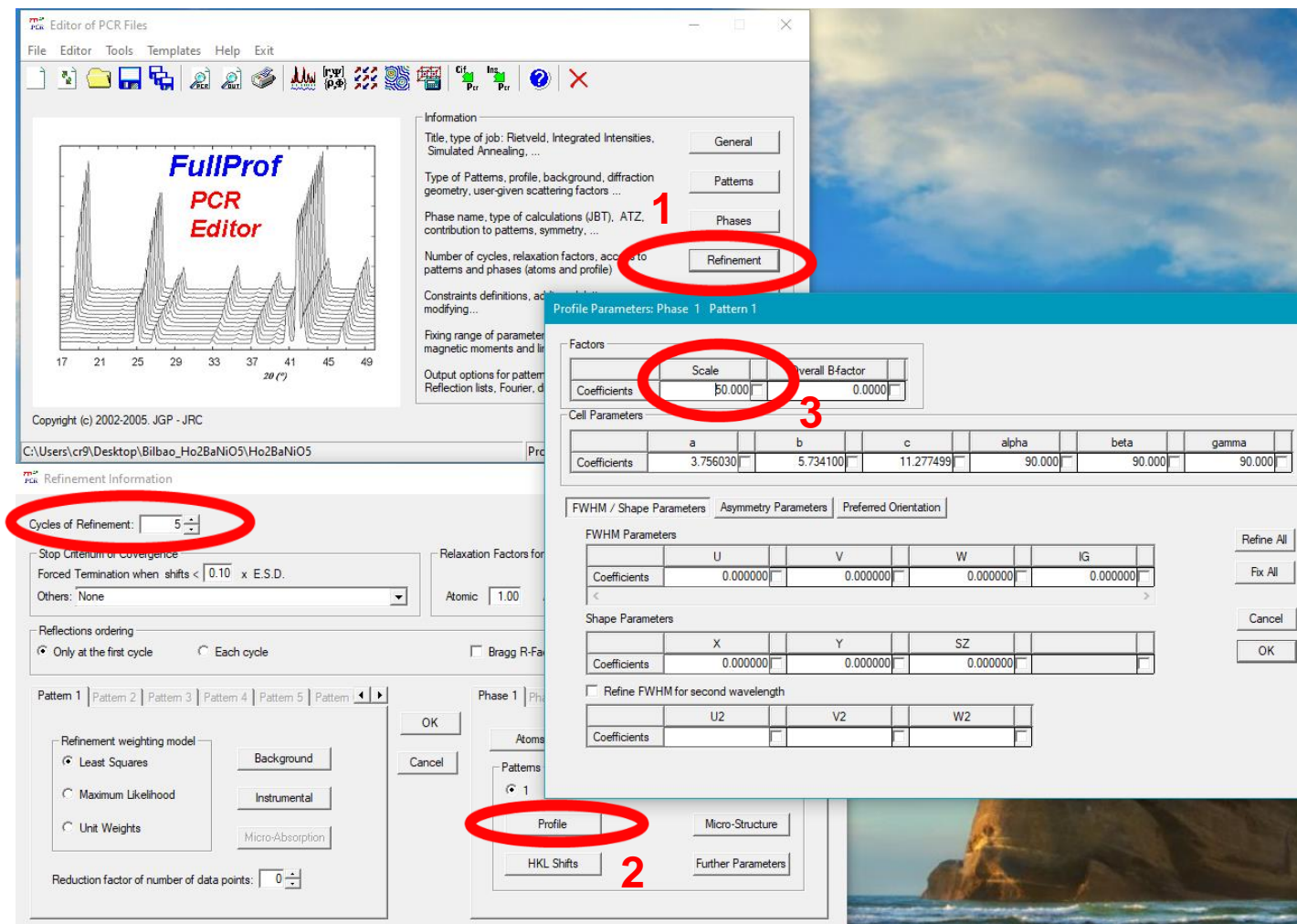
Step 1: Refine the crystal structure using FullProf

- 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"*
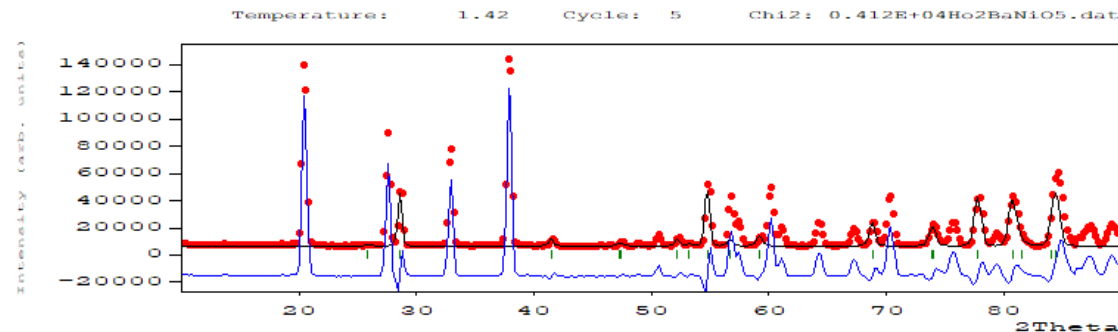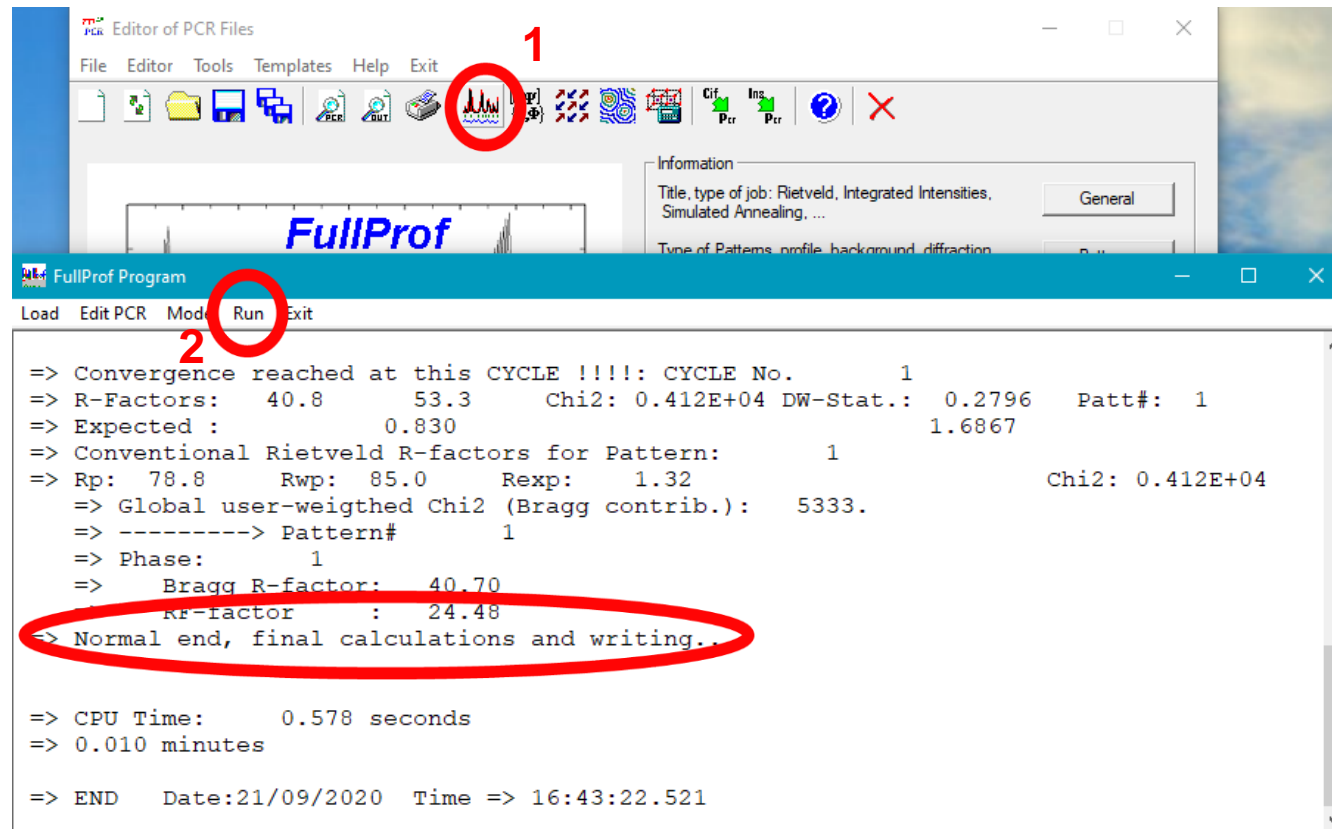
Step 1: Refine the crystal structure using FullProf

- 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	3.751845 ✔	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
Coefficents	7000.0 ✔	0.0000 ✔	0.0000 ✔	0.0000	0.0000	0.0000

	d_6	d_7	d_8	d_9	d_10	d_11
Coefficents						

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	Therm. 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

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Step 1: Refine the crystal structure using FullProf

Run refinement again
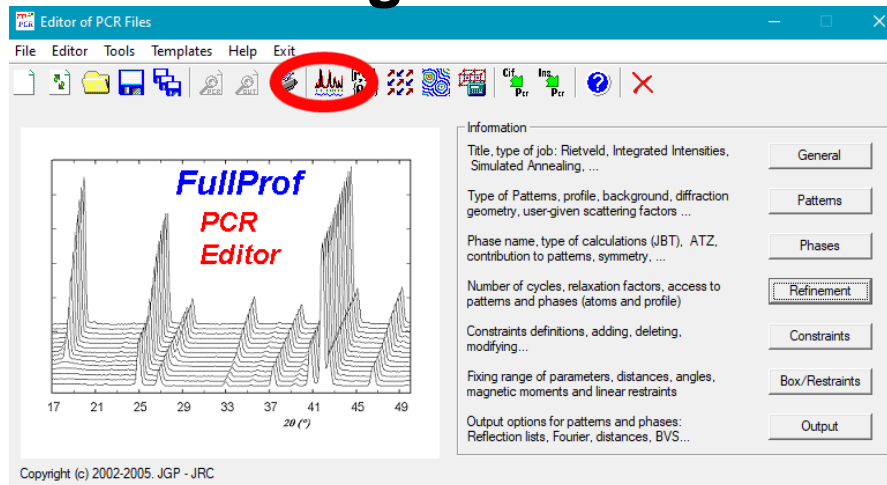
- Check refinement in WinPlotr

- 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.
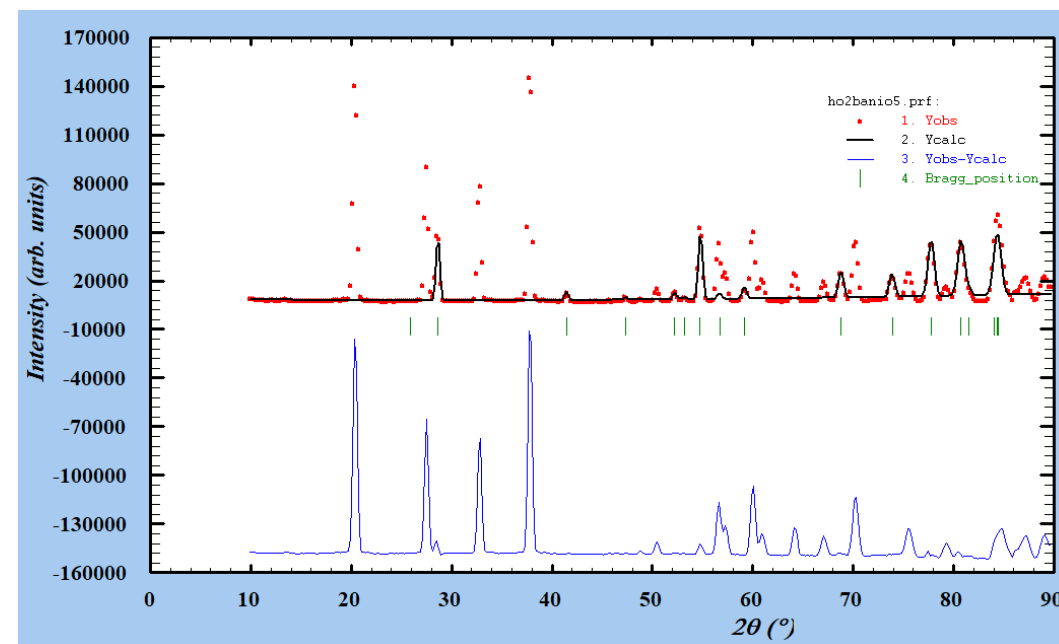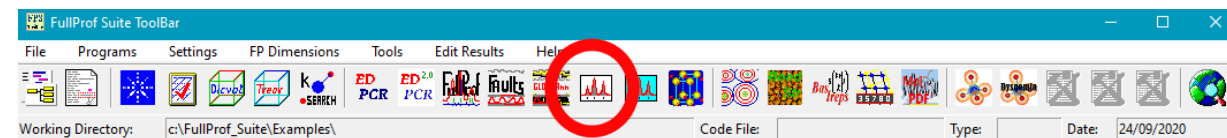
Ho$_2$BaNiO$_5$

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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.
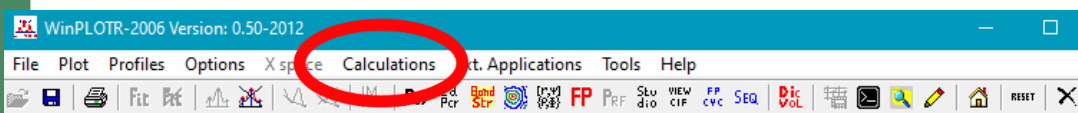
Select magnetic peaks
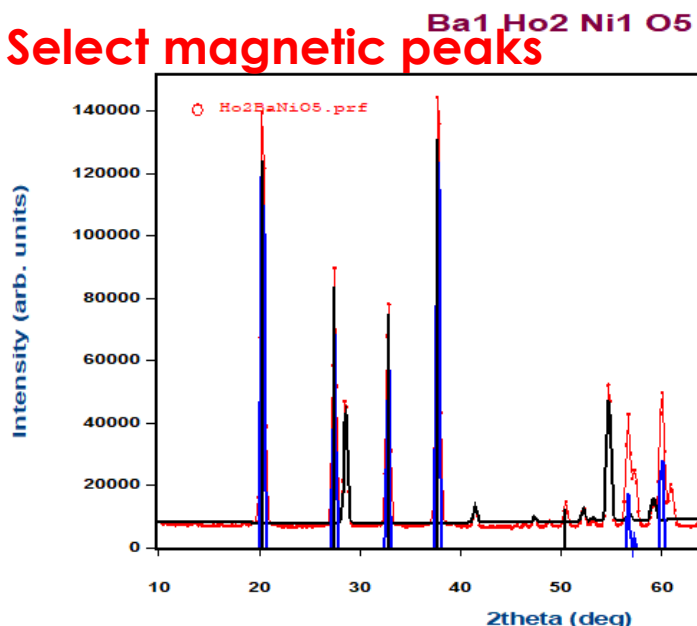
Input structural information

k=(0.5,0,0.5)

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Ho$_2$BaNiO$_5$

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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

Step 3: Creating mCIF file

- Then select "MAXMAGN"

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.

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"

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	☑
2	Ba1	Ba	2c	0.50000 0.50000 0.00000	☐
3	Ni1	Ni	2a	0.00000 0.00000 0.00000	☑
4	O1	O	8l	0.00000 0.24140 0.14950	☐
5	O2	O	2b	0.50000 0.00000 0.00000	☐

Submit

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

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)

- 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**

- Only Ho can contribute to magnetic structure.

- Spins only allowed along x and z (a-axis and c-axis)

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

- Both Ho and Ni can contribute to magnetic structure.

- Spins only allowed along x and z (a-axis and c-axis)

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

- Both Ho and Ni can contribute to magnetic structure.

- Spins only allowed along y (b-axis)

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

- Only Ho can contribute to magnetic structure.

- Spins only allowed along y (b-axis)

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Step 3: Creating mCIF file

- MVISUALIZE lets you quickly check magnetic structure.

- But we will use the downloaded mcif to fit data using fullprof.
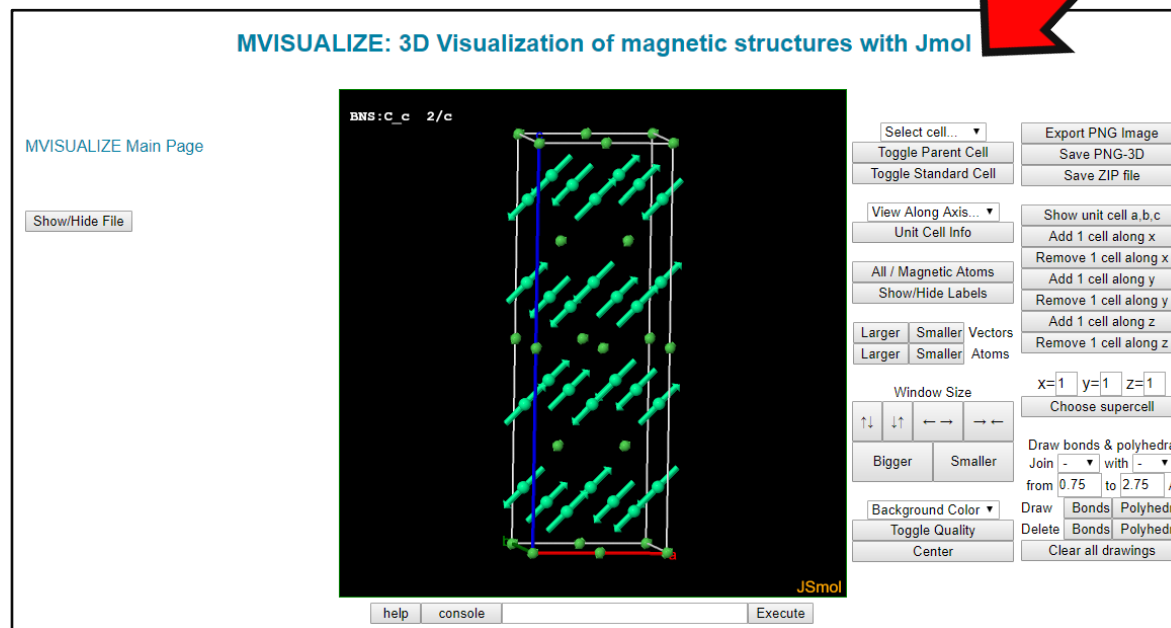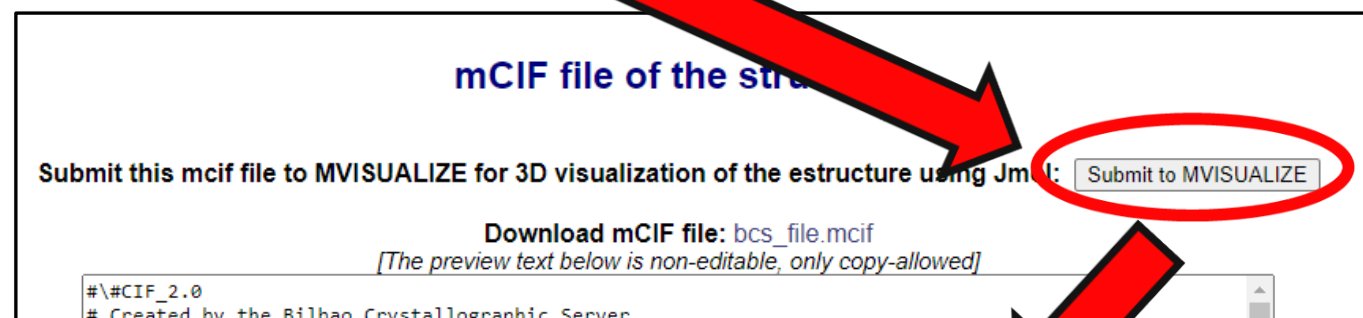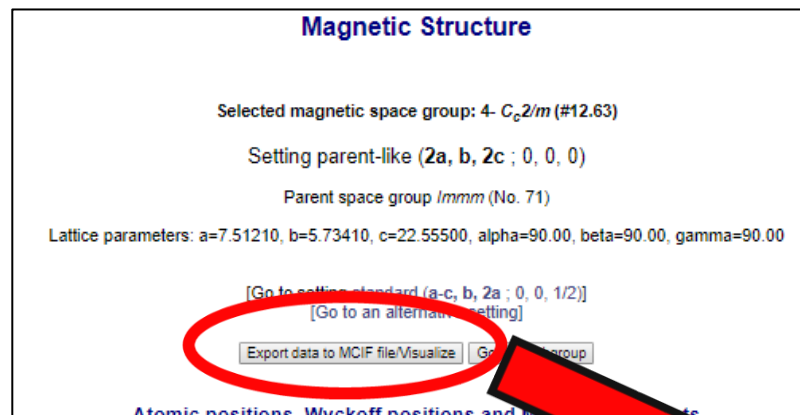
Step 3: Creating mCIF file:

- 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

- 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.

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

2. Click export/view

1. Input values for magnetic moment

Step 3: 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"

We now need
to go to Step 4

Ho$_2$BaNiO$_5$

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Step 4: Creating a pcr from an mcif file

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

Step 4: Creating a pcr from an mcif file

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

- **[2]** Click convert

- This will convert the file and "Click to download it" will download the .pcr file

- We will use this .pcr file in <u>Step 3</u>. Put it in the same folder as the data file "Ho2BaNiO5.dat"

Ho$_2$BaNiO$_5$

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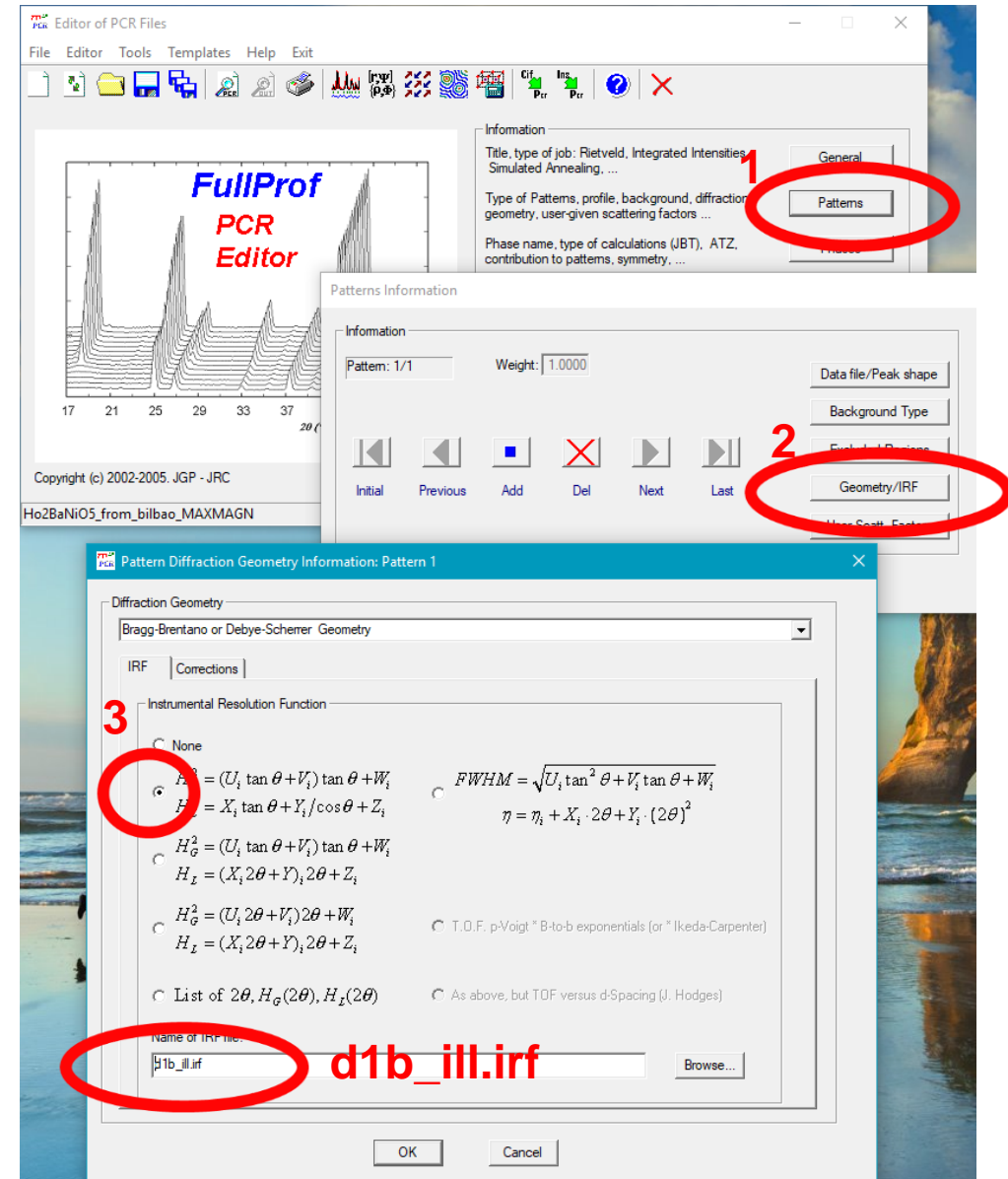
Step 5: Refining the magnetic structure with Fullprof

- 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**

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Step 5: Refining the magnetic structure with Fullprof

- Open pcr file

- Load instrument parameters (irf file)

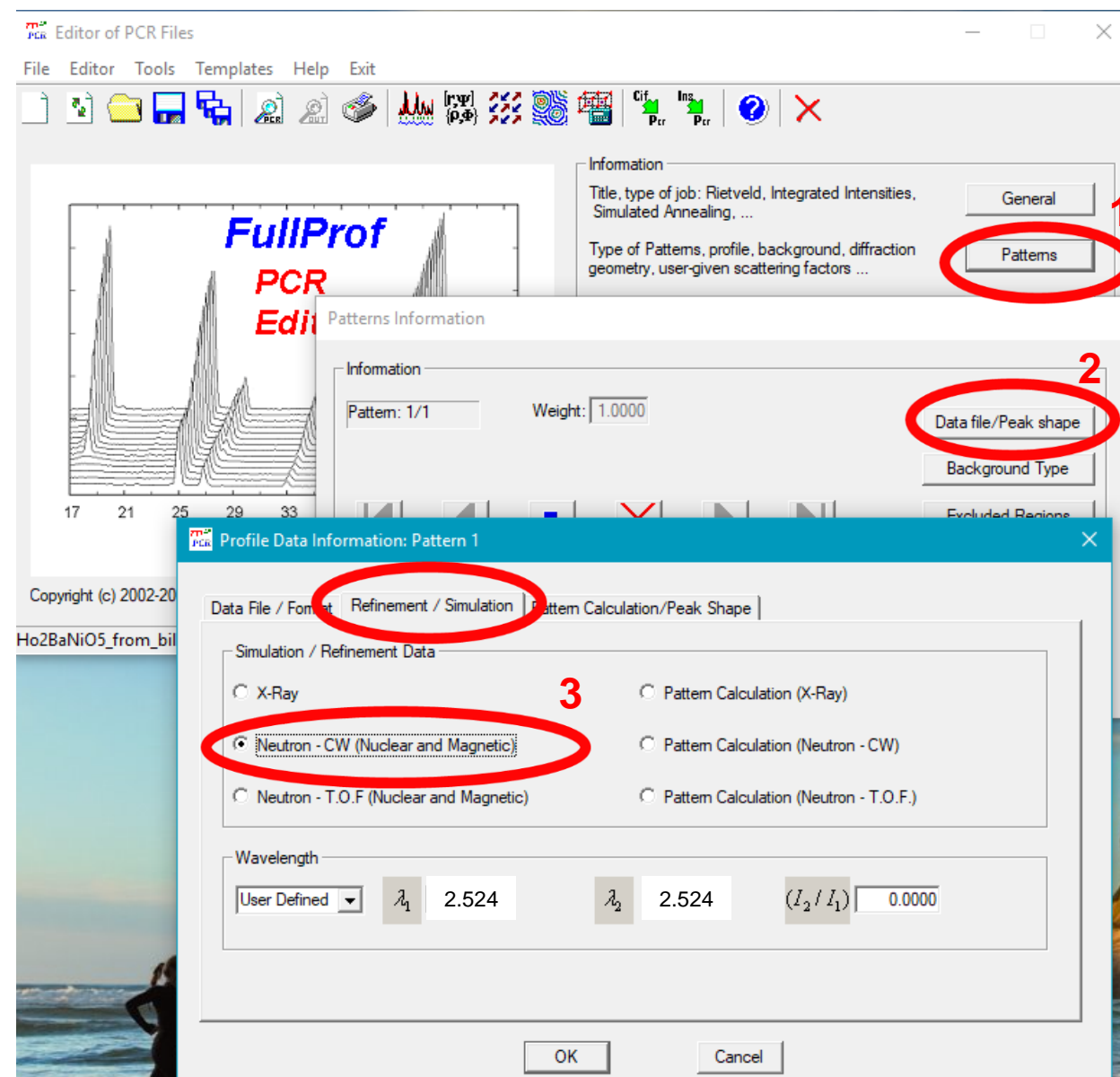- Patterns → Geometry/irf→ d1b_ill.irf

Step 5: Refining the magnetic structure with Fullprof

- Open pcr file

- Select the format of the data file Fullprof should refine.
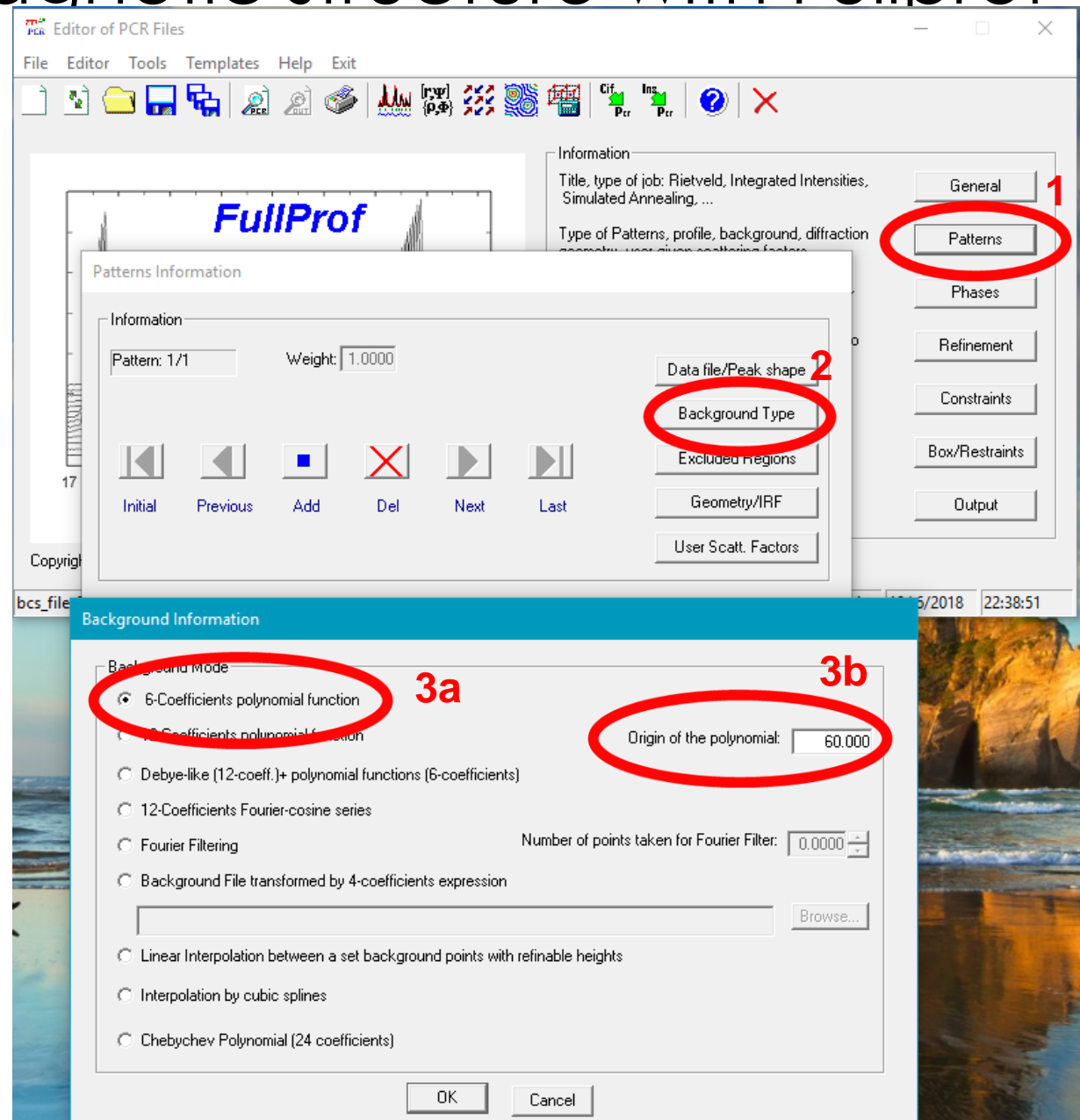
- Patterns → Data file/Peak Shape → D1B/D20
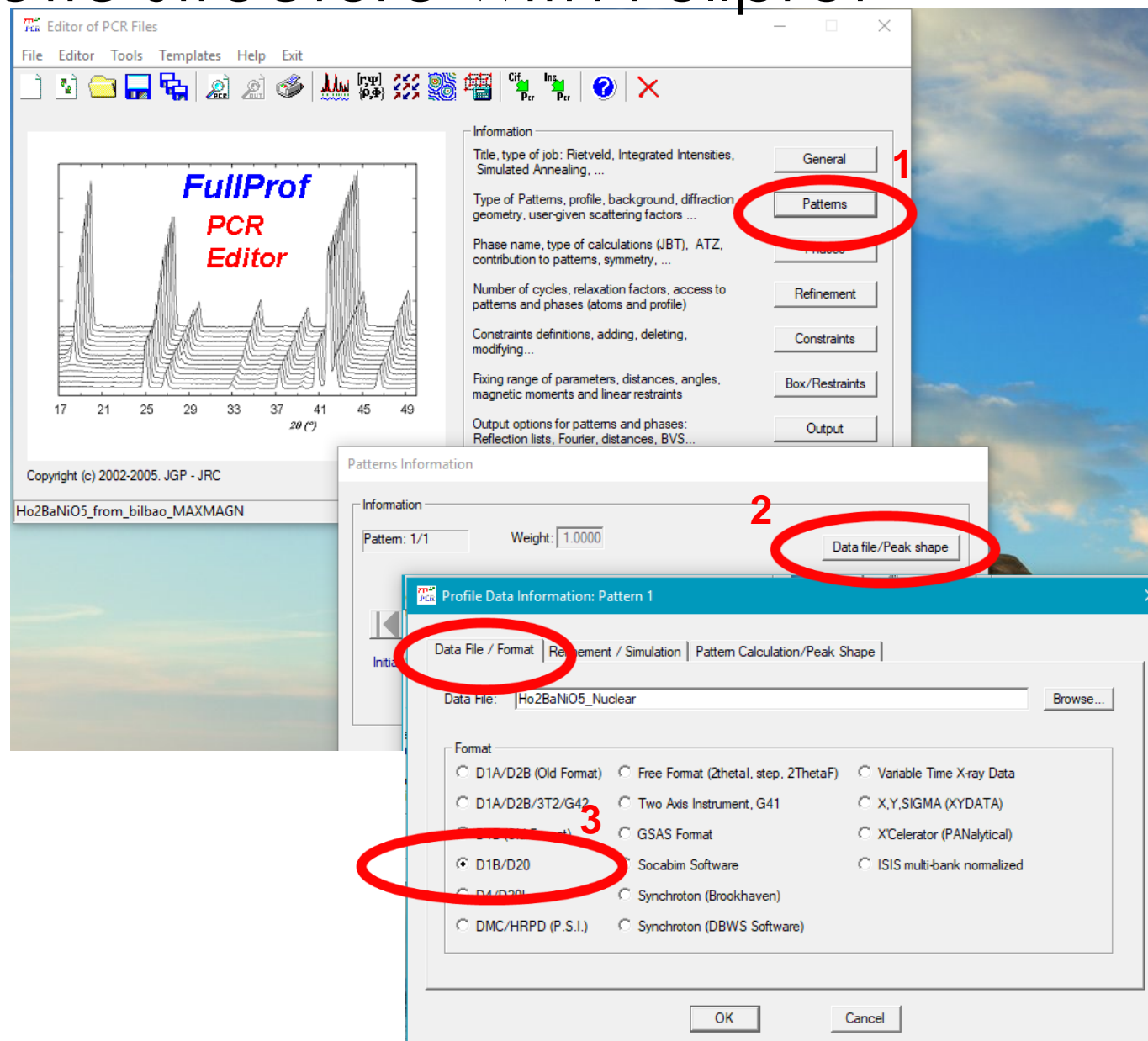
Step 5: Refining the magnetic structure with Fullprof

- 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

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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
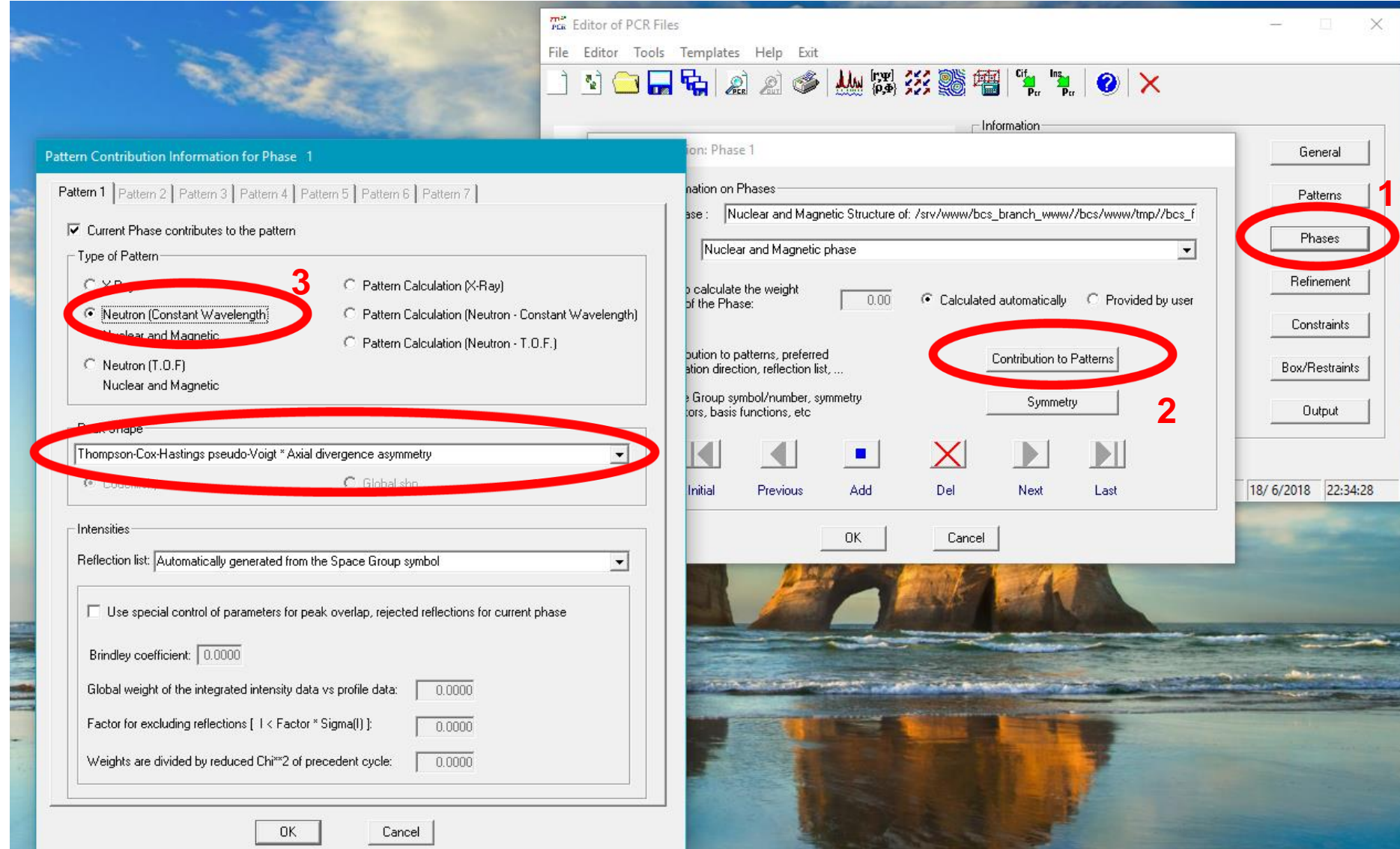
Step 5: Refining the magnetic structure with Fullprof

- 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

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
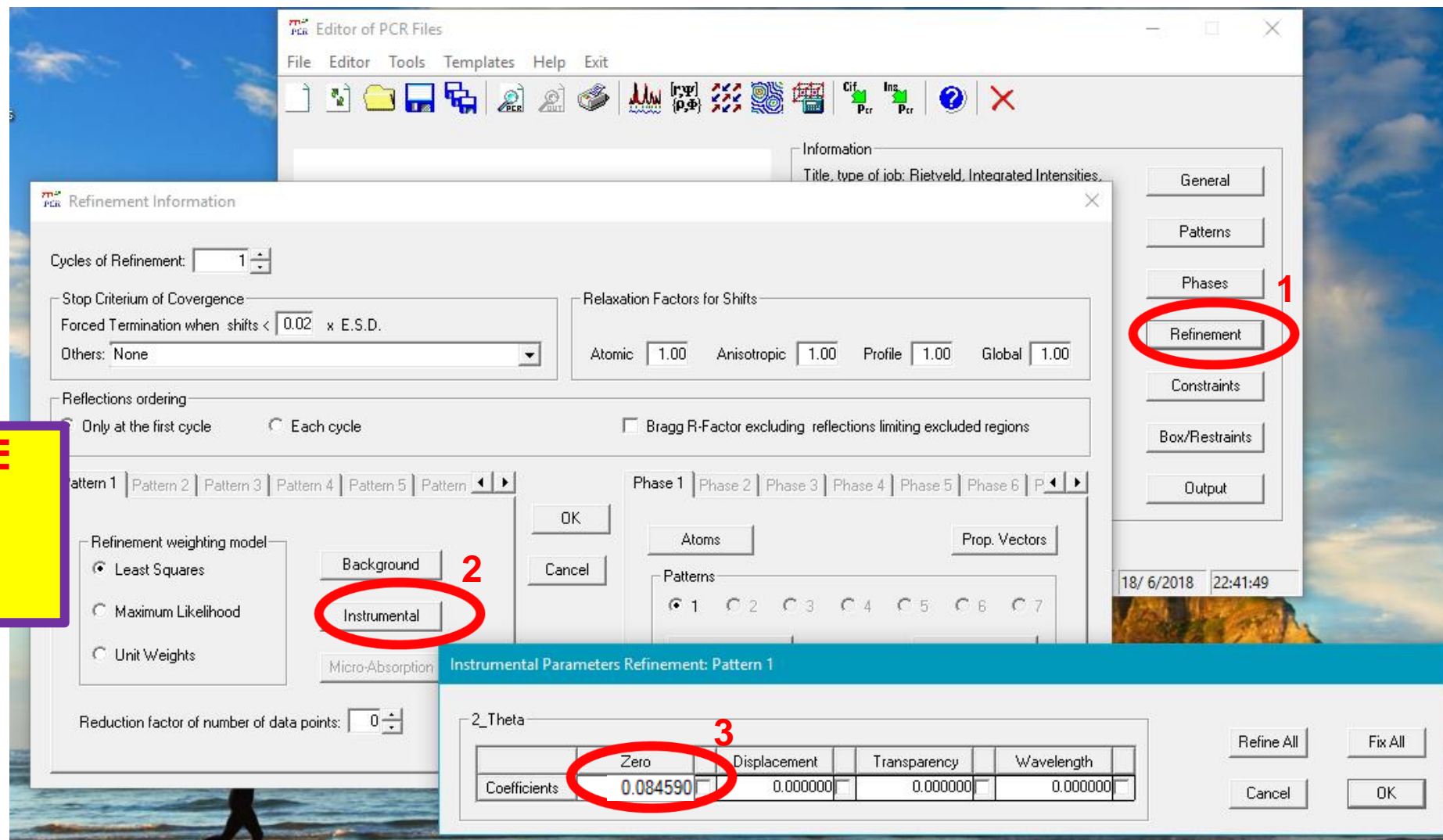
Step 5: Refining the magnetic structure with Fullprof

- 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= (½ 0 ½) the a and c-unit cell values are doubled.
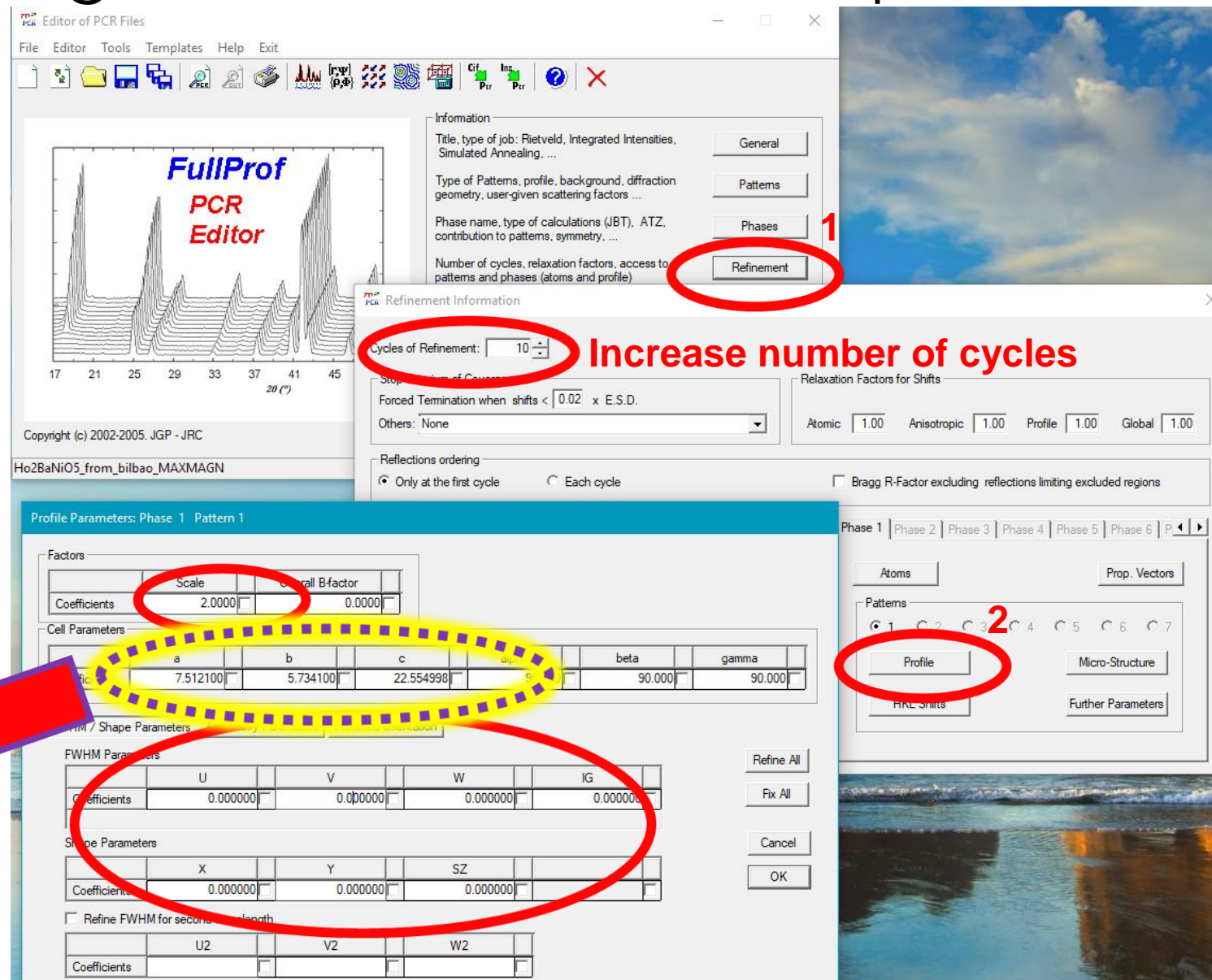
Step 5: Refining the magnetic structure with Fullprof

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

- Note that Re(x) and Re(z) are set to refine.

- This is a default in files from mcif to pcr that we will turn off in next slide.

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

Delete this to stop auto refinements of moments

Step 5: Refining the magnetic structure with Fullprof

Refine background

Refine scale and lattice constants

Refine moments

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Step 5: Refining the magnetic structure with Fullprof

- Run the refinement.

- Select the "Ho2BaNiO5.dat" neutron data file.
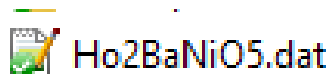
Ho2BaNiO5.dat

- Refinement models most of the data well.

- Notice high chi2 (due to instrument and background)

- But R-factor and Rf-factor low.
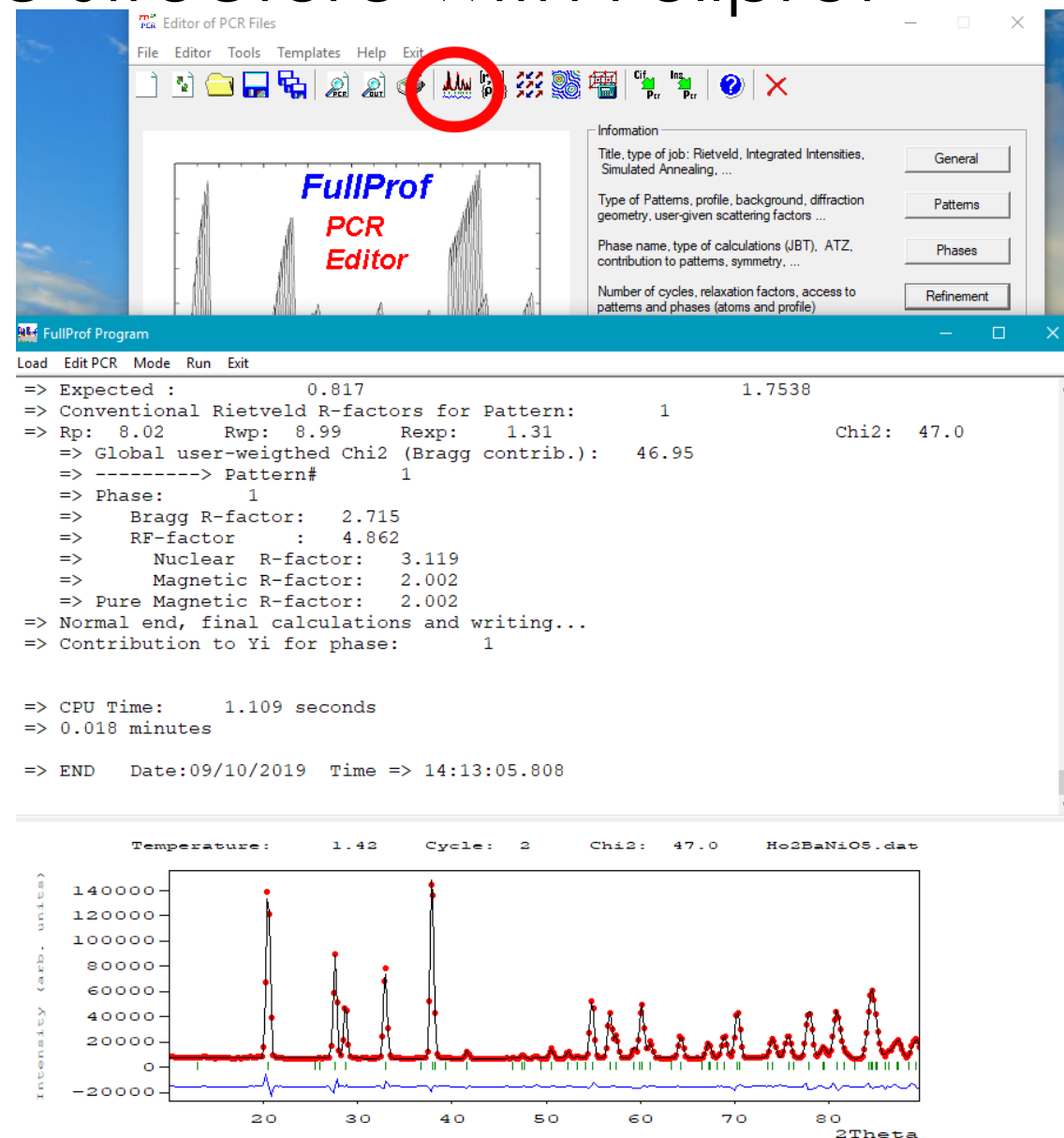
Step 5: Refining the magnetic structure with Fullprof

- List of files output

Name

- Ho2BaNiO5_from_bilbao_MAXMAGN.pcr
- Ho2BaNiO5_from_bilbao_MAXMAGN.out
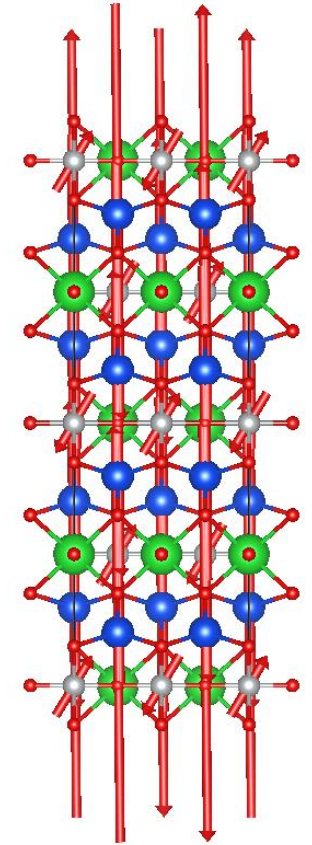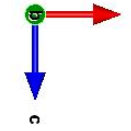- Ho2BaNiO5_from_bilbao_MAXMAGN.prf
- Ho2BaNiO5_from_bilbao_MAXMAGN.sum
- Ho2BaNiO5_from_bilbao_MAXMAGN1.fst
- Ho2BaNiO5_from_bilbao_MAXMAGN1.mcif
- Ho2BaNiO5_from_bilbao_MAXMAGN1.mic
- Ho2BaNiO5_from_bilbao_MAXMAGN1.sub
- Ho2BaNiO5_from_bilbao_MAXMAGN1.vesta

- Check magnetic structure with .fst file (Fpstudio) or .vesta or .mcif outputs.

- Values with errors in .sum file

  Ho: $M_x=0.11(6)$ μ_B; $M_z=9.02(5)$ μ_B

  Ni: $M_x=0.7(1)$ μ_B; $M_z=-1.30(5)$ μ_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	

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