

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

Stuart Calder

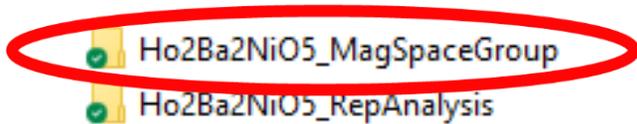
MagStr 2022, ORNL

- 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	

Ho₂BaNiO₅

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



- There is a Ho₂BaNiO₅ 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 Ho₂BaNiO₅ using FullProf Suite and SARAh

Ho₂BaNiO₅

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

NiO₆ 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

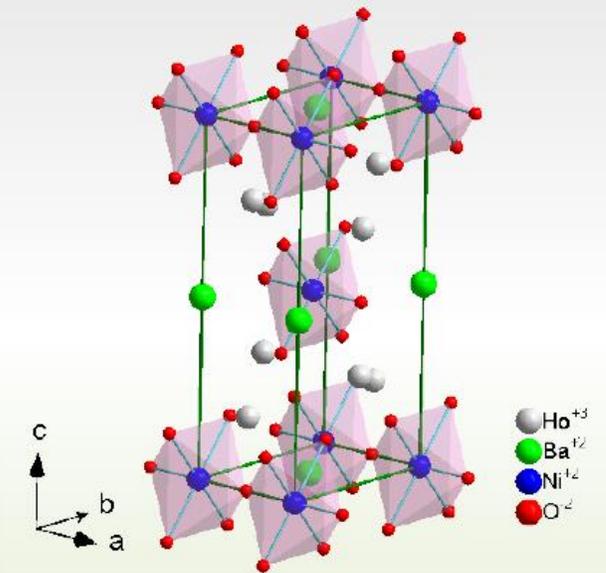
Neutron diffraction study of the magnetic ordering in the series R₂BaNiO₅ (R = Rare Earth)

E. García-Matres^{1,a}, J.L. Martínez², and J. Rodríguez-Carvajal^{3,b}

¹ Institut Laue-Langevin, BP 156, 38042, Grenoble Cedex, France

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

³ 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

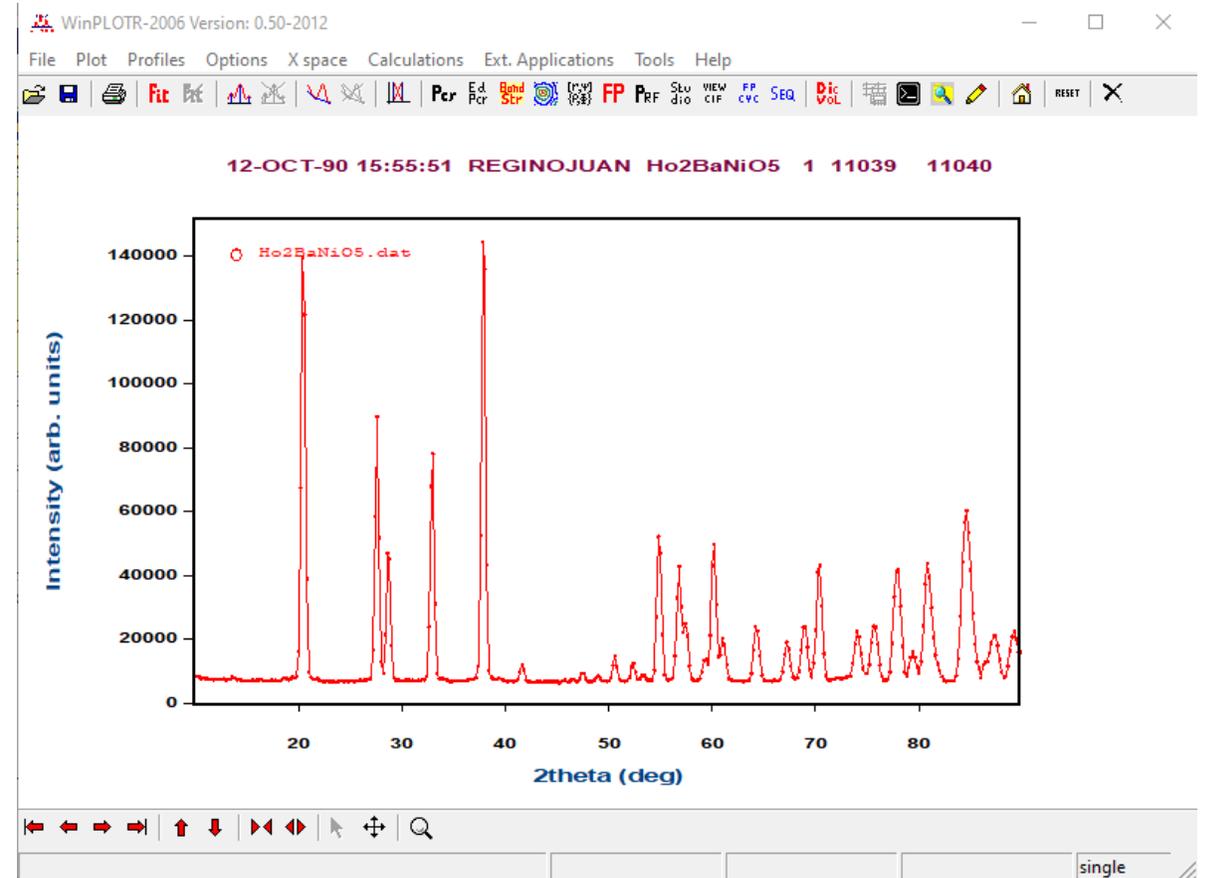


MAGSTR Workshop, Knoxville, TN 2014



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**



Ho₂BaNiO₅

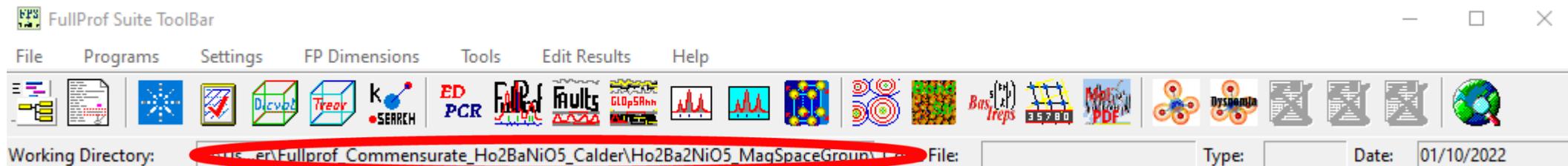
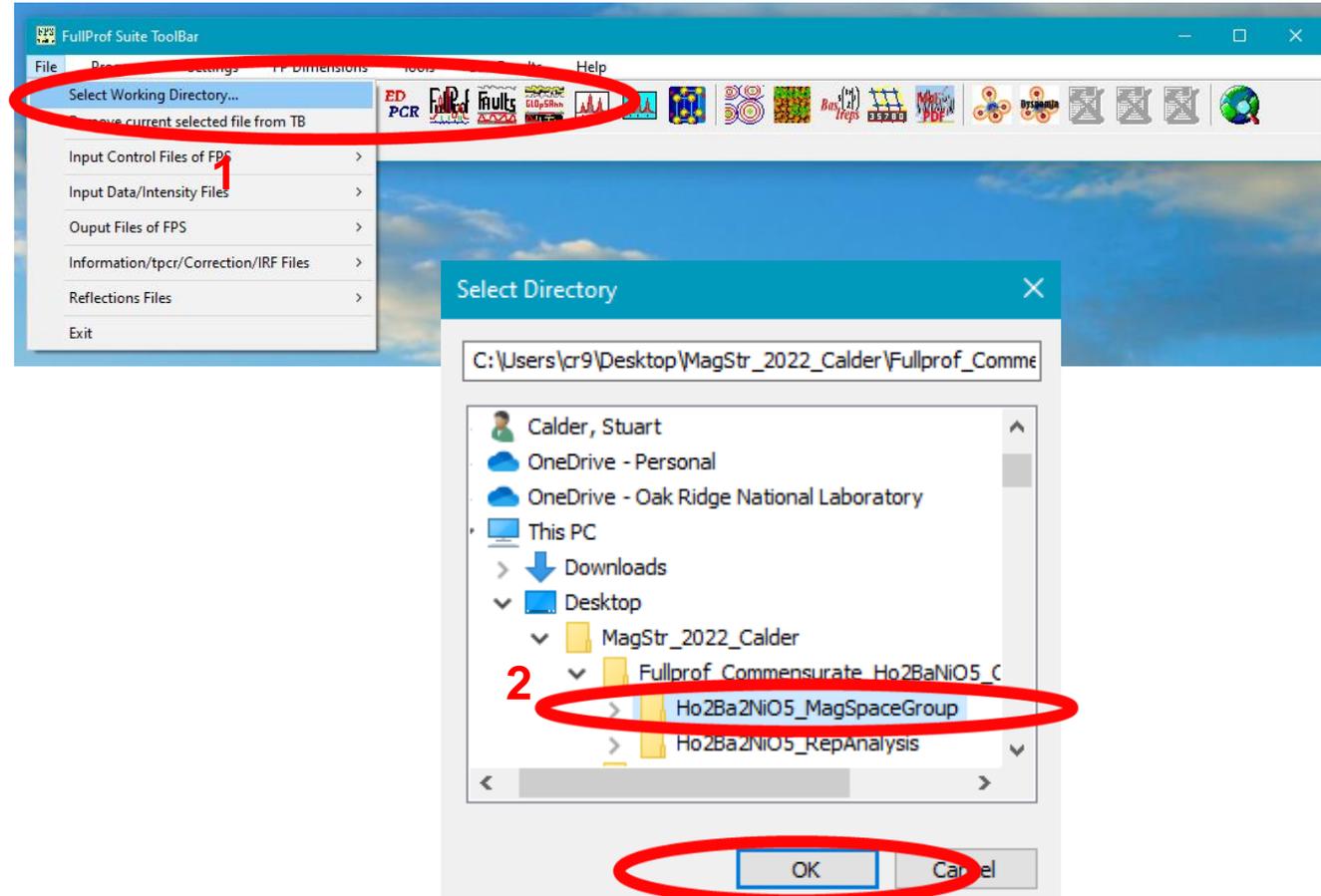
- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
 - Step 1: Refine the crystal structure using FullProf
 - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
 - Step 3: Create test magnetic space groups using 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.

Ho₂BaNiO₅

- 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 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"

The image shows two screenshots of the FullProf Suite software. The top screenshot is the 'FullProf Suite Toolbar' with the 'Ed PCR' button circled in red and labeled '1'. A large red arrow points from this button to the 'Editor of PCR Files' window. In the 'Editor of PCR Files' window, the 'Cif Pcr' button is circled in red and labeled '2'. A second red arrow points from this button to a file explorer window. In the file explorer, the file 'Ho2BaNiO5.cif' is circled in red and labeled '3'. The 'Editor of PCR Files' window also displays a plot of intensity versus 2θ (degrees) with the text 'FullProf PCR Editor' overlaid. The plot shows several sharp peaks. The file explorer window shows a list of files and folders, including 'Bilbao_Ho2BaNiO5_backup', 'Ho2BaNiO5_backup', and 'Ho2BaNiO5.cif'.

File Name	Date	Type
Bilbao_Ho2BaNiO5_backup	9/21/2020 3:43 PM	File folder
Ho2BaNiO5_backup	9/21/2020 3:43 PM	File folder
Ho2BaNiO5.cif	5/28/2014 5:08 PM	CIF File

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”

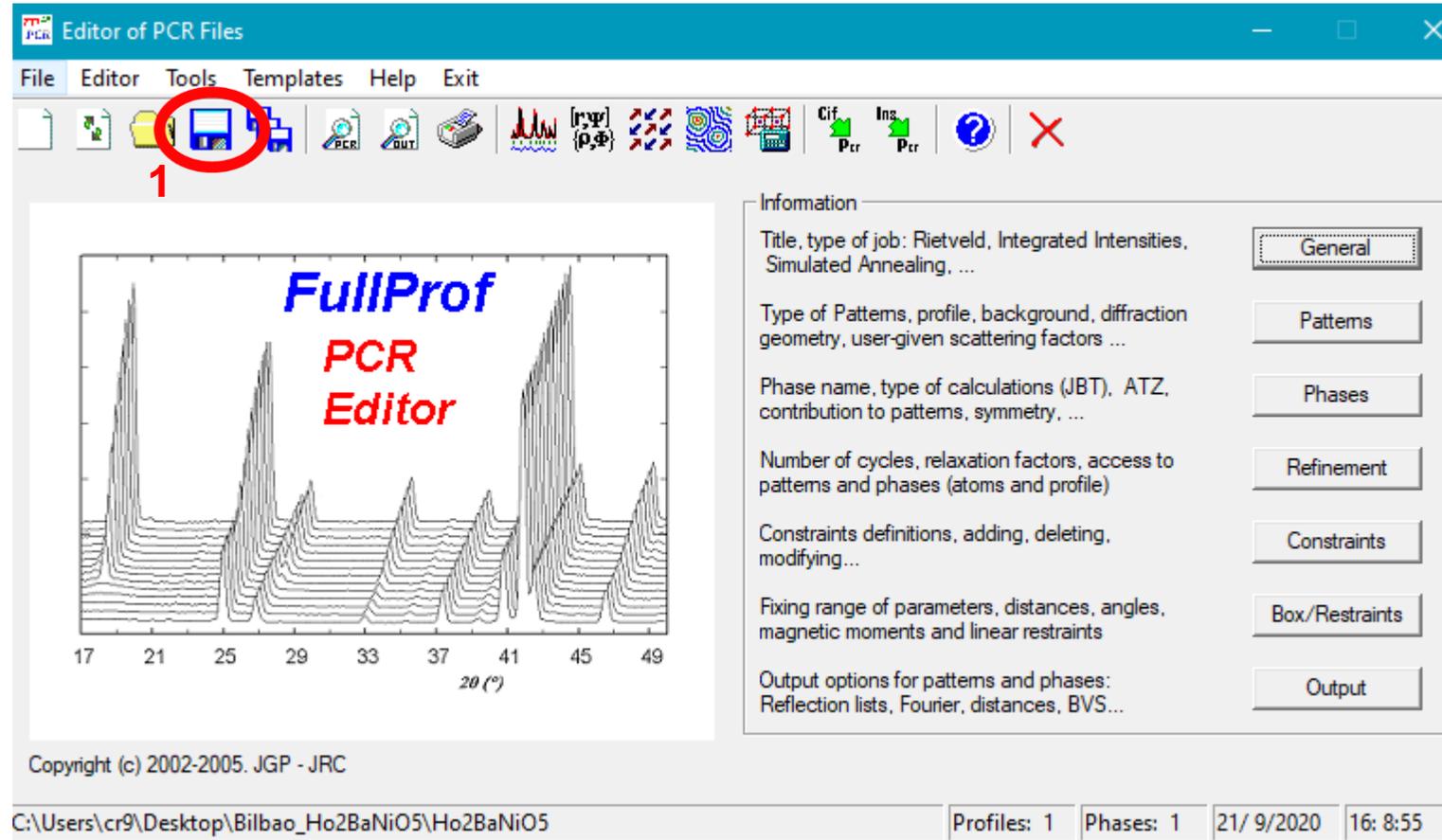
The screenshot shows the FullProf software interface. The 'Simple Calculation Template' dialog box is open, with the following settings:

- Type:** Neutron (circled in red with a '2')
- Instrumental Resolution File:** IRF File d1b_ill.irf (circled in red with a '1')
- Cell Parameters/ SpaceGroup:** I m m m
- Atoms Information:** A table with columns for a, b, c, alpha, beta, and gamma.
- Number of total Operators:** 0
- OK** button (circled in red with a '3')

a	b	c	alpha	beta	gamma
3.756030	5.734100	11.277499	90.000	90.000	90.000

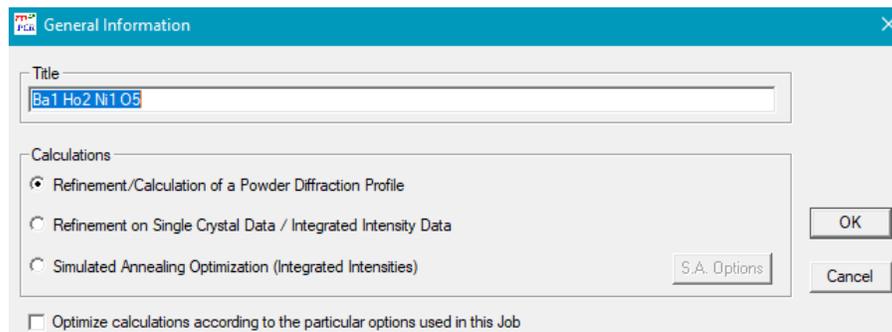
Step 1: Refine the crystal structure using FullProf

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



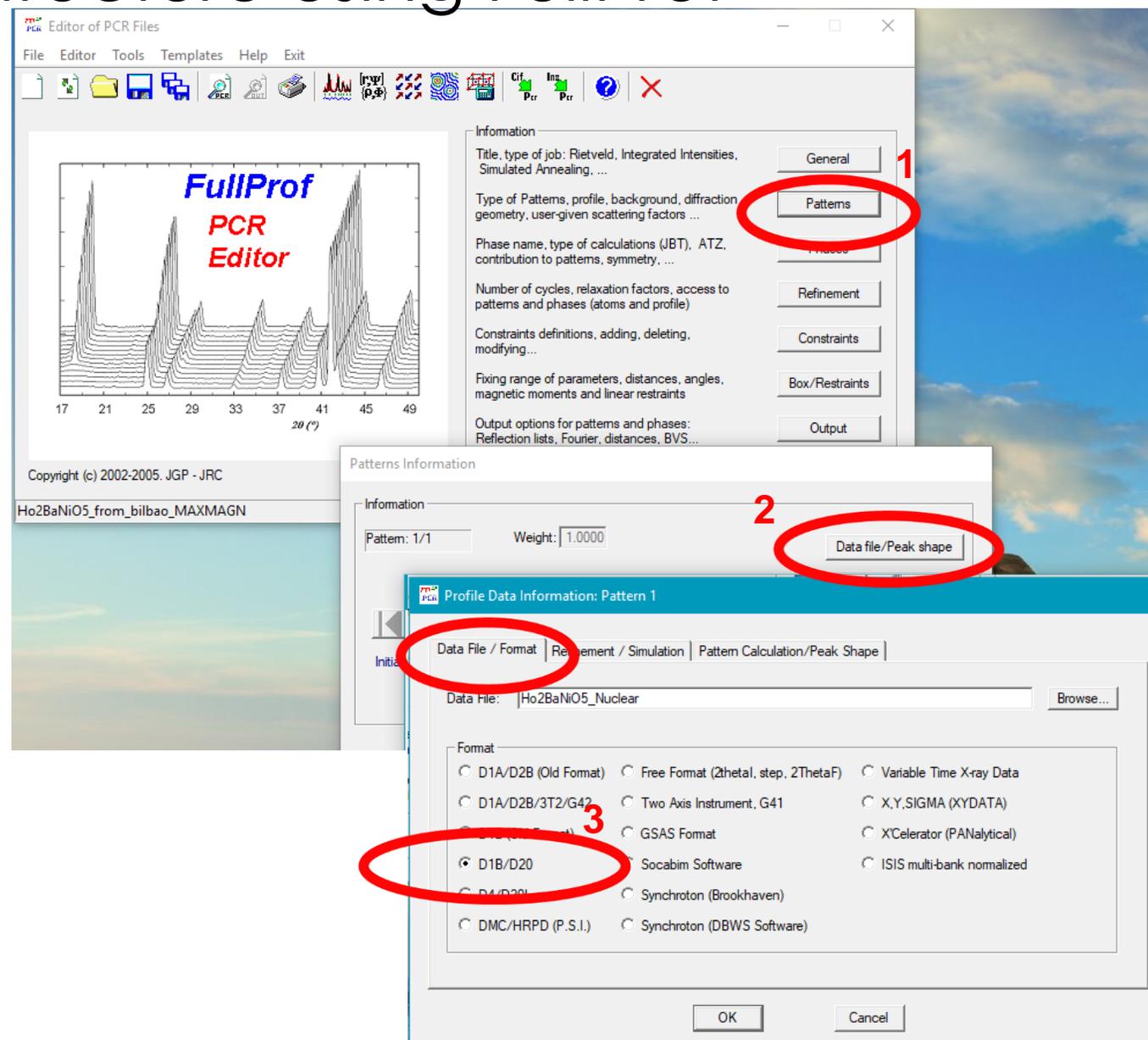
Step 1: Refine the crystal structure using FullProf

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



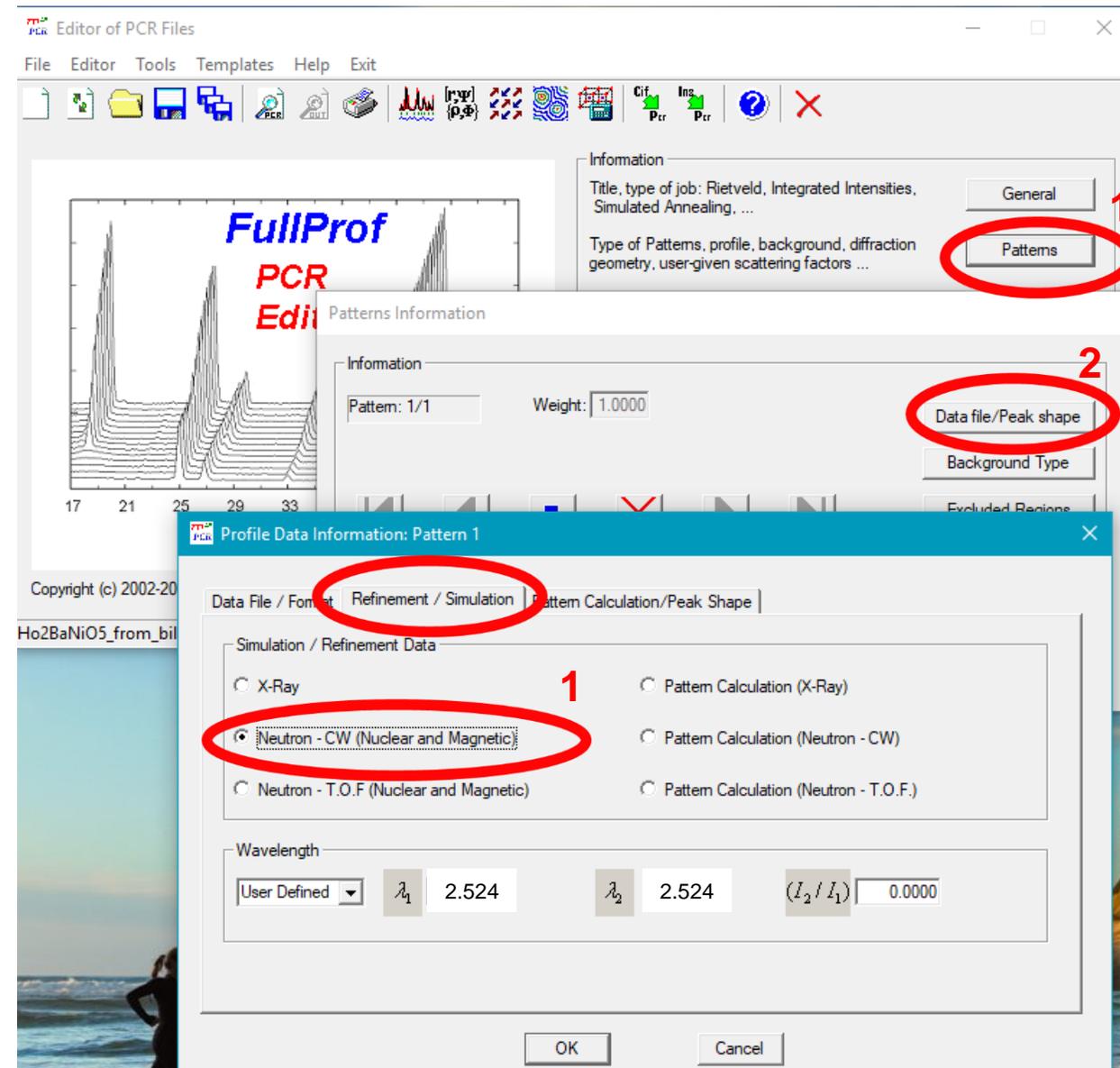
1. “Patterns” tab

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



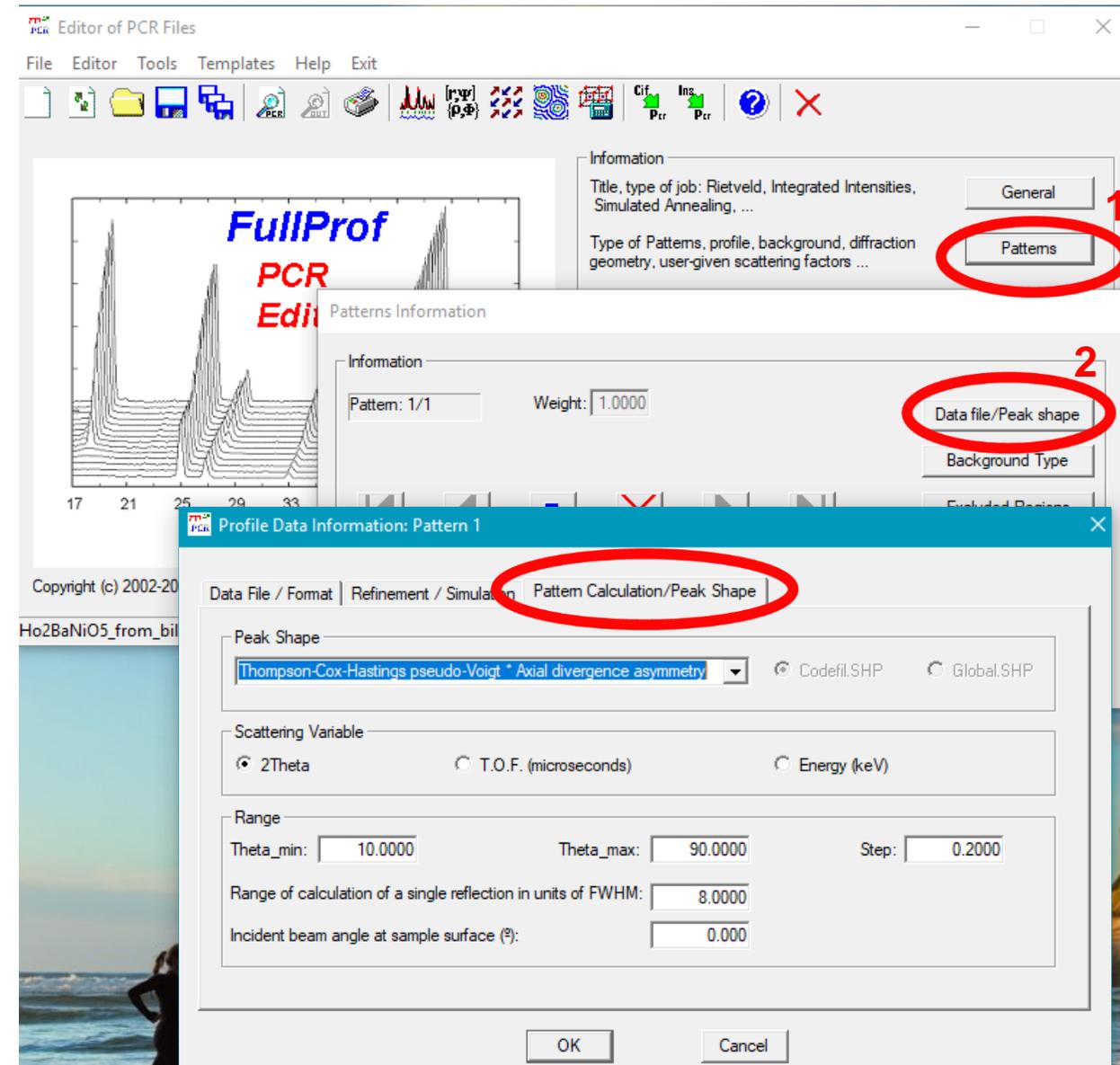
Step 1: Refine the crystal structure using FullProf

- 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.



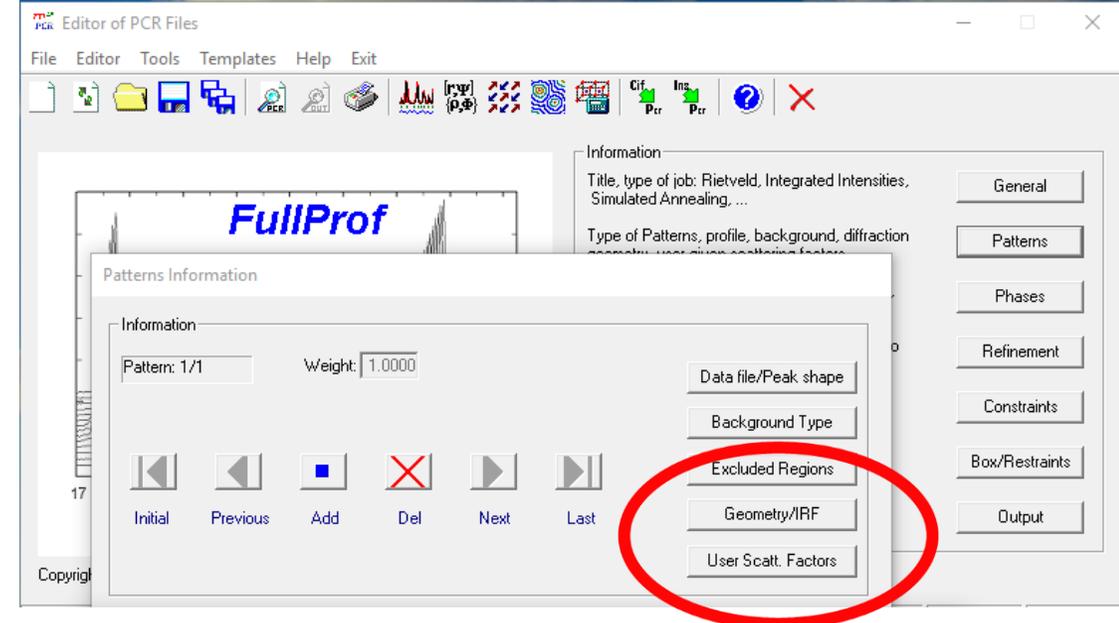
Step 1: Refine the crystal structure using FullProf

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

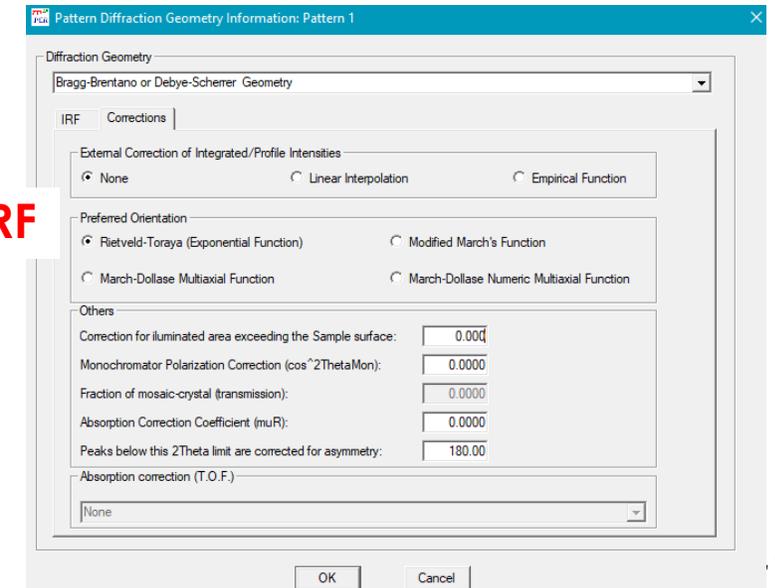
The screenshot shows the FullProf software interface. The main window is titled 'Editor of PCR Files'. A 'Patterns Information' dialog box is open, showing 'Pattern: 1/1' and 'Weight: 1.0000'. The 'Background Type' button is circled in red and labeled '2'. To the right, a vertical menu has the 'Patterns' button circled in red and labeled '1'. Below the 'Patterns Information' dialog, a 'Background Information' dialog box is open. The '6-Coefficients polynomial function' radio button is circled in red and labeled '3a'. The 'Origin of the polynomial' text box, containing the value '60.000', is circled in red and labeled '3b'. The 'Background Information' dialog also shows 'Number of points taken for Fourier Filter: 0.0000' and 'OK' and 'Cancel' buttons at the bottom.

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



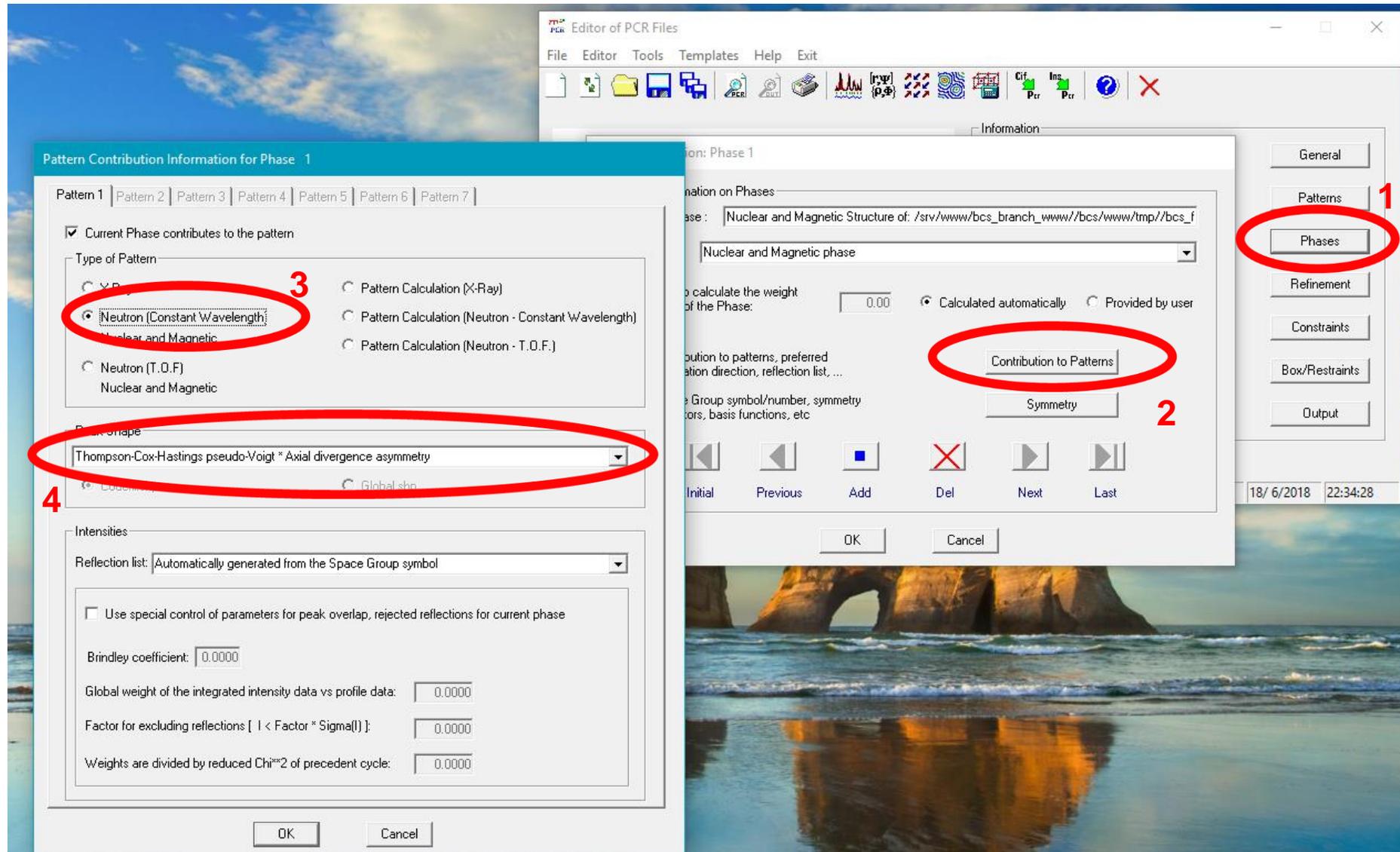
Geometry/IRF



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”**



Step 1: Refine the crystal structure using FullProf

REFINEMENT tab:

- Setting starting values for refinements
- Starting background value of 7000 (check data)

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 menu is circled in red (1). The 'Background' button in the 'Refinement weighting model' section is circled in red (2). The '6 Coefficients Polynomial Background: Pattern 1' dialog box is also open, showing a table of coefficients. The value '7000' in the 'd_0' column is circled in red (3).

	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						

Intensity (arb. units)

13600
12800
12000
11200
10400
9600
8800
8000
7200
6400
5600

6 15 24 33 42 51 60 69 78 87 96

2θ (°)

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.

The screenshot displays the FullProf Editor interface. The main window shows a plot of intensity versus 2θ (degrees) with several peaks. The plot is titled "FullProf PCR Editor".

The "Refinement Information" panel is visible, showing the following settings:

- Cycles of Refinement: 5
- Stop Criterion of convergence: Forced Termination when shifts < 0.10 x E.S.D.
- Others: None
- Reflections ordering: Only at the first cycle
- Refinement weighting model: Least Squares
- Reduction factor of number of data points: 0

The "Profile Parameters: Phase 1 Pattern 1" dialog box is open, showing the following parameters:

Factors	
Scale	50.000
Overall Bfactor	0.0000

Cell Parameters						
a	b	c	alpha	beta	gamma	
3.756030	5.734100	11.277499	90.000	90.000	90.000	

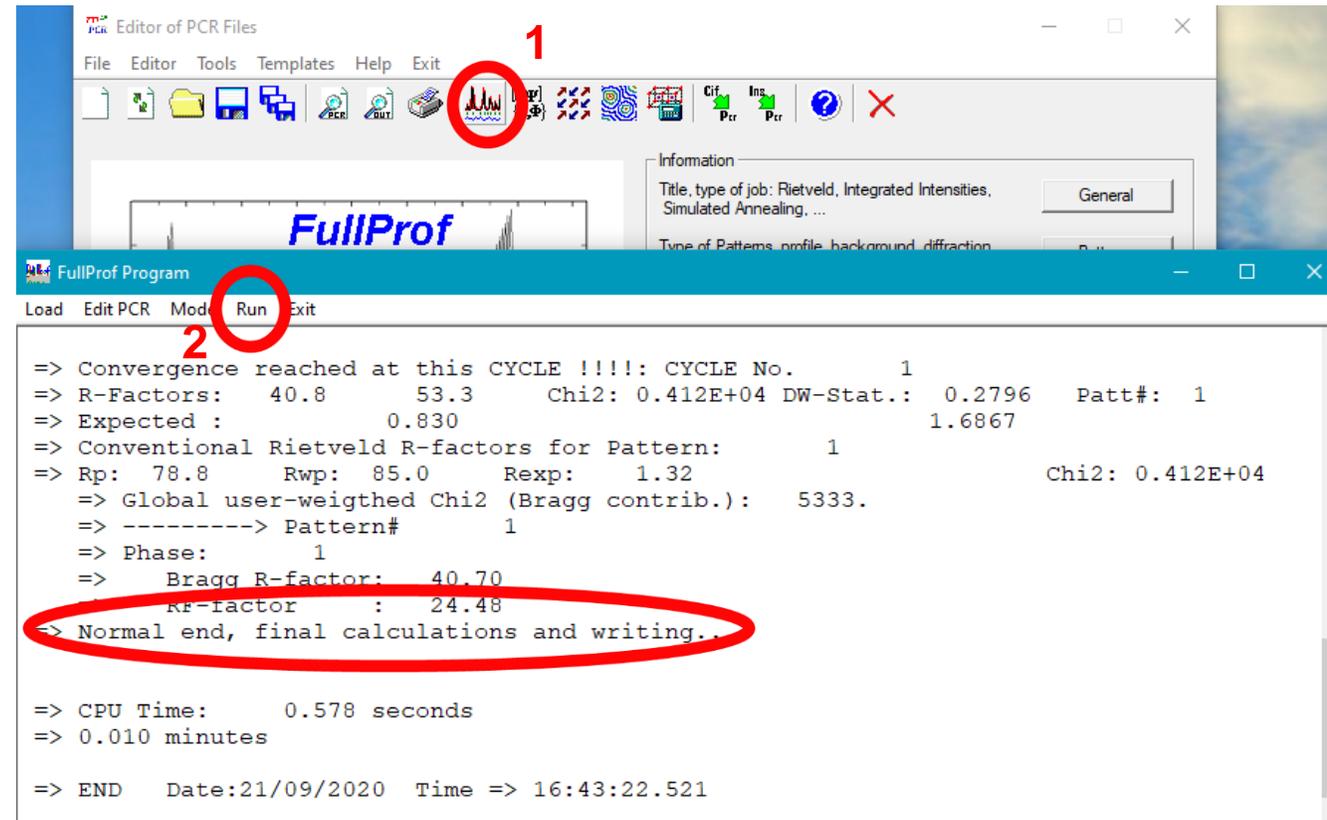
FWHM / Shape Parameters			
FWHM Parameters			
U	V	W	IG
0.000000	0.000000	0.000000	0.000000

Shape Parameters		
X	Y	SZ
0.000000	0.000000	0.000000

The "Profile" button in the "Refinement" tab is highlighted with a red circle. The "Scale" parameter in the "Profile Parameters" dialog is also highlighted with a red circle. The "Cycles of Refinement" field in the "Refinement Information" panel is highlighted with a red circle.

Step 1: Refine the crystal structure using FullProf

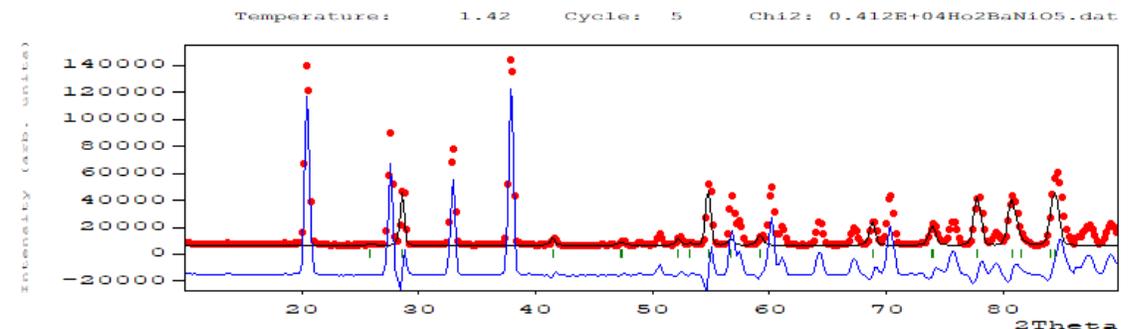
- 1. Can now run the refinement
Select the “*Ho2BaNiO5.dat*” data
 - Note: we have not set anything to refine yet. It is good to check your model is close to the data and makes sense before refining.
- 2. Refinement runs for the number of cycles (in this case 5). You can repeat this by pushing run until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



```
=> Convergence reached at this CYCLE !!!!: CYCLE No.      1
=> R-Factors:   40.8   53.3   Chi2: 0.412E+04 DW-Stat.:  0.2796   Patt#:  1
=> Expected :           0.830                               1.6867
=> Conventional Rietveld R-factors for Pattern:           1
=> Rp:  78.8   Rwp:  85.0   Rexp:  1.32                               Chi2: 0.412E+04
=> Global user-weighted Chi2 (Bragg contrib.):  5333.
=> -----> Pattern#      1
=> Phase:           1
=> Bragg R-factor:   40.70
=> Rp-factor       :  24.48
=> Normal end, final calculations and writing...

=> CPU Time:       0.578 seconds
=> 0.010 minutes

=> END   Date:21/09/2020   Time => 16:43:22.521
```



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

Buttons: 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						

Buttons: Refine All, Fix All

Instrumental Parameters Refinement: Pattern 1

2_Theta

	Zero	Displacement	Transparency	Wavelength
Coefficients	0.000000 ✓	0.000000	0.000000	0.000000

Buttons: Refine All, Fix All, Cancel, OK

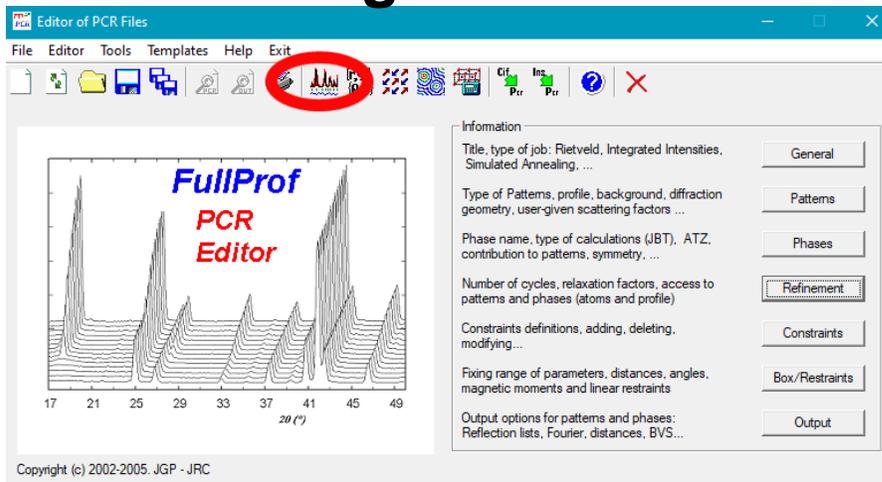
List of Atoms

Number of Atoms: 5

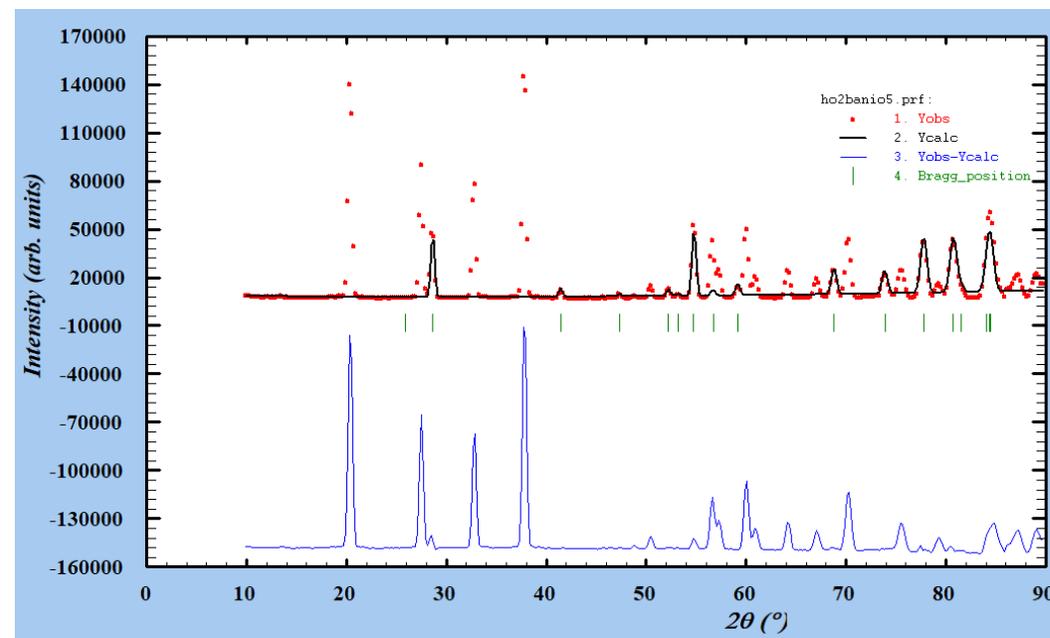
	Label	Ntyp	X	Y	Z	B	Occ	Them. Fact.
Atom # 1	Ho1	Ho	0.50000	0.00000	0.20250 ✓	0.00000	0.25000	Isotropic
Atom # 2	Ba1	Ba	0.50000	0.50000	0.00000	0.00000	0.12500	Isotropic
Atom # 3	Ni1	Ni	0.00000	0.00000	0.00000	0.00000	0.12500	Isotropic
Atom # 4	O1	O	0.00000	0.24140 ✓	0.14950 ✓	0.00000	0.50000	Isotropic

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.

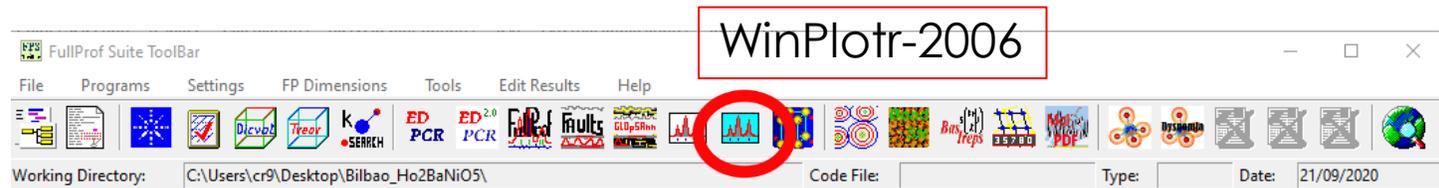


Ho₂BaNiO₅

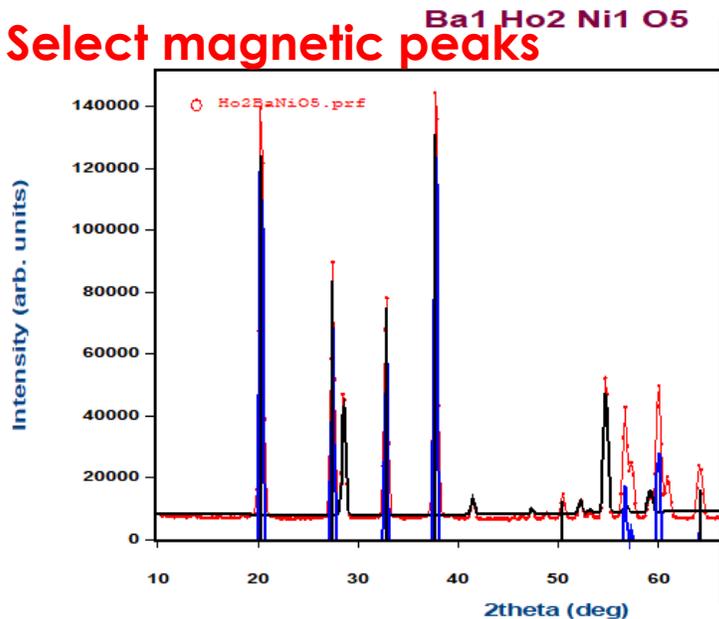
- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
 - Step 1: Refine the crystal structure using FullProf
 - **Step 2: Determine the k-vector by indexing the magnetic reflections using k-search**
 - Step 3: Create test magnetic space groups 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.

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|

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)

Ho₂BaNiO₅

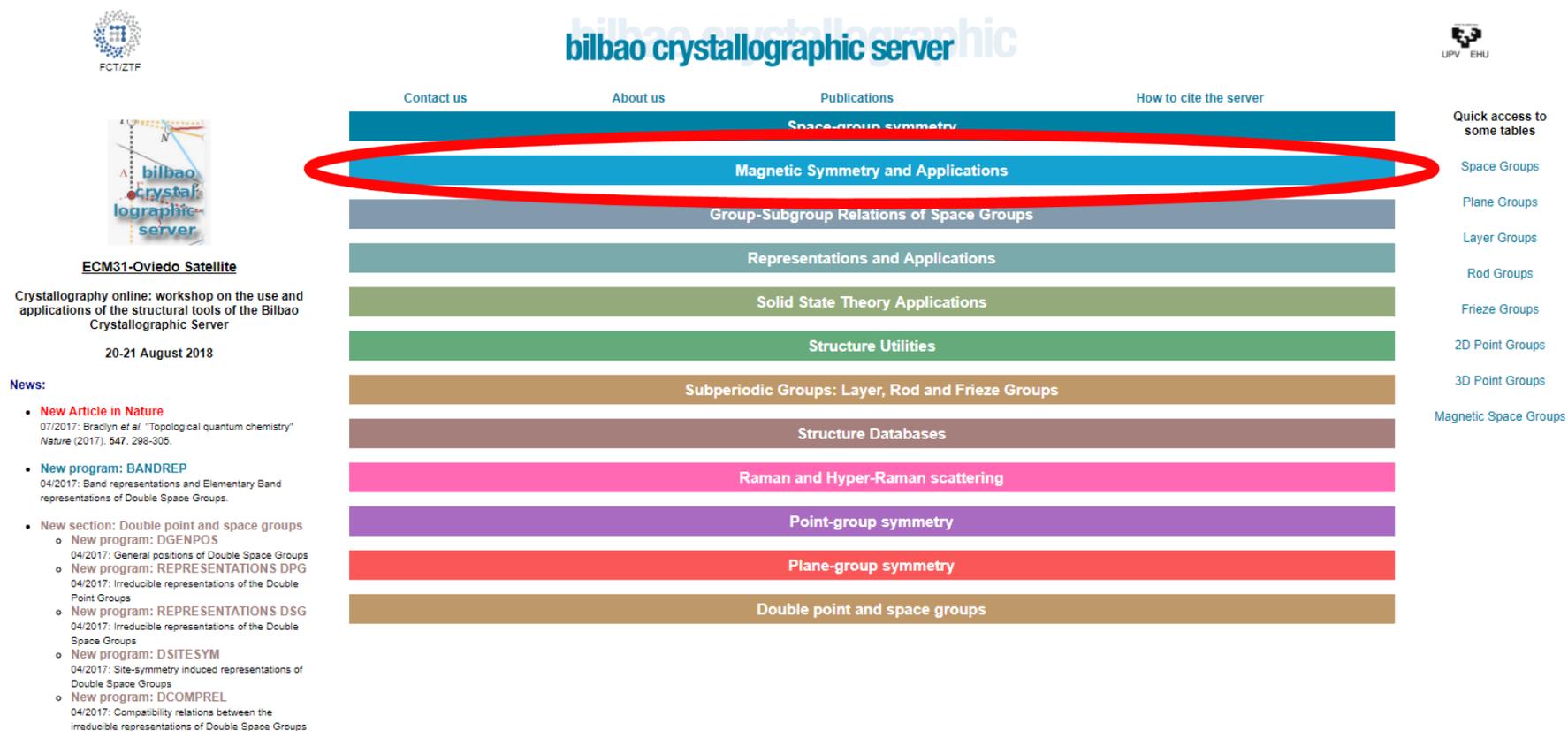
- This example will use the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/>) and follow these steps:
 - Step 1: Refine the crystal structure using FullProf
 - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
 - **Step 3: Create test magnetic space groups using 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 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 website. The main navigation bar includes links for Contact us, About us, Publications, and How to cite the server. A dropdown menu is open, listing various topics. The item "Magnetic Symmetry and Applications" is highlighted with a red oval. To the right of the dropdown menu, there is a "Quick access to some tables" section with links to Space Groups, Plane Groups, Layer Groups, Rod Groups, Frieze Groups, 2D Point Groups, 3D Point Groups, and Magnetic Space Groups. On the left side of the page, there is a logo for FCT/ZTF and a news section titled "ECM31-Oviedo Satellite" with a date of 20-21 August 2018. Below the news section, there are several bullet points under the heading "News:".

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

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

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

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

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

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

Examples and further information can be found in the following paper:
J.M. Perez-Mato, S.V. Gallego, E.S. Tasci, L. 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

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 $k = (1/2, 0, 1/2)$

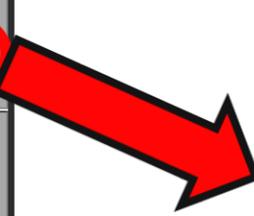
Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	<i>C_c2/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_c2/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_c2/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_c2/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_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

- 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_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, 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

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

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]

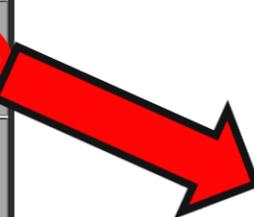
Export data to MCIF file/Visualize Go to a subgroup

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	-	-

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

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: 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	-	-

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

Step 3: Creating mCIF file

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

Magnetic Structure

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 parent space group]

Atomic positions, Wyckoff positions and ...

mCIF file of the structure

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

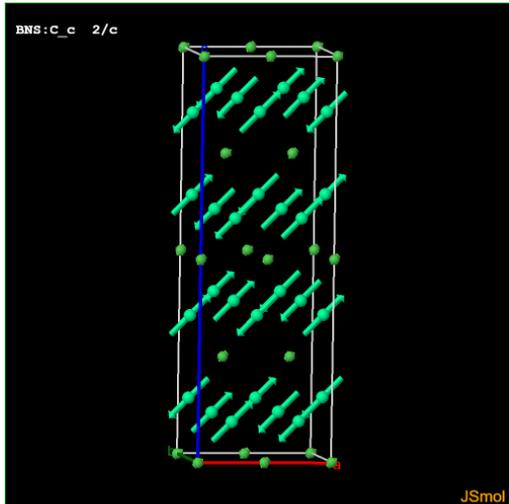
Download mCIF file: bcs_file.mcif
[The preview text below is non-editable, only copy-allowed]

```
##CIF_2.0  
# Created by the Bilbao Crystallographic Server
```

MVISUALIZE: 3D Visualization of magnetic structures with Jmol

MVISUALIZE Main Page

Show/Hide File



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

help console Execute

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_c2/c (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	C_c2/c (#15.90) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	C_c2/m (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	C_c2/m (#12.63) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/2 \end{pmatrix}$	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

2. Click export/view

Magnetic Structure

Selected magnetic space group: $2-C_c2/c$ (#15.90)

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

Parent space group $Immm$ (No. 71)

=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 CIF file/Visualize Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

- 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

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 $(M_x,0,M_x)$.

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Ho1 Ho 0.25000 0.00000 0.10125	$(1/4, 0, z m_x, 0, m_z)$ $(1/4, 0, -z -m_x, 0, -m_z)$ $(0, 1/2, z+1/4 m_x, 0, m_z)$ $(0, 1/2, -z+1/4 -m_x, 0, -m_z)$ $(1/4, 0, z+1/2 -m_x, 0, -m_z)$ $(1/4, 0, -z+1/2 m_x, 0, m_z)$ $(0, 1/2, z+3/4 -m_x, 0, -m_z)$ $(0, 1/2, -z+3/4 m_x, 0, m_z)$ $(3/4, 0, z -m_x, 0, -m_z)$ $(1/2, 1/2, z+1/4 -m_x, 0, -m_z)$ $(3/4, 0, z+1/2 m_x, 0, m_z)$ $(1/2, 1/2, z+3/4 m_x, 0, m_z)$	8	$(M_x, 0, M_z)$	$M_x = 4$ $M_z = 5$
2	Ba1 Ba 0.25000 0.50000 0.00000	$(1/4, 1/2, 0 0, 0, 0)$ $(1/4, 1/2, 1/2 0, 0, 0)$ $(3/4, 1/2, 0 0, 0, 0)$ $(3/4, 1/2, 1/2 0, 0, 0)$	8	-	-
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 MVISUALIZE”

We now need to go to Step 4

Submit this mcif file to MVISUALIZE 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

data_5yOhtAoR
_audit_creation_date      2019-10-09
_audit_creation_method    "Bilbao Crystallographic Server"

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

loop_
_citation_author_name    ?

_atomic_positions_source_database_code_ICSD ?
_atomic_positions_source_other ?

_transition_temperature ?
_experiment_temperature ?

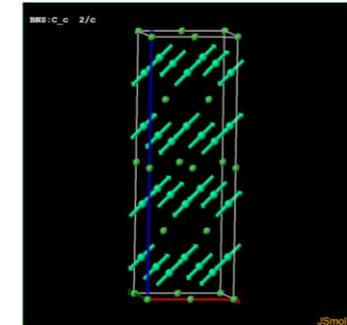
loop_
_irrep_id                ?
_irrep_dimension         ?
_irrep_small_dimension   ?
_irrep_direction_type    ?
_irrep_action            ?
_irrep_modes_number      ?
_irrep_presence          ?
? ? ? ? ? ? ?

_exptl_crystal_magnetic_properties_details
;
;

_active_magnetic_irreps_details
;
k-maximal magnetic symmetry
;

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

MVISUALIZE: 3D Visualization of magnetic structures with Jmol



Ho₂BaNiO₅

- 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

Contact us

About us

Publications

How to cite the server

Space-group symmetry

Magnetic Symmetry and Applications

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

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):

Ho2BaNiO5_...MAGN.mcif

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”

Ho₂BaNiO₅

- 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.**

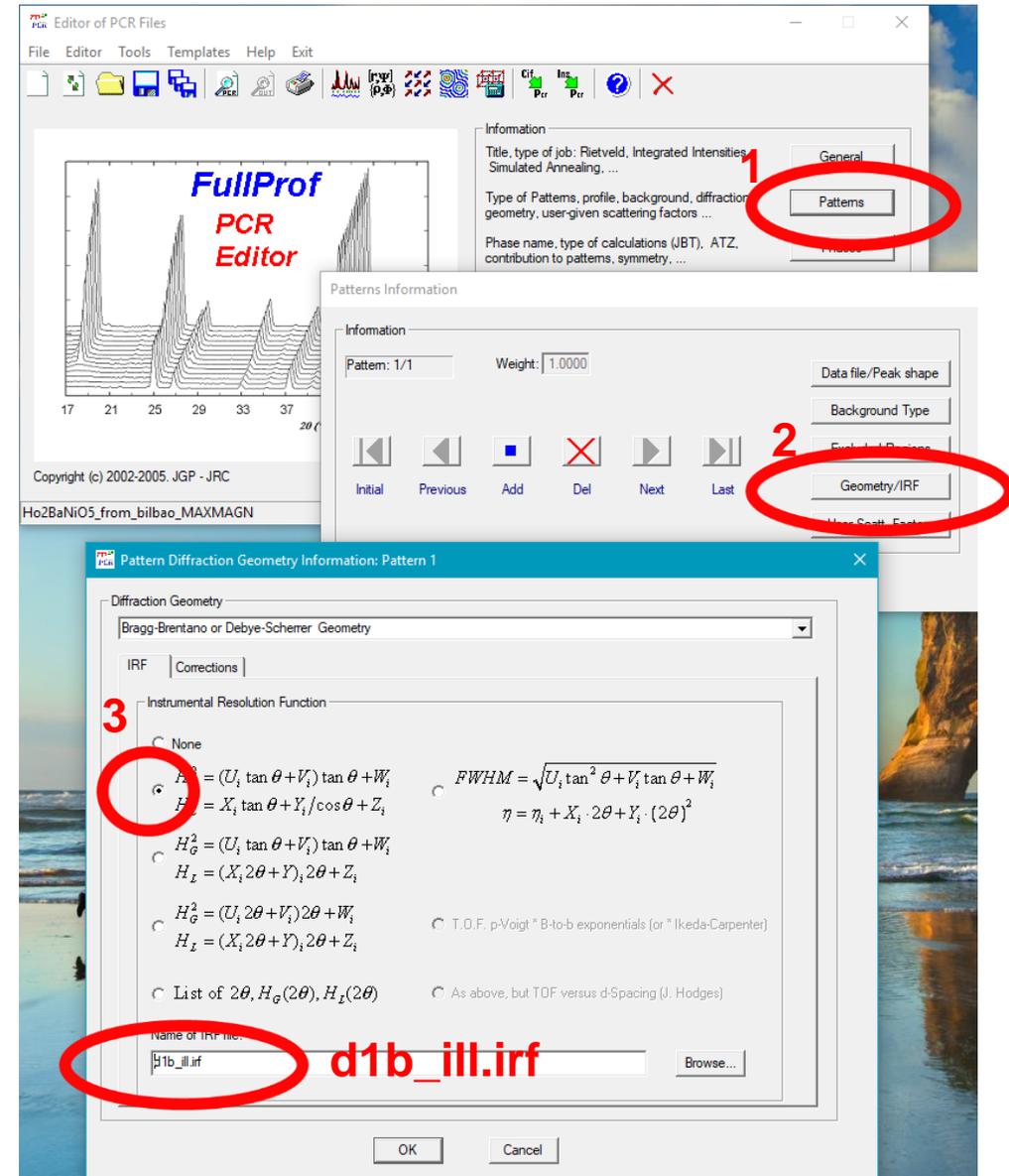
Step 5: Refining the magnetic structure with Fullprof

- 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



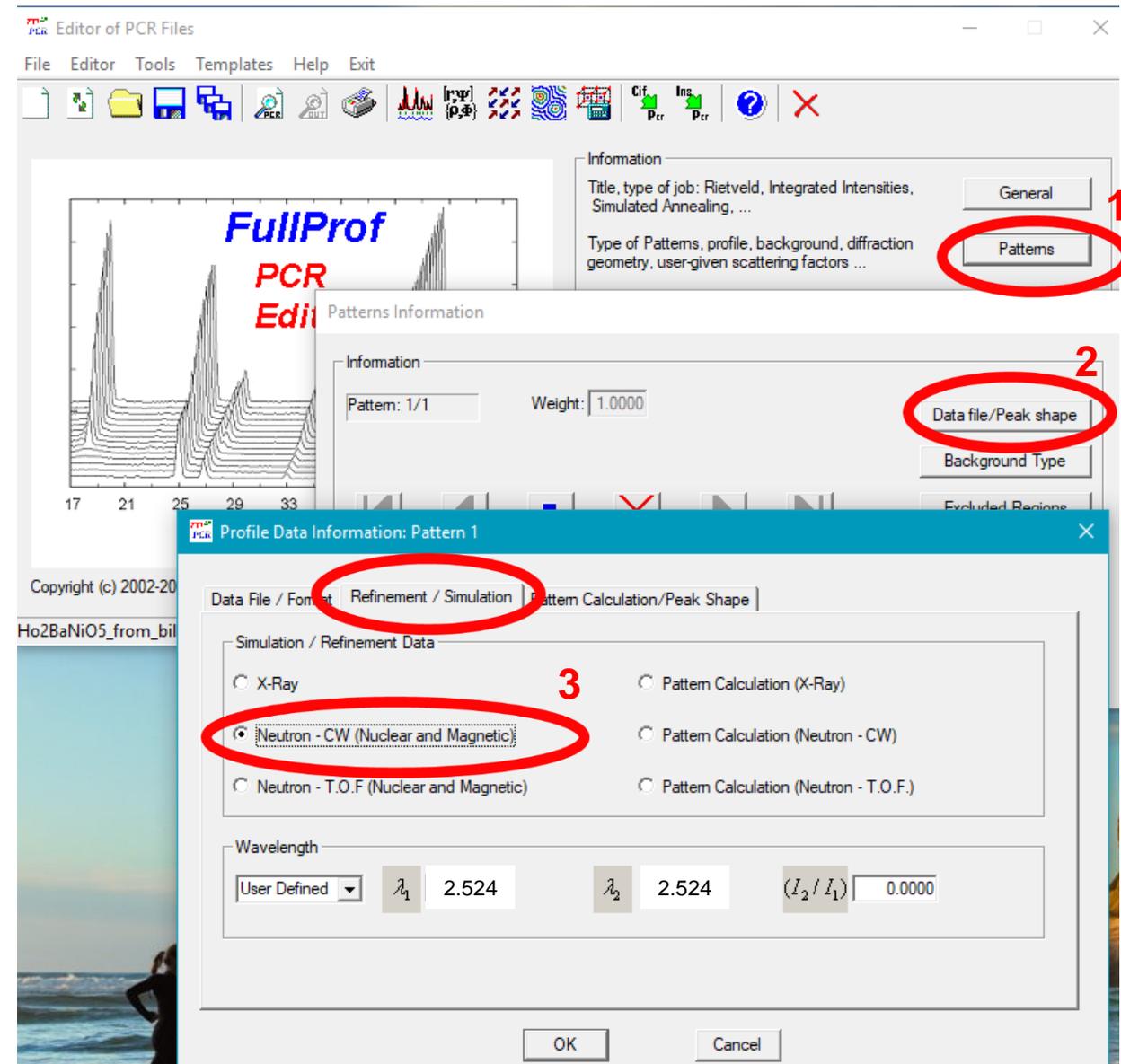
Step 5: Refining the magnetic structure with Fullprof

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

The screenshot displays the FullProf PCR Editor software interface. The main window shows a plot of intensity versus 2θ (degrees) with the text "FullProf PCR Editor" overlaid. The plot shows several peaks, with the x-axis ranging from 17 to 49 degrees. The main window has a menu bar (File, Editor, Tools, Templates, Help, Exit) and a toolbar. On the right side, there is an "Information" panel with several tabs: General, Patterns, Phases, Refinement, Constraints, Box/Restrains, and Output. The "Patterns" tab is selected and circled in red, with a red "1" next to it. Below the main window, there is a "Patterns Information" dialog box. It shows "Pattern: 1/1" and "Weight: 1.0000". The "Data file/Peak shape" button is circled in red, with a red "2" next to it. Below that, there is a "Profile Data Information: Pattern 1" dialog box. It has three tabs: "Data File / Format", "Refinement / Simulation", and "Pattern Calculation/Peak Shape". The "Data File / Format" tab is selected and circled in red, with a red "3" next to it. Under the "Format" section, the "D1B/D20" radio button is selected and circled in red. Other options include "D1A/D2B (Old Format)", "Free Format (2theta, step, 2ThetaF)", "Variable Time X-ray Data", "D1A/D2B/3T2/G42", "Two Axis Instrument, G41", "X,Y,SIGMA (XYDATA)", "D1B/D20 (Socabim)", "GSAS Format", "XCelerator (PANalytical)", "D1B/D20", "Socabim Software", "ISIS multi-bank normalized", "D1B/D20", "Synchrotron (Brookhaven)", "DMC/HRPD (P.S.I.)", and "Synchrotron (DBWS Software)". The "OK" and "Cancel" buttons are at the bottom.

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

The screenshot shows the FullProf software interface. The main window displays a plot of the diffraction pattern. The 'Patterns Information' dialog box is open, showing the 'Background Type' button circled in red with a '2'. The 'Background Information' dialog box is also open, showing the '6-Coefficients polynomial function' radio button circled in red with a '3a', and the 'Origin of the polynomial' text box containing '60.000' circled in red with a '3b'. The 'Patterns' button in the main window is circled in red with a '1'. The 'Background Information' dialog box has 'OK' and 'Cancel' buttons at the bottom.

Step 5: Refining the magnetic structure with Fullprof

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

The screenshot displays the Fullprof software interface. The 'Pattern Contribution Information for Phase 1' dialog box is open, showing the 'Type of Pattern' section with the 'Neutron (Constant Wavelength)' option selected and circled in red (labeled '3'). The 'Peak shape' dropdown menu is also circled in red (labeled '2'). The 'Information' dialog box is open in the background, with the 'Contribution to Patterns' button circled in red (labeled '2'). The 'Phases' button in the right sidebar is circled in red (labeled '1').

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.)

Refinement Information

Cycles of Refinement: 1

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

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

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

Refinement weighting model
 Least Squares Maximum Likelihood Unit Weights
 Background Instrumental Micro-Absorption

6 Coefficients Polynomial Background: Pattern 1

	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients	7000	0.0000	0.0000	0.0000	0.0000	0.0000
Coefficients	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

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)

Refinement Information

Cycles of Refinement: 1

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

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

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

Refinement weighting model
 Least Squares Maximum Likelihood Unit Weights

Background Instrumental Micro-Absorption

Instrumental Parameters Refinement: Pattern 1

	Zero	Displacement	Transparency	Wavelength
Coefficients	0.084590	0.000000	0.000000	0.000000

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.

The screenshot shows the FullProf PCR Editor interface. The main window displays a diffraction pattern plot with the text "FullProf PCR Editor" overlaid. The plot shows several sharp peaks. The x-axis is labeled "2θ (°)" with values 17, 21, 25, 29, 33, 37, 41, 45. The y-axis represents intensity. The plot is titled "Ho2BaNiO5_from_bilbao_MAXMAGN".

On the right side, there is an "Information" panel with tabs for "General", "Patterns", "Phases", and "Refinement". The "Refinement" tab is selected and circled in red, with a red "1" next to it. Below this is a "Refinement Information" dialog box. The "Cycles of Refinement" field is set to "10" and is circled in red. A red arrow points to this field with the text "Increase number of cycles".

Below the "Refinement Information" dialog is a "Profile Parameters: Phase 1 Pattern 1" dialog box. The "Scale" field is set to "2.0000" and is circled in red. The "Profile" field is set to "1" and is circled in red, with a red "2" next to it. A red arrow points from the "Profile" field to the "Profile" button in the "Patterns" section of the dialog box.

At the bottom of the "Profile Parameters" dialog, there are several tables for "FWHM Parameters" and "Shape Parameters". The "FWHM Parameters" table has columns for U, V, W, and IG, with coefficients all set to 0.000000. The "Shape Parameters" table has columns for X, Y, and SZ, with coefficients all set to 0.000000. There are also buttons for "Refine All", "Fix All", "Cancel", and "OK".

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 $Re(x)$ 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.

The screenshot shows the FullProf PCR Editor interface. The main window displays a diffraction pattern plot with the text "FullProf PCR Editor" overlaid. The plot shows intensity versus 2θ (degrees) from 17 to 49. The interface includes a menu bar (File, Editor, Tools, Templates, Help, Exit) and a toolbar with various icons. On the right side, there is an "Information" panel with tabs for General, Patterns, Phases, and Refinement. The "Refinement" tab is selected and circled in red, with a red "1" next to it. Below this is the "Refinement Information" panel, which includes a "Cycles of Refinement" field set to 10, a "Stop Criterion of Coverage" dropdown set to "Forced Termination when shifts < 0.02 x E.S.D.", and "Relaxation Factors for Shifts" for Atomic, Anisotropic, Profile, and Global, all set to 1.00. There is also a "Reflections ordering" section with radio buttons for "Only at the first cycle" (selected) and "Each cycle", and a checkbox for "Bragg R-Factor excluding reflections limiting excluded regions".

At the bottom of the main window, there is a "Atoms Information: Phase 1" section. It contains a "List of Atoms" table with columns for Label, Ntyp, Mag. Rot., Prog. V..., X, Y, Z, B, and Occ. Below this is a table for thermal parameters with columns for $Re[x]$, $Re[y]$, $Re[z]$, $Im[x]$, $Im[y]$, $Im[z]$, and MPhase. The "Number of Atoms" is set to 5. The $Re[x]$ and $Re[z]$ columns for Atom #1 and Atom #3 are circled in red, with a red "2" next to the "Atoms" button in the "Refinement Information" panel. The "B" column for Atom #3 is also circled in red, with a red "3" next to it.

Atom #	Label	Ntyp	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

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

```
!
!
! 4 ?Number of refined parameters
!
! Zero Code SyCos Code SySin Code Lambda Code MORE ->Patt# 1
! 0.00459 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
! 0.00 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/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
!
! C_2/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 Vek X Y Z Biso Occ N_type Spc/FFtype /Line below:Codes
! ? beta11 beta22 beta33 beta12 beta13 beta23 / Line below:Codes
! Ho1 JHO2 1 0 0.25000 0.00000 0.10125 0.30000 0.50000 1 0 #
! 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
! Ba Ba 1 0 0.25000 0.50000 0.00000 0.30000 0.25000 0 0 #
! 0.00 0.00 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 #
! 1.00000 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 <--MagPar
! 41.00 0.00 21.00 0.00 0.00 0.00 0.00
! O1 O 1 0 0.00000 0.24140 0.07475 0.30000 1.00000 0 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! O2 O 1 0 0.00000 0.50000 0.25000 0.30000 0.25000 0 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
```

Delete this to stop auto refinements of moments

Step 5: Refining the magnetic structure with Fullprof

Refine background

Refinement Information

Cycles of Refinement: 10

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

Others: None

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

Reflections ordering
Only at the first cycle

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

Profile Parameters: Phase 1 Pattern 1

Factors

Scale	Overall B-factor
2.0000	0.0000

Parameters

a	b	c	alpha	beta	gamma
7.512101	5.734099	22.554998	90.0000	90.0000	90.0000

FWHM / Shape Parameters

U	V	W	IG
0.000000	0.000000	0.000000	0.000000

Shape Parameters

X	Y	SZ
0.000000	0.000000	0.000000

Refine FWHM for second wavelength

U2	V2	W2

Atoms

Refine moments

Atoms Information: Phase 1

List of Atoms

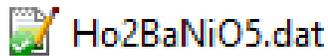
Atom #	Label	Ntyp	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Ho1	JHO3	1	0	0.25000	0.00000	0.10125	0.30000	0.50000
Atom # 2	Ba1	Ba	1	0	0.25000	0.50000	0.00000	0.30000	0.25000
Atom # 3	Ni1	MNI2	1	0	0.00000	0.00000	0.00000	0.30000	0.25000
Atom # 4	O1	O	1	0	0.00000	0.24140	0.07475	0.30000	1.00000

Refine Moments

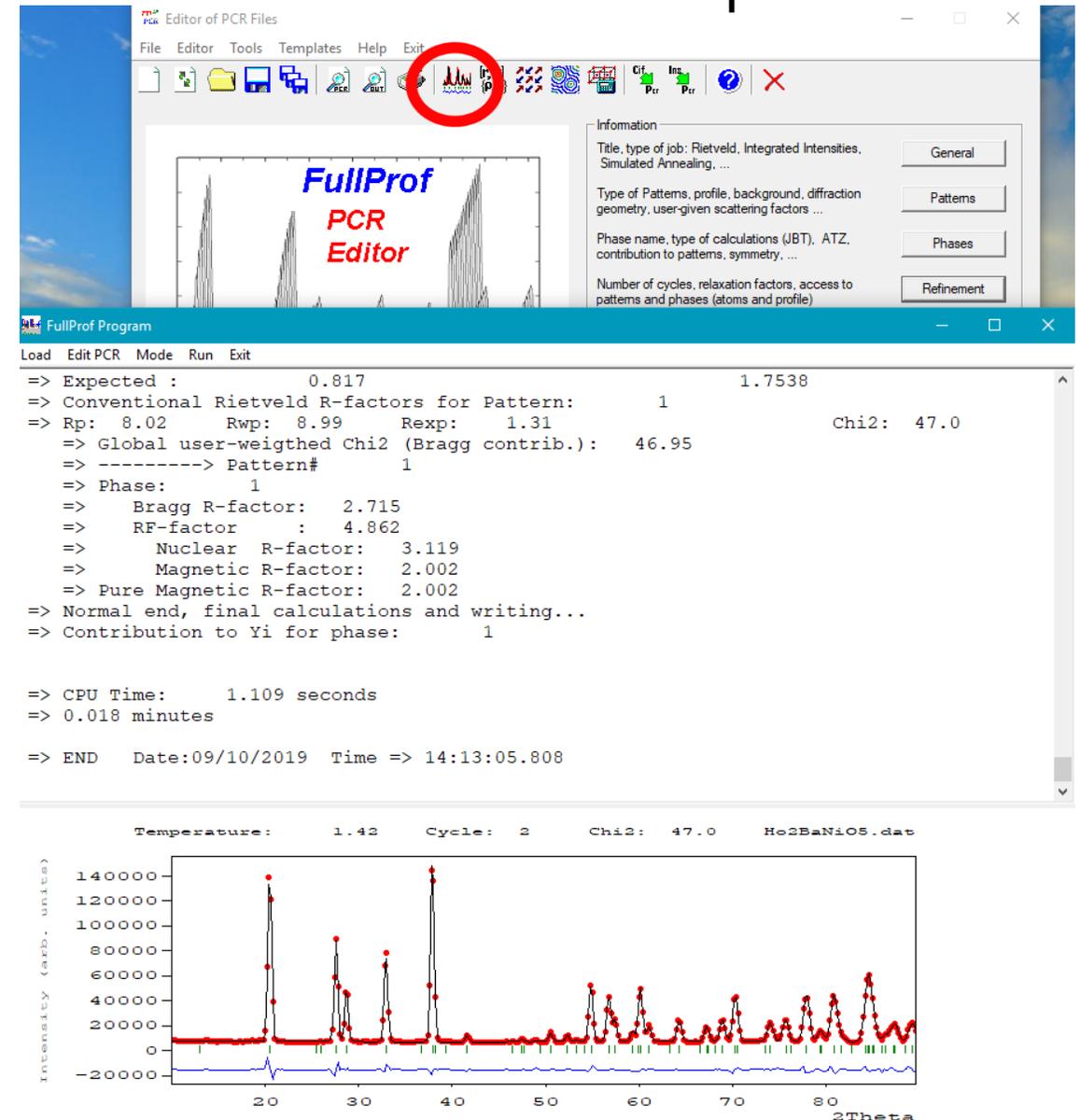
Atom #	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom # 1	5.00000	0.00000	5.00000	0.00000	0.00000	0.00000	0.00000
Atom # 2	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00000

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

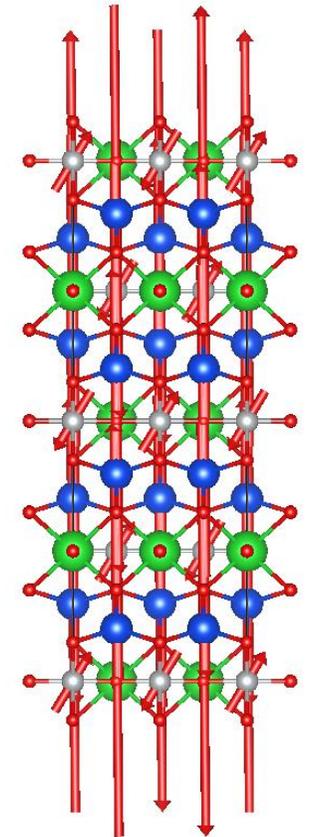
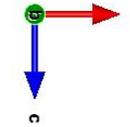
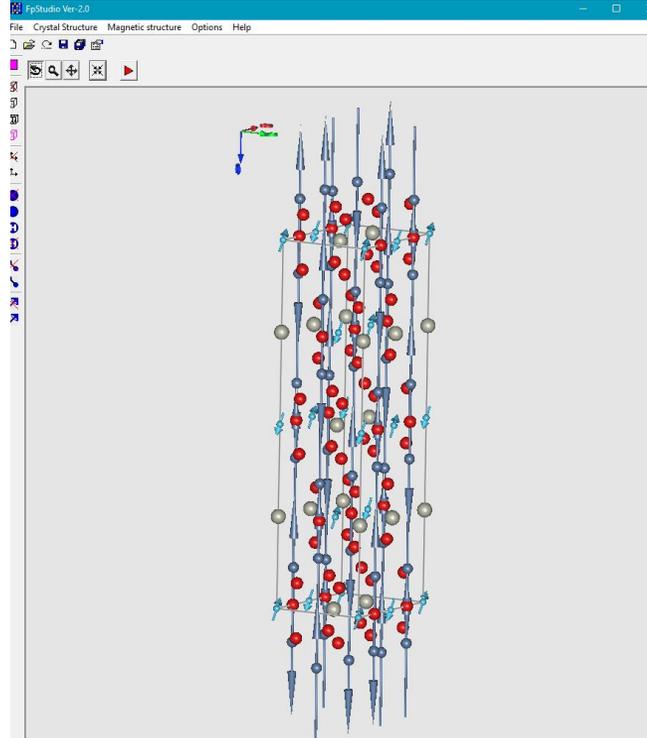
Name

- 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	