

A visual guide for crystal and magnetic structure refinement using Mag2Pol

Naveen Kumar Chogondahalli Muniraju

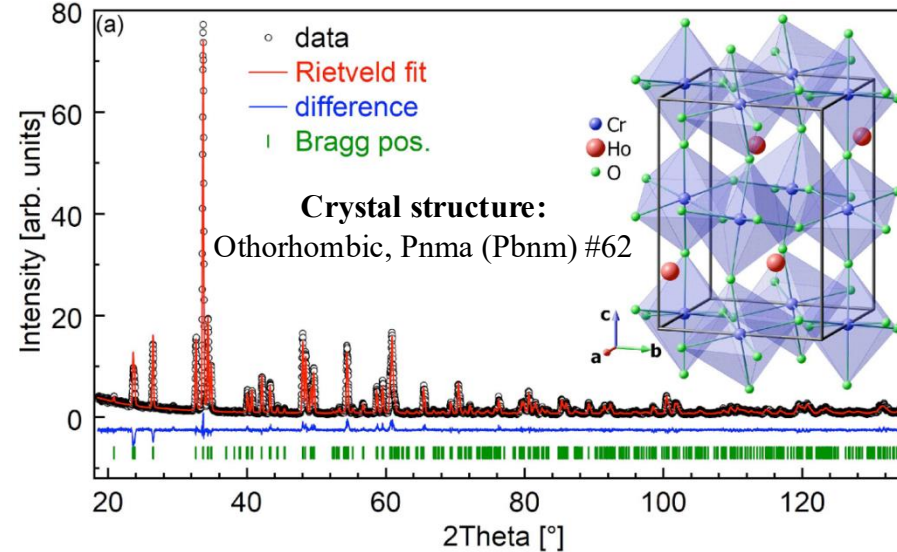
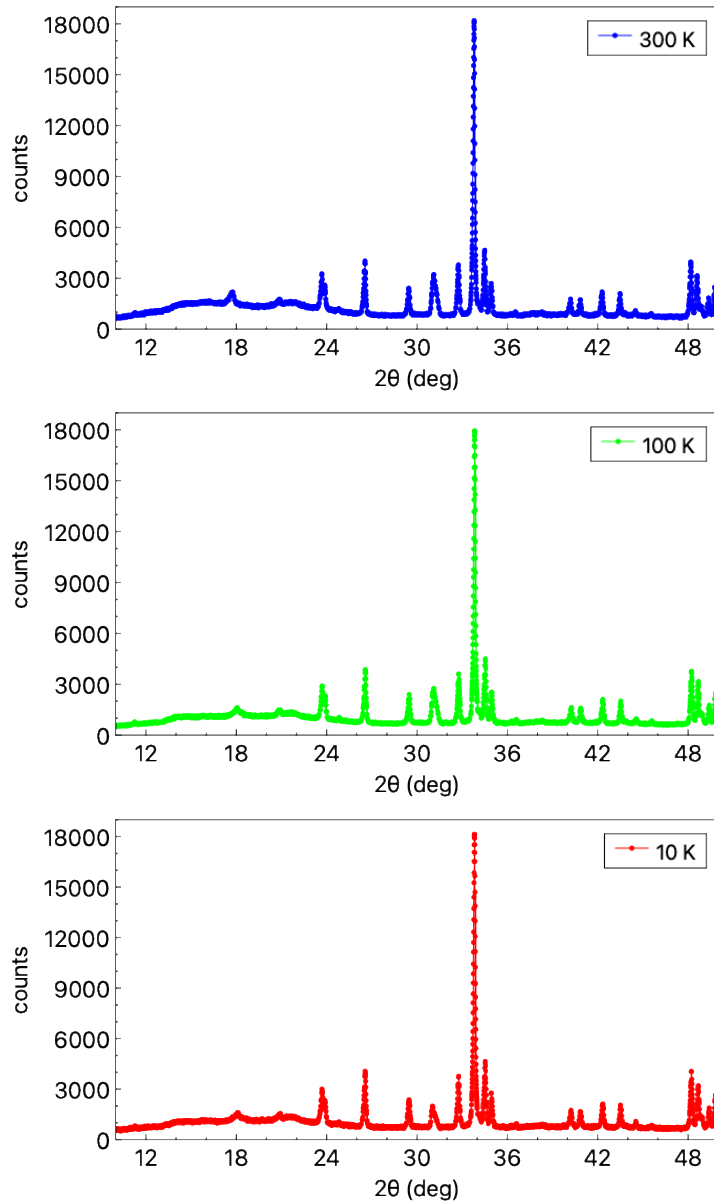
Institute of Nuclear Physics, PAN
31-342 Kraków, ul. Radzikowskiego 152

Session 2

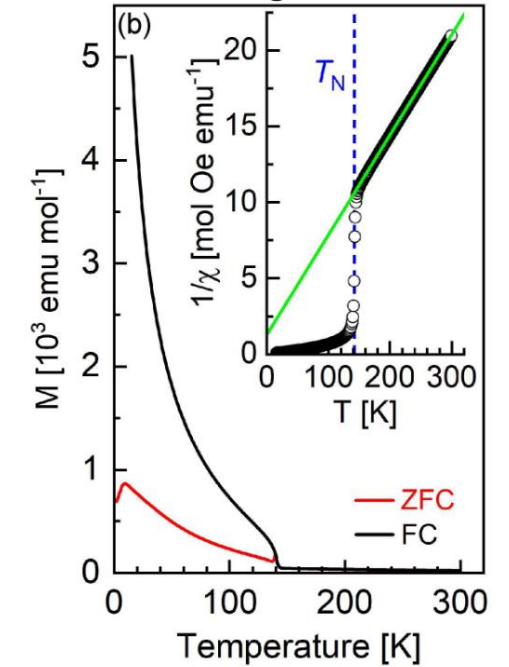
Refinement of crystal structure from NPD data

Inhouse and Macroscopic characterizations of HoCrO_3

X-ray powder diffraction



DC magnetization



$$T_N \approx 142 \text{ K}$$

From Curie-Weiss fit:

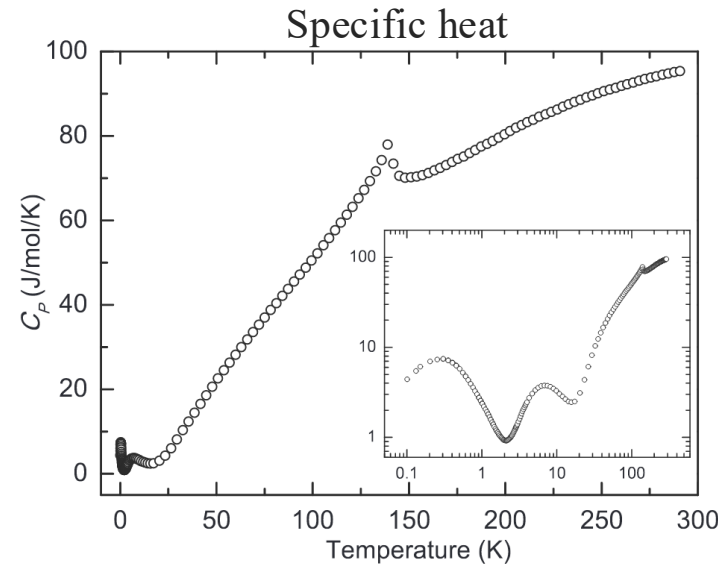
$$\mu_{\text{eff}} = 11.01 \pm 0.02 \mu_B$$

This corresponds to magnetic ions:

Cr^{3+} (spin only $S = 3/2$)

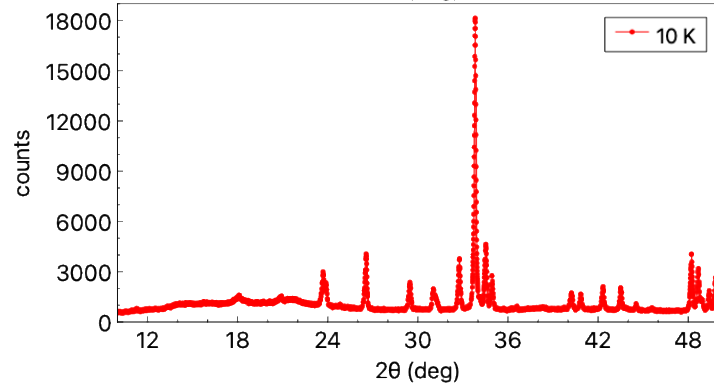
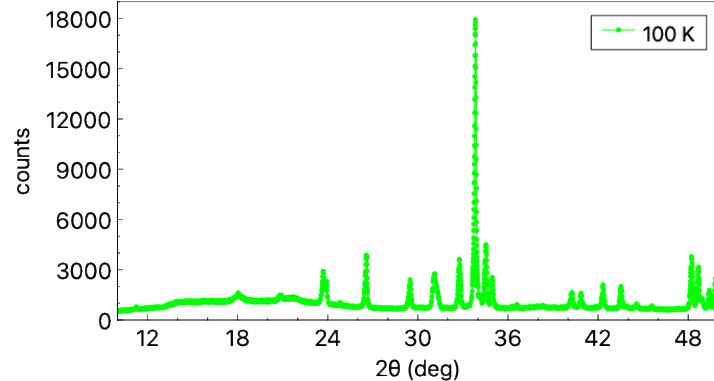
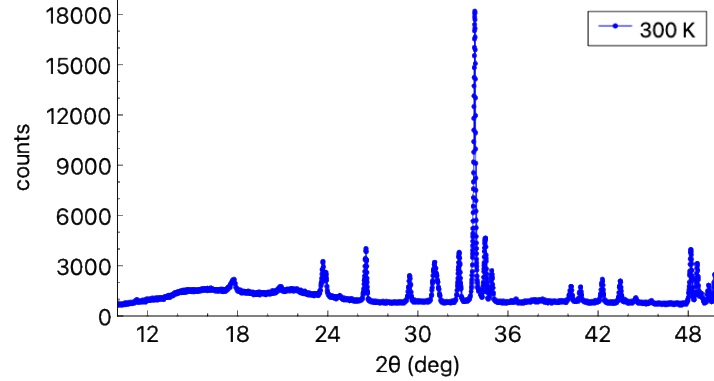
Ho^{3+} (strong spin-orbit, $J=8$)

Neutrons can tell us if both ions order simultaneously. The moment size and directions for each magnetic site in the lattice.

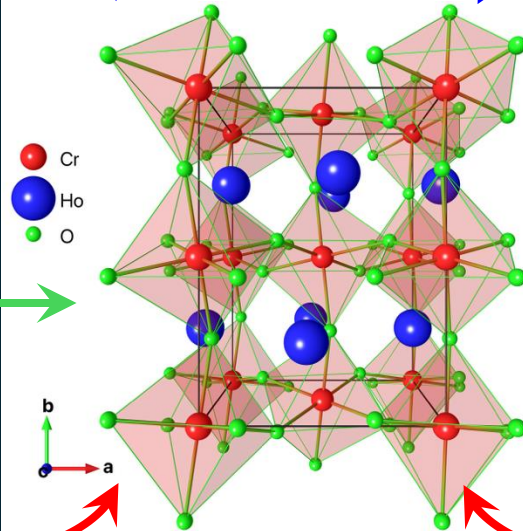


X-ray vs. Neutron powder diffraction

X-ray powder diffraction

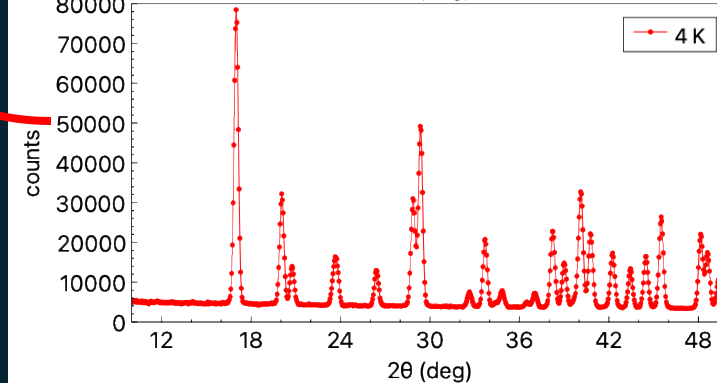
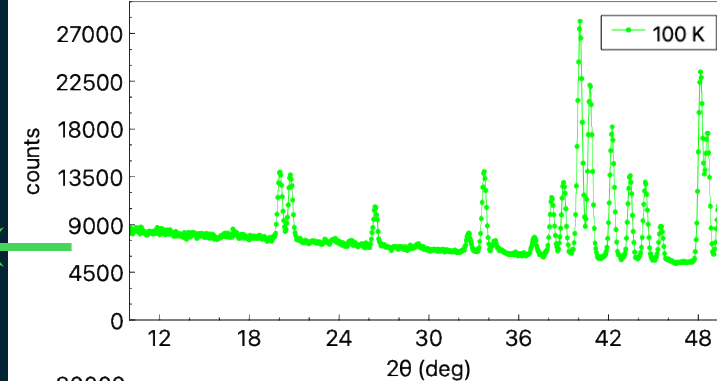
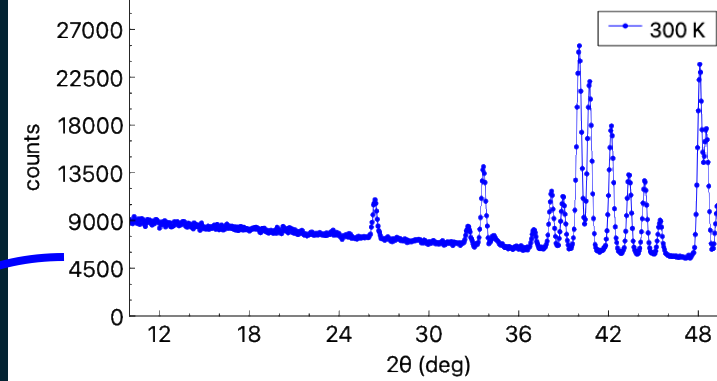


Orthorhombic space group:
Pnma (*Pbnm*) #62



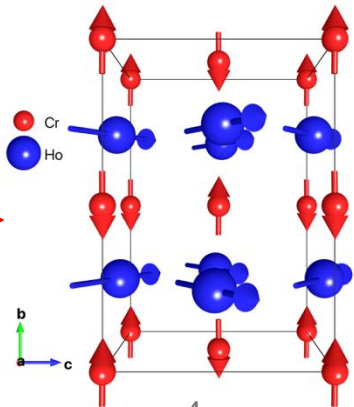
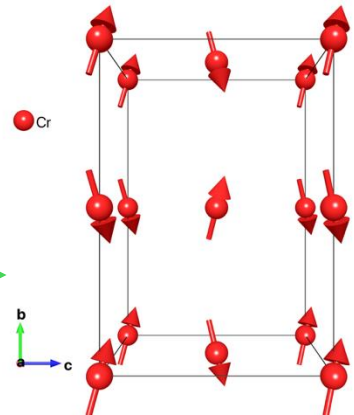
Atom	x	y	z
Cr (4a)	0.0000	0.0000	0.0000
Ho(4c)	0.43449	0.25000	0.00670
O1(4c)	0.53340	0.25000	0.58885
O2(8d)	0.19680	0.05420	0.30450

Neutron powder diffraction

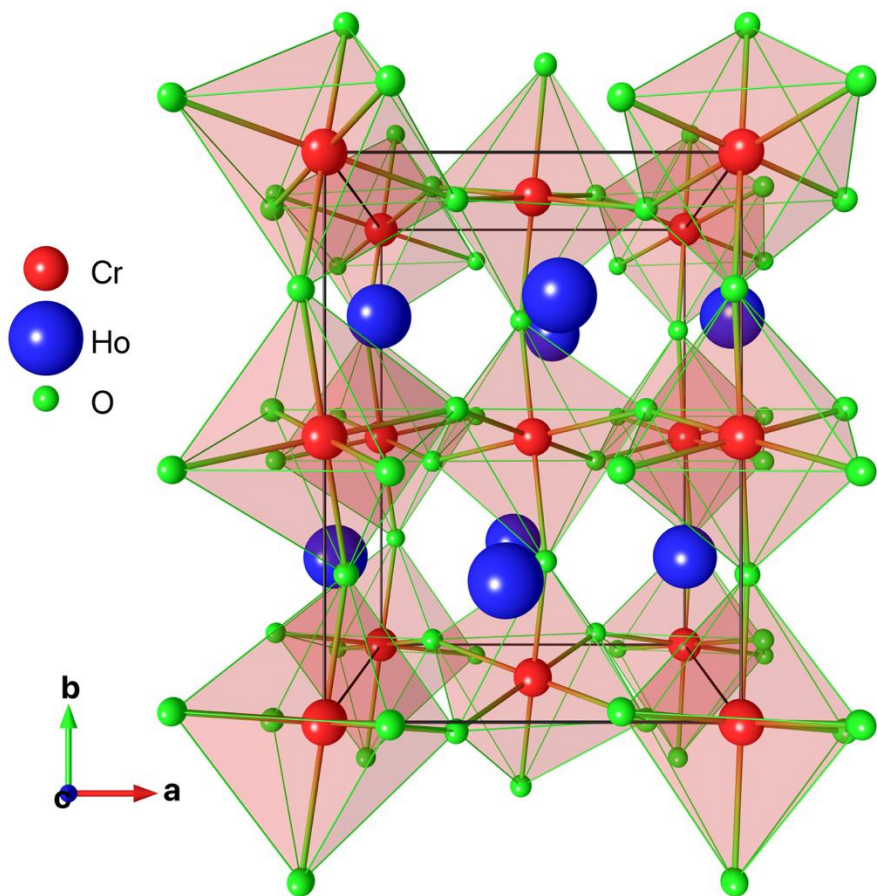


X-ray diffraction:
Lattice structure

Neutron diffraction:
Lattice + Magnetic



Measurement and data details



Orthorhombic structure: *Pnma* (No. 62)

Instrument: Neutron powder diffractometer SPODI at FRM II
research reactor, Garching, Germany

Wavelength: 1.5482 Å

Data files:

Data collected at 300 K: HCO_300K.dat

Data collected at 100 K: HCO_100K.dat (→ HCO_100K.m2p)

Data collected at 4 K: HCO_4K.dat

Crystal Information File for crystal structure:

[HoCrO3_300K.cif](#)

Mag2Pol version used: [7.2.2](#)

The main interface of Mag2Pol

Is the sample a good scatterer or an absorber?

Neutron Activation and Scatt

ncnr.nist.gov/resources/activation/

Guest

NIST CENTER FOR NEUTRON RESEARCH

NIST

Material

HoCrO3

Neutron Activation

Thermal flux

1e8

Cd ratio

0

Thermal/fast ratio

0

Mass

Exposure

10

Decay

1 y

For rabbit system

Calculate

Absorption and Scattering

Density

5

Thickness

1

Calculate

Source neutrons

1.5 Ang

Source X-rays

Cu Ka

Thickness

Units: cm

The material thickness in cm is used to determine sample transmission, or how much beam will be absorbed by the sample or scattered incoherently. Leave it at 1 cm if you do not need this information.

Source neutrons

Units: Ang, meV or m/s

The energy of the source neutrons will affect the absorption cross section and hence the penetration depth and sample attenuation. Energy can be expressed as wavelength in Å, as energy in meV, or as

Scattering from HoCrO3

Source neutrons: 1.500 Å = 36.36 meV = 2637 m/s

Source X-rays: 1.542 Å = 8.042 keV

Sample in beam: HoCrO₃ at 5.00 g/cm³

1/e penetration depth (cm)		Scattering length density (10 ⁻⁶ /Å ²)		Scattering cross section (1/cm)		X-ray SLD (10 ⁻⁶ /Å ²)	
abs	1.557	real	3.351	coh	0.248	real	31.848
abs+incoh	1.484	imag	-0.002	abs	0.642	imag	-2.098
abs+incoh+coh	1.085	incoh	1.190	incoh	0.031		

Neutron transmission is 50.98% for 1 cm of sample (after absorption and incoherent scattering).

Transmitted flux is 5.098e+7 n/cm²/s for a 1e8 n/cm²/s beam.

Contrast match point: 56.3% D₂O by volume (real SLD = 3.351×10⁻⁶/Å²)

Questions?

Neutron activation: NCNR Health Physics <hp@nist.gov>

Scattering calculations: Paul Kienzle <paul.kienzle@nist.gov>

Using [periodictable v2.0.0](#)

Low transmittance (<20%):

Heavy absorption → distorted intensities, surface scattering, need strong absorption corrections

High transmittance (>90%):

Weak scattering → poor S/N, long counting time, weak magnetic peaks

Aim for 30 – 70 % transmittance

7

The main interface of Mag2Pol

The main window of Mag2Pol - GUI

Running the Mag2Pol application, the main window 'Mag2Pol' will open. By default, the interface may look slightly different. You can modify this under the menu 'View'

This window should remain open as long as any other Mag2Pol utility or window is running. The current version of Mag2Pol will not save the project automatically, so make sure to save any project before closing this window.

The screenshot displays the Mag2Pol GUI with the following sections:

- Symmetry Panel:**
 - Space group:
 - Cell: a = 0.00000 b = 0.00000 c = 0.00000
α = 90.000 β = 90.000 γ = 90.000
 - Number of symmetry operators: 1 Number of irreps: 1
 - Table:

	x	y	z	u	v	w	φ
1	x	y	z	u	v	w	0.000
- Atoms Panel:**
 - Number of sites: 1
 - Table:

Atom	x	y	z	B	occ	plot	color	R	S
1	0.00000	0.00000	0.00000	0.000	1.000	<input checked="" type="checkbox"/>	blue	10	1.0
- Spins Panel:**
 - Propagation vector: q = 0.000 0.000 0.000 ☐ +q ≠ -q
 - Table:

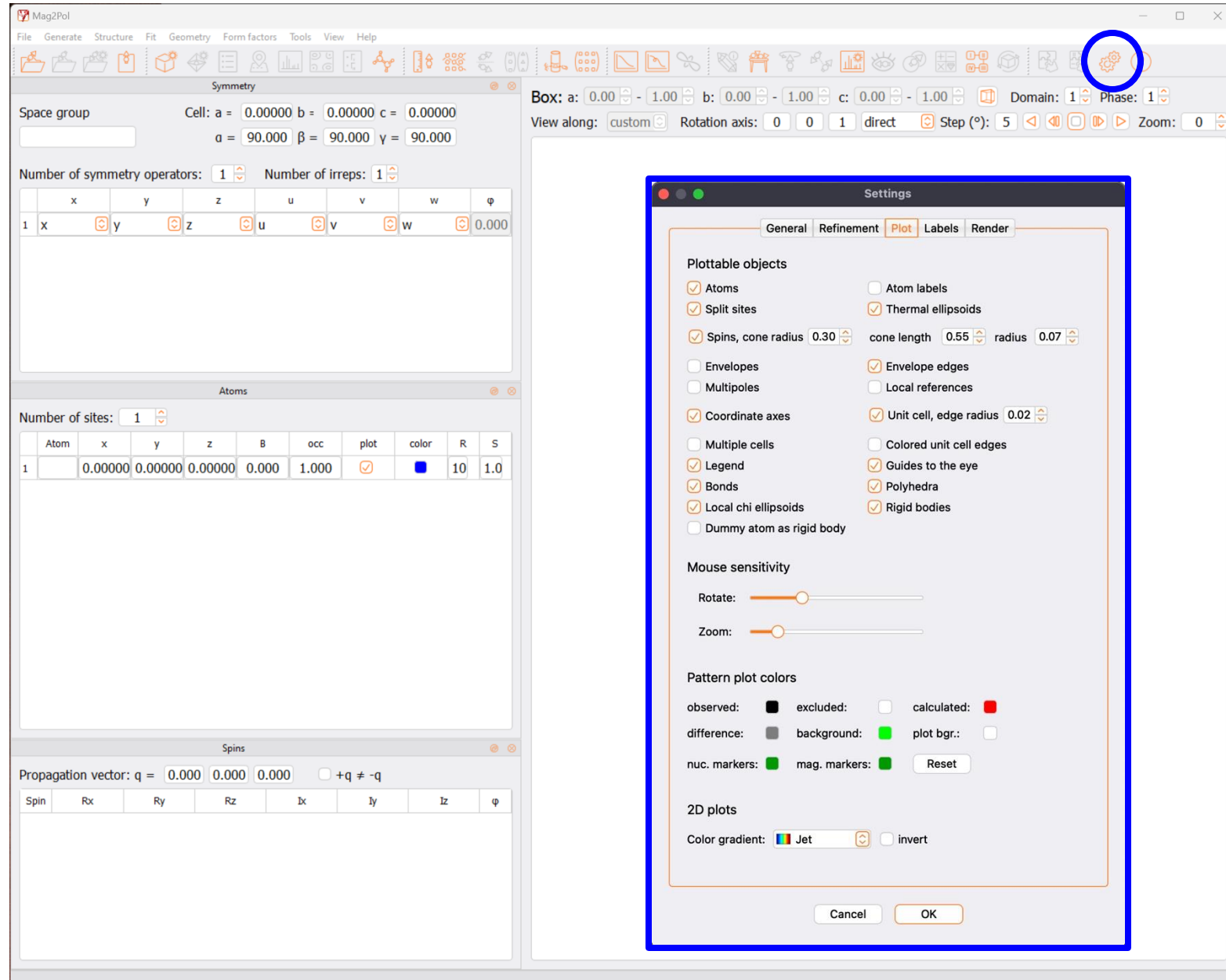
Spin	Rx	Ry	Rz	Ix	Iy	Iz	φ
------	----	----	----	----	----	----	---

On the right side, there are controls for the visualization:

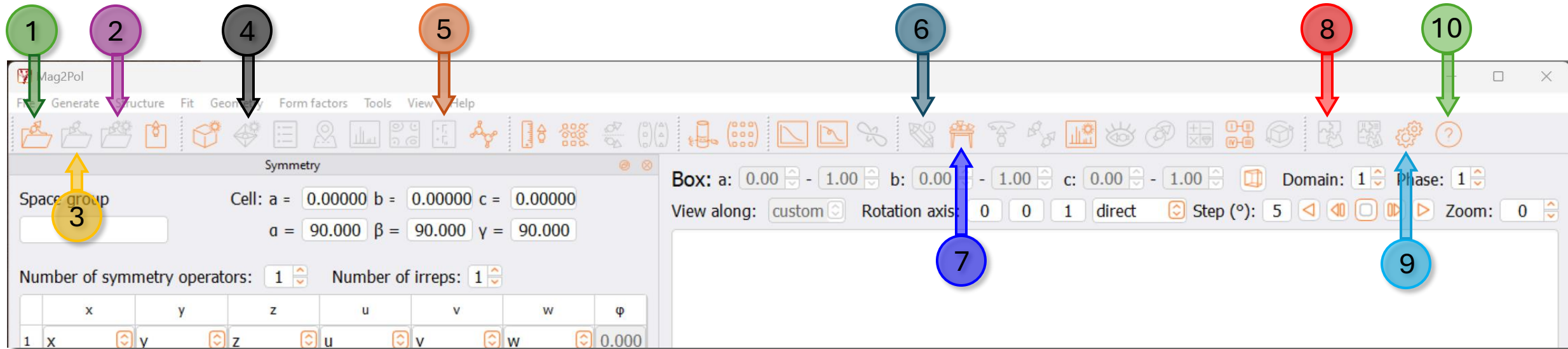
- Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1
- View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 0

The main window of Mag2Pol - GUI

Some key plot elements that needs to be activated under settings for the purpose of this hands-on. (*For purely aesthetic reasons*)



Menu items (icons) on the main window relevant for this tutorial



1 Open: Load a structure file (cif) or an existing Mag2Pol project (xml).

2 Save as: Save as a new Mag2Pol project (as *.xml).

3 Save: Append the currently working project with the same name.

4 Bonds: Opens a new window that is used to modify the visuals of the structural model [active after loading the structure file, if it is not active even after loading the cif file, press *Ctrl+U* (on Windows) or *Cmd+U* (on Mac)].

5 Irreducible representations: Opens a new window that provides details of irreps and lets you select one or more irreps for the refinement of magnetic structure (active when at least one magnetic ion is defined)

6 Sample info: Opens a new window that provides details of, lattice and magnetic structures and the results of the last refinements.

7 Spacegroup tables: Opens a window on which you can select magnetic space group (Shubnikov group) instead of irreps, to refine the magnetic structure.

8 Fit: Opens the window where you can choose the data file, and instrument resolution file, and perform the refinements.

9 Settings: Opens a new window that lets you modify a few important settings about GUI, a graphical rendering of plots and figures, and also the refinement procedure.

10 Manual: Opens Mag2Pol manual in pdf format.

Refining high temperature NPD data, collected in paramagnetic phase

Try to find a reported structure (Crystal Information File)

Search for the structure in multiple free and subscription-based sources. For example, *COD* or in the *Materials Project* database.

HoCrO₃ is not available in COD but can be found in Materials Project (you can sign in by linking your Google, GitHub, and many more accounts, or sign up using your email account).

Download symmetrized CIF and save as:

HoCrO3_mp-756834.cif

Other free structure databases:

<https://www.rruff.net/>

<https://www.crystallography.net/cod/search.php>

<https://next-gen.materialsproject.org/>

Materials Explorer

HoCrO₃
mp-756834

TABLE OF CONTENTS

- Summary
- Crystal Structure
- Properties
- Contributed Data
- Literature References
- External Links
- More
- Related Materials

Energy Above Hull: 0.000 eV/atom
Space Group: Pnma
Band Gap: 2.50 eV
Predicted Formation Energy: -3.227 eV/atom
Magnetic Ordering: Ferromagnetic
Total Magnetization: 3.00 μB/f.u.
Experimentally Observed: Yes

Description (Auto-generated)
HoCrO₃ is Orthorhombic Perovskite structured and crystallizes in the orthorhombic Pnma space group. Ho³⁺ is bonded in a 8-coordinate geometry to eight O²⁻ atoms. There are a spread of Ho-O bond distances ranging from ...

Export Materials Details

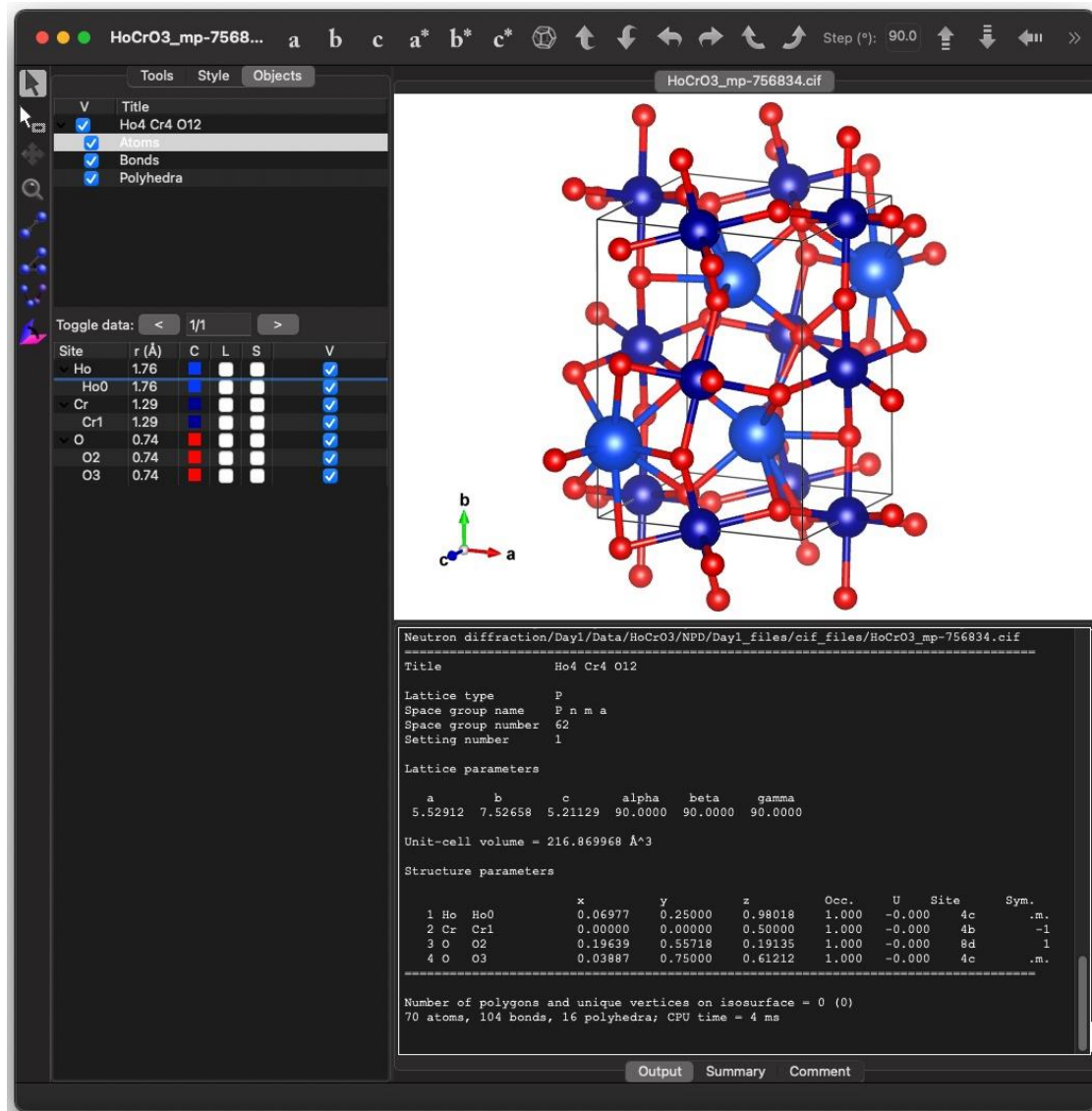
Crystal Structure

Lattice (Primitive)	
a	5.21 Å
b	5.53 Å
c	7.53 Å

Atomic Positions			
Wyckoff	Element	x	y
4b	Cr	0	1/2
4c	Ho	0.519819	0.569775

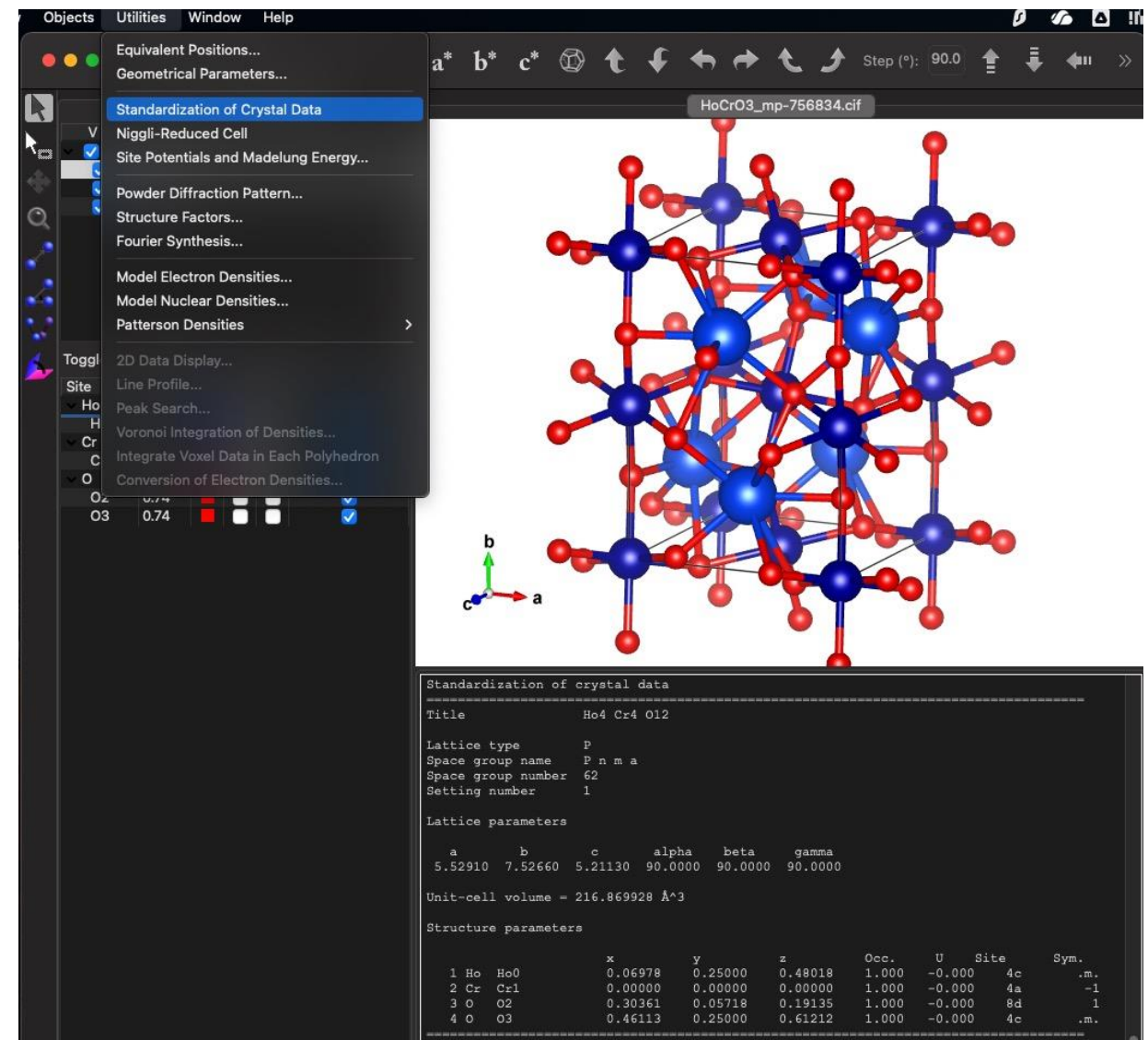
Open the CIF file in VESTA and standardize (optional)

HoCrO3_mp-756834.cif



Utilities→Standardization of Crystal Data...

File→ Export Data → HoCrO3_mp-756834_Standardized.cif



Step 1: Loading the structure or an existing project in Mag2Pol

The structure file (*.cif, *.mcif) or existing Mag2Pol project file (*.xml) can be loaded by clicking this icon or through the menu tree: File→Open

In this case:
HoCrO3_mp-756834_Standardized.cif

1

Space group: **Pnma** Cell: a = 5.52910 b = 7.52660 c = 5.21130
a = 90.000 β = 90.000 γ = 90.000

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	φ
1	x	y	z	u	v	w	0.000

Atoms

Atom	x	y	z	B	occ	plot	color	R	S
1 Ho	0.06978	0.25000	0.48018	0.000	1.000	<input checked="" type="checkbox"/>	blue	10	1.0
2 Cr	0.00000	0.00000	0.00000	0.000	1.000	<input checked="" type="checkbox"/>	red	10	1.0
3 O	0.30361	0.05718	0.19135	0.000	1.000	<input checked="" type="checkbox"/>	green	10	1.0
4 O	0.46113	0.25000	0.61212	0.000	1.000	<input checked="" type="checkbox"/>	green	10	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ≠ -q

Spin	Rx	Ry	Rz	lx	ly	lz	φ
------	----	----	----	----	----	----	---

Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1
View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 34

Legend: blue Ho, red Cr, green O

If the structure file is loaded properly, several sections in the main window are populated automatically.

Step 1: Editing structure, plot it your way!

Mag2Pol

Symmetry

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130
 $\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

plot	color	R	S
<input checked="" type="checkbox"/>	blue	20	1.0
<input checked="" type="checkbox"/>	red	12	1.0
<input checked="" type="checkbox"/>	green	7	1.0
<input checked="" type="checkbox"/>	green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q \neq -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
------	----	----	----	----	----	----	--------

Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10

Domain: 1 Phase: 1

View along: custom Rotation axes: 0 0 1 direct Step/81: 5 Zoom: 26

2 Extended the cell (box) to show

Here, R and S change the radius of the atom and S length of the spin vector (just cosmetic, has no effect on the refinement)

4

After making changes, press **Ctrl+U** (on Windows) or **Cmd+U** (on Mac) to append the structure on the screen.

Step 1: Editing structure - bond and the octahedra

Left-click on the 'bonds' icon to open the 'Bonds and polyhedral' editing window.

Bonds and polyhedra

Bonds

1 Number of bonds

Atom 1	Atom 2	dmin Å	dmax Å	add	style	Color 1	Color 2	alpha	radius	show
1 CR	O	0.10	3.00	<input checked="" type="checkbox"/>	Gradient	■	■	<input type="checkbox"/>	0.04	<input checked="" type="checkbox"/>

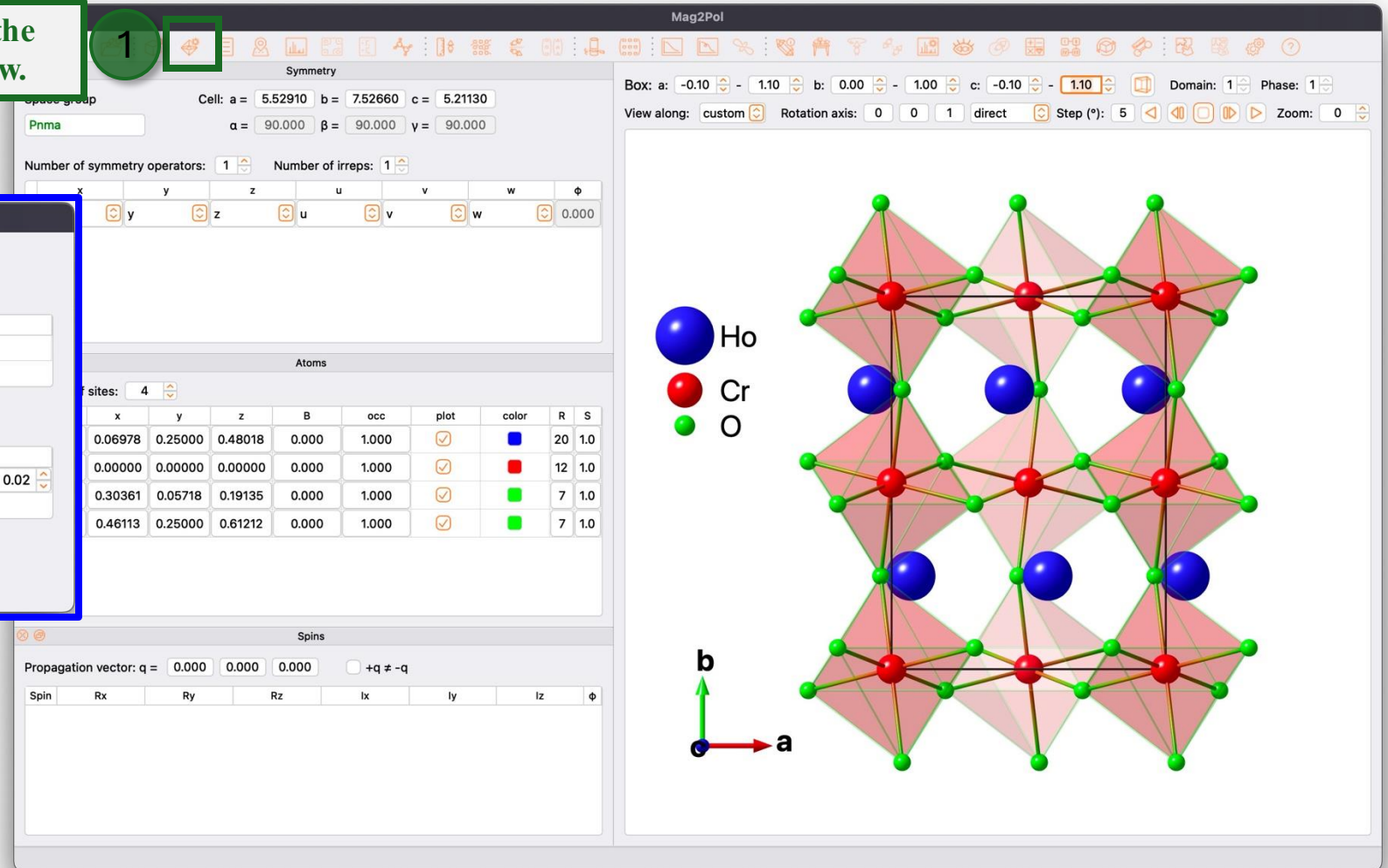
Polyhedra

Atom 1	Atom 2	polyhedra	face color	alpha	min. d Å	edge color	alpha	radius
1 CR	O	face Color 1, edge Color2	■	<input type="checkbox"/>	0.30	■	<input type="checkbox"/>	0.02

Apply Cancel OK

2

Create 1 set of bonds between Cr and O, which creates CrO₆ octahedra. Use the drop-down menu, values, and dials to create the desired crystal lattice view. The structure in the main window will be updated when you press 'Apply' in this window.



Step 2: Enter the refinement (Fit) window and load experimental data

To load the experimental data we need to open the 'Fit' window, by clicking on the icon as shown in the screenshot below (or the keyboard shortcut 'Ctrl+F').

The screenshot displays the Mag2Pol software interface. The main window is divided into several panels. On the left, the 'Symmetry' panel shows the space group 'Pnma' and unit cell parameters. Below it, the 'Atoms' panel lists four sites: Ho, Cr, and two O atoms, with their respective coordinates and occupancies. The 'Spins' panel at the bottom left shows the propagation vector and spin components. The central panel displays a 3D model of the crystal structure with atoms represented by colored spheres (blue for Ho, red for Cr, green for O) and bonds. A legend on the left identifies the atoms. The 'Fit' window is open on the right, showing tabs for 'Data', 'Moments', 'Domains', 'Constraints', and 'Fit'. The 'Data' tab is active, displaying 'Polarization data' and buttons for 'Load *.fli', 'Load *.int', and 'Load Numors'. Below this, the 'Integrated intensities' section has buttons for 'Load *.int' and 'Load *.col/*.*.fsq/*.*.sf/*.*.bra'. The 'Powder patterns' section has buttons for 'Load pattern' and 'Mag2Pol format'. At the bottom, there are 'View data' and 'Save data' buttons for both sections. A blue arrow points from the 'Fit' icon in the top toolbar to the 'Fit' window.

Within the 'Fit' window, you can load the data, load the instrument resolution file, and perform Le Bail Profile fit or Rietveld refinement.

Load the experimental data collected at 300 K

The data can be loaded under the 'Data' tab of the 'Fit' window. Mag2Pol can accept three kinds of data sets. In this example, we will start with 'Powder diffraction data' of HoCrO_3 collected at 300 K (Paramagnetic phase). **Follow the numerical order indicated below.**

The screenshot shows the 'Fit' window in Mag2Pol. The 'Data' tab is selected, indicated by a red circle with the number 1. The window is divided into two main sections: 'Polarization data' and 'Powder patterns'. In the 'Polarization data' section, there are buttons for 'Load *.fli', 'Load *.int', and 'Load Numors'. A text box explains that the user should click on 'Load pattern' and select the data file 'HCO_300K.dat'. In the 'Powder patterns' section, there is a 'Load pattern' button and a dropdown menu for 'x y sigma (Ins 10)', which is highlighted by a green circle with the number 2. A text box explains that the user should select the data format 'x y Sigma (Ins 10)'. Below the dropdown, the file 'HCO_300K.dat (weight = 1)' is listed. In the 'Integrated intensities' section, there are buttons for 'Load *.int' and 'Load *.col/*.fsq/*.sf/*.bra'. At the bottom, there is a checkbox for 'Refine nuclear structure' which is checked, and a radio button for 'Purely magnetic scattering'. A text box explains that the user should activate 'Refine nuclear structure', indicated by a black circle with the number 4. The window also has 'View data' and 'Save data' buttons in both sections.

1 We are under the 'Data' tab

Polarization data

Load *.fli Load *.int Load Numors

Click on 'Load pattern' and select the data file when prompted. In this case: **HCO_300K.dat**

You can load more than one pattern. For example, if you have collected data with different wavelengths, or want to refine XRD data collected at same temperature. Or even single crystal diffraction data (polarized unpolarized)

Integrated intensities

Load *.int Load *.col/*.fsq/*.sf/*.bra

Powder patterns

Load pattern x y sigma (Ins 10)

2 Select the data format 'x y Sigma (Ins 10)'

HCO_300K.dat (weight = 1)

3

4 Activate 'Refine nuclear structure'

View data Save data

View data Save data

☒ Refine nuclear structure ☐ Purely magnetic scattering

Step 2b: Confirm all the atoms are loaded properly

Activate 'Atoms' tab: Check if all the atoms are loaded properly and the occupancies nominally follow the chemical formula. Do not select any of these parameters for refinement at this stage.

Fit

Data **Atoms** Moments Domains Constraints Patterns Fit

	Atom	x	y	z	B	occ
A1	HO	0.06978	0.25000	0.48018	0.000	1.000
A2	CR	0.00000	0.00000	0.00000	0.000	1.000
A3	O	0.30361	0.05718	0.19135	0.000	1.000
A4	O	0.46113	0.25000	0.61212	0.000	1.000

Scale factor and $\lambda/2$: 1.00000 0.00000

Extinction parameters:
☒ anisotropic ShelX-like model

x_{11} x_{12} x_{13}
0.00000 0.00000 0.00000

x_{22} x_{23}
0.00000 0.00000

x_{33}
0.00000

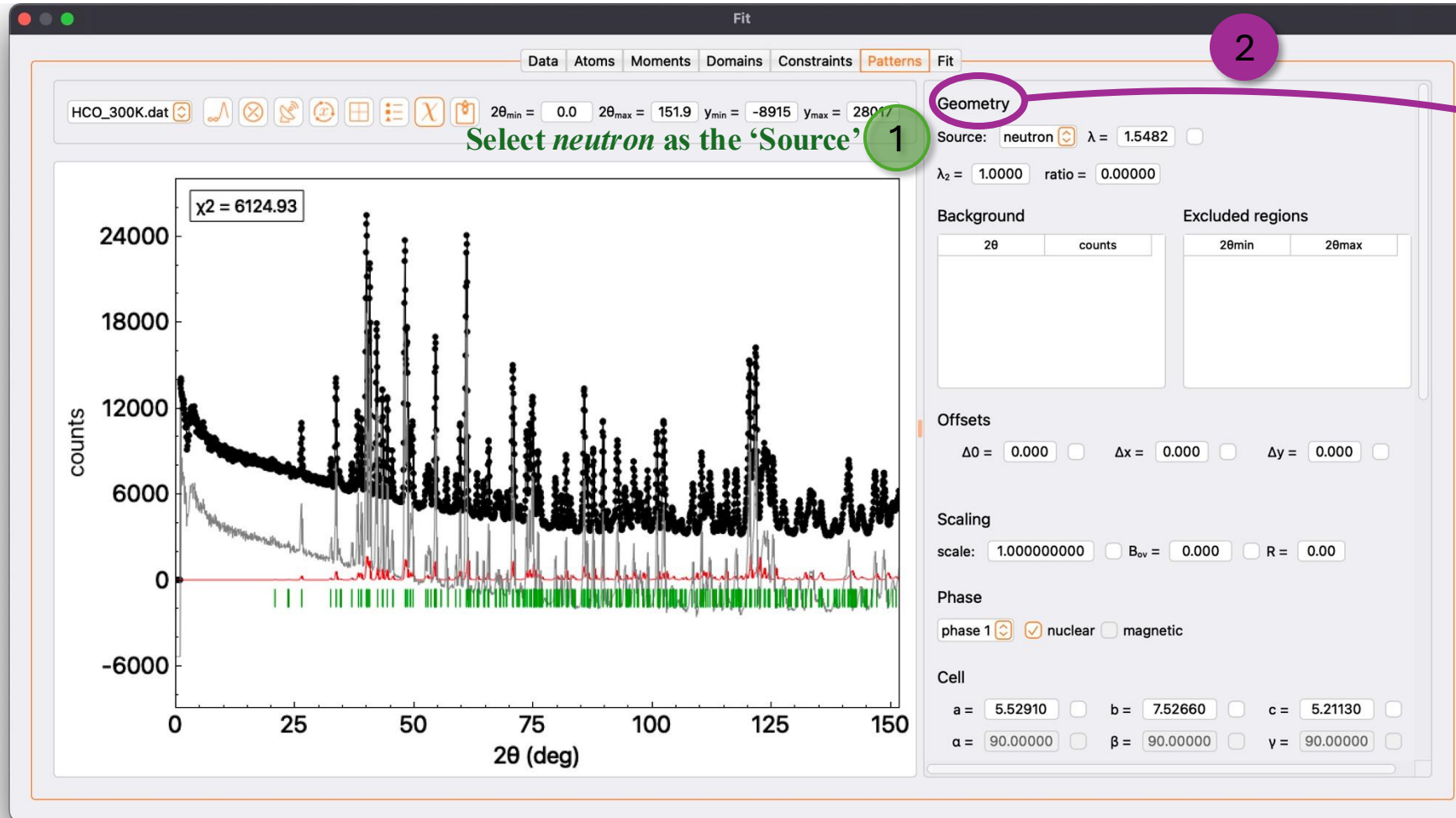
☐ Becker-Coppens model

r_D : 0.000

θ_D : 0.000 Lorentzian

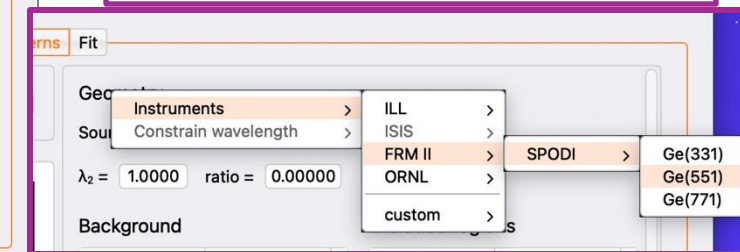
Step 2c: Edit source, instrument, and wavelength parameters

Activate 'Patterns' tab

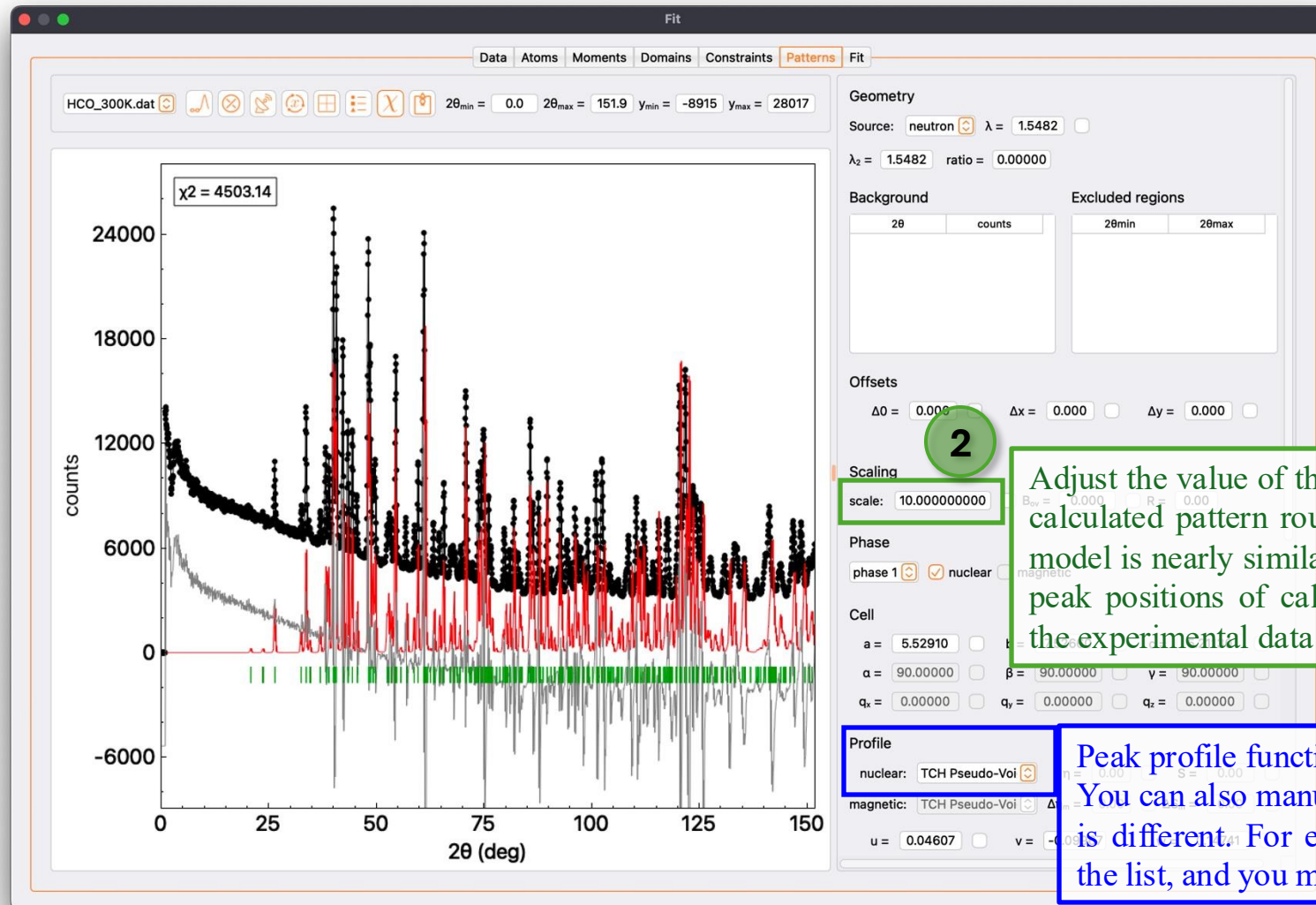


Right-click on the text 'Geometry' and follow the menu items as shown in the screenshot below, to select the neutron facility, instrument, and the appropriate monochromator (which is used for the experiment).

In this case, it is Ge(551) was is used to select neutrons of wavelength 1.5482 Å



Step 2d: Check the peak function and set an appropriate scale factor



Adjust the value of the 'scale' factor so that the intensities of the calculated pattern roughly match those of observed data. If the model is nearly similar and the wavelength choice is correct then peak positions of calculated patterns (red curve) should match the experimental data (black curve)

Peak profile function is automatically updated here. You can also manually select it if, for any reason, it is different. For example, the instrument is not in the list, and you manually entered the wavelength.

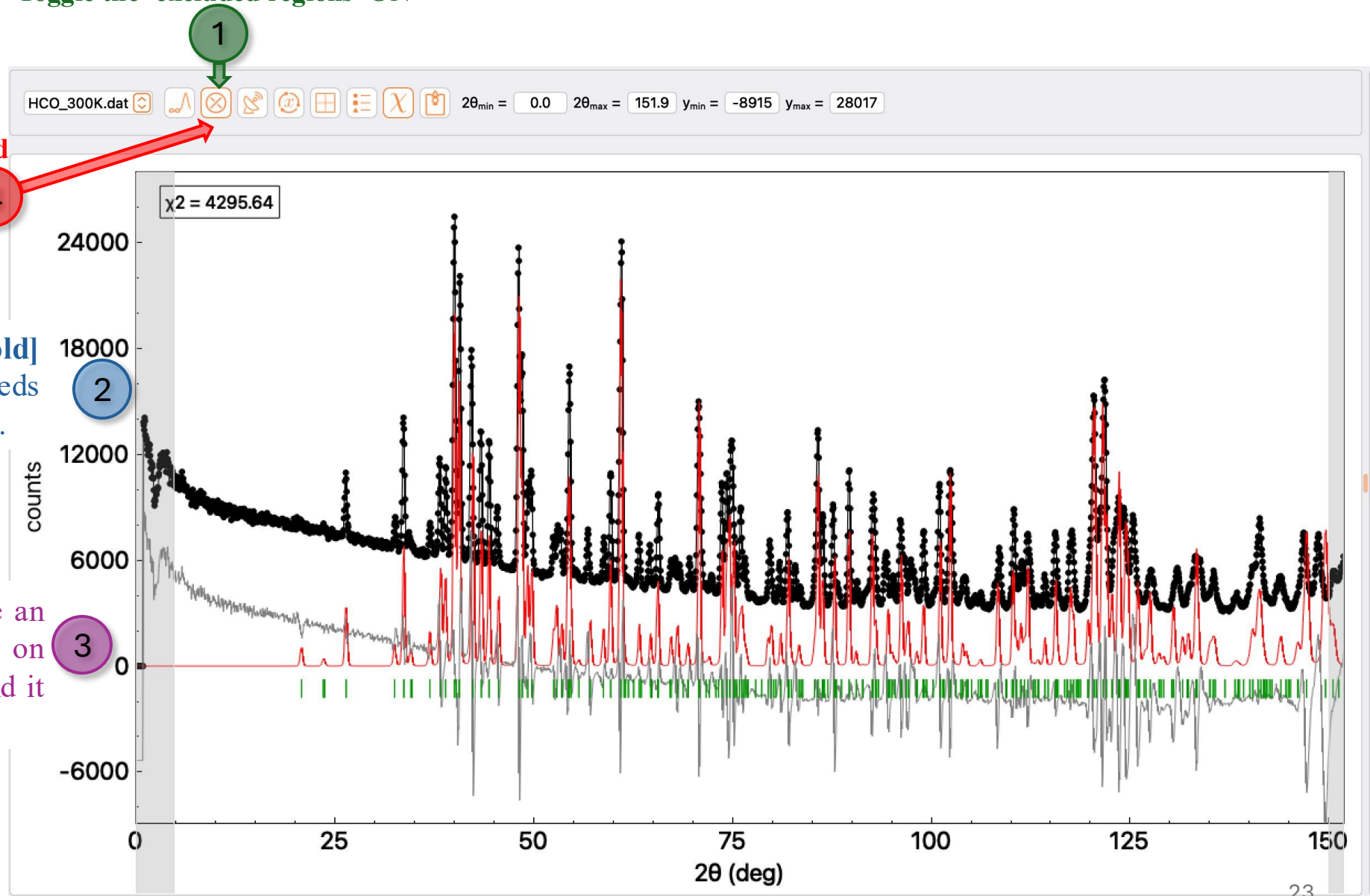
Step 2e: Select the region to exclude from the fit 'Excluded region'

Toggle the 'excluded regions' ON

Toggle the 'excluded regions' OFF

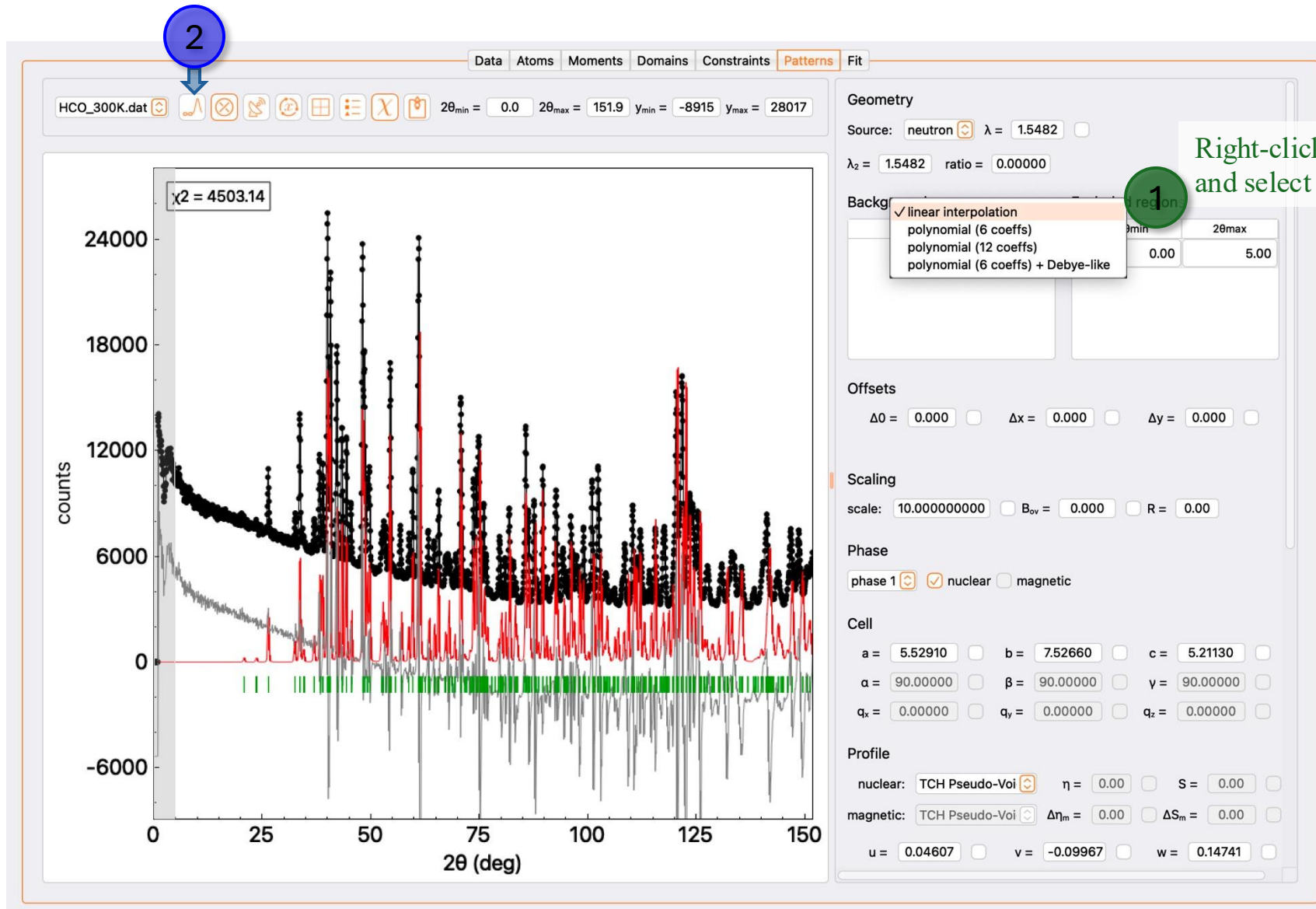
On the plot, [Left click + hold] and drag on the region that needs to be excluded. Grey area here.

If it is necessary to remove an excluded region, right-click on the (grey) excluded area, and it will be removed



Step 2f: Select the background type

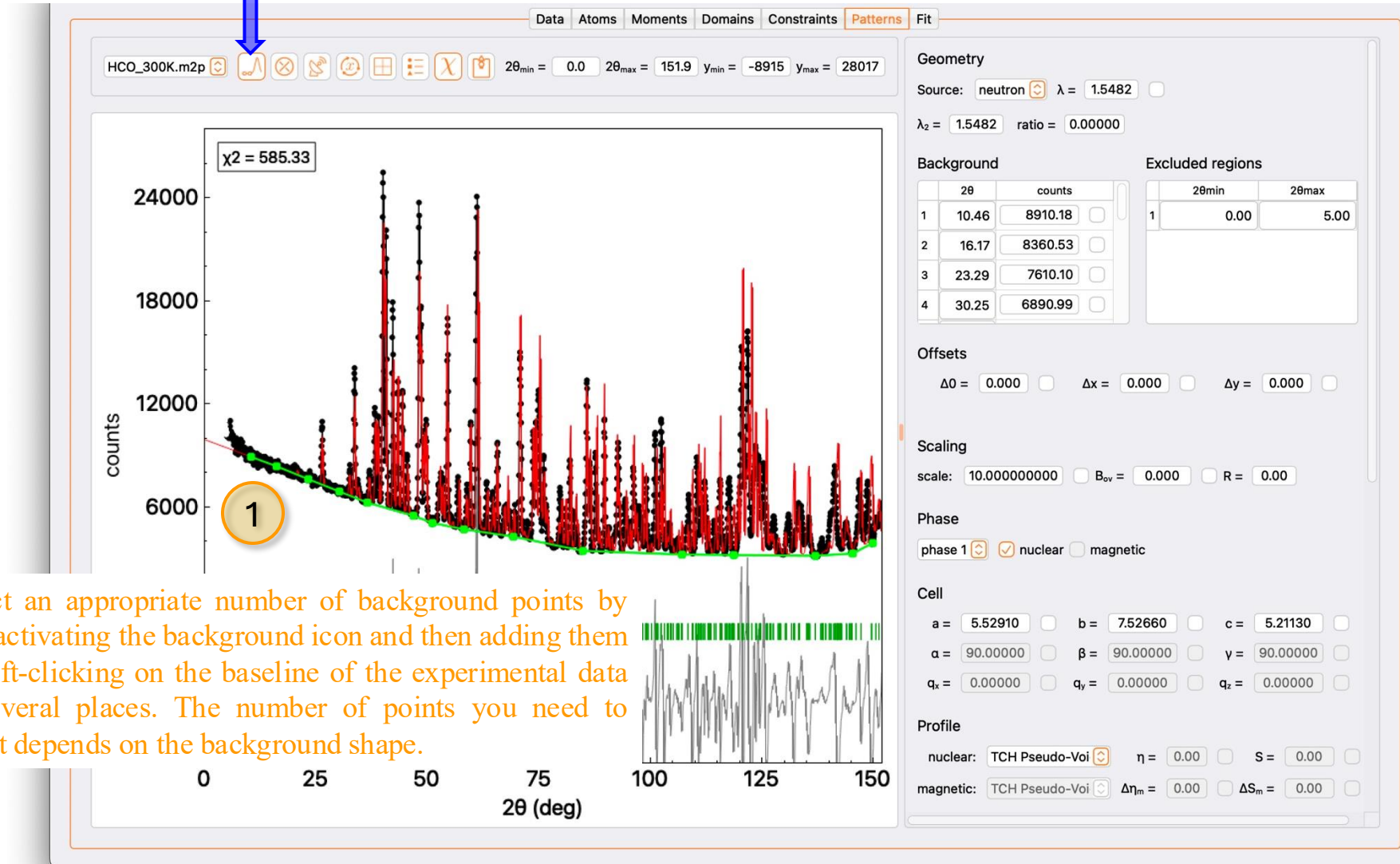
For manual background selection, toggle this ON



Step 2f: Select the background

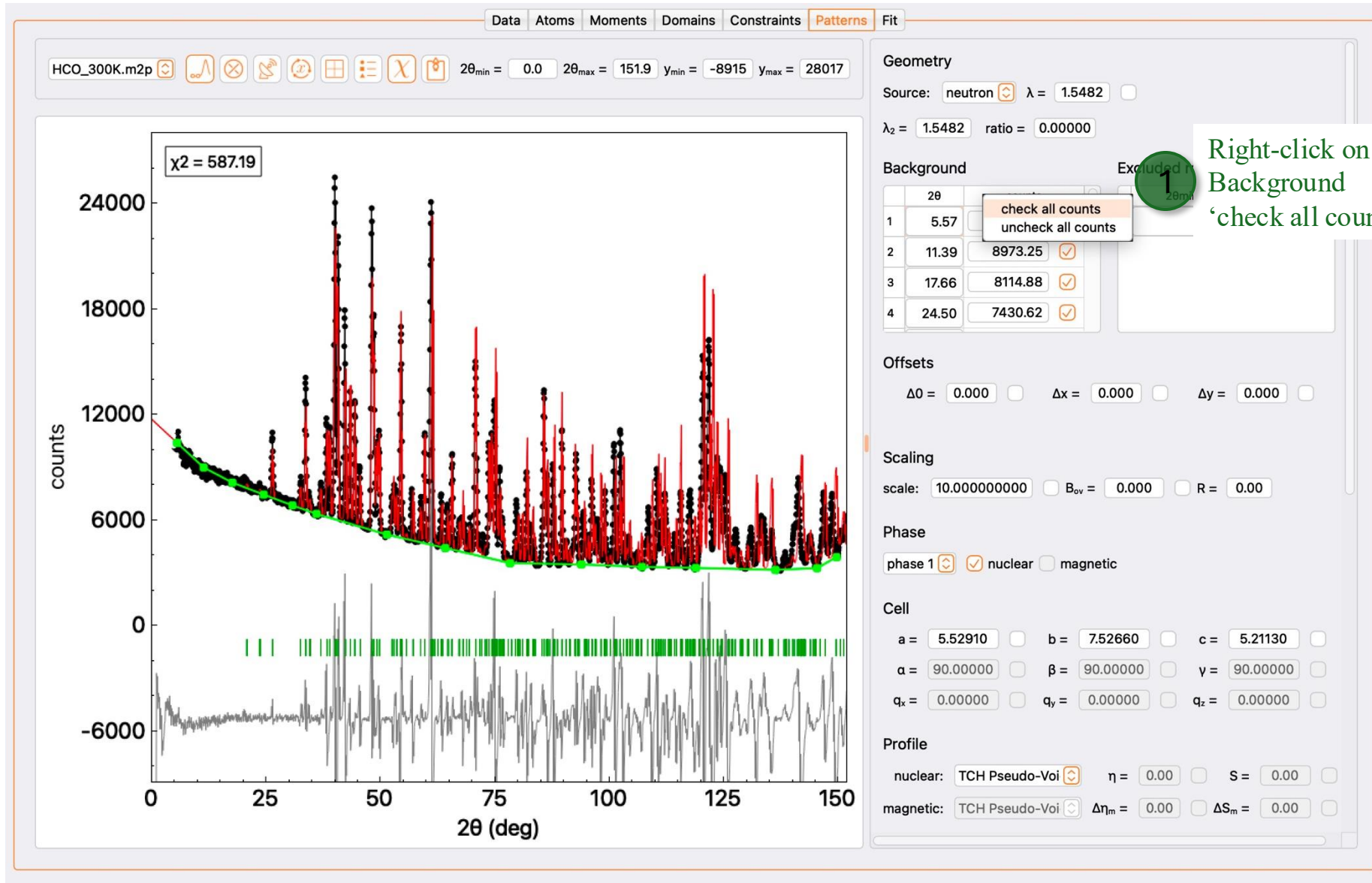
Toggle it off after selecting all the background points

2



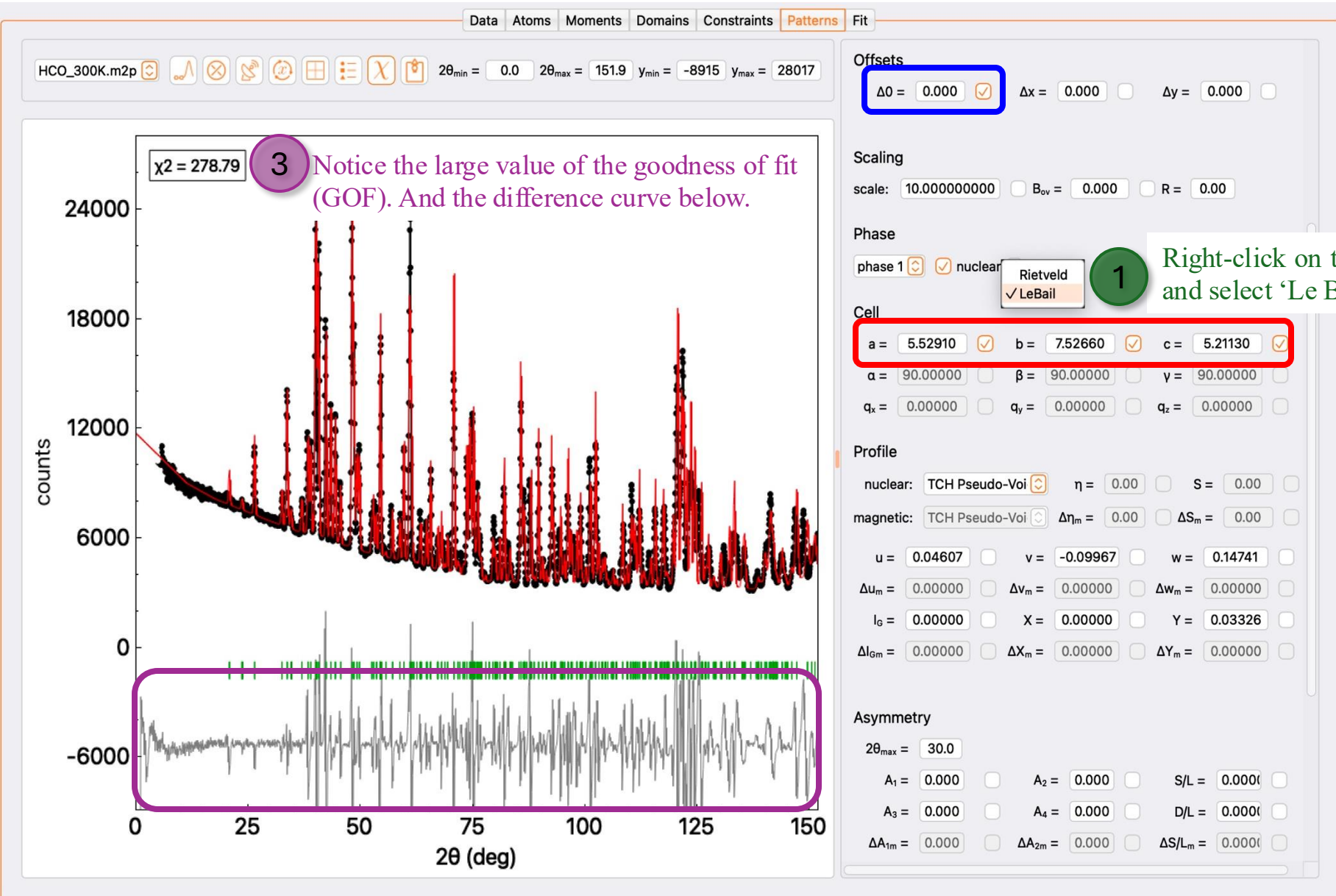
Select an appropriate number of background points by first activating the background icon and then adding them by left-clicking on the baseline of the experimental data at several places. The number of points you need to select depends on the background shape.

Activate the refinement of background



Right-click on the text 'counts' in the Background section and select 'check all counts'

Le Bail fit



Activate the refinement of:

$\Delta 0$, A constant shift added to all calculated Bragg angles:

$$2\theta_{\text{calc}} \rightarrow 2\theta_{\text{calc}} + \Delta 0$$

Influenced by:

- mis-calibration of detector zero
- instrument alignment

a , b , c : Lattice parameters

Run Le Bail fit

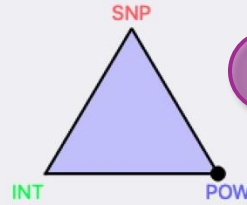
1 Activate 'Fit' tab

Data Atoms Moments Domains Constraints Patterns **Fit**

weight SNP: 0.000

weight intensities: 0.000

weight powder: 1.000



2

Fit

POW nucle

Left-click on 'Fit'.

While the fit is running, this tab appears with the text 'Stop', if you see that the fit is diverging, stop the fitting by right-clicking on 'Stop'.

5

Refined parameters window

Background points:

point 1 at $2\theta = 5.57$: $1.015(6)e+4$
point 2 at $2\theta = 11.39$: $8.75(5)e+3$
point 3 at $2\theta = 17.66$: $8.17(4)e+3$
point 4 at $2\theta = 24.5$: $7.34(4)e+3$
point 5 at $2\theta = 30.79$: $6.88(4)e+3$
point 6 at $2\theta = 36.04$: $6.27(3)e+3$
point 7 at $2\theta = 51.43$: $5.14(3)e+3$
point 8 at $2\theta = 64.17$: $4.43(2)e+3$
point 9 at $2\theta = 78.34$: $3.55(2)e+3$
point 10 at $2\theta = 93.92$: $3.48(2)e+3$
point 11 at $2\theta = 107.14$: $3.35(2)e+3$
point 12 at $2\theta = 118.91$: $3.31(2)e+3$
point 13 at $2\theta = 136.34$: $3.16(2)e+3$
point 14 at $2\theta = 145.41$: $3.23(3)e+3$
point 15 at $2\theta = 149.69$: $3.90(3)e+3$

Offsets:

$\lambda = 1.548$ $\Delta 0 = 0.000101(0.000403)$ $\Delta x = 0.000$ $\Delta y = 0.000$

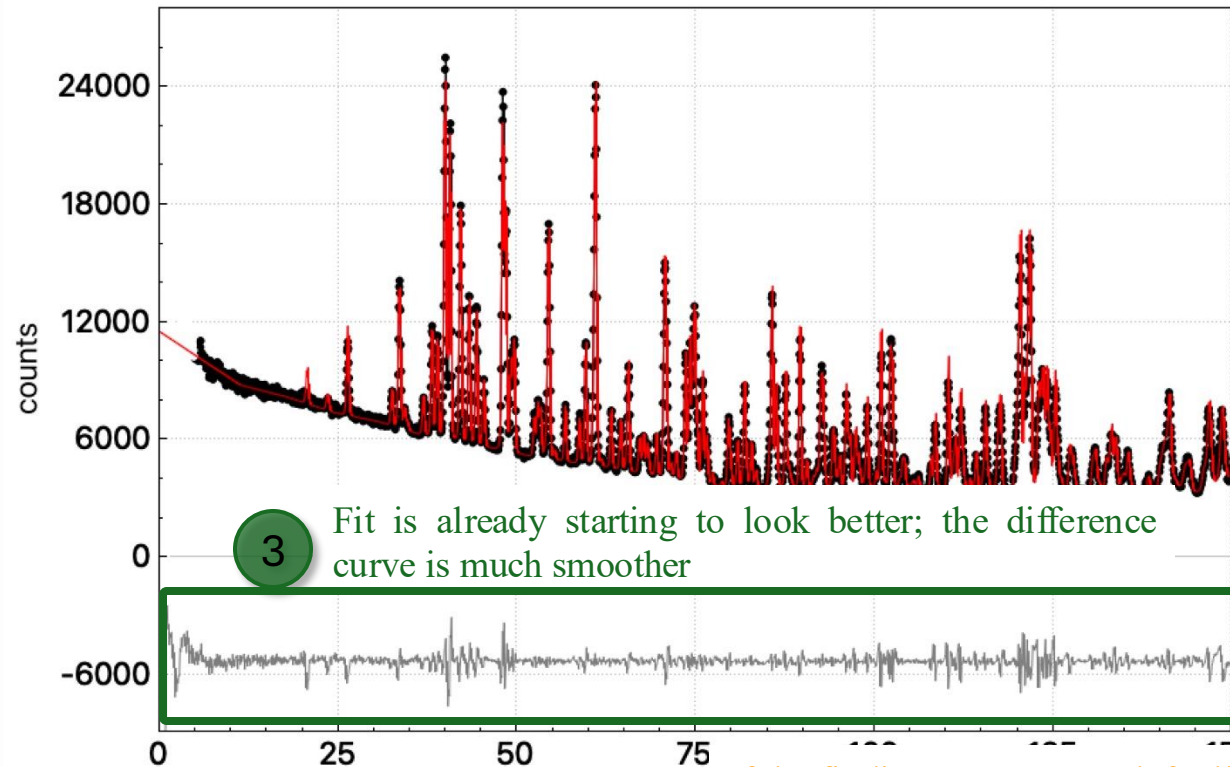
Profile:

$u = 0.046$ $v = -0.100$ $w = 0.147$ $I_0 = 0.000$
 $X = 0.000$ $Y = 0.033$
 $A_1 = 0.000$ $A_2 = 0.000$ $A_3 = 0.000$ $A_4 = 0.000$
 $S/L = 0.000$ $D/L = 0.000$
 $P_1 = 0.000$ $P_2 = 0.000$

Lattice:

$a = 5.51709(7)$ $b = 7.53673(7)$ $c = 5.242390(20.863946)$
 $\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$
Volume = $217.982949(867.540308)$

$B_{ov} = 0.000$



3

Fit is already starting to look better; the difference curve is much smoother

4

If the fit diverges, you can left-click on 'Undo' to retrieve the parameters with which you started the last fit.

View results

Export results

View correlations

Export graph

Undo (2)

Accept

Calculated diffraction intensity: Le Bail fit



iteration 29
 $\chi^2 = 17.1643$, $(\Delta / \epsilon\sigma)_{\max} (b) = 34.5467$
 iteration 30
 $\chi^2 = 17.118$, $(\Delta / \epsilon\sigma)_{\max} (b) = 18.773$
 iteration 31
 $\chi^2 = 17.0768$, $(\Delta / \epsilon\sigma)_{\max} (b) = 9.22227$
 iteration 32
 $\chi^2 = 17.0397$, $(\Delta / \epsilon\sigma)_{\max} (b) = 4.42354$
 iteration 33
 $\chi^2 = 17.0064$, $(\Delta / \epsilon\sigma)_{\max} (b) = 0.849272$

Fit converged after 33 iterations

$\chi^2 = 49641.70$
 $\chi_r^2 = 17.01$
 $R_F = 0.17$

Atoms:

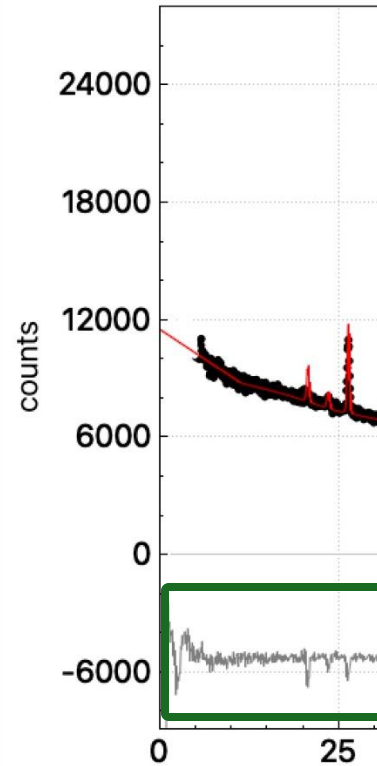
HO = [0.070 0.250 0.480]
 B = 0.000, occ = 1.000
 CR = [0.000 0.000 0.000]
 B = 0.000, occ = 1.000
 O = [0.304 0.057 0.191]
 B = 0.000, occ = 1.000
 O = [0.461 0.250 0.612]
 B = 0.000, occ = 1.000

POWDER PARAMETERS:

scale = 10.000

Background points:

point 1 at $2\theta = 5.57$: $1.033(6)e+4$
 point 2 at $2\theta = 11.39$: $8.92(5)e+3$



Least square minimization via:

$$\chi^2 = \sum_i \left[\frac{y_{\text{obs},i} - y_{\text{cal},i}}{\sigma_i} \right]^2$$

$$\chi_r^2 = \chi^2 / (m - n)$$

σ_i = statistical counting uncertainty of each observed point.

m = number of observations (data points),

n = number of refined parameters

Agreement is evaluated via:

$$R_F = 100 \cdot \frac{\sum_Q |F_{\text{obs},Q} - F_{\text{cal},Q}|}{\sum_Q F_{\text{obs},Q}}$$

$$F_{\text{obs},Q} = \sqrt{\frac{I_{\text{obs},Q}}{m_Q L_Q}}$$

Here $I_{\text{obs},Q} \approx I_Q$ after convergence

Calculated diffraction intensity Le Bail:

$$y_{\text{cal}}(2\theta_i) = \sum_{Q=(hkl)} \underbrace{I_Q}_{\text{refined reflection intensity}} \underbrace{\Phi(2\theta_i - 2\theta_Q - \Delta(2\theta)_{\text{disp}})}_{\text{profile function}} + \underbrace{b_i}_{\text{background}}$$

$Q = (hkl)$: reflection index

I_Q : refined integrated intensity of each reflection (free parameter; no structure factor)

$\Phi(\dots)$: peak profile (U, V, W, X, Y, asymmetry, sample displacement, etc.)

B_i : background intensity at point i (polynomial / point-interpolated / Debye-like), modeling all non-Bragg contributions.

$2\theta_Q$: Bragg angle obtained from lattice parameters via

$$2^*d^*\sin\theta_Q = \lambda$$

In Le Bail fit, $F_{\text{cal},Q}$ is not computed from structure factors, instead, refined reflection intensities serve as effective F^2

View results

Export results

View correlations

Export graph

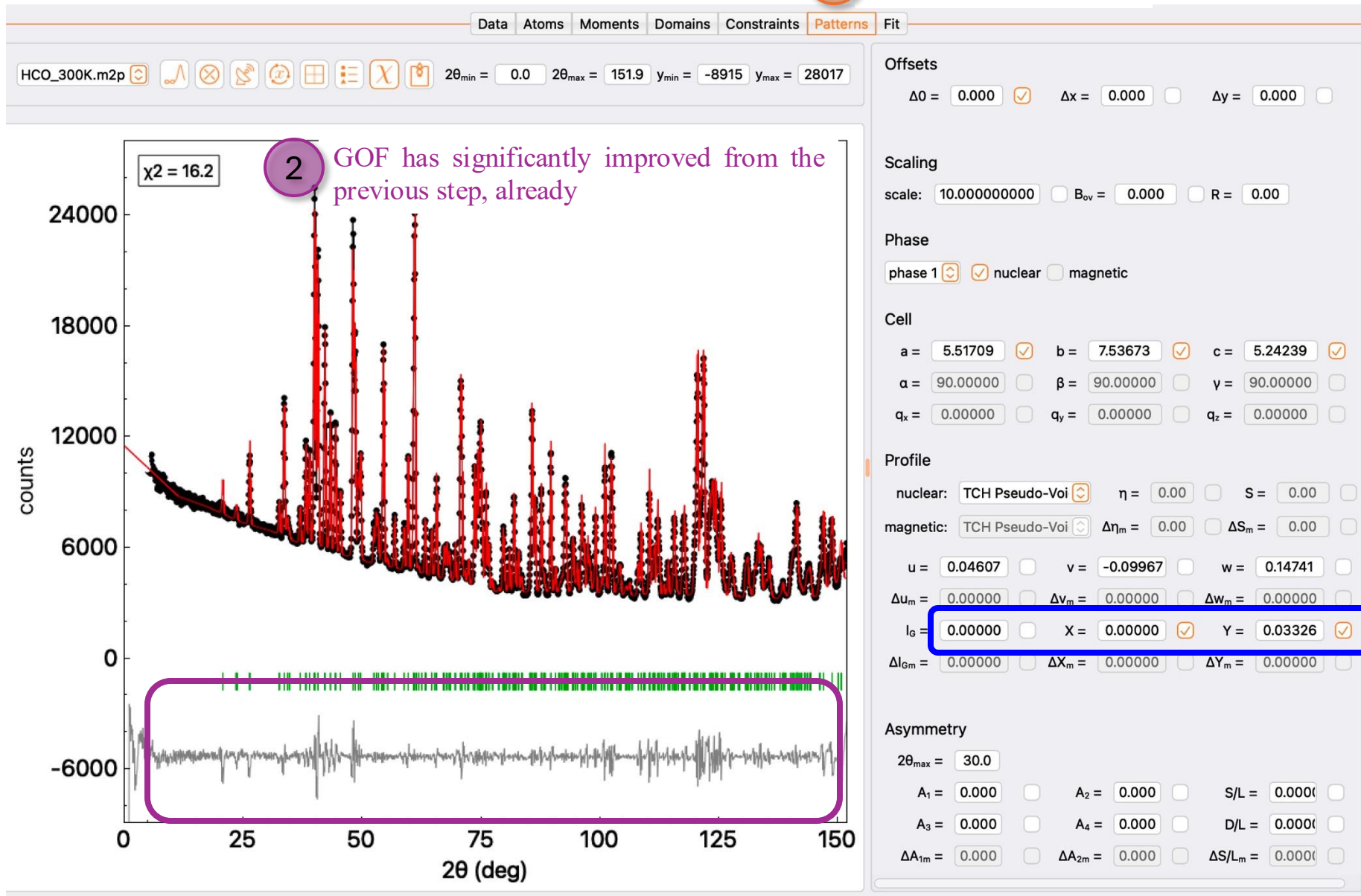
Undo (2)

Accept

Refine more profile parameters

1

Activate 'Patterns' tab



3

Activate refinement of X and Y

X and Y control the Lorentzian component of peak width:

$$H_L = X \tan \theta + Y / \cos \theta$$

Influenced by:

- crystallite size (Lorentzian term)
- strain broadening (high-angle broadening)
- instrument axial divergence (partially)

4

Go to the 'Fit' tab and run the refinement by left-clicking on the 'Fit' button. Then return back to 'Patterns' tab.

Refine more profile parameters

1

Activate 'Patterns' tab

3

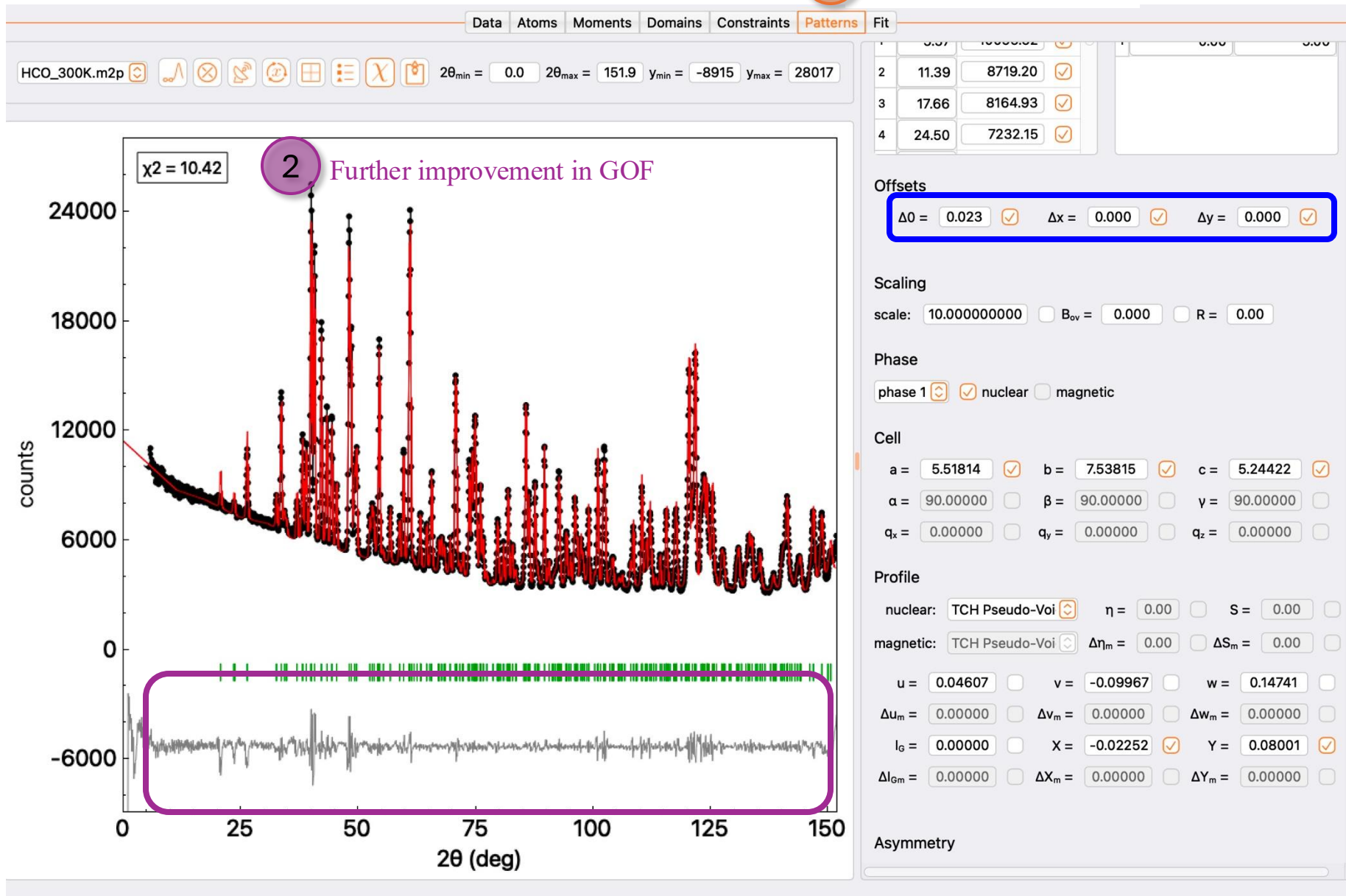
Activate refinement of ΔX and ΔY

ΔX : Sample height deviation

ΔY : lateral mis-positioning along the beam direction

4

Go to the 'Fit' tab and run the refinement by left-clicking on the 'Fit' button. Then return back to 'Patterns' tab.



Refine more profile parameters

1

Activate 'Patterns' tab

3

Fix: Offsets, ΔX and ΔY

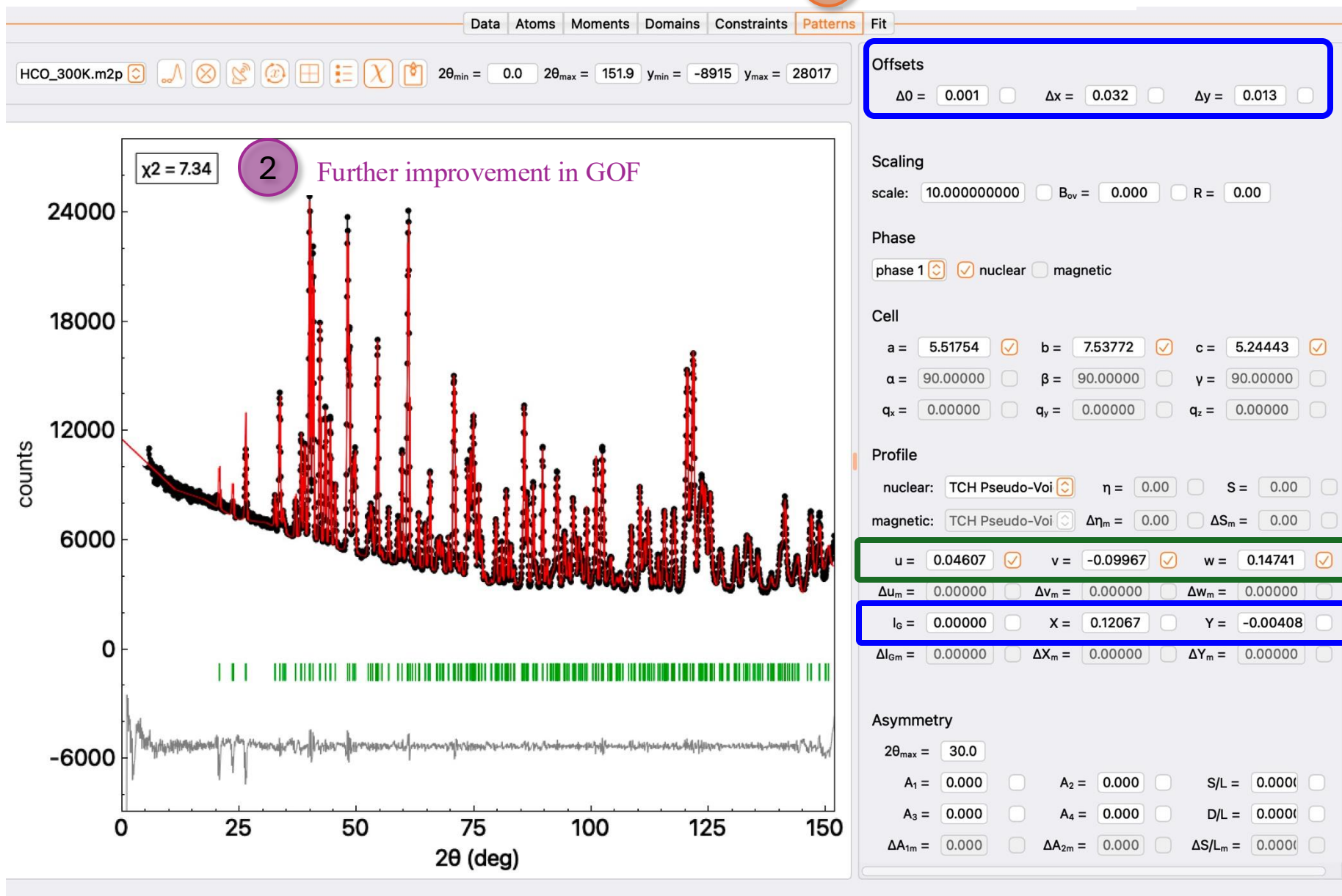
4

Refine: u , v , w , which control the Gaussian component of the peak function

$$H_G^2 = u \tan^2 \theta + v \tan \theta + w$$

5

Go to the 'Fit' tab and run the refinement by left-clicking on the 'Fit' button. Then return back to 'Patterns' tab.



Refine more profile parameters

1

Activate 'Patterns' tab

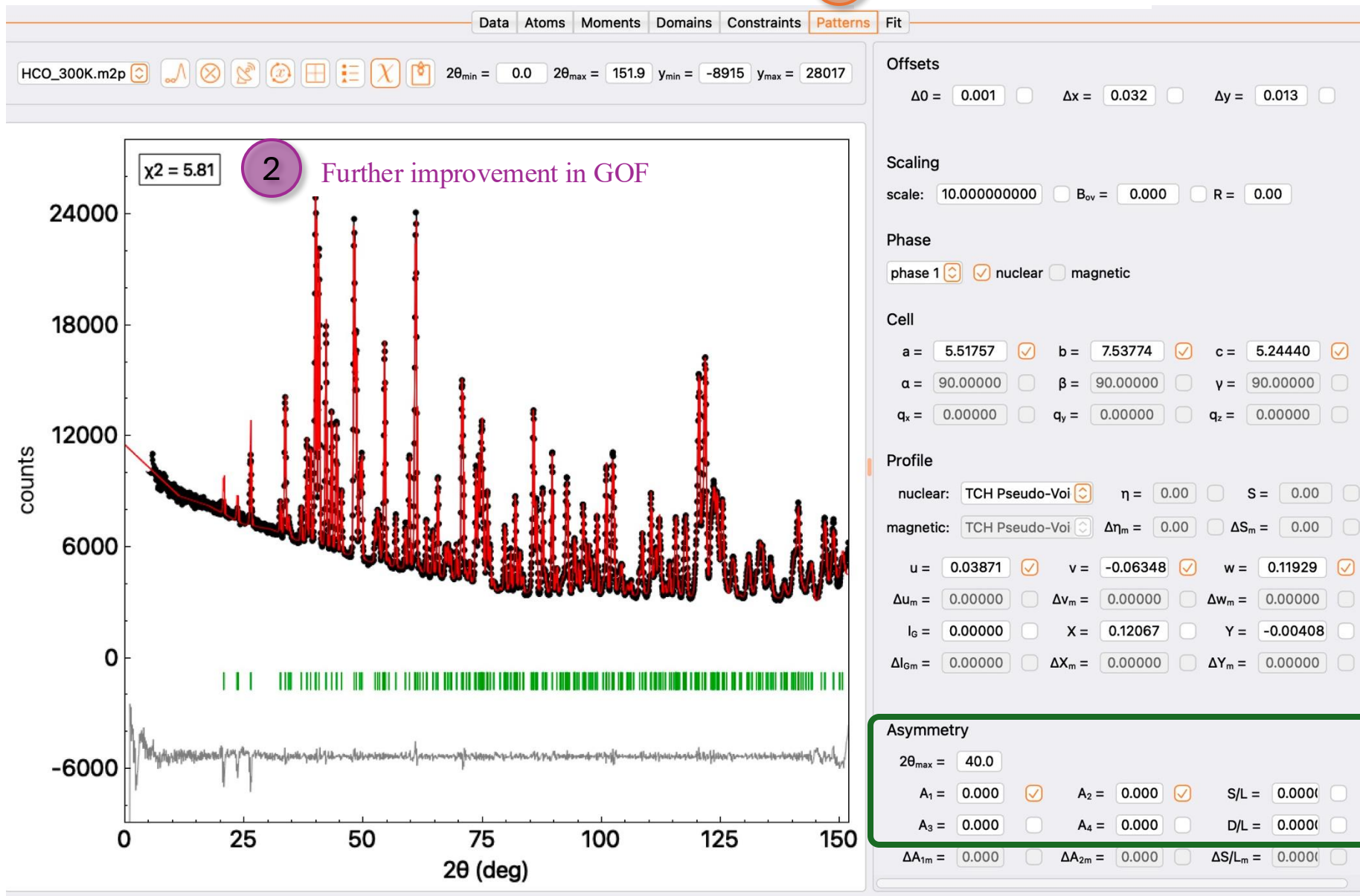
3

Refine: A_1, A_2 asymmetry correction coefficients describing peak tails on the low-angle side

$$\text{Asymmetry} = A_1 f_1(\theta) + A_2 f_2(\theta) + A_3 f_3(\theta) + A_4 f_4(\theta)$$

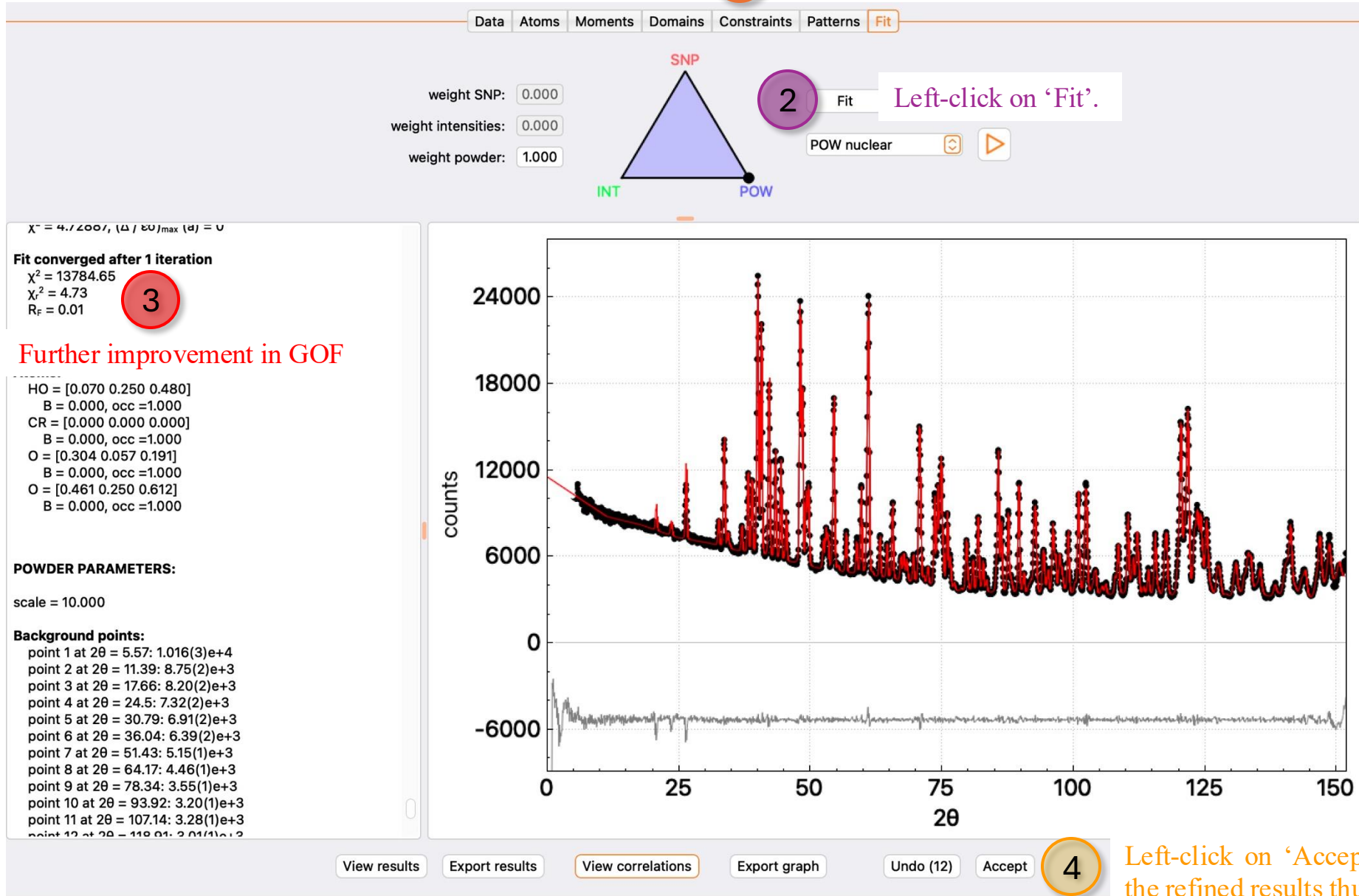
4

Go to the 'Fit' tab and run the refinement by left-clicking on the 'Fit' button.



Run final Le Bail fit

1 Activate 'Fit' tab



Save a copy of the project file

1 Go to the main Mag2Pol window

2 Save a copy of the project as 'HCO_300K_LeBail.xml'

Save as

Symmetry

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130
 $\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 HO	0.06978	0.25000	0.48018	0.000	1.000	<input checked="" type="checkbox"/>	blue	20	1.0
2 CR	0.00000	0.00000	0.00000	0.000	1.000	<input checked="" type="checkbox"/>	red	12	1.0
3 O	0.30361	0.05718	0.19135	0.000	1.000	<input checked="" type="checkbox"/>	green	7	1.0
4 O	0.46113	0.25000	0.61212	0.000	1.000	<input checked="" type="checkbox"/>	green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☐ -q

Spin	Rx	Ry	Rz	lx	ly	lz	ϕ
------	----	----	----	----	----	----	--------

Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10 Domain: 1 Phase: 1

View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 0

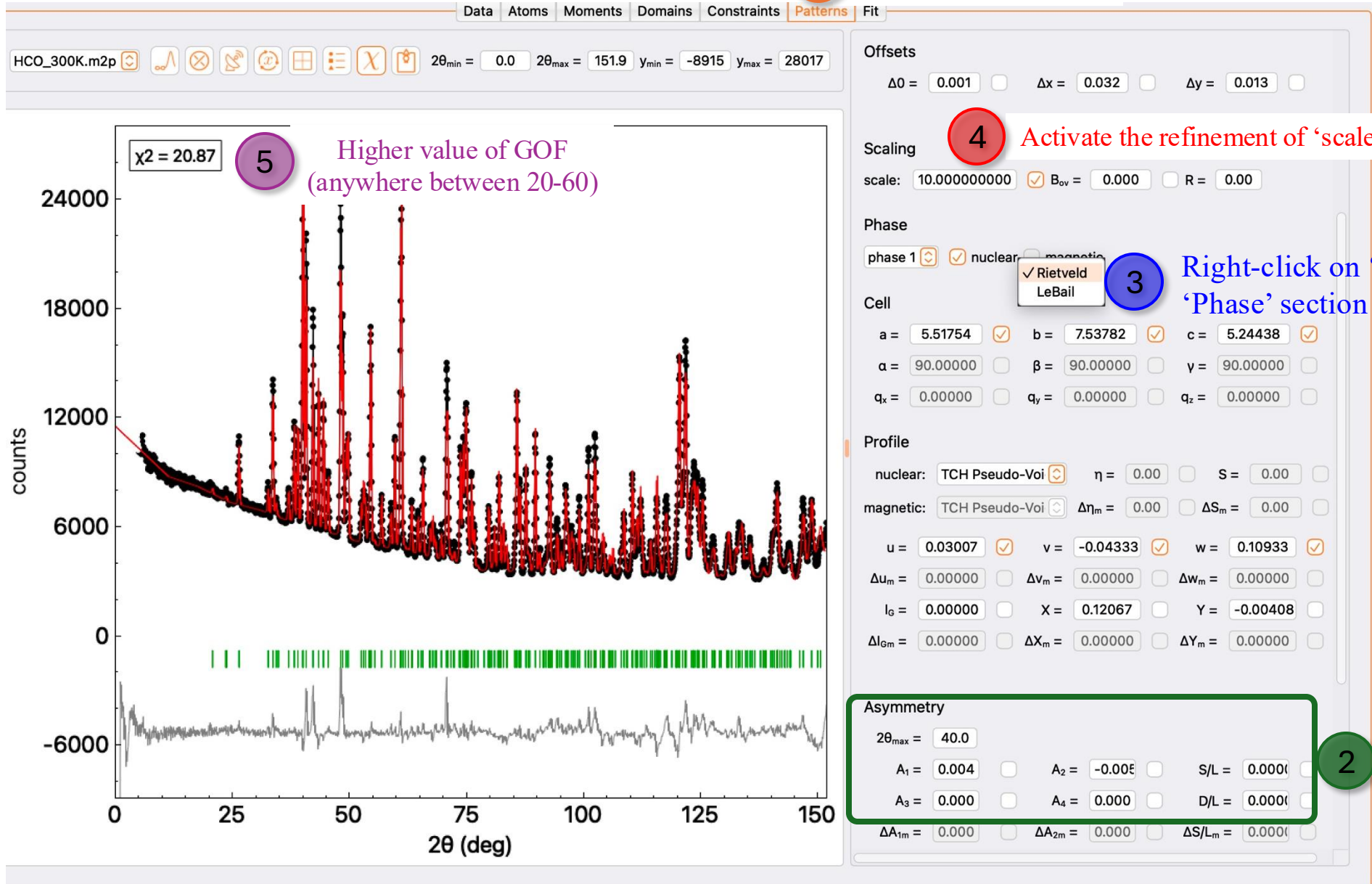
3

Go back to the 'Fit' window

Activate Rietveld refinement of lattice structure

1

Activate 'Patterns' tab



4

Activate the refinement of 'scale'

3

Right-click on 'nuclear' under the 'Phase' section and choose Rietveld.

2

Fix Asymmetry parameters

Rietveld refinement of lattice structure

1 Activate 'Atoms' tab

Atom	x	y	z	B	occ
A1 HO	0.06978 <input checked="" type="checkbox"/>	0.25000 <input checked="" type="checkbox"/>	0.00000 <input checked="" type="checkbox"/>	0.500 <input type="checkbox"/>	1.000 <input type="checkbox"/>
A2 CR	0.00000 <input type="checkbox"/>	0.00000 <input type="checkbox"/>	0.00000 <input type="checkbox"/>	0.500 <input type="checkbox"/>	1.000 <input type="checkbox"/>
A3 O	0.30361 <input checked="" type="checkbox"/>	0.05718 <input checked="" type="checkbox"/>	0.19135 <input checked="" type="checkbox"/>	0.500 <input type="checkbox"/>	1.000 <input type="checkbox"/>
A4 O	0.46113 <input checked="" type="checkbox"/>	0.25000 <input type="checkbox"/>	0.61212 <input checked="" type="checkbox"/>	0.500 <input type="checkbox"/>	1.000 <input type="checkbox"/>

2

Right-click on x and 'check all x' to select symmetry allowed refinable x co-ordinates of all atoms. Repeat this for y and z co-ordinates as well.

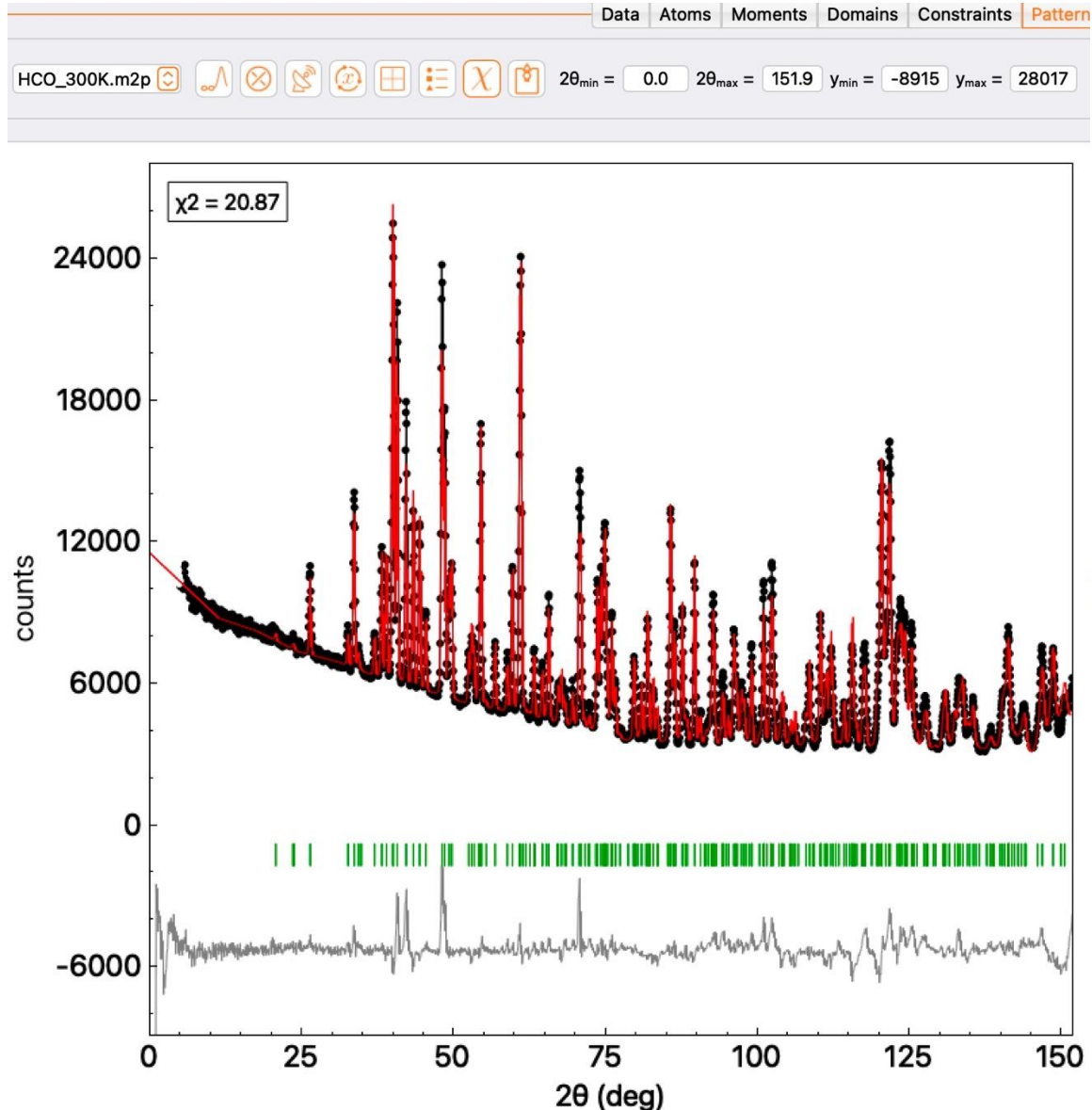
In some cases, starting the refinement of both positions and thermal parameters might lead to divergence or local minima, so refine positions (x, y, z) first and then activate and refine thermal parameters (B).

3 Set B (B_{iso}) isotropic thermal displacement parameter to be 0.5 for all atoms (a good starting point). Do not refine them together with atomic positions, to start with.

4

Go to the 'Fit' tab and run the refinement by left-clicking on the 'Fit' button. Then return to the 'Patterns' tab.

Calculated diffraction intensity: Rietveld fit



Least square minimization via:

$$\chi^2 = \sum_i \left[\frac{y_{\text{obs},i} - y_{\text{cal},i}}{\sigma_i} \right]^2$$

$$\chi_r^2 = \chi^2 / (m - n)$$

σ_i = statistical counting uncertainty of each observed point.

m = number of observations (data points),

n = number of refined parameters

Agreement is evaluated via:

$$R_F = 100 \cdot \frac{\sum_Q |F_{\text{obs},Q} - F_{\text{cal},Q}|}{\sum_Q F_{\text{obs},Q}}$$

$$F_{\text{obs},Q} = \sqrt{\frac{I_{\text{obs},Q}}{m_Q L_Q}}$$

Calculated diffraction intensity Rietveld:

$$y_{\text{cal}}(2\theta_i) = \sum_{Q=(hkl)} \underbrace{m_Q L_Q |F_{\text{cal},Q}|^2}_{\text{structure-factor term}} \underbrace{\Phi(2\theta_i - 2\theta_Q - \Delta(2\theta)_{\text{disp}})}_{\text{profile function}} + \underbrace{b_i}_{\text{background}}$$

$Q = (hkl)$: reflection index

m_Q : multiplicity

L_Q : Lorentz factor

$|F_{\text{cal},Q}|^2 = |N(Q)|^2 + |M_{\perp}(Q)|^2$ – from nuclear + magnetic structure factors

$\Phi(\dots)$ – peak profile (U, V, W, X, Y, asymmetry, sample displacement, etc.)

b_i – background intensity at point i (polynomial / point-interpolated / Debye-like), modeling all non-Bragg contributions.

Nuclear structure factor: $N(Q) = \sum_j o_j b_j e^{-2\pi i(hx_j + ky_j + lz_j)} e^{-B_j \sin^2 \theta / \lambda^2}$

Magnetic structure factor: $M(Q) = \sum_j p_n o_j S_j f_j(Q) e^{-2\pi i(hx_j + ky_j + lz_j)} e^{-B_j \sin^2 \theta / \lambda^2}$

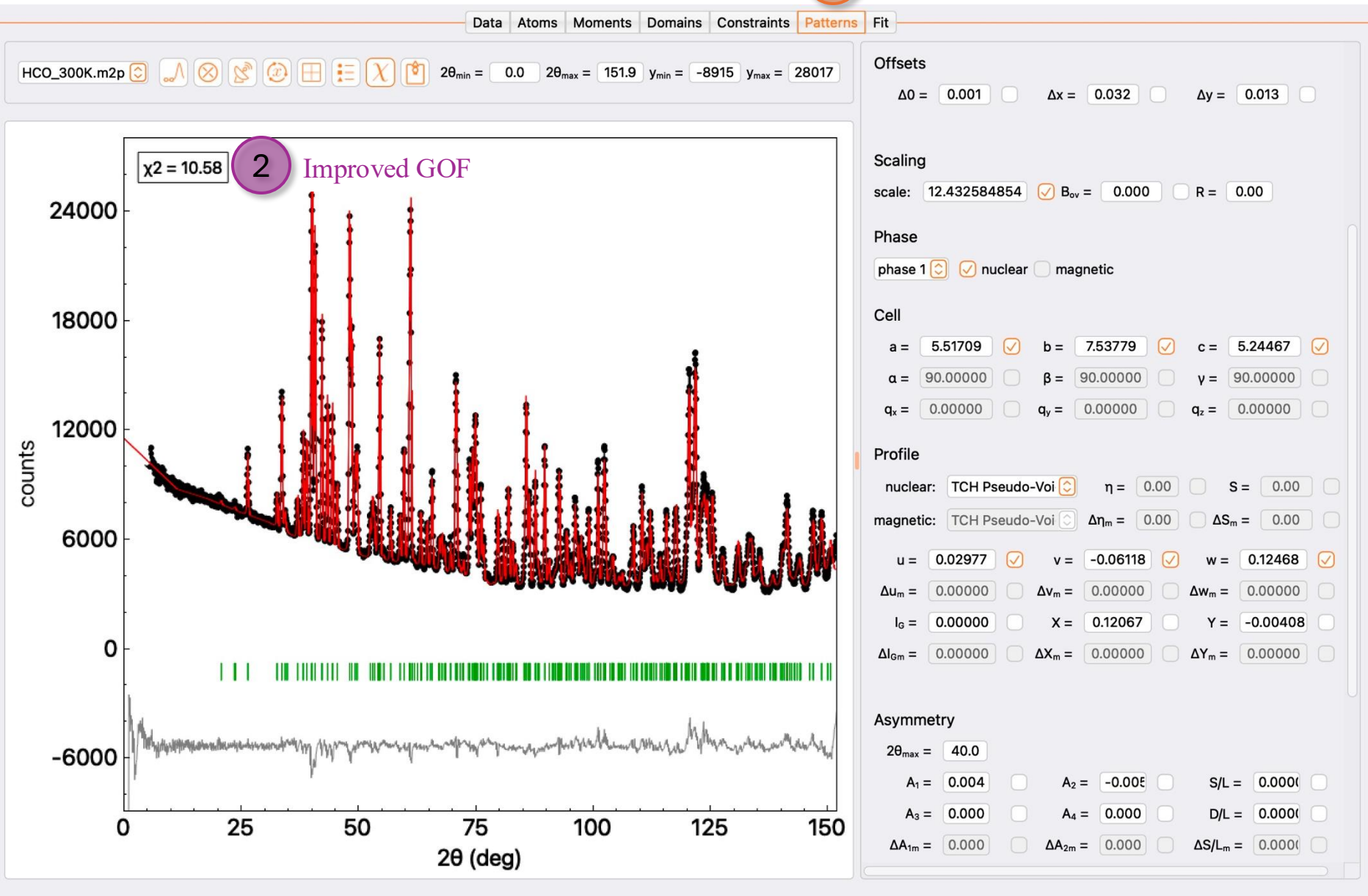
$$|M_{\perp}(Q)|^2 = |M(Q)|^2 - |M(Q) \cdot \hat{Q}|^2$$

Only the perpendicular component scatters

Activate Rietveld refinement of lattice structure

1

Activate 'Patterns' tab



Rietveld refinement of lattice structure

1 Activate 'Atoms' tab

Software interface for Rietveld refinement showing the 'Atoms' tab.

Navigation tabs: Data, **Atoms**, Moments, Domains, Constraints, Patterns, Fit.

x		y		z		B	
0.06441	<input checked="" type="checkbox"/>	0.25000	<input type="checkbox"/>	0.48407	<input checked="" type="checkbox"/>	0.500	
0.00000	<input type="checkbox"/>	0.00000	<input type="checkbox"/>	0.00000	<input type="checkbox"/>	0.500	<input checked="" type="checkbox"/>
0.30393	<input checked="" type="checkbox"/>	0.05311	<input checked="" type="checkbox"/>	0.19252	<input checked="" type="checkbox"/>	0.500	<input checked="" type="checkbox"/>
0.46462	<input checked="" type="checkbox"/>	0.25000	<input type="checkbox"/>	0.60403	<input checked="" type="checkbox"/>	0.500	<input checked="" type="checkbox"/>

Scale factor and $\lambda/2$: 1.00000 ☐ 0.0

Extinction parameters:

☒ anisotropic ☐ ShelX-like model

x_{11} x_{12} x_{13}

0.00000 ☐ 0.00000 ☐ 0.00000 ☐

x_{22} x_{23}

0.00000 ☐ 0.00000 ☐

x_{33}

0.00000 ☐

☐ Becker-Coppens model

r_D : 0.000 ☐

θ_D : 0.000 ☐ Lorentzian ☐

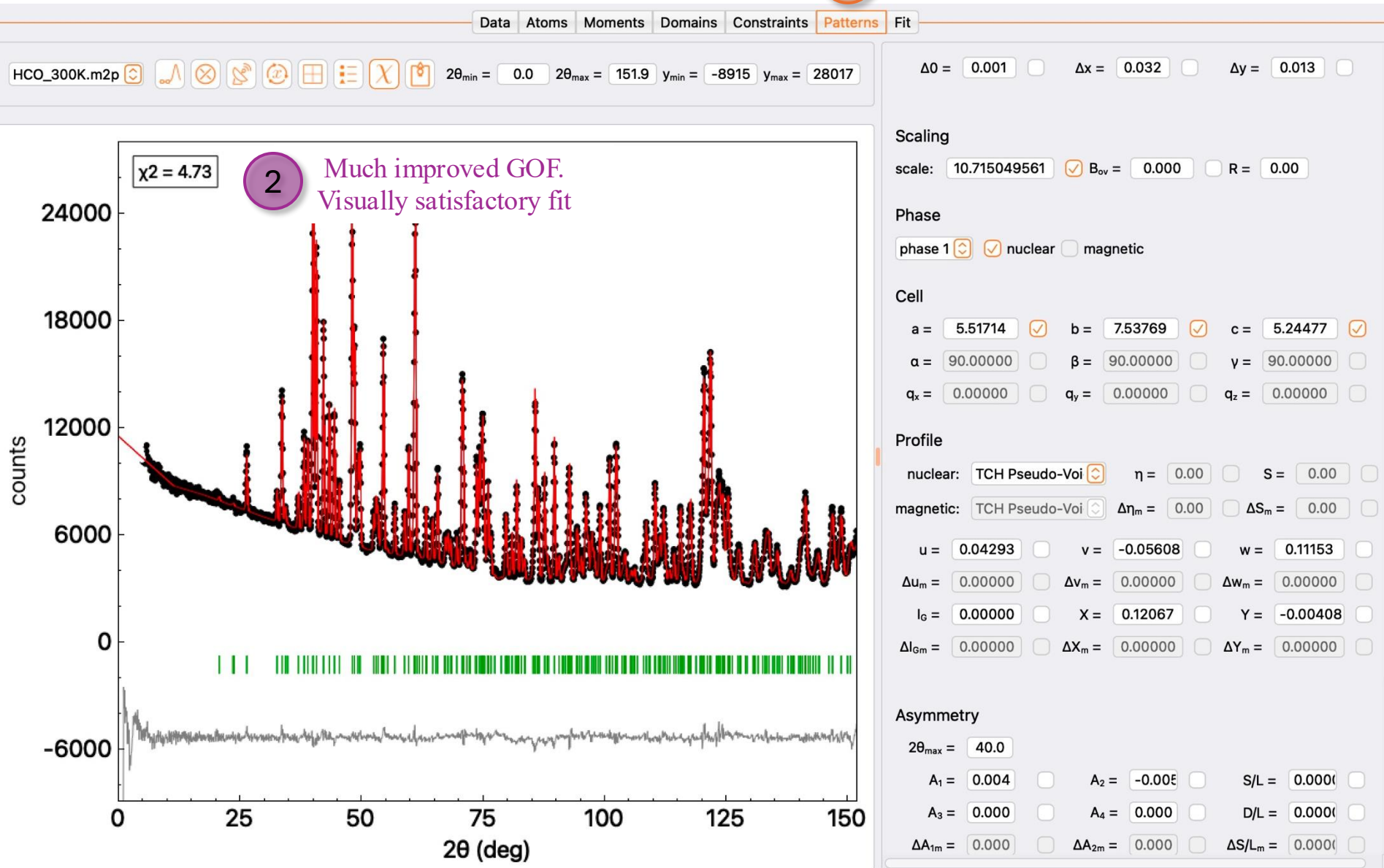
2 Activate all B (thermal parameters)

3

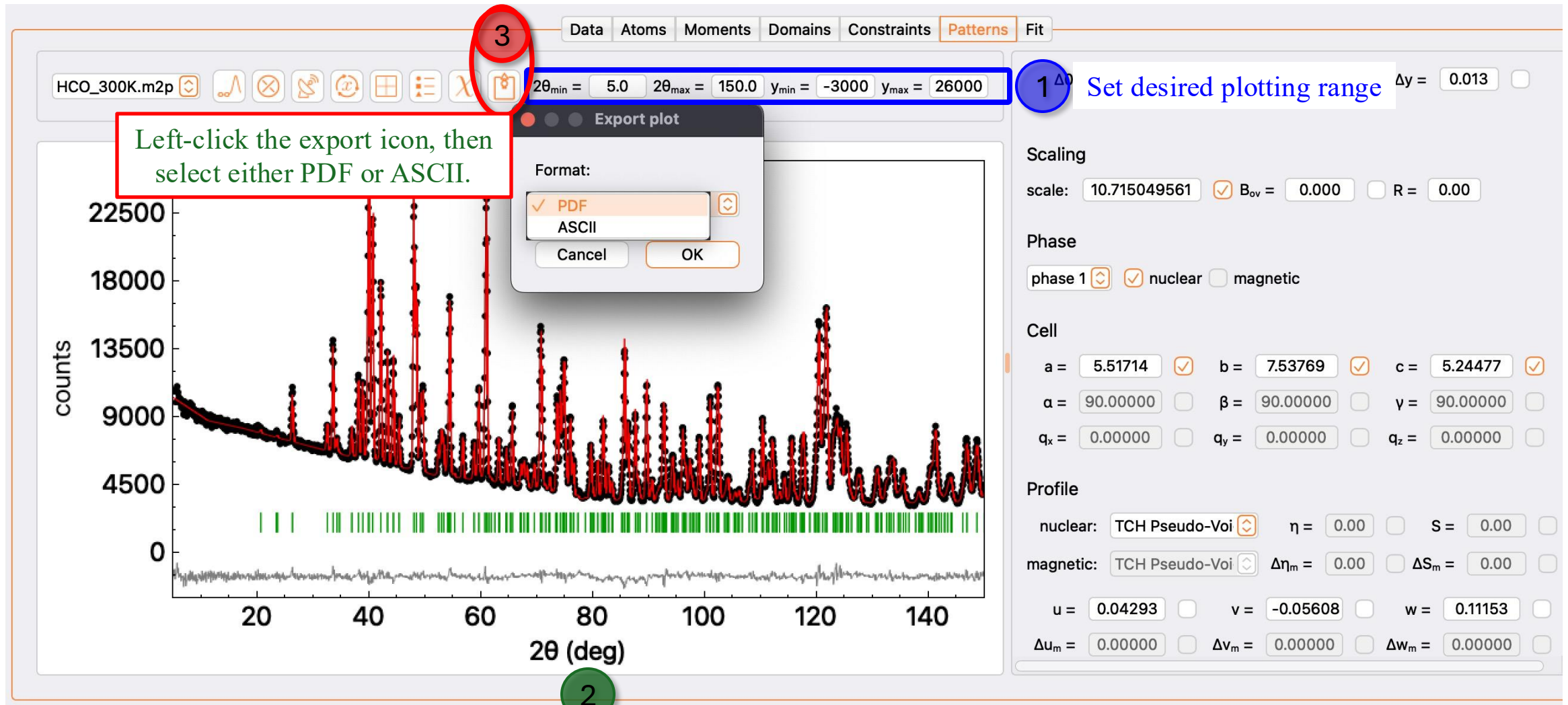
Go to the 'Fit' tab and run the refinement by left-clicking on the 'Fit' button. Then return to the 'Patterns' tab.

Rietveld refinement of lattice structure

1 Activate 'Patterns' tab



Rietveld refinement of lattice structure



Rearrange the plot window to a desired-looking aspect ratio and font size

Accept the final Rietveld refinement results

1 Activate 'Fit' tab

Data Atoms Moments Domains Constraints Patterns **Fit**

weight SNP: 0.000
weight intensities: 0.000
weight powder: 1.000

Fit

POW nuclear

INT SNP POW

Profile:

$u = 0.043$ $v = -0.056$ $w = 0.112$ $I_G = 0.000$
 $X = 0.121$ $Y = -0.004$
 $A_1 = 0.004$ $A_2 = -0.005$ $A_3 = 0.000$ $A_4 = 0.000$
 $S/L = 0.000$ $D/L = 0.000$
 $P_1 = 0.000$ $P_2 = 0.000$

Lattice:

$a = 5.51714(6)$ $b = 7.53769(6)$ $c = 5.24477(5)$
 $\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$
Volume = 218.112(4)

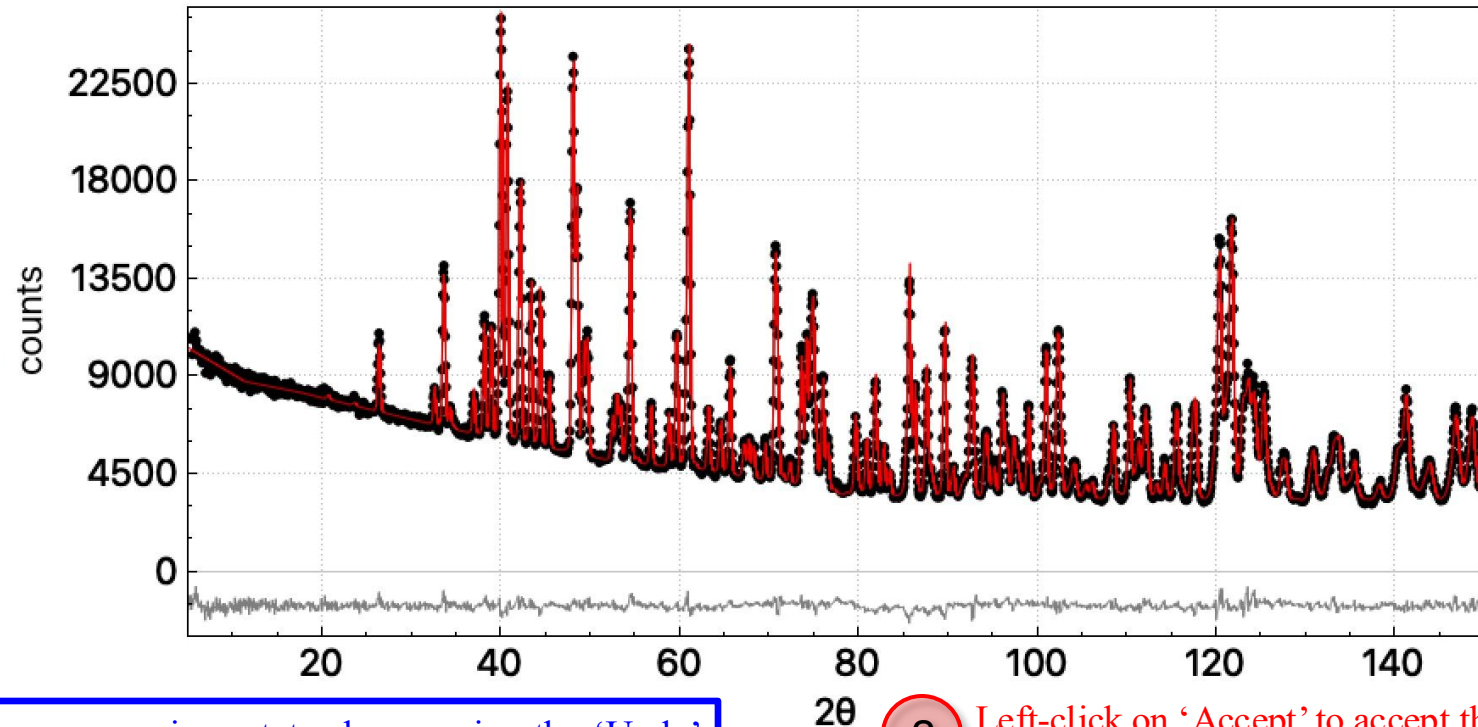
$B_{ov} = 0.000$

WARNINGS:

- negative temperature factor for atom 2, atom 1

Profile:

$u = 0.046$ $v = -0.100$ $w = 0.147$ $I_G = 0.000$
 $X = 0.000$ $Y = 0.033$
 $A_1 = 0.000$ $A_2 = 0.000$ $A_3 = 0.000$ $A_4 = 0.000$
 $S/L = 0.000$ $D/L = 0.000$
 $P_1 = 0.000$ $P_2 = 0.000$



2 Left-click on 'Accept' to accept the final refinement results and return to the main window

At any stage, if the fit diverges, you can recover previous states by pressing the 'Undo' button. It can go back as many steps as you want, all the way back to the initial state of the refinements of the current session.

Undo (18)

Accept

Save a copy of the project file

1 Go to the main Mag2Pol window

2 Save a copy of the project as 'HCO_300K_Lattice.xml'

Save as

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130
 $\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 HO	0.06978	0.25000	0.48018	0.000	1.000	<input checked="" type="checkbox"/>	blue	20	1.0
2 CR	0.00000	0.00000	0.00000	0.000	1.000	<input checked="" type="checkbox"/>	red	12	1.0
3 O	0.30361	0.05718	0.19135	0.000	1.000	<input checked="" type="checkbox"/>	green	7	1.0
4 O	0.46113	0.25000	0.61212	0.000	1.000	<input checked="" type="checkbox"/>	green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☒ -q

Spin	Rx	Ry	Rz	lx	ly	lz	ϕ
------	----	----	----	----	----	----	--------

Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10 Domain: 1 Phase: 1

View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 0

Legend:

- Ho (blue sphere)
- Cr (red sphere)
- O (green sphere)

Export the structure graphic and cif

1

Use the menu **File**→**Export**→**Graphic** to save the crystal structure exactly as seen on the main window.

Use the menu **File**→**Export**→**cif** to save the crystal information file for publication or to be plotted in external programs.

The screenshot displays the Mag2Pol software interface. The 'File' menu is open, showing the 'Export' option. The 'Export' submenu is also visible, showing 'Graphic', '3D model', 'cif', and 'mcif'. The main window shows a 3D crystal structure model of HoCrO, with atoms represented by spheres (Ho in blue, Cr in red, O in green) and bonds shown as lines. The structure is viewed along the 'a' axis, with the 'b' and 'c' axes indicated by arrows. The 'Atoms' table is visible, listing the positions and occupancies of the atoms.

Atoms

Atom	x	y	z	B	occ	plot	color	R	S
1 HO	0.06429	0.25000	0.48286	-0.158	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
2 CR	0.00000	0.00000	0.00000	-0.002	1.000	<input checked="" type="checkbox"/>	Red	12	1.0
3 O	0.30332	0.05297	0.19411	0.194	1.000	<input checked="" type="checkbox"/>	Green	7	1.0
4 O	0.46553	0.25000	0.60429	0.120	1.000	<input checked="" type="checkbox"/>	Green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ≠ -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	φ
------	----	----	----	----	----	----	---

Refining low temperature NPD data, collected in the magnetically ordered phase

Save another copy of the project file

We will use the 300 K refinement project as the starting point for the refinement of 4 K data

1 Save a copy of the project as 'HCO_4K_Lattice.xml'

1 Go to the 'Fit' window

Space group: **Pnma**

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 HO	0.06978	0.25000	0.48018	0.000	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
2 CR	0.00000	0.00000	0.00000	0.000	1.000	<input checked="" type="checkbox"/>	Red	12	1.0
3 O	0.30361	0.05718	0.19135	0.000	1.000	<input checked="" type="checkbox"/>	Green	7	1.0
4 O	0.46113	0.25000	0.61212	0.000	1.000	<input checked="" type="checkbox"/>	Green	7	1.0

Spins

Propagation vector: $q =$ 0.000 0.000 0.000 ☐ +q \neq -q

Spin	Rx	Ry	Rz	lx	ly	lz	ϕ
------	----	----	----	----	----	----	--------

Load the experimental data collected at 300 K

The data can be loaded/replaced under the 'Data' tab of the 'Fit' window. Mag2Pol can accept three kinds of data sets. In this example, we will start with 'Powder diffraction data' of CrSbSe_3 collected at 300 K (Paramagnetic phase). **Follow the order indicated below.**

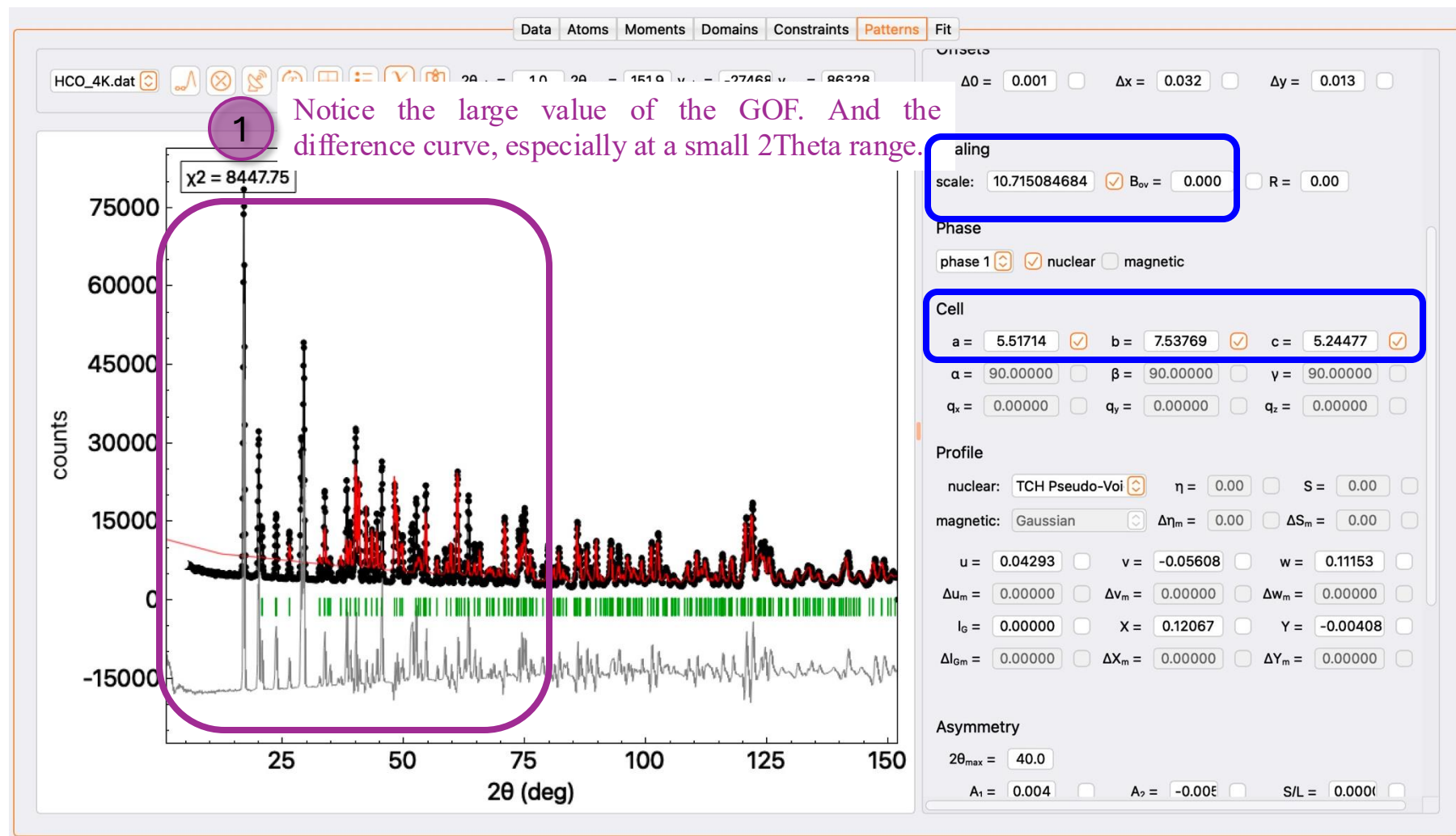
The screenshot shows the 'Fit' window in Mag2Pol with the 'Data' tab selected. The window is divided into two main sections: 'Polarization data' and 'Powder patterns'. The 'Data' tab is highlighted with a red circle and the number 1, with the text 'We are under the 'Data' tab'.

Under 'Polarization data', there are buttons for 'Load *.fli', 'Load *.int', and 'Load Numors'. Below these are 'View data' and 'Save data' buttons.

Under 'Powder patterns', there is a 'Load pattern' button and a dropdown menu showing 'x y sigma (Ins 10)'. A green circle with the number 2 points to this dropdown, with the text 'Select the data format 'x y Sigma (Ins 10)''. Below the dropdown is a list box containing 'HCO_300K.int'. A right-click context menu is open over this list box, showing options: 'Delete', 'Replace', and 'Change weight'. A purple circle with the number 3 points to the 'Replace' option, with the text 'Right-click on the data file name and choose 'Replace'. Select the file *HCO_4K.dat* when prompted.'

At the bottom, there is a section for 'Integrated intensities' with 'Load *.int' and 'Load *.hkl' buttons, and 'View data' and 'Save data' buttons. Below this, a text label says 'Make sure 'Refine nuclear structure' is active'. A blue circle with the number 4 points to the 'Refine nuclear structure' checkbox, which is checked. To its right is the 'Purely magnetic scattering' checkbox, which is unchecked. At the bottom right are 'View data' and 'Save data' buttons.

Rietveld fit of Lattice only contribution to 4 K data



2

Refine

Scale and lattice parameters (a , b , c)

4

a , b , c : Lattice parameters

Accept the Rietveld refinement results

4

Close this window and
return to the main window

1

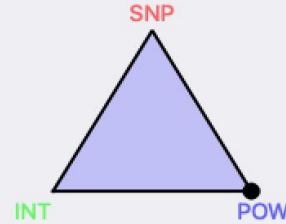
Activate 'Fit' tab

Data Atoms Moments Domains Constraints Patterns **Fit**

weight SNP: 0.000

weight intensities: 0.000

weight powder: 1.000



Fit

POW nuclear



Fit converged after 1 iteration

$\chi^2 = 1795636.09$
 $\chi_r^2 = 617.48$
 $R_F = 16.69$

2

Significant improvement in GOF.

Atoms:

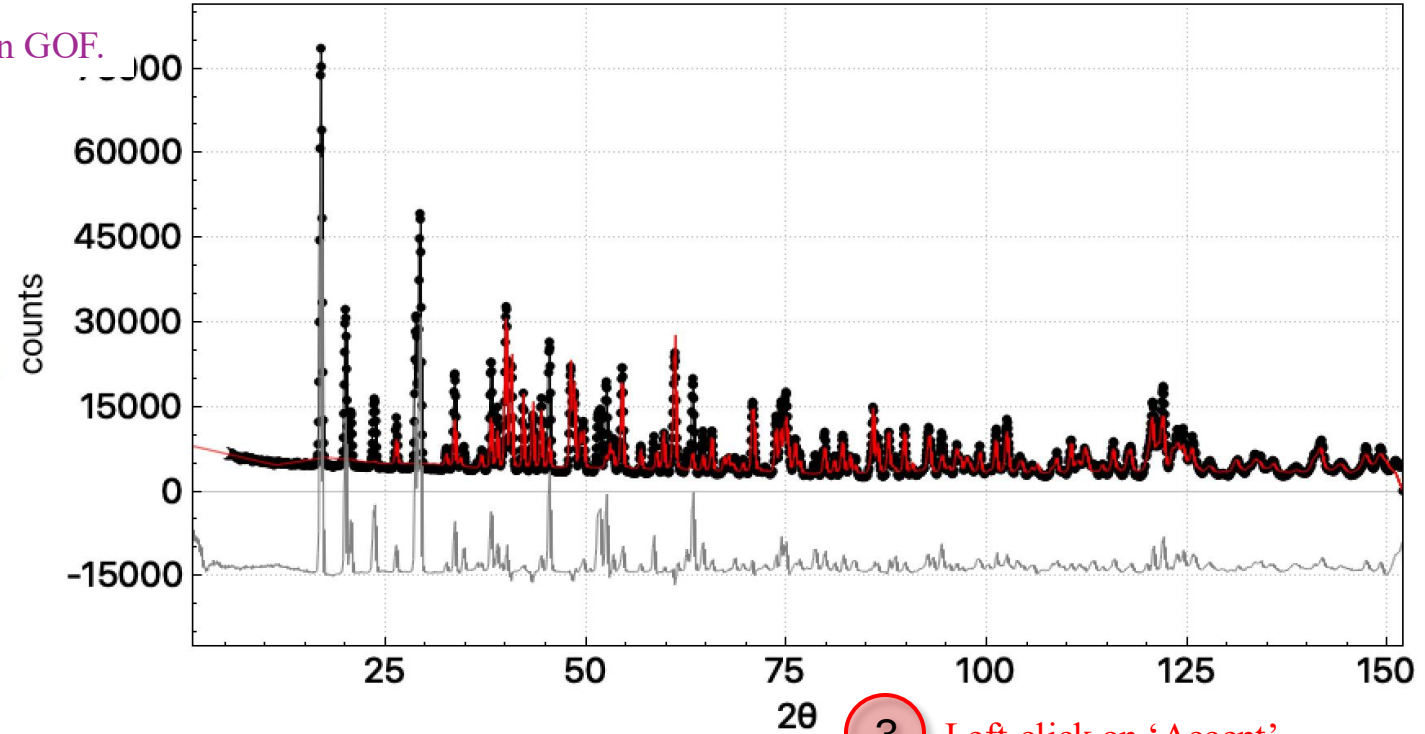
HO = [0.067(2) 0.250 0.482(2)]
B = 0.8(2), occ = 1.000
CR = [0.000 0.000 0.000]
B = 1.2(3), occ = 1.000
O = [0.304(2) 0.053(1) 0.185(2)]
B = 0.7(1), occ = 1.000
O = [0.460(2) 0.250 0.608(2)]
B = 0.5(2), occ = 1.000

POWDER PARAMETERS:

scale = 14.8(5)

Background points:

point 1 at $2\theta = 5.57$: $6.5(3)e+3$
point 2 at $2\theta = 11.39$: $4.6(2)e+3$
point 3 at $2\theta = 17.66$: $5.9(2)e+3$
point 4 at $2\theta = 24.5$: $4.9(2)e+3$
point 5 at $2\theta = 30.79$: $4.8(2)e+3$
point 6 at $2\theta = 36.04$: $4.1(2)e+3$
point 7 at $2\theta = 51.43$: $4.1(2)e+3$



3

Left-click on 'Accept'.

View results

Export results

View correlations

Export graph

Undo (2)

Accept

Save Rietveld fit of the Lattice only contribution to 4 K data

1

Left-click on the save icon

Save

Symmetry

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130
 $\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 HO	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
2 CR	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	Red	12	1.0
3 O	0.30427	0.05292	0.18465	0.736	1.000	<input checked="" type="checkbox"/>	Green	7	1.0
4 O	0.46025	0.25000	0.60812	0.505	1.000	<input checked="" type="checkbox"/>	Green	7	1.0

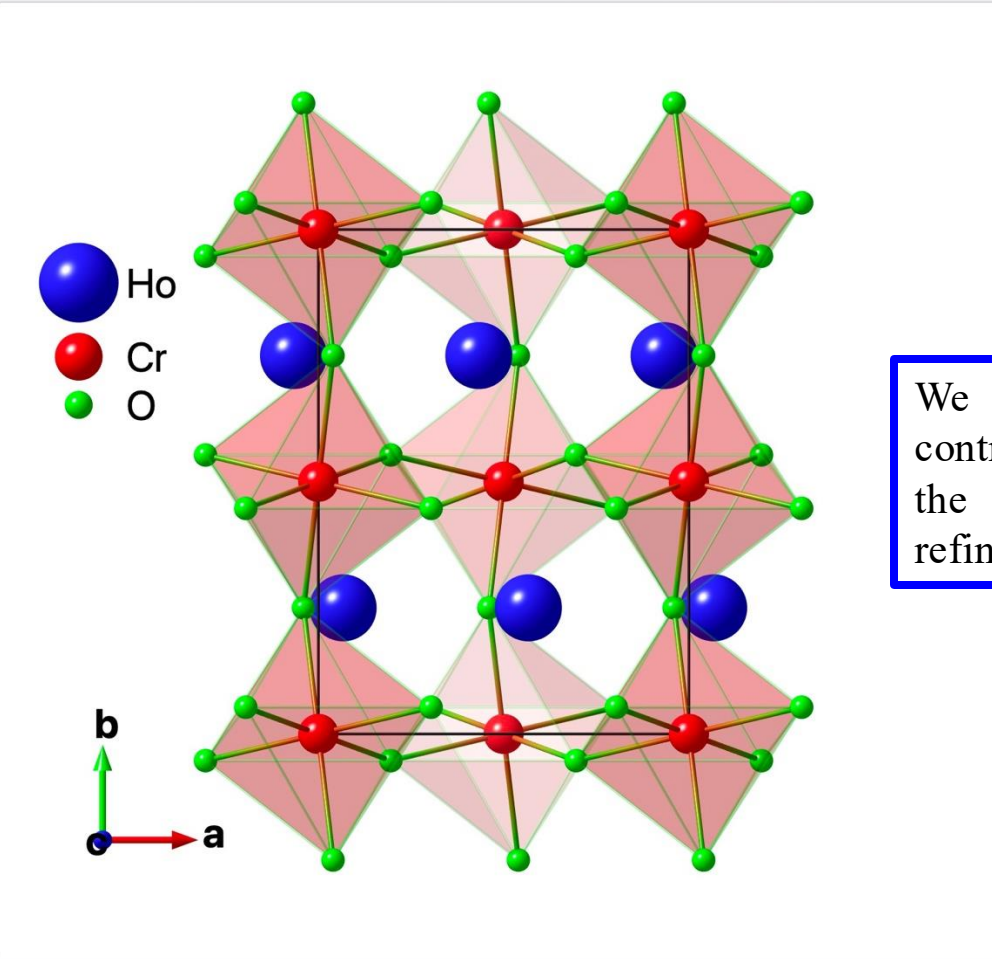
Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q \neq -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
------	----	----	----	----	----	----	--------

Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10 Domain: 1 Phase: 1

View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 0



We have refined only the lattice contribution so far, and now we can define the magnetic ion and proceed with the refinement of the magnetic structure.

Session 3

Refinement of magnetic structure

Activate (define) magnetic ions

Ion	Electronic configuration	S	L	J	Notes
Cr^{3+}	$3d^3$ ($t_{2g}^3, {}^4A_{2g}$)	$3/2$	≈ 0	$\approx 3/2$	3d ion; orbital moment quenched: → spin-only \mathbf{M}
Ho^{3+}	$4f^0$ (6I_8 term)	2	6	8	4f ion; strong spin-orbit: → total J form factor

Under the 'Atoms' section:

Depending on the type of magnetic contribution, simply add the prefix \mathbf{M} or \mathbf{J} to the magnetic ion, followed by the ionic state. In this case, only Cr^{3+} and Ho^{3+} are magnetic.

After this, update the structure by the keyboard shortcut [Ctrl+U] (on Windows) or [Cmd+U] (on Mac)

As soon as a Magnetic atom is defined under the 'Atoms' section, the 'Spins' section will be populated automatically with the Magnetic ions. By default, the Propagation vector is set to (0, 0, 0). Leave everything default for now. We will determine magnetic propagation vectors soon.

1

2

Mag2Pol

Symmetry

Space group: $Pnma$

Cell: a = 5.52910 b = 7.52660 c = 5.21130

$\alpha = 90.000^\circ \beta = 90.000^\circ \gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
JHO3	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
MCR3	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	Red	12	1.0
O	0.30427	0.05292	0.18465	0.736	1.000	<input checked="" type="checkbox"/>	Green	7	1.0
O	0.46025	0.25000	0.60812	0.505	1.000	<input checked="" type="checkbox"/>	Green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☐ -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
1 JHO3	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2 MCR3	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10 Domain: 1 Phase: 1

View along: custom Rotation axis: 0 0 1 direct Step (*): 5 Zoom: 22

Open the fit window 3

Legend: Ho (blue), Cr (red), O (green)

Coordinate system: a, b, c

Fix all the atomic parameters

1

Fit

Data **Atoms** Moments Domains Constraints Patterns Fit

	Atom	x	y	z	B	occ
A1	JHO3	0.06694	0.25000	0.48189	0.821	
A2	MCR3	0.00000	0.00000	0.00000	1.150	1.000
A3	O	0.30427	0.05292	0.18465	0.736	1.000
A4	O	0.46025	0.25000	0.60812	0.505	1.000

check all B
uncheck all B

2

At this stage, do not refine any of the atomic parameters. Fix them by unchecking one by one or by right-clicking on the column name and selecting 'uncheck all'

Scale factor and $\lambda/2$: 1.00000 0.00000

Extinction parameters:

☒ anisotropic ☐ ShelX-like model

x_{11} x_{12} x_{13}

0.00000 0.00000 0.00000

x_{22} x_{23}

0.00000 0.00000

x_{33}

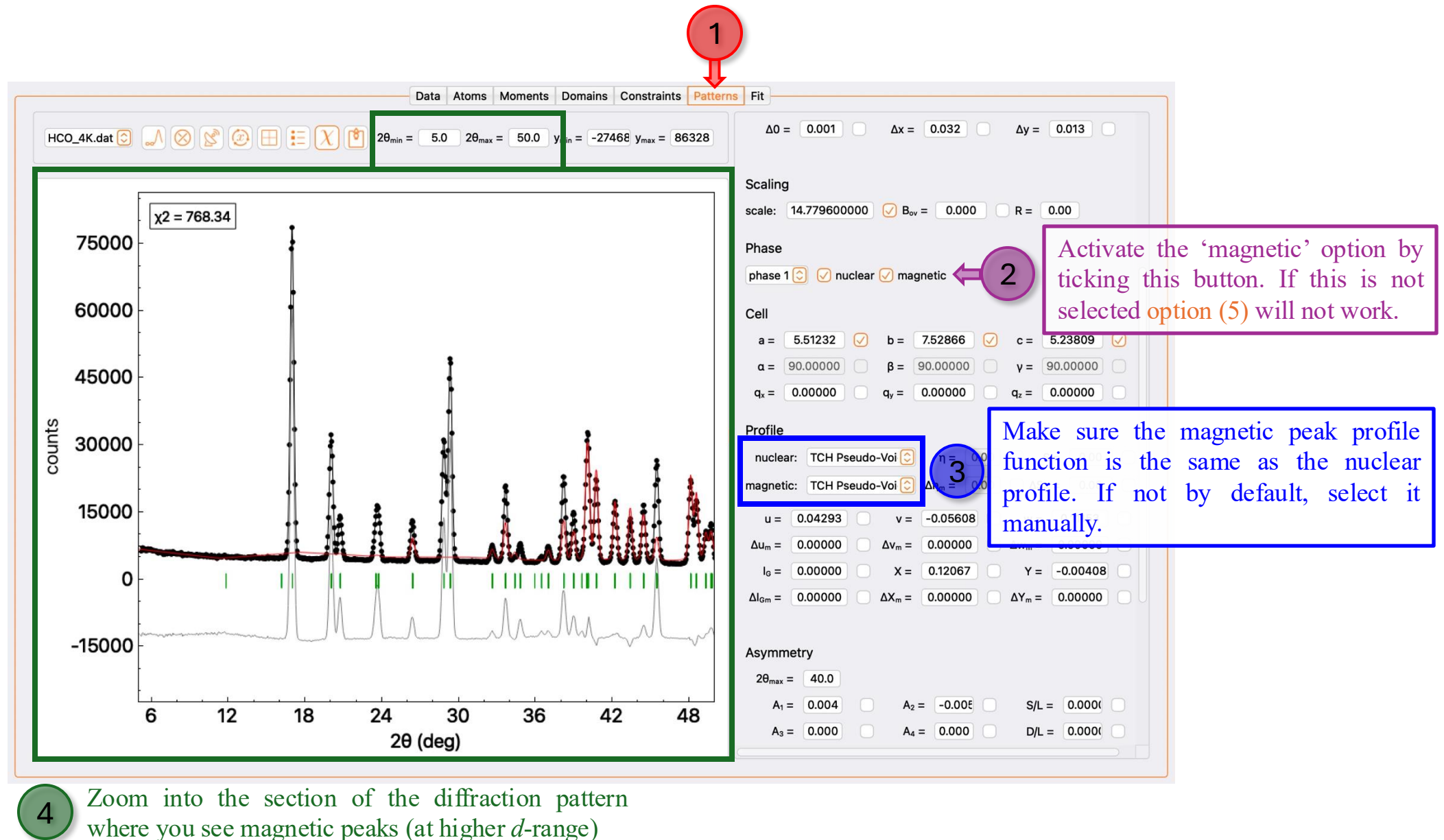
0.00000

☐ Becker-Coppens model

r_D : 0.000

θ_D : 0.000 Lorentzian

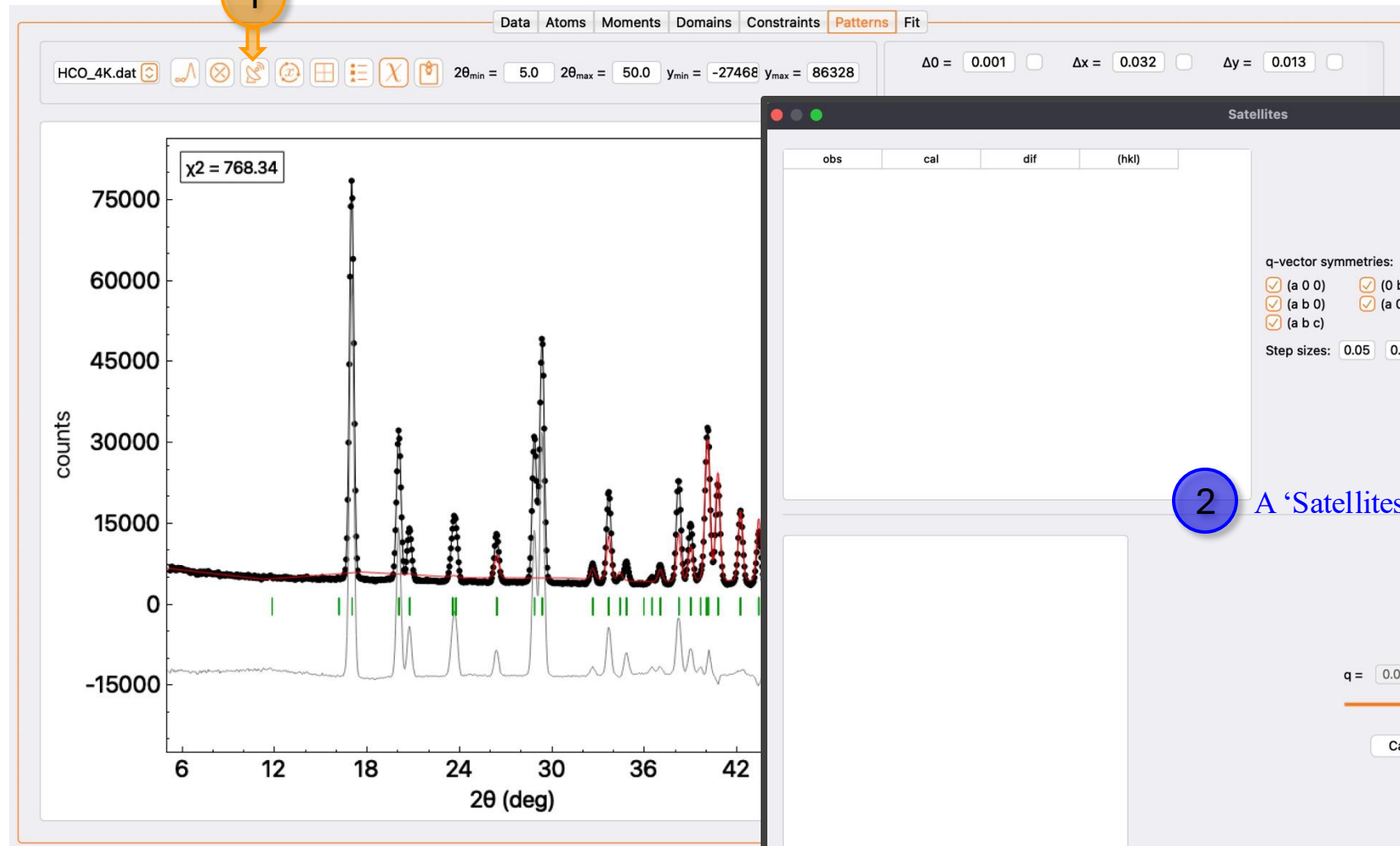
Determination of propagation vector



Determination of propagation vector

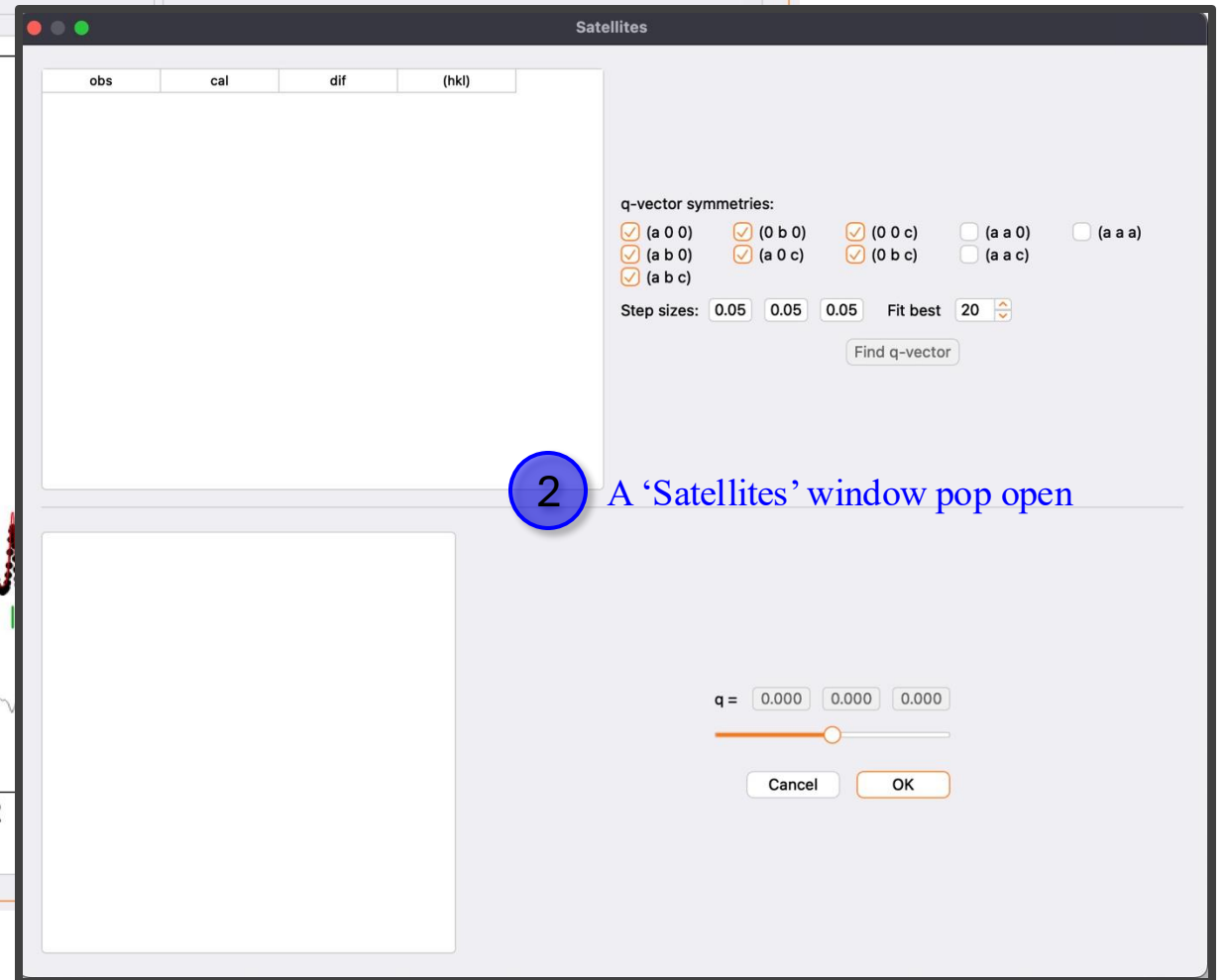
Click on the 'satellites' tab which
will open a new window

1

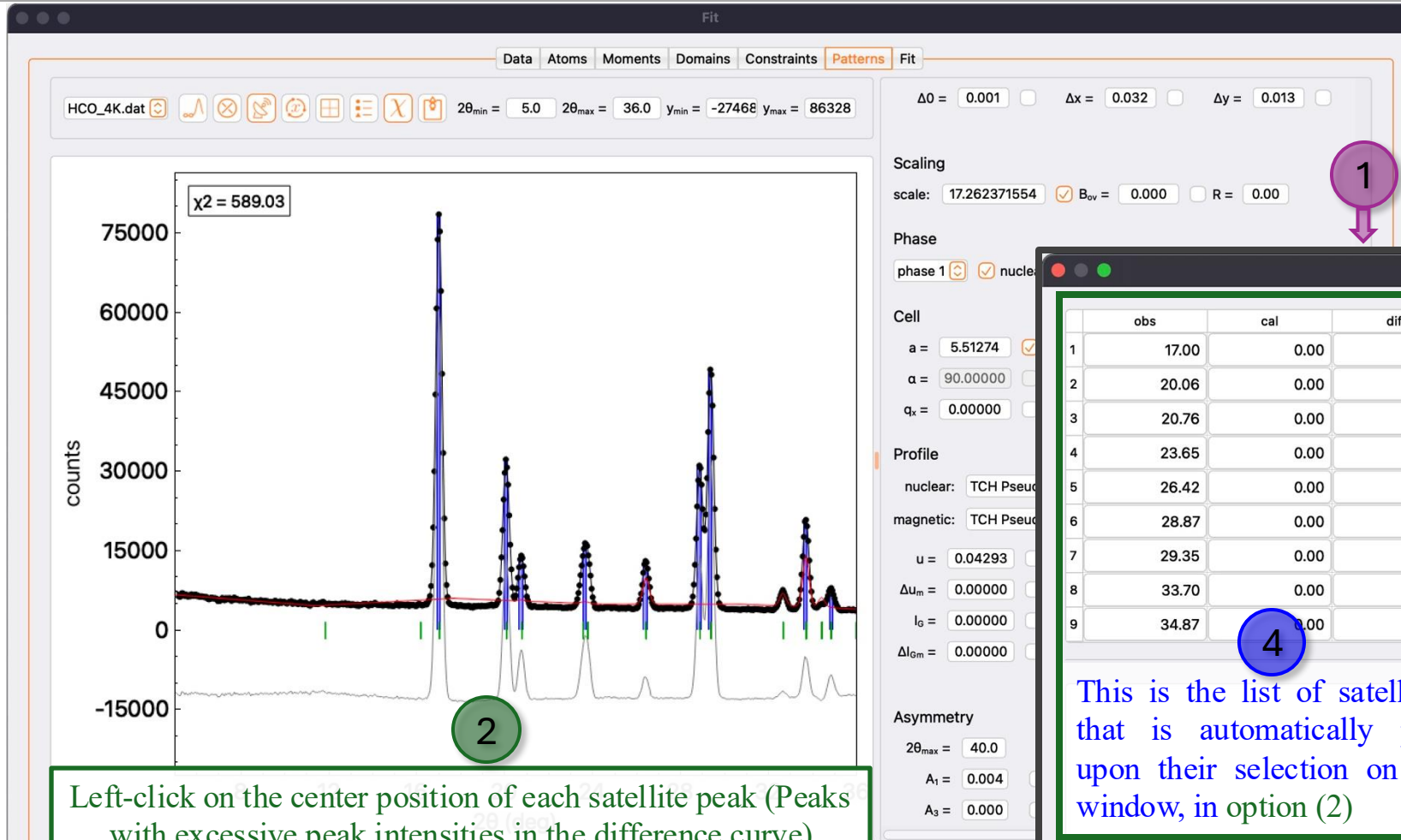


2

A 'Satellites' window pop open



Select satellite (magnetic) peaks and q-vector type



Move this 'Satellites' window away from the 'Fit' window so that the diffraction profile is accessible.

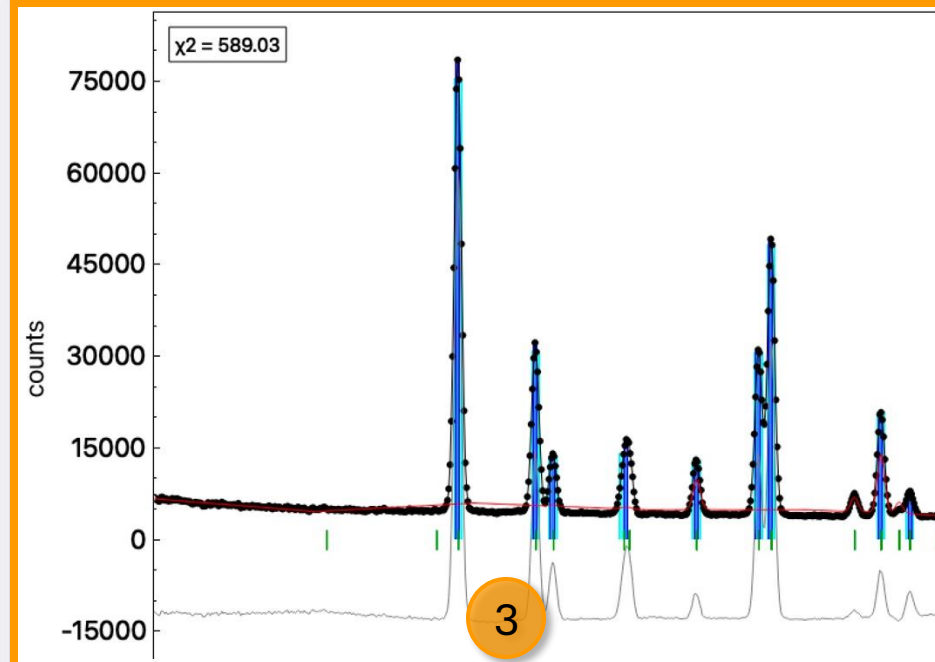
Left-click on the center position of each satellite peak (Peaks with excessive peak intensities in the difference curve)

This is the list of satellite peaks that is automatically populated upon their selection on the 'Fit' window, in option (2)

Select an appropriate q-vector type expected based on the lattice symmetry.

Each selected satellite peak will have a blue vertical column. The position of the blue vertical column can be altered using a mouse (left-click + hold + move) and can be removed by right-clicking on it

Select satellite (magnetic) peaks



The position indicated by Cyan columns here is the calculated peak position corresponding to the selected 'propagation vector' on the 'Satellites' window [section indicated in option (2) on this slide].

5 Note down all the propagation vectors that you wish to try out (typically is the case for incommensurate structures)

Scaling

scale: 17.26

Phase

phase 1

Cell

a = 5.512

α = 90.000

q_x = 0.000

Profile

nuclear: TO

magnetic: TO

u = 0.042

Δu_m = 0.000

I_0 = 0.000

ΔI_{0m} = 0.000

Asymmetry

$2\theta_{max}$ = 40

A_1 = 0.0

A_3 = 0.0

Satellites

	obs	cal	dif	(hkl)
1	17.00	17.04	-0.04	(0 0 1)+
2	20.06	20.09	-0.03	(1 1 0)+
3	20.76	20.78	-0.02	(0 1 1)+
4	23.65	23.56	0.09	(1 0 1)+
5	26.44	26.44	0.00	(1 1 1)+
6	28.87	28.88	-0.01	(1 2 0)+
7	29.35	29.38	-0.03	(0 2 1)+
8	33.70	33.71	-0.01	(1 2 1)+
9	34.87	34.84	0.03	(2 1 0)+

q-vector symmetries:

☒ (a 0 0) ☒ (0 b 0) ☒ (0 0 c) ☒ (a a 0) ☒ (a a a)

☐ (a b 0) ☐ (a 0 c) ☐ (0 b c) ☐ (a a c)

☐ (a b c)

Step sizes: 0.05 0.05 0.05 Fit best 20

1 → Find q-vector

Clicking on 'Find q-vector' will run the search routine.

propagation vector

	propagation vector	chisq
1	(0.000121(0.000593) 0.000 0.000)	0.01208
2	(0.196(2) 0.196 0.196)	0.11694
3	(0.047(4) 0.047 0.047)	0.21398
4	(0.000 0.000 0.302(6))	0.23324
5	(0.000 0.025(9) 0.000)	0.24532
6	(0.245(6) 0.000 0.000)	0.35079
7	(0.362(8) 0.362 0.000)	0.43633
8	(0.147(5) 0.147 0.147)	0.44015
9	(0.254(5) 0.254 0.254)	0.44852

2

4

q = 0.000 0.000 0.000

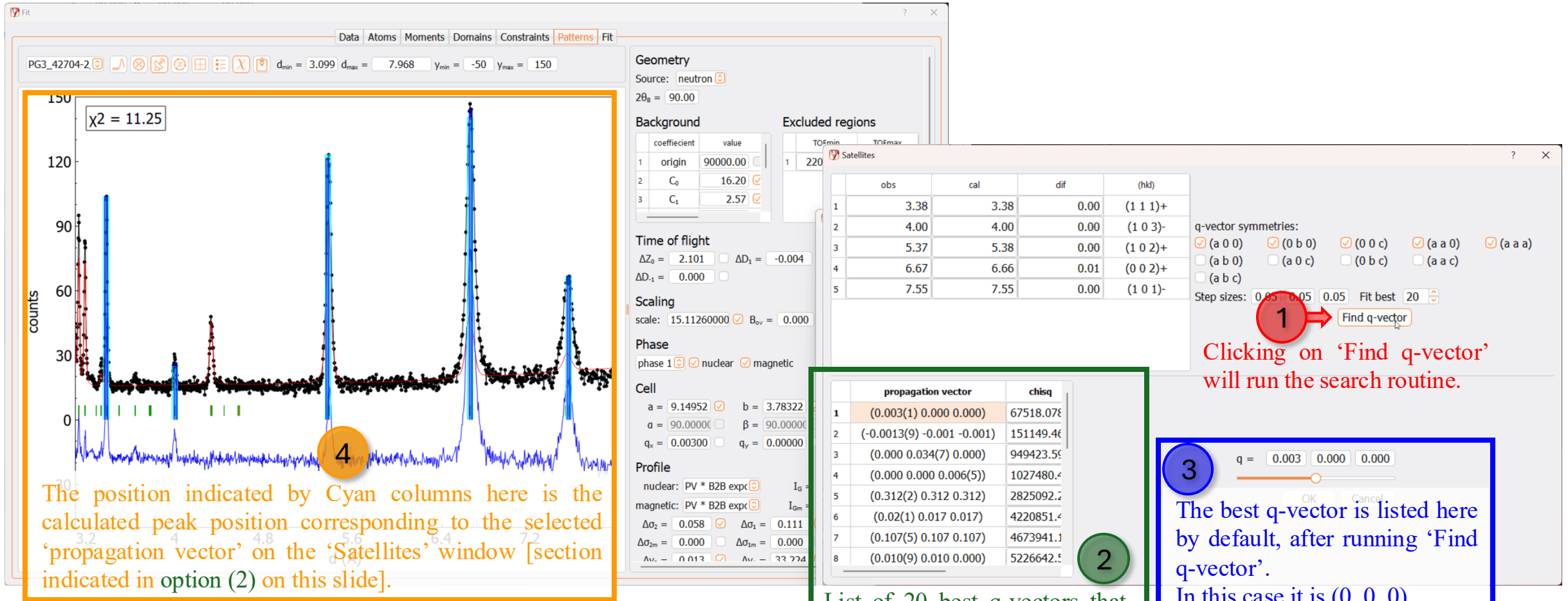
Cancel OK

The q-vector highlighted in (2) will appear here. We can modify these values and see how calculated satellite peak positions change, live on (3).

In this case, q-vector is (0, 0, 0)

List of up to 20 best q-vectors that fit the selected satellites, populated automatically after running 'Find q-vector'.

Step 5c: Run the q-vector search, and note down the best q-vectors



Clicking on 'Find q-vector' will run the search routine.

The best q-vector is listed here by default, after running 'Find q-vector'. In this case it is (0, 0, 0)

List of 20 best q-vectors that fit the selected satellites best, Populated automatically after running 'Find q-vector'.

Note down all the propagation vectors that you wish to try out. Close both the 'Satellites' and 'Fit' windows. And go back to the main window of Mag2Pol.

Refinement of magnetic structure using irreducible representations

Left-click on 'irreducible representations'

2

Space group: **Pnma** Cell: a = 5.52910 b = 7.52660 c = 5.21130
 $\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$
 Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

	Atom	x	y	z	B	occ	plot	color	R	S
1	JHO3	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
2	MCR3	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	Red	12	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☒ -q

	Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
1	JHO3	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	MCR3	0.000	0.000	0.000	0.000	0.000	0.000	0.000

1

4 If the propagation vector is other than (0,0,0), change it here. And update it by pressing the keyboard shortcut 'Ctrl + U' (Windows) or 'cmd + U' (on Mac). In the current case, it is the default value.

Irreducible representations

Symmetry Multiplication table Irreps Basis vectors

8 operators in little group with q = (0 0 0): Pnma (No. 62)

(1) x y z	1	
(2) -x+1/2 -y z+1/2	2(0,0,1/2)	1/4,0,z
(3) -x y+1/2 -z	2(0,1/2,0)	0,y,0
(4) x+1/2 -y+1/2 -z+1/2	2(1/2,0,0)	x,1/4,1/4
(5) -x -y -z	-1 0,0,0	
(6) x+1/2 y -z+1/2	a x,y,1/4	
(7) x -y+1/2 z	m x,1/4,z	
(8) -x+1/2 y+1/2 z+1/2	n(0,1/2,1/2)	1/4,y,z

Atomic positions:

Site 1

(1.1) JHO3 (0.06694 0.25 0.48189)
 (1.2) JHO3 (0.43306 0.75 0.98189)
 (1.3) JHO3 (0.93306 0.75 0.51811)
 (1.4) JHO3 (0.56694 0.25 0.01811)

Site 2

(2.1) MCR3 (0 0 0)
 (2.2) MCR3 (0.5 0 0.5)
 (2.3) MCR3 (0 0.5 0)
 (2.4) MCR3 (0.5 0.5 0.5)

Atoms within primitive unit cell:

Site 1

(1.1) JHO3 (0.06694 0.25 0.48189)
 (1.2) JHO3 (0.43306 0.75 0.98189)
 (1.3) JHO3 (0.93306 0.75 0.51811)
 (1.4) JHO3 (0.56694 0.25 0.01811)

Decomposition of the magnetic representation:

$$\Gamma = 1\Gamma_1 + 2\Gamma_2 + 2\Gamma_3 + 1\Gamma_4 + 1\Gamma_5 + 2\Gamma_6 + 2\Gamma_7 + 1\Gamma_8$$

Site 2

(2.1) MCR3 (0 0 0)
 (2.2) MCR3 (0.5 0 0.5)
 (2.3) MCR3 (0 0.5 0)
 (2.4) MCR3 (0.5 0.5 0.5)

Decomposition of the magnetic representation:

$$\Gamma = 3\Gamma_1 + 3\Gamma_3 + 3\Gamma_5 + 3\Gamma_7$$

For k = 0,
the little group = full space group
(all 8 symmetry operators)

Both Ho and Cr have 4
positions per unit cell.

These orbits define how the
spin components on each atom
are linked by symmetry

In the newly opened 'Irreducible
representations' window, the 'Symmetry'
tab provides details of symmetry analysis
and magnetic representation.

Ho can order according to any of
the 8 irreps, some with multiple
independent basis vectors.

Cr can order only via $\Gamma_1, \Gamma_3, \Gamma_5, \Gamma_7$
($\Gamma_2, \Gamma_4, \Gamma_6, \Gamma_8$ are not allowed for Cr).

Refinement of magnetic structure using irreducible representations

Space group: **Pnma** (No. 62)

Cell: a = 5.52910 b = 7.52660 c = 5.21130
 $\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

	Atom	x	y	z	B	occ	plot	color	R	S
1	JHO3	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
2	MCR3	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	Red	12	1.0
3	O	0.30427	0.05292	0.18465	0.736	1.000	<input checked="" type="checkbox"/>	Green	7	1.0
4	O	0.46025	0.25000	0.60812	0.505	1.000	<input checked="" type="checkbox"/>	Green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☒ -q

	Spin	Rx	Ry	Rz	lx	ly	lz	ϕ
1	JHO3	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	MCR3	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Irreducible representations

Symmetry Multiplication table Irreps Basis vectors

8 operators in little group with q = (0 0 0): Pnma (No. 62)

(1) x y z	1
(2) -x+1/2 -y z+1/2	2(0,0,1/2) 1/4,0,z
(3) -x y+1/2 -z	2(0,1/2,0) 0,y,0
(4) x+1/2 -y+1/2 -z+1/2	2(1/2,0,0) x,1/4,1/4
(5) -x -y -z	-1 0,0,0
(6) x+1/2 y -z+1/2	a x,y,1/4
(7) x -y+1/2 z	m x,1/4,z
(8) -x+1/2 y+1/2 z+1/2	n(0,1/2,1/2) 1/4,y,z

Atomic positions:

Site 1

(1.1) JHO3 (0.06694 0.25 0.48189)
 (1.2) JHO3 (0.43306 0.75 0.98189)
 (1.3) JHO3 (0.93306 0.75 0.51811)
 (1.4) JHO3 (0.56694 0.25 0.01811)

Site 2

(2.1) MCR3 (0 0 0)
 (2.2) MCR3 (0.5 0 0.5)
 (2.3) MCR3 (0 0.5 0)
 (2.4) MCR3 (0.5 0.5 0.5)

Atoms within primitive unit cell:

Site 1

(1.1) JHO3 (0.06694 0.25 0.48189)
 (1.2) JHO3 (0.43306 0.75 0.98189)
 (1.3) JHO3 (0.93306 0.75 0.51811)
 (1.4) JHO3 (0.56694 0.25 0.01811)

Decomposition of the magnetic representation:

$$\Gamma = 1\Gamma_1 + 2\Gamma_2 + 2\Gamma_3 + 1\Gamma_4 + 1\Gamma_5 + 2\Gamma_6 + 2\Gamma_7 + 1\Gamma_8$$

Site 2

(2.1) MCR3 (0 0 0)
 (2.2) MCR3 (0.5 0 0.5)
 (2.3) MCR3 (0 0.5 0)
 (2.4) MCR3 (0.5 0.5 0.5)

Decomposition of the magnetic representation:

$$\Gamma = 3\Gamma_1 + 3\Gamma_3 + 3\Gamma_5 + 3\Gamma_7$$

Practical refinement strategy

1. Choose irreps allowed for both Ho(4c) and Cr(4a)

Only $\Gamma_1, \Gamma_3, \Gamma_5, \Gamma_7$ appear in the Cr decomposition \rightarrow

These are the only viable magnetic irreps for the whole structure.

2. Refine each candidate irrep

Load the basis vectors for Ho(4c) and Cr(4a) in Mag2Pol.

Refine the basis-vector amplitudes and compare fit quality.

3. Select the irrep that fits best

The irrep giving the best agreement with the magnetic Bragg intensities is the common irrep for both Ho and Cr.

4. (Later) Convert this irrep solution into the corresponding MSG to impose the same ordering via symmetry constraints.

On the 'Irreducible representation' window select an irrep (Γ_n) for the refinement

The 'Symmetry' tab provides details of symmetry analysis and magnetic representation

1

Irreducible representations

Symmetry Multiplication table Irreps Basis vectors

Γ_1 Γ_2 Γ_3 Γ_4 Γ_5 Γ_6 Γ_7 Γ_8

(8) $-x+1/2$ $y+1/2$ $z+1/2$ $n(0,1/2,1/2)$ $1/4,y,z$

Atomic positions:

Site 1

(1.1) JHO3 (0.06694 0.25 0.48189)
(1.2) JHO3 (0.43306 0.75 0.98189)
(1.3) JHO3 (0.93306 0.75 0.51811)
(1.4) JHO3 (0.56694 0.25 0.01811)

Site 2

(2.1) MCR3 (0 0 0)
(2.2) MCR3 (0.5 0 0.5)
(2.3) MCR3 (0 0.5 0)
(2.4) MCR3 (0.5 0.5 0.5)

Atoms within primitive unit cell:

Site 1

(1.1) JHO3 (0.06694 0.25 0.48189)
(1.2) JHO3 (0.43306 0.75 0.98189)
(1.3) JHO3 (0.93306 0.75 0.51811)
(1.4) JHO3 (0.56694 0.25 0.01811)

Decomposition of the magnetic representation:

$\Gamma = 1\Gamma_1 + 2\Gamma_2 + 2\Gamma_3 + 1\Gamma_4 + 1\Gamma_5 + 2\Gamma_6 + 2\Gamma_7 + 1\Gamma_8$

Site 2

(2.1) MCR3 (0 0 0)
(2.2) MCR3 (0.5 0 0.5)
(2.3) MCR3 (0 0.5 0)
(2.4) MCR3 (0.5 0.5 0.5)

Decomposition of the magnetic representation:

$\Gamma = 3\Gamma_1 + 3\Gamma_3 + 3\Gamma_5 + 3\Gamma_7$

The 'Basis vectors' tab provides details of the Basis vectors of all magnetic sites for an irrep.

Choose an irrep to see the Basis vector details for each magnetic ion

2

3

Symmetry Multiplication table Irreps Basis vectors

Basis vectors of Γ_1

Display of basis vectors: normalized

Site 1 Site 2

	(0 0 0)	(1/2 0 1/2)	(0 1/2 0)	(1/2 1/2 1/2)
ψ_1	1 0 0	-1 0 0	-1 0 0	1 0 0
ψ_2	0 1 0	0 -1 0	0 1 0	0 -1 0
ψ_3	0 0 1	0 0 1	0 0 -1	0 0 -1

The 'Irreps' tab lists all irreps.

Right-click on one of the irreps symbols (Γ_1 in this example), and consequently click on 'Use Γ_1 '

Go back to the main window of Mag2Pol

4

Symmetry Multiplication table Irreps Basis vectors

	1	21z	21y	21x	-1	az	my	nx
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1	-1	-1
Γ_3	1	1	-1	-1	1	1	-1	-1
Γ_4	1	1	-1	-1	-1	-1	1	1
Γ_5	1	-1	1	-1	1	-1	1	-1
Γ_6	1	-1	1	-1	-1	1	-1	1
Γ_7	1	-1	-1	1	1	-1	-1	1
Γ_8	1	-1	-1	1	-1	1	1	-1

Use Γ_1

62

Save the project with an appropriate name that indicates the irrep

2 Save as 'HCO_4K_Mag-G1.xml'

Mag2Pol

Symmetry

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130

$\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

	Atom	x	y	z	B	occ	plot	color	R	S
1	JHO3	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	blue	20	1.0
2	MCR3	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	red	12	1.0
3	O	0.30427	0.05292	0.18465	0.736	1.000	<input checked="" type="checkbox"/>	green	7	1.0
4	O									

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q \neq -q

	Spin	C1	C2	C3	C4	C5	C6	ϕ
1	JHO3	8.000	0.000	0.000	0.000	0.000	0.000	0.000
2	MCR3	2.000	2.000	2.000	0.000	0.000	0.000	0.000

1 Set a reasonable value for the coefficients of the allowed number of basis functions. And update it by pressing the keyboard shortcut 'Ctrl + U' (Windows) or 'cmd + U' (on Mac).

3 Right-click to open refinement window

Fix all atomic parameters

On the 'Fit' window, under the 'Atoms' tab, make sure all the atomic parameters are fixed.



Software interface showing the 'Fit' window, specifically the 'Atoms' tab. The interface includes a table of atomic parameters and various adjustment options.

	Atom	x	y	z	B	occ
A1	JHO3	0.06694	0.25000	0.48189	0.821	1.000
A2	MCR3	0.00000	0.00000	0.00000	1.150	1.000
A3	O	0.30427	0.05292	0.18465	0.736	1.000
A4	O	0.46025	0.25000	0.60812	0.505	1.000

Scale factor and $\lambda/2$: 1.00000 ☐ 0.00000 ☐

Extinction parameters:

☒ anisotropic ☐ ShelX-like model

x_{11} x_{12} x_{13}

0.00000 ☐ 0.00000 ☐ 0.00000 ☐

x_{22} x_{23}

0.00000 ☐ 0.00000 ☐

x_{33}

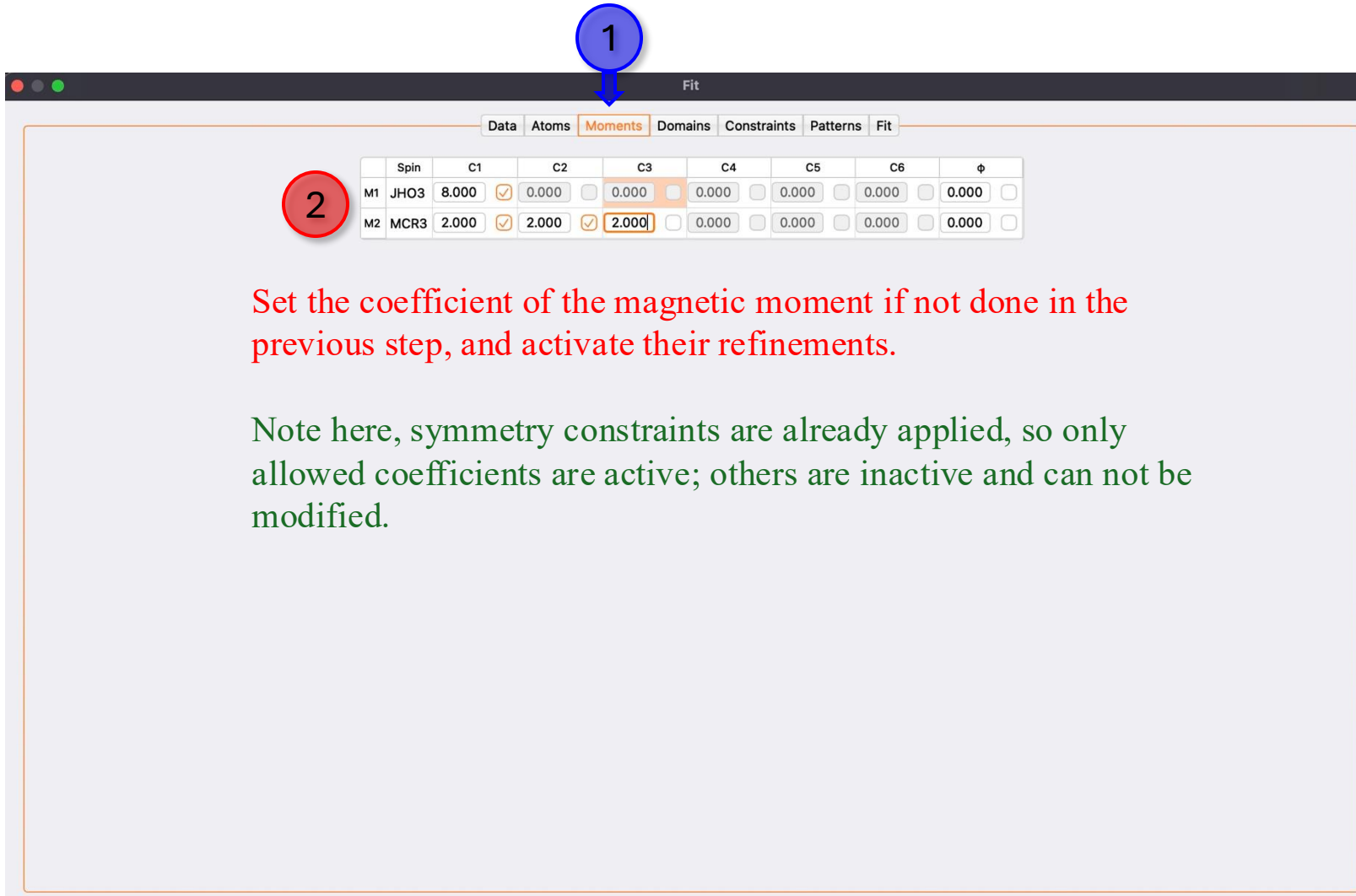
0.00000 ☐

☐ Becker-Coppens model

r_D : 0.000 ☐

θ_D : 0.000 ☐ Lorentzian

Activate refinement of magnetic moments



1

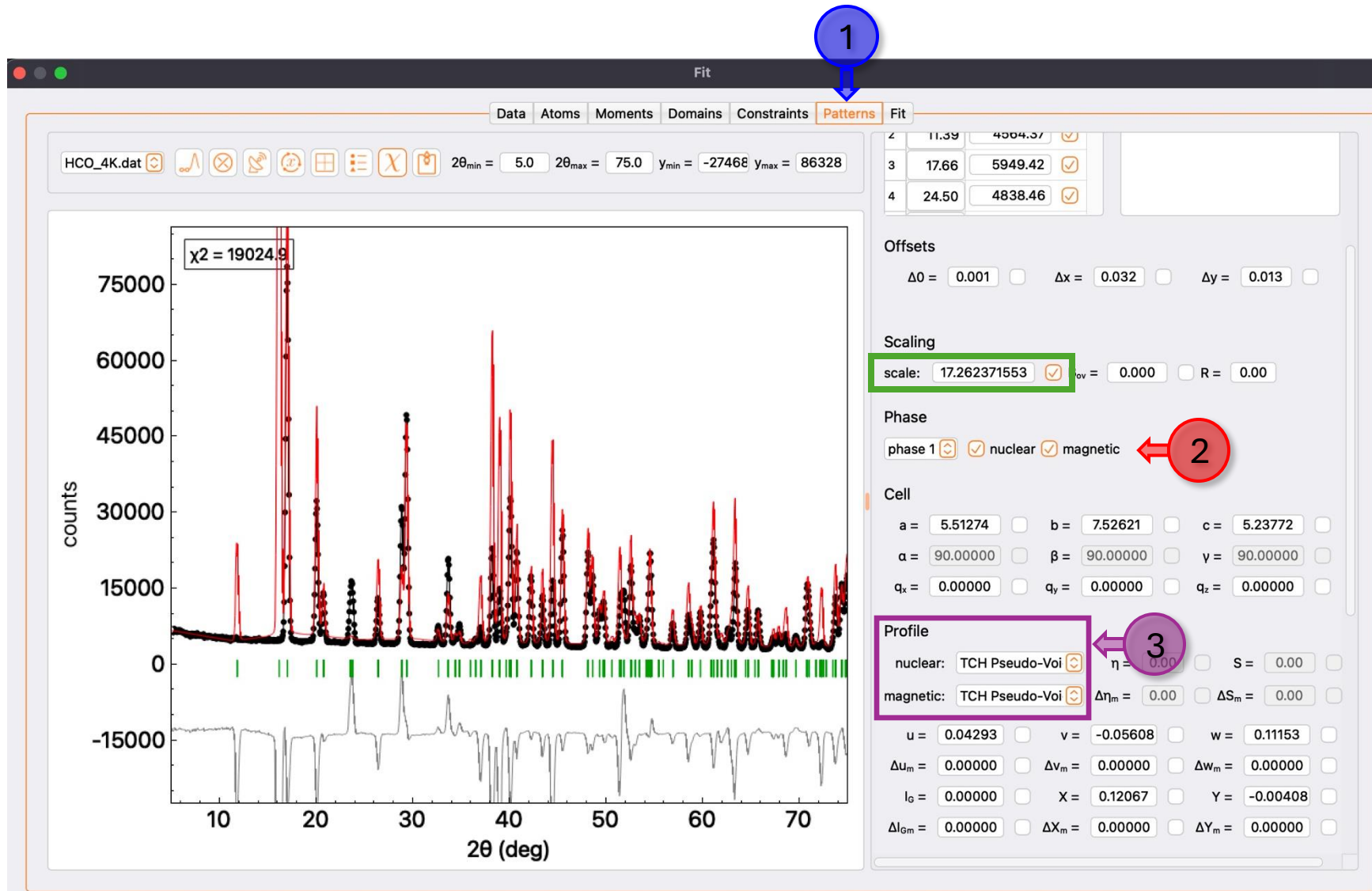
2

	Spin	C1	C2	C3	C4	C5	C6	ϕ
M1	JHO3	8.000 <input checked="" type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>
M2	MCR3	2.000 <input checked="" type="checkbox"/>	2.000 <input checked="" type="checkbox"/>	2.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>

Set the coefficient of the magnetic moment if not done in the previous step, and activate their refinements.

Note here, symmetry constraints are already applied, so only allowed coefficients are active; others are inactive and can not be modified.

Fix all parameters but the scale



Fix all parameters except the 'scale' parameter.

Also, make sure both 'nuclear' and 'magnetic' phases are active

Nuclear and magnetic phases should have the same Peak functions

Run the Rietveld fit

1

2

3

5

4

The fitting of magnetic peaks is rather poor with the irrep Γ_1 . We should test other irreps.

After accepting the refinement results on the 'Fit' window (keep this window open), go to the main window and click on the save button, which appends the previously saved project, **HCO_4K_Mag-G1.xml**

iteration 6
 $\chi^2 = 305.817$, $(\Delta / \epsilon\sigma)_{\max}$ (M2C2) = 1.01526
iteration 7
 $\chi^2 = 305.817$, $(\Delta / \epsilon\sigma)_{\max}$ (M2C2) = -0.272234

Fit converged after 7 iterations

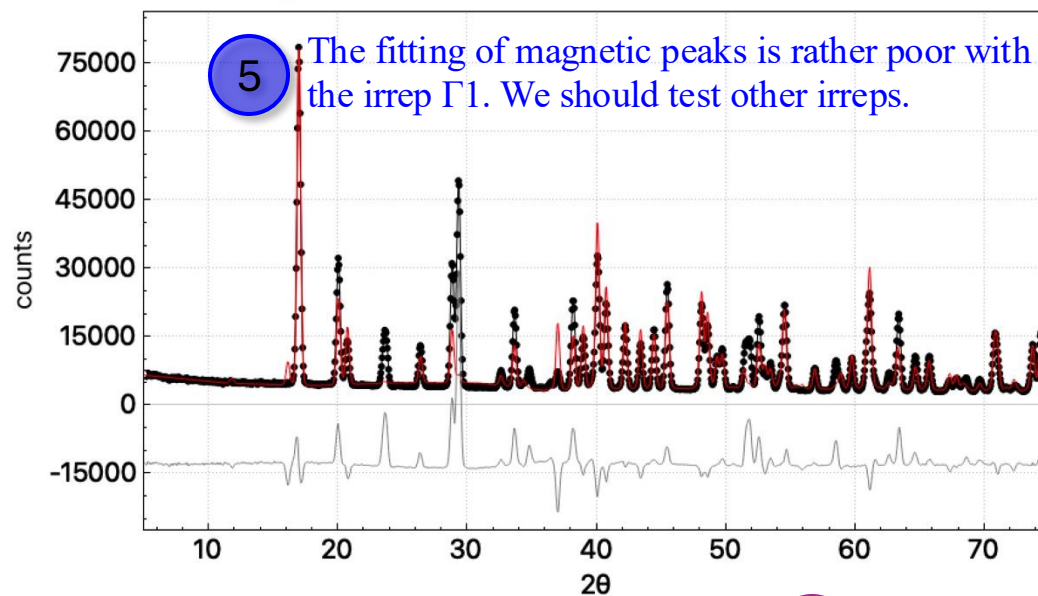
$\chi^2 = 892374.09$
 $\chi^2 = 305.82$
 $R_F = 9.95$ $R_{F,mag} = 18.58$

Atoms:

JHO3 = [0.067 0.250 0.482]
B = 0.821, occ = 1.000
MCR3 = [0.000 0.000 0.000]
B = 1.150, occ = 1.000
O = [0.304 0.053 0.185]
B = 0.736, occ = 1.000
O = [0.460 0.250 0.608]
B = 0.505, occ = 1.000

Magnetic moments:

JHO3: $C_1 = 3.76(6)$
 $\phi = 0.000$
 $|\mu| = 3.76(6) \mu_B$
MCR3: $C_1 = 2.26(7)$ $C_2 = -2.12(5)$ $C_3 = 0.5(1)$
 $\phi = 0.000$
 $|\mu| = 3.14(6) \mu_B$



View results

Export results

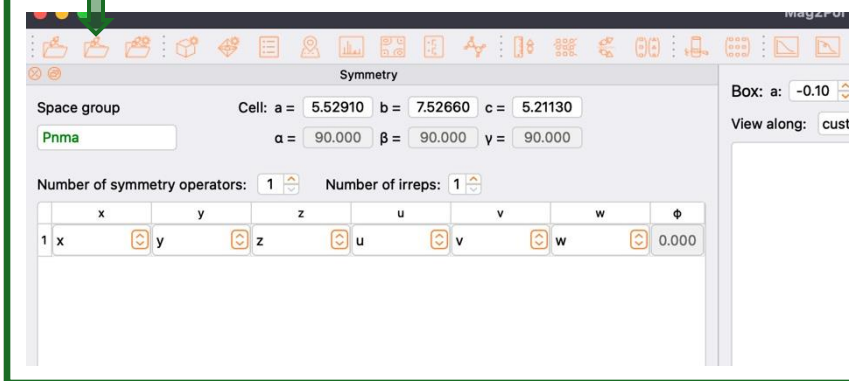
View correlations

Export graph

Undo (3)

Accept

Once the convergence is reached, accept the fit results by clicking this button.



Test all irreps by running built-in *Fit macros*

We can test each irrep one by one by selecting them in the main window of the Mag2Pol. But this can also be done much faster using the built-in fit macro 'Test irreps'.

The irrep 3 (Γ_3) looks best and is applied to the model at the end of the test. At this stage, we can refine Cell and profile parameters and atomic parameters in steps, which can further improve the refinements.

The screenshot shows the 'Fit' window of the Mag2Pol software. The 'Fit' tab is selected, showing a list of fit macros. A blue arrow labeled '1' points to the 'Test irreps' macro. A red arrow labeled '2' points to the 'Run' button (a yellow triangle). A green arrow labeled '3' points to the 'SUMMARY' table. A purple arrow labeled '4' points to the 'Accept' button.

1 Select the macro 'Test irreps'

2 Click on this arrow to run the macro

3

4

Fit

Data Atoms Moments Domains Constraints Patterns **Fit**

weight SNP: 0.000
weight intensities: 0.000
weight powder: 1.000

SNP
INT POW

Test irreps
POW nuclear
INT B --> Baniso
Test irreps
Fit macro 4
Fit macro 5
Fit macro 6
Fit macro 7
Fit macro 8
Fit macro 9
Fit macro 10

Profile:
u = 0.043 v = -0.056 w = 0.112 I₀ = 0.000
X = 0.121 Y = -0.004
A₁ = 0.004 A₂ = -0.005 A₃ = 0.000 A₄ = 0.000
S/L = 0.000 D/L = 0.000
P₁ = 0.000 P₂ = 0.000
 $\Delta u_m = 0.000 \Delta v_m = 0.000 \Delta w_m = 0.000 \Delta I_{0m} = 0.000$
 $\Delta X_m = 0.000 \Delta Y_m = 0.000$
 $\Delta A_{1m} = 0.000 \Delta A_{2m} = 0.000 \Delta A_{3m} = 0.000 \Delta A_{4m} = 0.000$
 $\Delta S/L_m = 0.000 \Delta D/L_m = 0.000$
 $\Delta P_{1m} = 0.000 \Delta P_{2m} = 0.000$

Lattice:
a = 5.513 b = 7.526 c = 5.238
 $\alpha = 90.000 \beta = 90.000 \gamma = 90.000$
Volume = 217.313
q_x = 0.000 q_y = 0.000 q_z = 0.000
B_{ov} = 0.000

SUMMARY
 $\chi^2 = 85.60$, irrep 3
 $\chi^2 = 304.05$, irrep 1
 $\chi^2 = 444.64$, irrep 7
 $\chi^2 = 520.29$, irrep 5
 $\chi^2 = 536.23$, irrep 2
 $\chi^2 = 562.70$, irrep 8
 $\chi^2 = 579.27$, irrep 6
 $\chi^2 = 613.82$, irrep 4

counts

75000
60000
45000
30000
15000
0
-15000

10 20 30 40 50 60 70

2 θ

View results Export results View correlations Export graph Undo (4) **Accept**

Save the project with an appropriate name that indicates the new irrep used

1 Save as 'HCO_4K_Mag-G7.xml'

3 Back to the fit-window

2 Click this to change the perspective of the structure

The screenshot displays the Mag2Pol software interface. The left panel contains three sections: Symmetry, Atoms, and Spins. The Symmetry section shows the space group 'Pnma' and unit cell parameters. The Atoms section lists four sites: JHO3, MCR3, O, and O. The Spins section shows the propagation vector and spin parameters. The right panel shows a 3D visualization of the crystal structure with magnetic moments represented by blue arrows. A legend identifies the atoms: Ho (blue sphere), Cr (red sphere), and O (green sphere). A coordinate system (a, b, c) is shown at the bottom left.

Symmetry

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130

$\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 JHO3	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	blue	20	1.0
2 MCR3	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	red	12	1.0
3 O	0.30427	0.05292	0.18465	0.736	1.000	<input checked="" type="checkbox"/>	green	7	1.0
4 O	0.46025	0.25000	0.60812	0.505	1.000	<input checked="" type="checkbox"/>	green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☒ -q

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 JHO3	5.667	2.338	0.000	0.000	0.000	0.000	0.000
2 MCR3	-0.083	2.084	-0.307	0.000	0.000	0.000	0.000

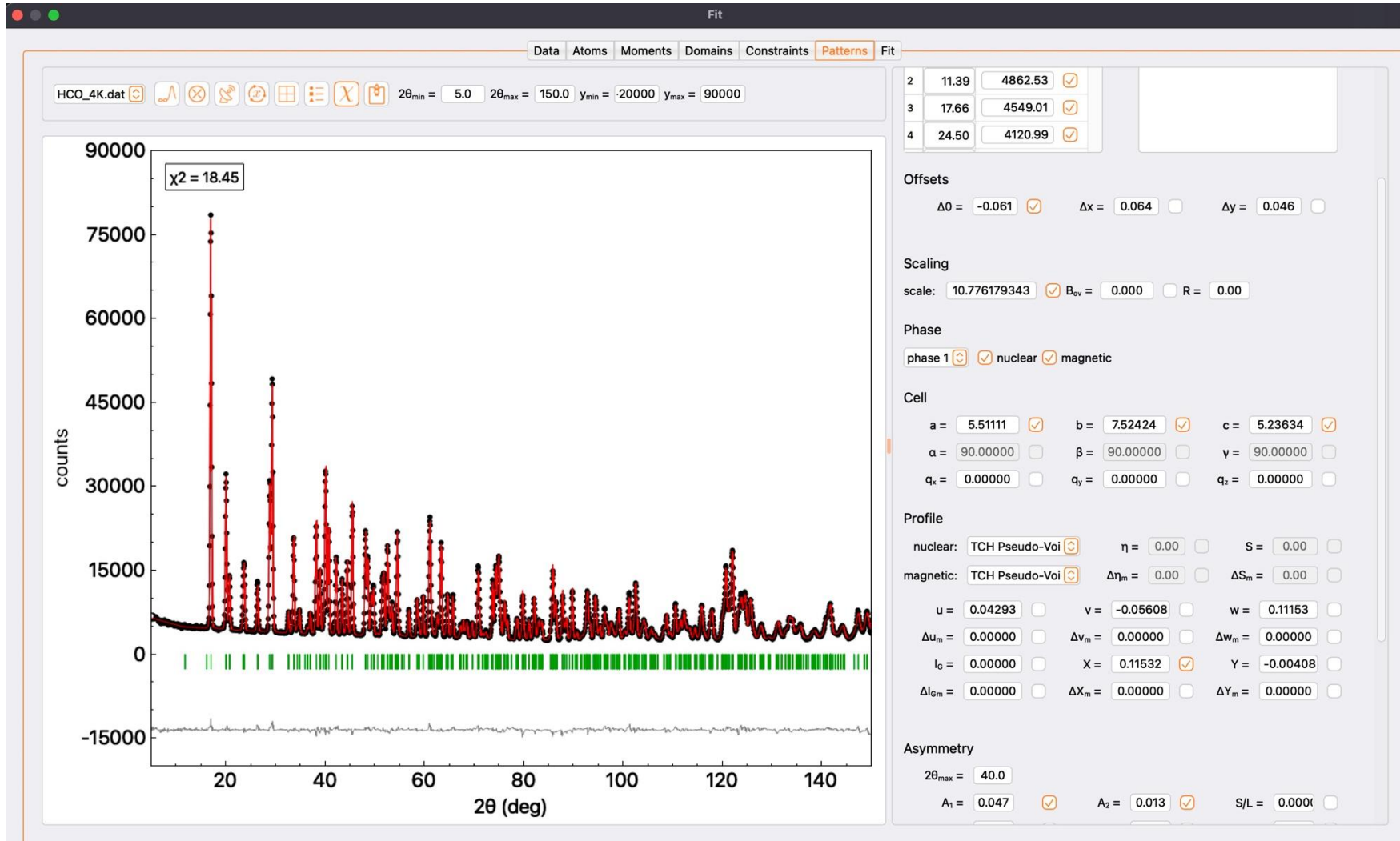
Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10

View along: custom Rotation axis: 0 0 1 direct Step (°): 5

Legend: Ho (blue sphere), Cr (red sphere), O (green sphere)

Coordinate system: a (red arrow), b (green arrow), c (blue arrow)

In steps activate and refine all necessary parameters



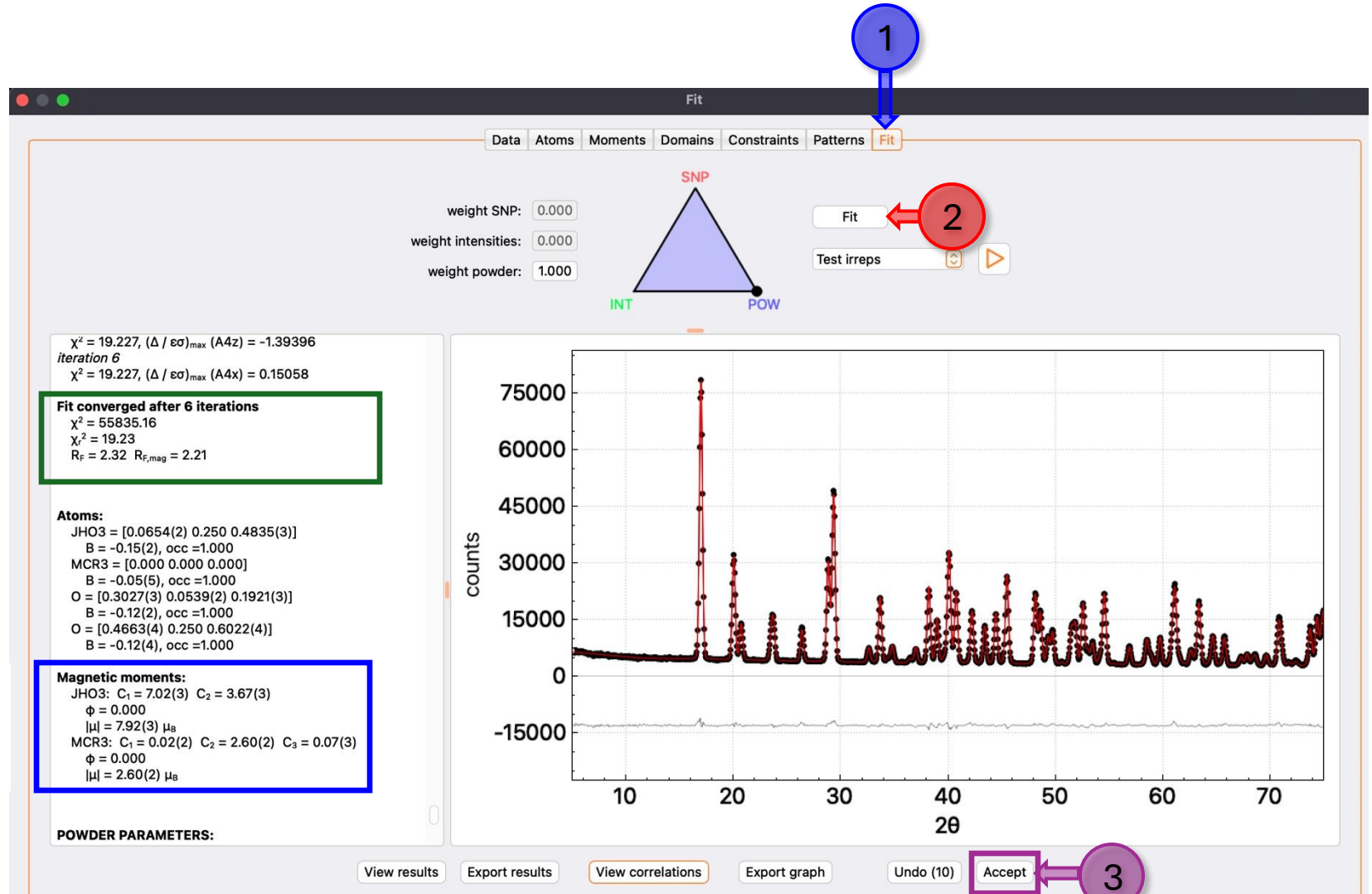
Activate refinement of different parameters in steps. Run the fit during each step.

1. BG
2. Offsets and Asymmetry parameters
3. Profile parameters
4. Atomic positions
5. Thermal parameters (B)

Final refinement results for irrep 3

Magnetic R-factor, $R_{F,\text{mag}}$ is a good indicator to pick the best irrep (along with the visual fit)

Note that coefficients C_1 and C_3 are quite small and can be fixed to zero during the final refinements



After accepting the refinement results here, do not forget to save the project from the main window!

It is recommended to save versioned copies of the project often. If the program crashes, it is easy to start over from the saved versions.

Inspecting full refinement results

Click this icon to open the 'Sample info' window, which contains detailed information on the refined Crystal structure, Magnetic structure, and Fit results. Also indicates the path and name of the current project file.

1

2

'Sample info' window, with the 'Crystal Structure' tab active.

Sample info (/Users/dinkleberry/Library/CloudStorage/OneDrive-Personal/Research/Workshops/2025/Neutron diffraction/Da...)

Crystal structure | Magnetic structure | Absorption | Fit results

Chemical formula: HoCrO_3 ($Z = 4$, $M = 264.923$ g/mol)

Space group: Pnma

Real lattice: $a = 5.5291 \text{ \AA}$ $b = 7.5266 \text{ \AA}$ $c = 5.2113 \text{ \AA}$ Reciprocal lattice: $a^* = 0.180861 \text{ \AA}^{-1}$ $b^* = 0.132862 \text{ \AA}^{-1}$ $c^* = 0.191891 \text{ \AA}^{-1}$

$\alpha = 90^\circ$ $\beta = 90^\circ$ $\gamma = 90^\circ$ $\alpha^* = 90^\circ$ $\beta^* = 90^\circ$ $\gamma^* = 90^\circ$

$V = 216.87 \text{ \AA}^3$ $V^* = 0.00461106 \text{ \AA}^{-3}$

List of atoms

	Atom	Wyckoff site	x	y	z
1.1	JHO3	4c	0.06539	1/4	0.48336
1.2	JHO3	4c	0.43461	3/4	0.98336
1.3	JHO3	4c	0.93461	3/4	0.51664
1.4	JHO3	4c	0.56539	1/4	0.01664
2.1	MCR3	4a	0	0	0
2.2	MCR3	4a	1/2	0	1/2
2.3	MCR3	4a	0	1/2	0

Inspecting full refinement results

‘Magnetic structure’ tab information of the magnetic model used in the last fit.

1

Sample info (/Users/dinkleberry/Library/CloudStorage/OneDrive-Personal/Research/Workshops/2025/Neutron diffraction/Day1/D...)

Crystal structure **Magnetic structure** Absorption Fit results

Magnetic symmetry: irrep Γ_3

Propagation vector: $q = (0\ 0\ 0)$

List of spins for domain **1**

	Spin	x	y	z	Mx	My	Mz	Sx	Sy	Sz
1.1	JHO3	0.06539	0.25	0.48336	7.01	0	3.65	7.01	0	3.65
1.2	JHO3	0.43461	0.75	0.98336	-7.01	0	3.65	-7.01	0	3.65
1.3	JHO3	0.93461	0.75	0.51664	7.01	0	3.65	7.01	0	3.65
1.4	JHO3	0.56539	0.25	0.01664	-7.01	0	3.65	-7.01	0	3.65
2.1	MCR3	0	0	0	0	2.61	0	0	2.61	0
2.2	MCR3	0.5	0	0.5	0	-2.61	0	0	-2.61	0
2.3	MCR3	0	0.5	0	0	-2.61	0	0	-2.61	0
2.4	MCR3	0.5	0.5	0.5	0	2.61	0	0	2.61	0

Inspecting full refinement results

Sample info (/Users/dinkleberry/Library/CloudStorage/OneDrive-Personal/Research/Workshops/2025/Neutron diffraction/Day1/Data/HoCrO3/NPD/HCO_4K_Magn_G...)

Crystal structure Magnetic structure Absorption **Fit results**

Fit converged after 4 iterations
 $\chi^2 = 54363.08$
 $\chi_r^2 = 18.74$
 $R_F = 2.35$ $R_{F,mag} = 2.23$

Atoms:
JHO3 = [0.0654(2) 0.250 0.4834(3)]
B = -0.13(2), occ = 1.000
MCR3 = [0.000 0.000 0.000]
B = -0.07(5), occ = 1.000
O = [0.3028(3) 0.0540(2) 0.1918(3)]
B = -0.10(2), occ = 1.000
O = [0.4665(4) 0.250 0.6020(4)]
B = -0.09(3), occ = 1.000

Magnetic moments:
JHO3: $C_1 = 7.01(3)$ $C_2 = 3.65(3)$
 $\phi = 0.000$
 $|\mu| = 7.91(3) \mu_B$
MCR3: $C_2 = 2.61(2)$
 $\phi = 0.000$
 $|\mu| = 2.61(2) \mu_B$

POWDER PARAMETERS:
scale = 10.80(7)

Background points:
point 1 at $2\theta = 5.57$: 6.33(5)e+3
point 2 at $2\theta = 11.39$: 4.86(4)e+3
point 3 at $2\theta = 17.66$: 4.55(4)e+3
point 4 at $2\theta = 24.5$: 4.11(4)e+3
point 5 at $2\theta = 30.79$: 3.81(4)e+3
point 6 at $2\theta = 36.04$: 3.65(3)e+3
point 7 at $2\theta = 51.43$: 3.09(3)e+3
point 8 at $2\theta = 64.17$: 2.94(2)e+3
point 9 at $2\theta = 78.34$: 2.32(2)e+3
point 10 at $2\theta = 93.92$: 2.32(3)e+3
point 11 at $2\theta = 107.14$: 2.54(2)e+3
point 12 at $2\theta = 118.91$: 2.27(3)e+3
point 13 at $2\theta = 136.53$: 2.58(3)e+3
point 14 at $2\theta = 145.41$: 2.44(3)e+3
point 15 at $2\theta = 149.94$: 3.30(6)e+3
point 16 at $2\theta = 151.18$: 9.2(2)e+2

Offsets:
 $\lambda = 1.548$ $\Delta\theta = -0.061(1)$ $\Delta x = 0.064$ $\Delta y = 0.046$

Profile:
 $u = 0.043$ $v = -0.056$ $w = 0.112$ $l_0 = 0.000$
 $X = 0.115(2)$ $Y = -0.004$
 $A_1 = 0.046(8)$ $A_2 = 0.012(3)$ $A_3 = 0.000$ $A_4 = 0.000$
 $S/L = 0.000$ $D/L = 0.000$
 $P_1 = 0.000$ $P_2 = 0.000$
 $\Delta u_m = 0.000$ $\Delta v_m = 0.000$ $\Delta w_m = 0.000$ $\Delta l_{0m} = 0.000$
 $\Delta X_m = 0.000$ $\Delta Y_m = 0.000$
 $\Delta A_{1m} = 0.000$ $\Delta A_{2m} = 0.000$ $\Delta A_{3m} = 0.000$ $\Delta A_{4m} = 0.000$
 $\Delta S/L_m = 0.000$ $\Delta D/L_m = 0.000$
 $\Delta P_{1m} = 0.000$ $\Delta P_{2m} = 0.000$

Lattice:
 $a = 5.5111(1)$ $b = 7.5242(1)$ $c = 5.23634(9)$
 $\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$
Volume = 217.135(6)
 $q_x = 0.000$ $q_y = 0.000$ $q_z = 0.000$
 $B_{av} = 0.000$

1

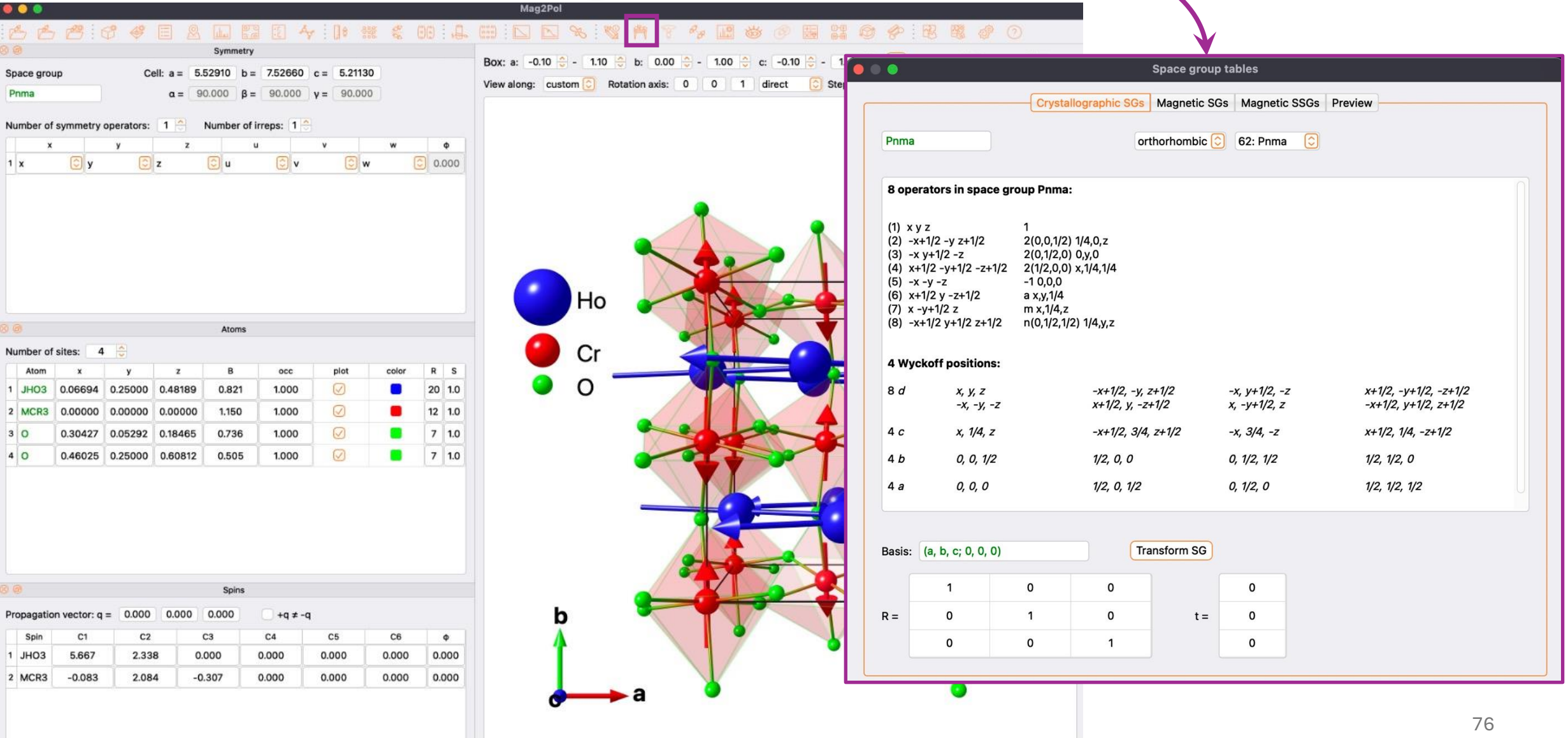
The 'Fit results' tab contains detailed refinement results of the last fit.

Refining magnetic structure using Shubnikov groups (Magnetic space groups)

Set up a Magnetic Space Group (MSG)

1

Click on the 'Space group tables' icon to open the new window with the same name.



Symmetry

Space group: **Pnma**

Cell: a = 5.52910 b = 7.52660 c = 5.21130

$\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

	Atom	x	y	z	B	occ	plot	color	R	S
1	JHO3	0.06694	0.25000	0.48189	0.821	1.000	<input checked="" type="checkbox"/>	blue	20	1.0
2	MCR3	0.00000	0.00000	0.00000	1.150	1.000	<input checked="" type="checkbox"/>	red	12	1.0
3	O	0.30427	0.05292	0.18465	0.736	1.000	<input checked="" type="checkbox"/>	green	7	1.0
4	O	0.46025	0.25000	0.60812	0.505	1.000	<input checked="" type="checkbox"/>	green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☒ -q

	Spin	C1	C2	C3	C4	C5	C6	ϕ
1	JHO3	5.667	2.338	0.000	0.000	0.000	0.000	0.000
2	MCR3	-0.083	2.084	-0.307	0.000	0.000	0.000	0.000

Space group tables

Crystallographic SGs Magnetic SGs Magnetic SSGs Preview

Pnma orthorhombic 62: Pnma

8 operators in space group Pnma:

(1) x y z	1
(2) -x+1/2 -y z+1/2	2(0,0,1/2) 1/4,0,z
(3) -x y+1/2 -z	2(0,1/2,0) 0,y,0
(4) x+1/2 -y+1/2 -z+1/2	2(1/2,0,0) x,1/4,1/4
(5) -x -y -z	-1 0,0,0
(6) x+1/2 y -z+1/2	a x,y,1/4
(7) x -y+1/2 z	m x,1/4,z
(8) -x+1/2 y+1/2 z+1/2	n(0,1/2,1/2) 1/4,y,z

4 Wyckoff positions:

8 d	x, y, z -x, -y, -z	-x+1/2, -y, z+1/2 x+1/2, y, -z+1/2	-x, y+1/2, -z x, -y+1/2, z	x+1/2, -y+1/2, -z+1/2 -x+1/2, y+1/2, z+1/2
4 c	x, 1/4, z	-x+1/2, 3/4, z+1/2	-x, 3/4, -z	x+1/2, 1/4, -z+1/2
4 b	0, 0, 1/2	1/2, 0, 0	0, 1/2, 1/2	1/2, 1/2, 0
4 a	0, 0, 0	1/2, 0, 1/2	0, 1/2, 0	1/2, 1/2, 1/2

Basis: [a, b, c; 0, 0, 0] Transform SG

	1	0	0
R =	0	1	0
	0	0	1

	0
t =	0
	0

Set up a Magnetic Space Group

1

Activate the 'Magnetic SGs' tab

2

Type the notation of an appropriate Magnetic Space Group or select it from the drop-down menu.

For this example, let's choose one of the first allowed magnetic space groups *Pnma* (62.441).

Space group tables

Crystallographic SGs **Magnetic SGs** Magnetic SSGs Preview

8 operators in space group Pnma:

(1) $x y z +1$	1
(2) $-x+1/2 -y z+1/2 +1$	$2(0,0,1/2) 1/4,0,z$
(3) $-x y+1/2 -z +1$	$2(0,1/2,0) 0,y,0$
(4) $x+1/2 -y+1/2 -z+1/2 +1$	$2(1/2,0,0) x,1/4,1/4$
(5) $-x -y -z +1$	$-1 0,0,0$
(6) $x+1/2 y -z+1/2 +1$	$a x,y,1/4$
(7) $x -y+1/2 z +1$	$m x,1/4,z$
(8) $-x+1/2 y+1/2 z+1/2 +1$	$n(0,1/2,1/2) 1/4,y,z$

4 Wyckoff positions:

8 d	$x, y, z [u, v, w]$ $-x, -y, -z [u, v, w]$	$-x+1/2, -y, z+1/2 [-u, -v, w]$ $x+1/2, y, -z+1/2 [-u, -v, w]$	$-x, y+1/2, -z [-u, v, -w]$ $x, -y+1/2, z [-u, v, -w]$	$x+1/2, -y+1/2, -z+1/2 [u, -v, -w]$ $-x+1/2, y+1/2, z+1/2 [u, -v, -w]$
4 c	$x, 1/4, z [0, v, 0]$	$-x+1/2, 3/4, z+1/2 [0, -v, 0]$	$-x, 3/4, -z [0, v, 0]$	$x+1/2, 1/4, -z+1/2 [0, -v, 0]$
4 b	$0, 0, 1/2 [u, v, w]$	$1/2, 0, 0 [-u, -v, w]$	$0, 1/2, 1/2 [-u, v, -w]$	$1/2, 1/2, 0 [u, -v, -w]$
4 a	$0, 0, 0 [u, v, w]$	$1/2, 0, 1/2 [-u, -v, w]$	$0, 1/2, 0 [-u, v, -w]$	$1/2, 1/2, 1/2 [u, -v, -w]$

Information based on (please cite accordingly):
H. T. Stokes, D. M. Hatch, and B. J. Campbell, ISO-MAG, ISOTROPY Software Suite, iso.byu.edu.

Basis:

R =	1	0	0	t =	0
	0	1	0		0
	0	0	1		0

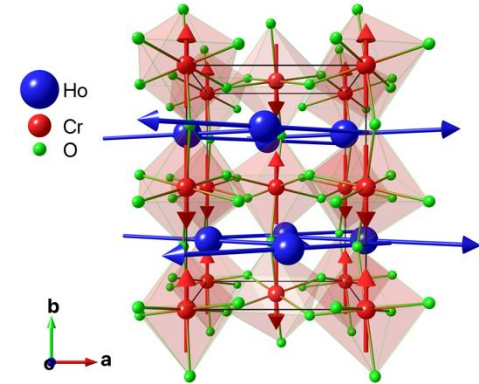
Set up a Magnetic Space Group

1

Switch to the 'Preview' tab

2

Keep an eye on the magnetic structure in the main window



3

Click on the button 'Transfer MSG'

Atom	Wyckoff position	parameter	value
1 JHO3	4c	x	0.06539
1 JHO3	4c	z	0.48336
3 O	8d	x	0.30276
3 O	8d	y	0.05395
3 O	8d	z	0.19180
4 O	4c	x	0.46645
4 O	4c	z	0.60197

5

The MSG **Pnma₋** is not a suitable magnetic model

Reset symmetry

1

Reset symmetry

4

In the main window of the Mag2Pol, the space group is appended to **Pnma₋** (underscore indicates it is a MSG)

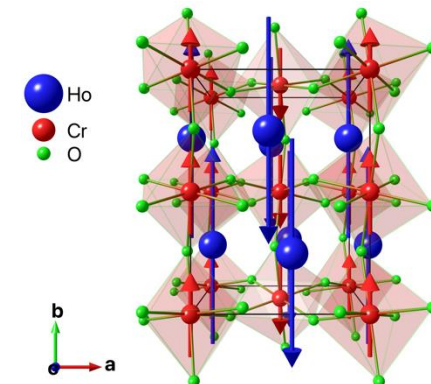
Symmetry

Space group: **Pnma₋**

Cell: a = 5.52910 b = 7.52660 c = 5.21130

α = 90.000 β = 90.000 γ = 90.000

The spin arrangement in MSG **Pnma₋** (which is appended now on the main window) looks very different from the irrep 3 above



Set up a Magnetic Space Group

1

Activate the 'Magnetic SGs' tab

Space group tables

Crystallographic SGs **Magnetic SGs** Magnetic SSGs Preview

Pn'm'a orthorhombic 62.446: Pn'm'a

8 operators in space group Pn'm'a:

(1) $x y z +1$	1
(2) $-x+1/2 -y z+1/2 +1$	$2(0,0,1/2) 1/4,0,z$
(3) $-x y+1/2 -z -1$	$2'(0,1/2,0) 0,y,0$
(4) $x+1/2 -y+1/2 -z+1/2 -1$	$2'(1/2,0,0) x,1/4,1/4$
(5) $-x -y -z +1$	$-1 0,0,0$
(6) $x+1/2 y -z+1/2 +1$	$a x,y,1/4$
(7) $x -y+1/2 z -1$	$m' x,1/4,z$
(8) $-x+1/2 y+1/2 z+1/2 -1$	$n'(0,1/2,1/2) 1/4,y,z$

4 Wyckoff positions:

8 d	$x, y, z [u, v, w]$ $-x, -y, -z [u, v, w]$	$-x+1/2, -y, z+1/2 [-u, -v, w]$ $x+1/2, y, -z+1/2 [-u, -v, w]$	$-x, y+1/2, -z [u, -v, w]$ $x, -y+1/2, z [u, -v, w]$	$x+1/2, -y+1/2, -z+1/2 [-u, v, w]$ $-x+1/2, y+1/2, z+1/2 [-u, v, w]$
4 c	$x, 1/4, z [u, 0, w]$	$-x+1/2, 3/4, z+1/2 [-u, 0, w]$	$-x, 3/4, -z [u, 0, w]$	$x+1/2, 1/4, -z+1/2 [-u, 0, w]$
4 b	$0, 0, 1/2 [u, v, w]$	$1/2, 0, 0 [-u, -v, w]$	$0, 1/2, 1/2 [u, -v, w]$	$1/2, 1/2, 0 [-u, v, w]$
4 a	$0, 0, 0 [u, v, w]$	$1/2, 0, 1/2 [-u, -v, w]$	$0, 1/2, 0 [u, -v, w]$	$1/2, 1/2, 1/2 [-u, v, w]$

Information based on (please cite accordingly):
H. T. Stokes, D. M. Hatch, and B. J. Campbell, ISO-MAG, ISOTROPY Software Suite, iso.byu.edu.

Basis: (a, b, c; 0, 0, 0) Transform MSG

R =

1	0	0
0	1	0
0	0	1

t =

0
0
0

2

Try other MSGs within the Pnma setting of the parent.

But for the exercise, let's now choose Pn'm'a (62.446).

Set up a Magnetic Space Group

1

Switch to the 'Preview' tab

Space group tables

Crystallographic SGs Magnetic SGs Magnetic SSGs **Preview**

Transfer SG Transfer MSG Transfer MSSG

☐ convert lattice constants ☐ convert atomic positions ☐ split sites in subgroup

Crystal structure Magnetic structure

	Atom	Wyckoff position	parameter	value
1	JHO3	4c	x	0.06539
1	JHO3	4c	z	0.48336
3	O	8d	x	0.30276
3	O	8d	y	0.05395
3	O	8d	z	0.19180
4	O	4c	x	0.46645
4	O	4c	z	0.60197

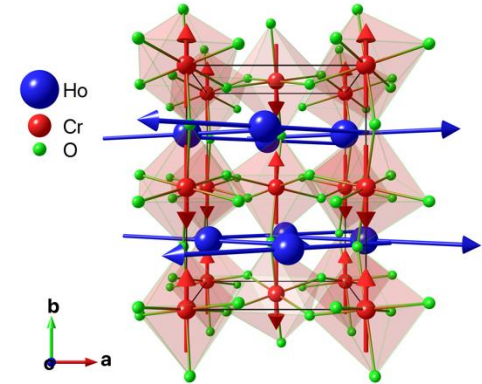
Reset parameters Reset symmetry

3

Click on the button 'Transfer MSG'

2

Keep an eye on the magnetic structure in the main window



4

In the main window of the Mag2Pol, the space group is appended to **Pn'm'a**

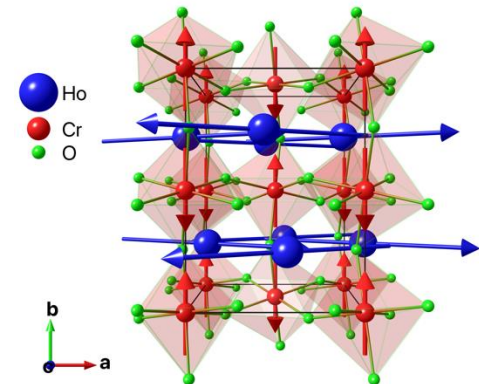
Symmetry

Space group **Pn'm'a**

Cell: a = 5.52910 b = 7.52660 c = 5.21130

α = 90.000 β = 90.000 γ = 90.000

The spin arrangement in MSG **Pn'm'a** is identical to irrep 3. This could be actual MSG



Save the project with MSG Pn'm'a

1 Save the project as 'HCO_4K_Mag-Pn'm'a.xml'

2

Software interface for crystal structure visualization and data management.

Symmetry

Space group: **Pn'm'a**

Cell: a = 5.52910 b = 7.52660 c = 5.21130

$\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 JHO3	0.06539	0.25000	0.48336	-0.133	1.000	<input checked="" type="checkbox"/>	Blue	20	1.0
2 MCR3	0.00000	0.00000	0.00000	-0.067	1.000	<input checked="" type="checkbox"/>	Red	12	1.0
3 O	0.30276	0.05395	0.19180	-0.103	1.000	<input checked="" type="checkbox"/>	Green	7	1.0
4 O	0.46645	0.25000	0.60197	-0.095	1.000	<input checked="" type="checkbox"/>	Green	7	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 ☐ +q ☒ -q

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 JHO3	7.014	3.649	0.000	0.000	0.000	0.000	0.000
2 MCR3	0.000	2.609	0.000	0.000	0.000	0.000	0.000

Box: a: -0.10 - 1.10 b: 0.00 - 1.00 c: -0.10 - 1.10 Domain: 1 Phase: 1

View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: -35

Legend:
Blue sphere: Ho
Red sphere: Cr
Green sphere: O

Coordinate system:
a: red arrow
b: green arrow
c: blue arrow

Save the project with MSG Pn'm'a

1

Fit

Data Atoms Moments Domains Constraints Patterns Fit

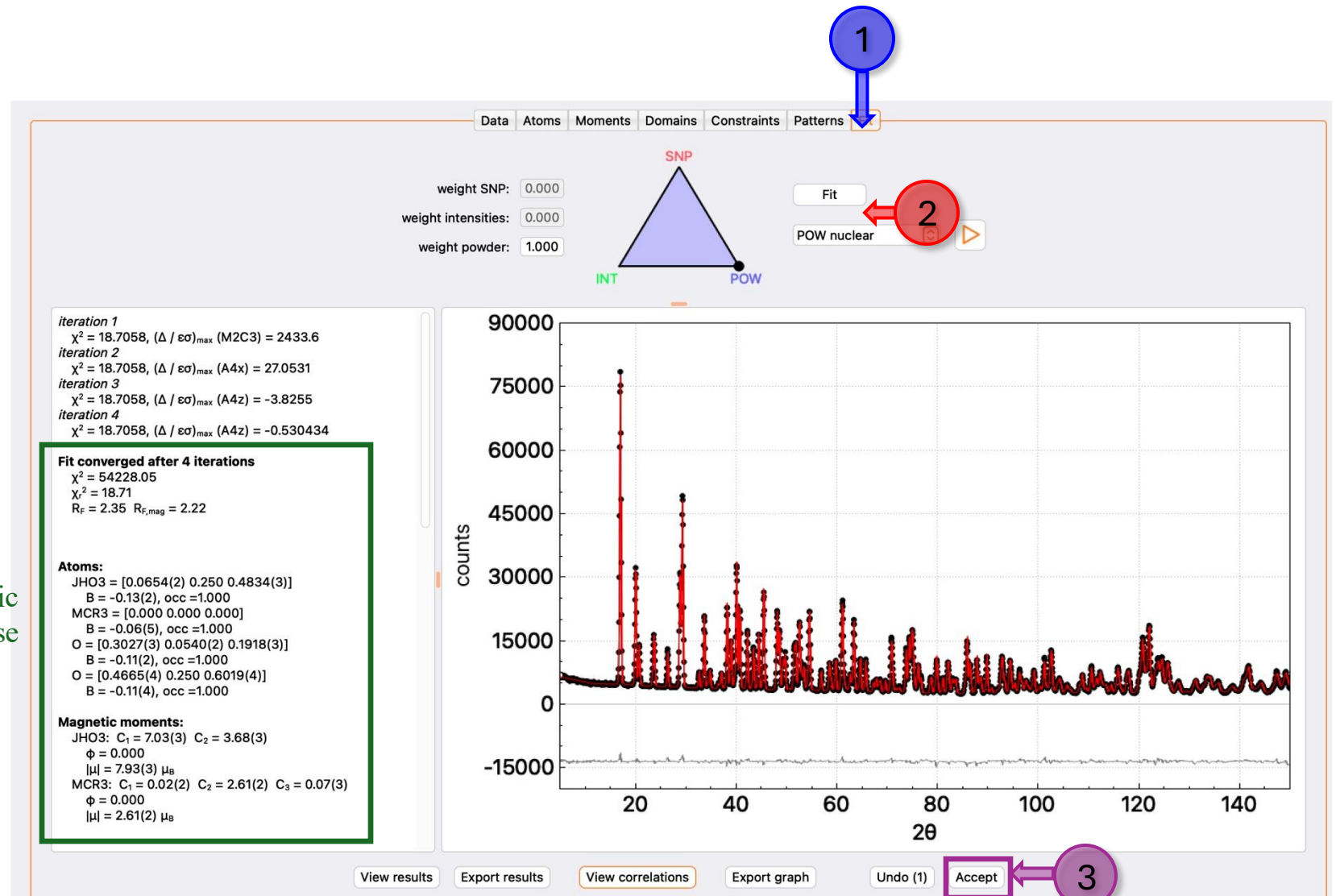
	Spin	C1	C2	C3	C4	C5	C6	ϕ
M1	JHO3	7.014 <input checked="" type="checkbox"/>	3.649 <input checked="" type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>
M2	MCR3	0.000 <input checked="" type="checkbox"/>	2.609 <input checked="" type="checkbox"/>	0.000 <input checked="" type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>	0.000 <input type="checkbox"/>

BV1: (1 0 0) + i(0 0 0)

Activate the refinements of all allowed basis vectors (BV)

Save the project with MSG Pn'm'a

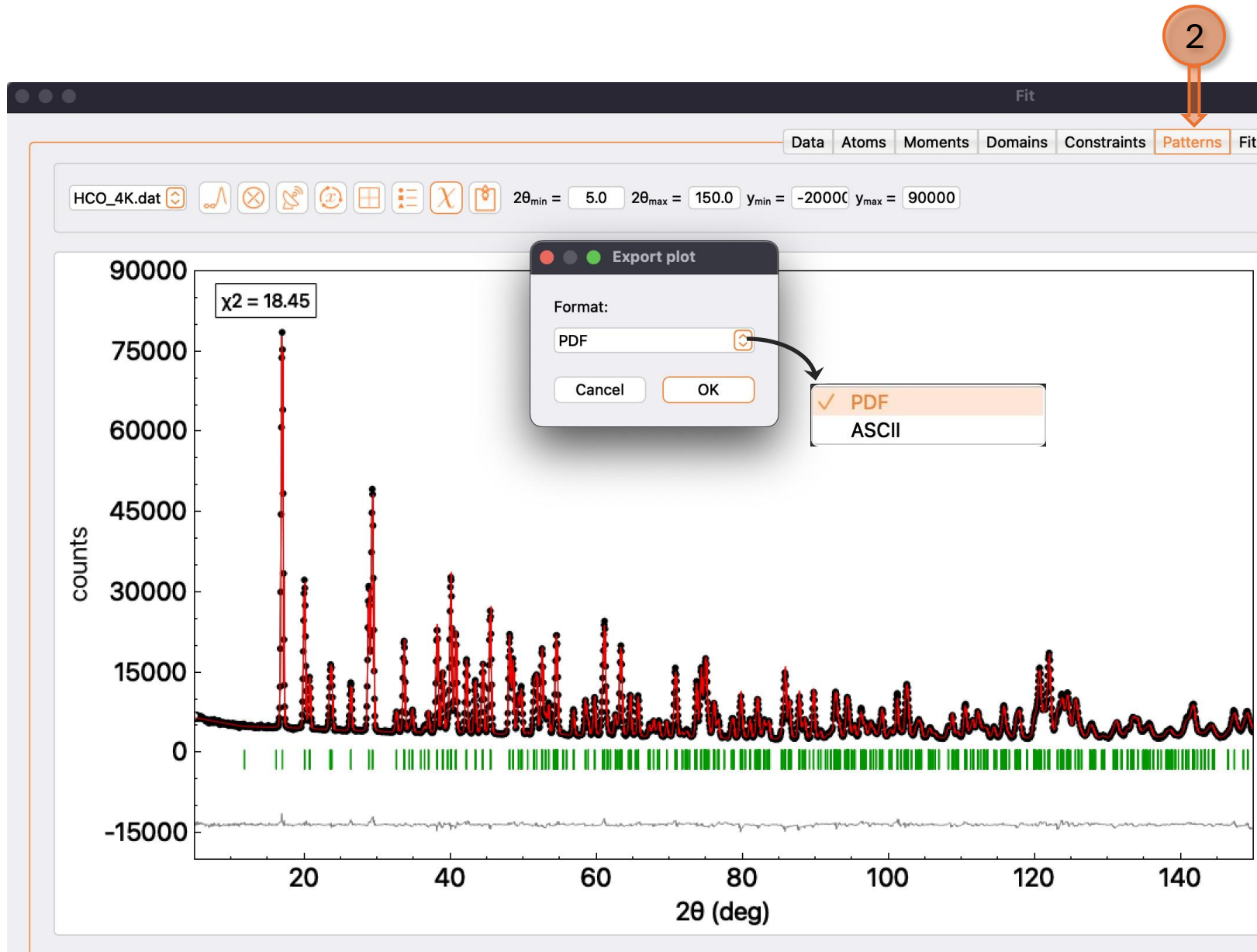
The refinement results using the Magnetic Space Group Pn'm'a are identical to those obtained using irrep Γ_3 .



After accepting the refinement results here, do not forget to save the project from the main window!

Exporting the refined structures, parameters and patterns

Export refined pattern as PDF or ASCII



While exporting it as a PDF rearrange the window to a desired aspect ratio. What you see is what you get.

Export the Graphic and structure models

2

Plot tweaks

1

The screenshot shows the Mag2Pol software interface. The 'File' menu is open, showing options like 'Open', 'Open recent', 'Save', 'Save as', 'Import', 'Export', 'Reset', and 'Check for updates'. The 'Export' option is highlighted, and a submenu is visible with options: 'Graphic', '3D model', 'cif', and 'mcif'. A red box labeled 'Plot tweaks' highlights a table with 4 columns: Atom, x, y, z, B, occ, plot, color, R, S. The table contains 4 rows of data for atoms JHO3, MCR3, O, and O. A red box labeled '1' highlights the 'plot' column. The main window displays a 3D model of a crystal structure with blue spheres (Ho) and red spheres (Cr) and red arrows representing magnetic moments. The axes are labeled a, b, and c.

Atom	x	y	z	B	occ	plot	color	R	S
1 JHO3	0.06542	0.25000	0.48340	-0.129	1.000	<input checked="" type="checkbox"/>	blue	20	0.6
2 MCR3	0.00000	0.00000	0.00000	-0.062	1.000	<input checked="" type="checkbox"/>	red	12	0.6
3 O	0.30274	0.05395	0.19180	-0.110	1.000	<input type="checkbox"/>	green	7	1.0
4 O	0.46650	0.25000	0.60191	-0.108	1.000	<input type="checkbox"/>	green	7	1.0

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 JHO3	7.030	3.677	0.000	0.000	0.000	0.000	0.000
2 MCR3	0.021	2.609	0.067	0.000	0.000	0.000	0.000

The structure model can be exported as:

*.png (Graphic)

*.cif

*.mcif

by following the menu tree:

File→Export→

Step 7e: Export refinement results as latex tables

1

The screenshot shows the Mag2Pol software interface. The 'Tools' menu is open, displaying a list of options. The 'LaTeX export' option is highlighted, which has opened a sub-menu. In this sub-menu, the 'Nuclear structure table' option is highlighted. The main window displays a 3D visualization of a crystal structure with red spheres representing atoms and blue arrows representing magnetic moments. The left panel shows the 'Symmetry' section with space group 'Pn'm'a' and unit cell parameters. Below that is the 'Atoms' section with a table of atom positions. At the bottom is the 'Spins' section with a table of spin parameters.

Symmetry

Space group: $Pn'm'a$

Cell: $a = 5.52910$ $b = 7.52660$ $c = 5.21130$

$\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w
1	x	y	z	u	v	w

Atoms

Number of sites: 4

Atom	x	y	z	B	occ	plot	color	R	S
1 JHO3	0.06542	0.25000	0.48340	-0.129	1.000	<input checked="" type="checkbox"/>	blue	20	0.6
2 MCR3	0.00000	0.00000	0.00000	-0.062	1.000	<input checked="" type="checkbox"/>	red	12	0.6
3 O	0.30274	0.05395	0.19180	-0.110	1.000	<input type="checkbox"/>	green	7	1.0
4 O	0.46650	0.25000	0.60191	-0.108	1.000	<input type="checkbox"/>	green	7	1.0

Spins

Propagation vector: $q = 0.000$ 0.000 0.000 ☐ $+q \neq -q$

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 JHO3	7.030	3.677	0.000	0.000	0.000	0.000	0.000
2 MCR3	0.021	2.609	0.067	0.000	0.000	0.000	0.000

Tools

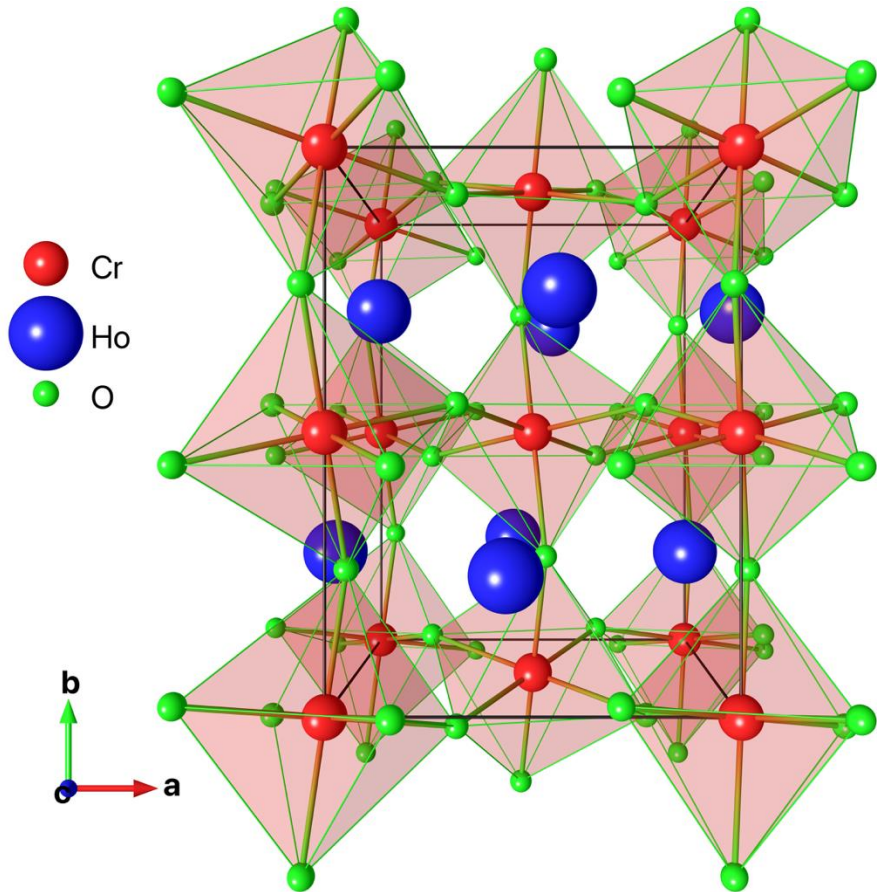
- Sample info
- Space group tables
- Multi-q structure
- Spin correlations
- Pattern editor
- Guides to the eye
- Phase transitions
- Crystal calculator
- Fit macros
- Cell animation
- Bond distances
- Data converter
- LaTeX export
 - Nuclear structure table
 - Magnetic structure table
 - Multiplication table
 - Irreps table
 - Basis vector table

A variety of fit results can be copied directly in LaTeX format by following the menu tree:

Tools \rightarrow LaTeX export

Exercise

Refine the lattice and magnetic structure of HoCrO_3 at 100 K



Orthorhombic structure: $Pnma$ (No. 62)

Instrument: Neutron powder diffractometer SPODI at FRM II research reactor, Garching, Germany

Wavelength: 1.5482 Å

Data files:

Data collected at 100 K: HCO_100K.dat (\rightarrow HCO_100K.m2p)

Hint:

Only Cr^{3+} is magnetically ordered at this temperature

Before you go!

- Our tutorial on the refinement of time-of-flight data is available on the website for the ToF Neutron Diffractometer POWGEN, Oak Ridge National Laboratory: [Link here](#)
- Polish users who performed measurements at ILL, please acknowledge the financing in the publications by including the following statement:
The authors {name of specific author(s) if necessary} acknowledge(s) the Polish Ministry of Education and Science decision no. 2023/WK/08 to fund the scientific membership of Poland at the ILL, which made this research possible.
- Cite the use of Mag2Pol as follows:
*Mag2Pol: a program for the analysis of spherical neutron polarimetry, flipping ratio and integrated intensity data, N. Qureshi, [J. Appl. Cryst.](#) **52** (2019) 175-185.*

If you have any questions:

Regarding Mag2Pol and need to report bugs.

Contact:

Navid Qureshi
Institute Laue Langevin,
Grenoble, France
Email: qureshi@ill.fr

Regarding this tutorial, or need a collaborator on
the lattice and magnetic structure refinement.

Contact:

Naveen Kumar Chogondahalli Muniraju
Institute of Nuclear Physics, PAN
Krakow, Poland
Email: naveen.chogondahalli@ifj.edu.pl

Good luck with your next refinement project!