

Single Crystal diffraction and Magnetic Structure Determination Examples using Fullprof

Yiqing Hao

Neutron Scattering Division

Magnetic Structure Determination From Neutron Diffraction Data 2026

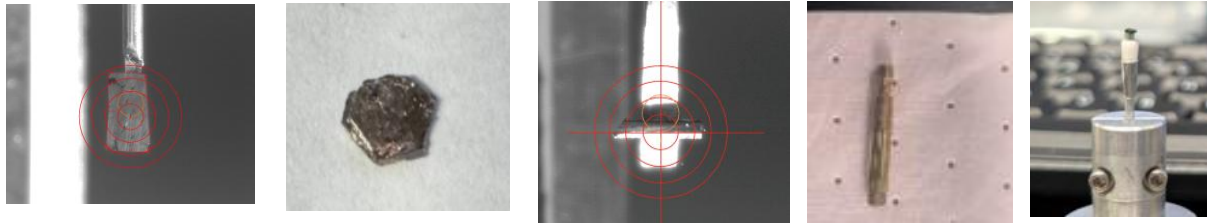
Duke University, North Carolina

2026 July

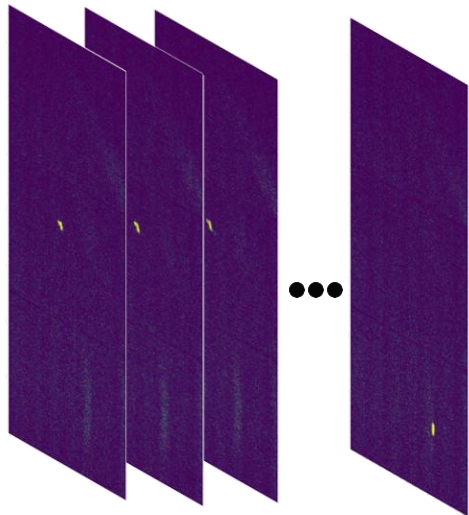


ORNL is managed by UT-Battelle, LLC for the US Department of Energy

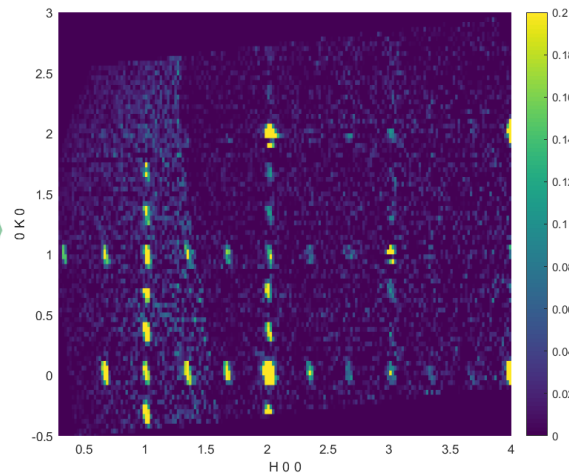
What Single-crystal diffraction?



Detector images
(raw data)



Reciprocal space
(processed data)



Lattice parameters,
k-vectors

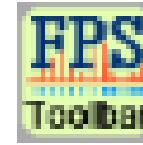
Peak intensities
(reduced data)

autoreduced peaks
(3i4,2f8.2,i6)
1.5424 0 0

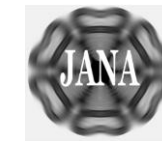
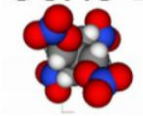
0	3	0	183.23	4.19	1
-1	3	1	67.76	2.01	1
2	2	-2	118.54	1.00	1
3	1	-2	8.47	0.23	1
3	2	-1	48.70	0.60	1
2	3	-1	51.90	1.04	1
4	0	-0	38.47	0.74	1
4	1	0	56.73	0.80	1
3	2	0	6.64	0.22	1
2	3	0	6.94	0.34	1
3	2	1	52.29	0.58	1
2	2	2	138.33	1.06	1
3	3	0	97.08	0.92	1
4	2	0	41.57	0.55	1
5	1	0	40.01	0.54	1
4	2	1	46.49	0.55	1
3	3	2	52.80	0.56	1
3	2	3	50.47	0.54	1
3	-0	4	215.50	1.37	1
2	0	-1	0.85	0.08	1
1	2	-1	46.29	0.87	1
1	3	-1	21.19	1.11	1
2	-0	-0	5.96	0.20	1
3	0	-0	136.83	1.40	1
1	2	0	15.89	0.46	1
2	-0	1	0.84	0.10	1



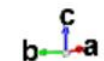
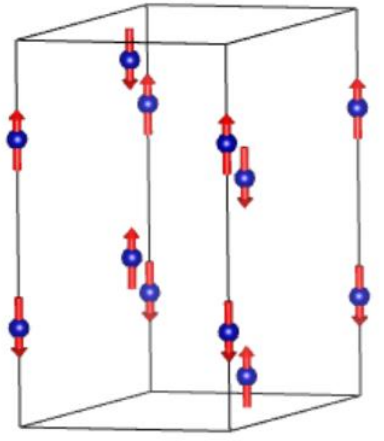
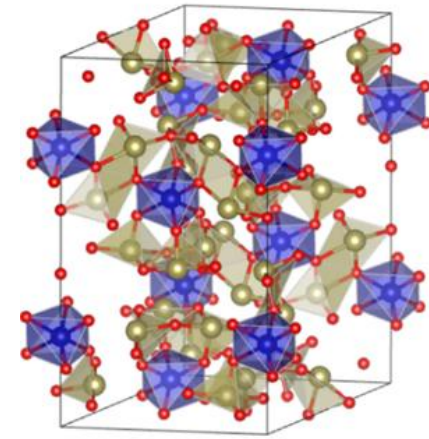
Crystal and
magnetic structure



GSAS-2



MAG2POL



Why Single-crystal diffraction?

Advantage:

- More information by measuring Bragg peaks in 3D reciprocal space: $\mathbf{Q} = (H, K, L)$ vs $|\mathbf{Q}|$. Easier to determine **Complex magnetic structures**
- **Unambiguously determine the k-vector** – superlattice or satellite peaks
- Less samples – mg vs g
- Faster **order parameter measurement**
- **Less neutron absorption** due to small size, no isotope needed for H, Li, even Eu, Sm, (sometimes Gd) et al,
- Magnetic field phase diagram – know the field orientation

Disadvantage:

- **You need a single crystal**
- Data collection can be more time consuming
- Extinction, domain, twining, etc.

Always **Good to combine** both X-ray Neutron powder and single-crystal diffraction!

DEMAND HB-3A at HFIR



Yan Wu (IS)



Yiqing Hao (IS)



Xiao Hu (CIS)



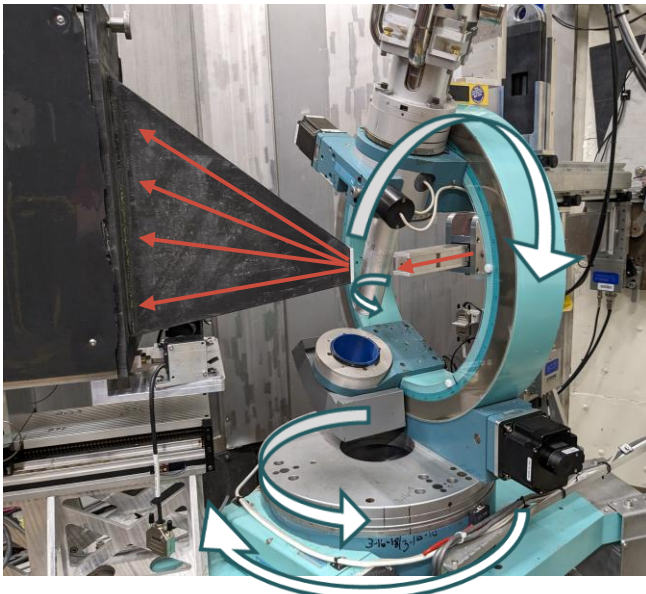
Emily Kroll (SA)



Jie Xing (SA)

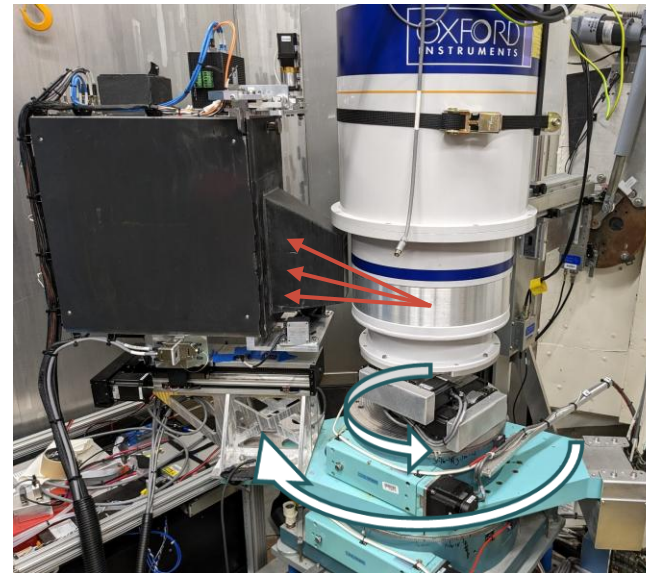
Topics: magnetic structures, magnetic phase transitions and possible accompanied structural changes, order parameters and phase diagrams.

Four-circle mode



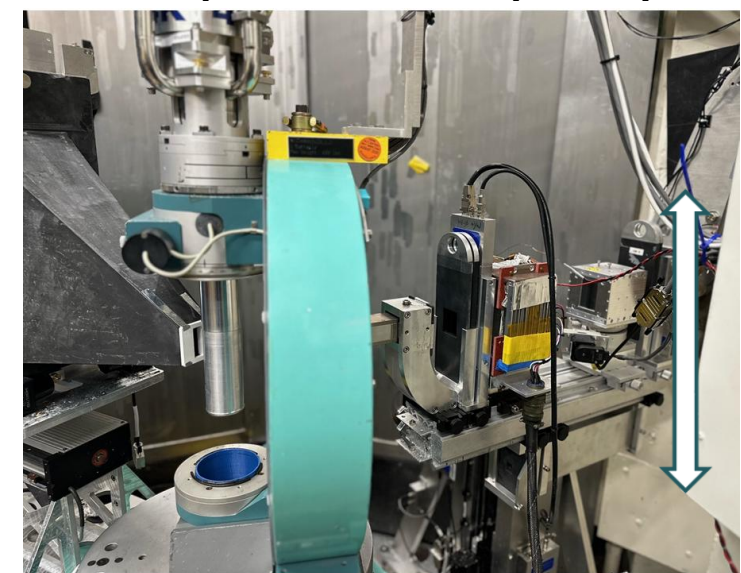
CCR
 $4\text{ K} < T < 700\text{ K}$
 $H < 0.7\text{ T}$ (permanent magnet)
Hemisphere Q-space coverage

Two-axis mode



Orange Cryostat/ Cyromagnet,
 ^3He / Dilution insert
 $60\text{ mK} < T < 300\text{ K}$
 $H < 6\text{ T}$
Smaller Q-coverage

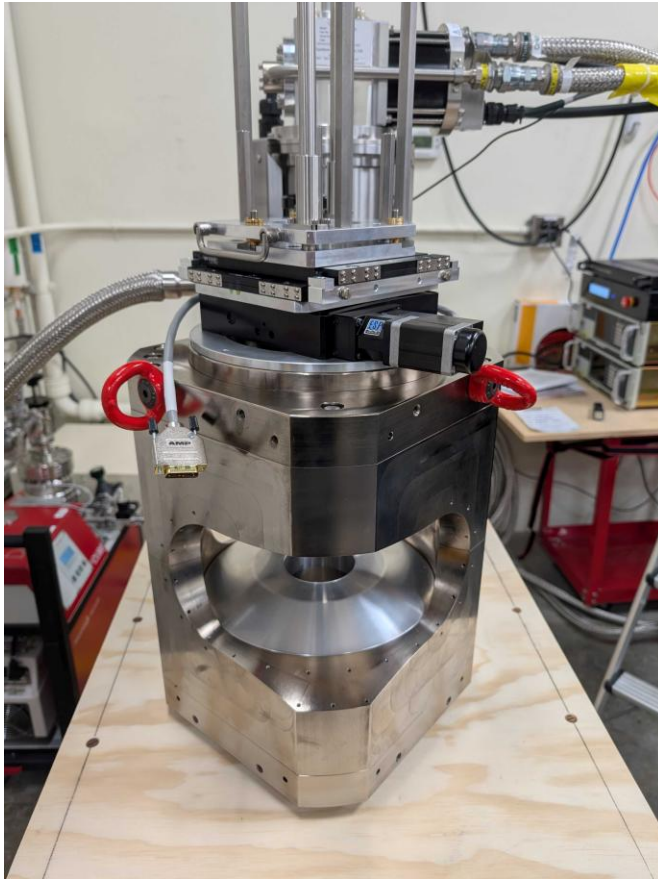
Half-polarization capability



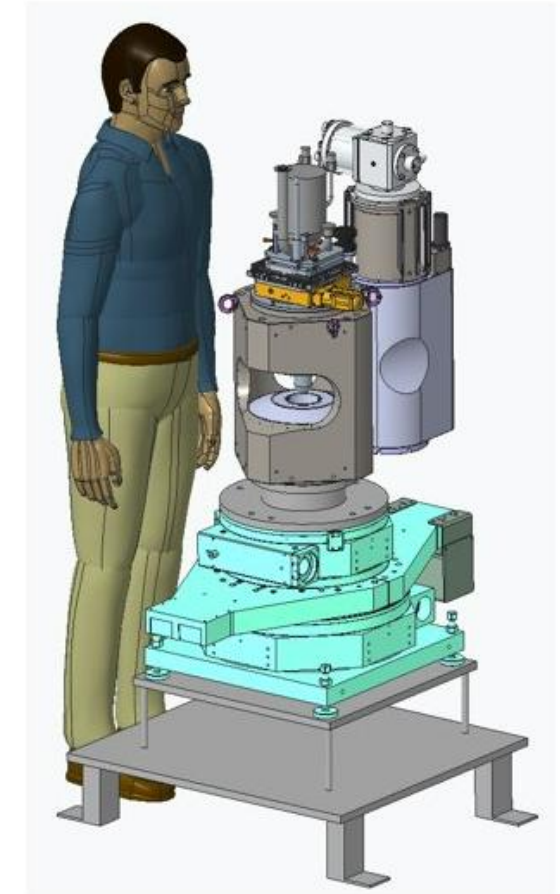
Polarized incident beam using S-bender
Polarization ratio 93% to 98%
Motorized optical rack to switch between polarized / nonpolarized neutrons

Capability of HB-3A DEMAND: New Magnet

High-temperature dry superconducting magnet (2.5 T, under commissioning)



Paired with the 4 K - CCR.
Maximum field 2.5 T.
Vertical coverage +/- 20 deg.

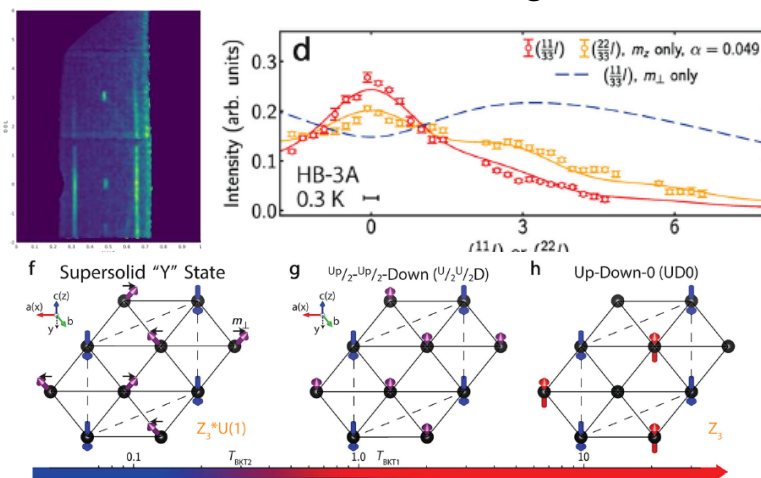


Mounting stack engineering & design:
Gregory Warren, Rudy Thermer

Recent Highlights of HB-3A DEMAND

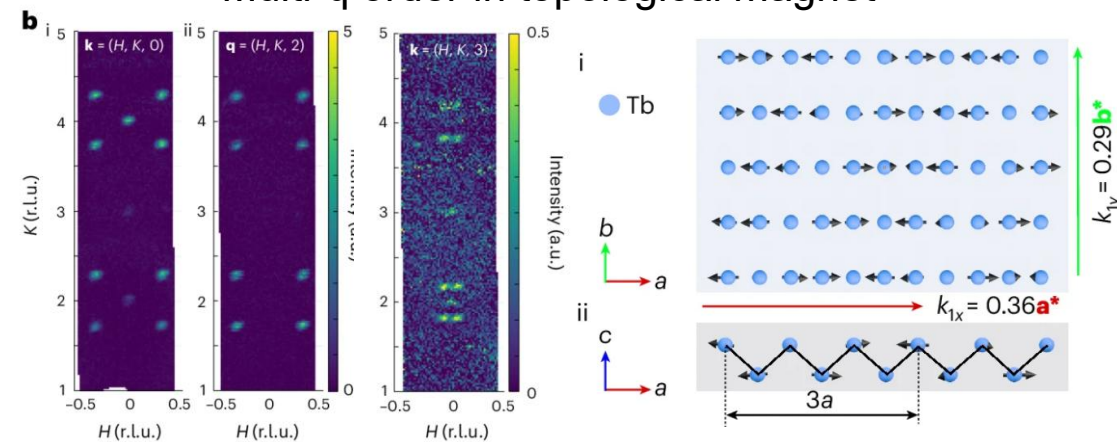
- ❖ Complex magnetism and structure
- ❖ New materials and phenomena
- ❖ Order parameter and phase transitions
- ❖ Long/short range magnetic order, local magnetic susceptibility, magnetic anisotropy
- ❖ Extreme condition tuning

Diffuse scattering



T. Chen et al., Nature Communication, 17, 2914 (2026)

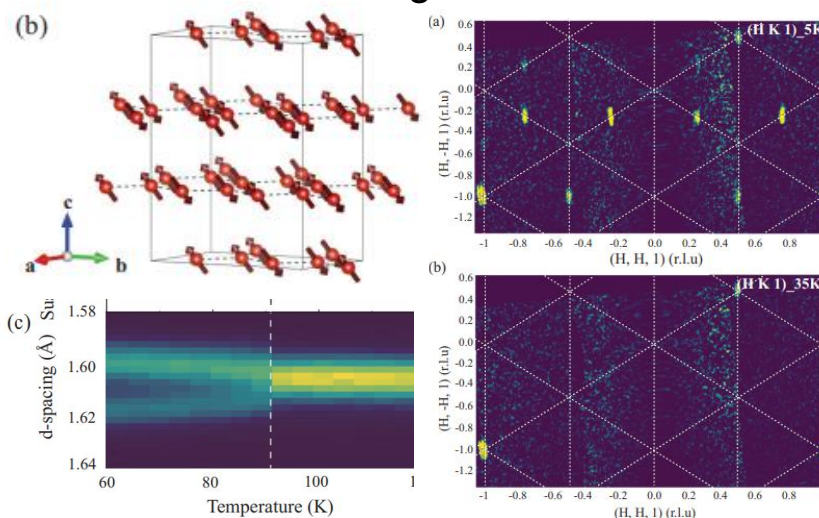
Multi-q order in topological magnet



E. Cheng et al., Nature Materials, 25, 602 (2025)

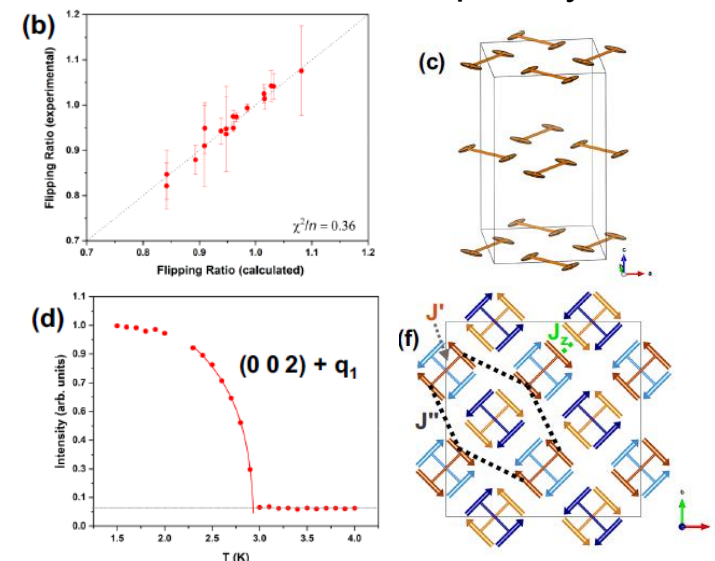
Magnetic structure studies use 80% beam time.

Structure and magnetism in vdW material



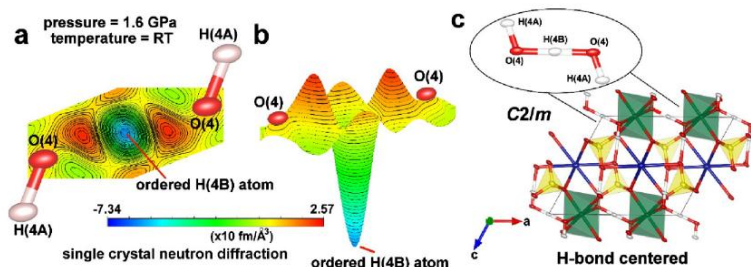
Y. Gu et al., Phys. Rev. B, 110, 064403 (2024)

Local site susceptibility



M. Marshall et al., Nature Communication, 14:3641 (2023)

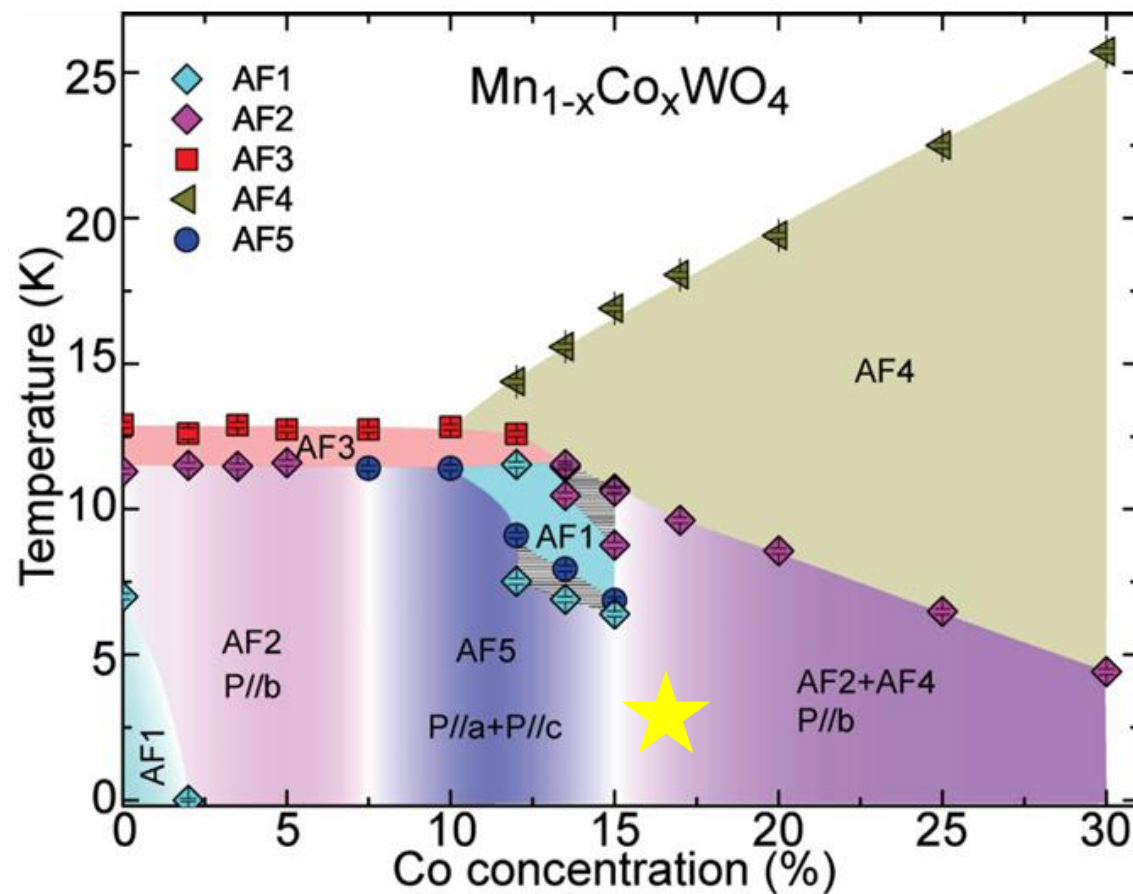
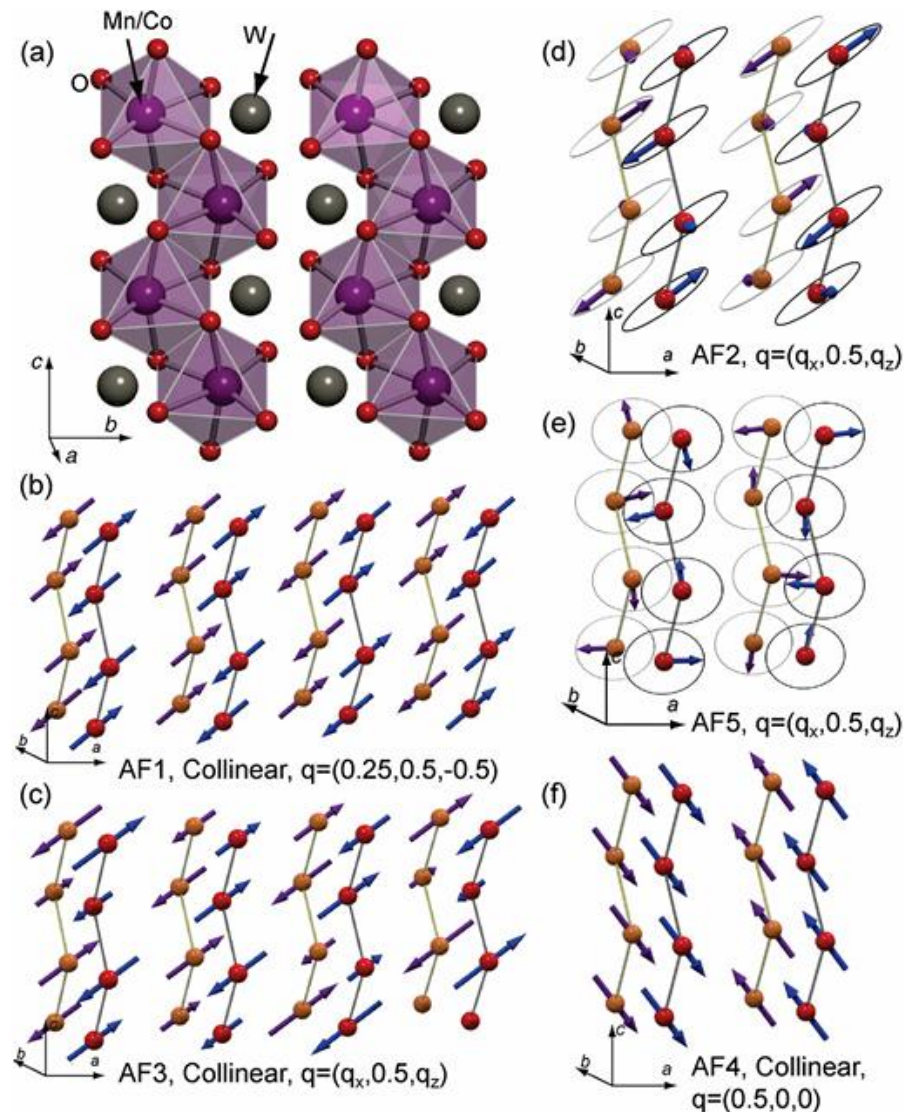
High pressure hydrogen bond



P. Reinhardt et al., JACS, 147, 26830 (2025)

Example: Incommensurate/commensurate structure of (Mn,Co)WO₄

Example: Magnetic structure in 17% Co-doped MnWO₄



SG: P 1 2/c 1
 $a=4.77 \text{ \AA}$ $b=5.72 \text{ \AA}$ $c=4.92 \text{ \AA}$ $\beta=90.9^\circ$

Explanation to Fullprof single crystal data file (k = 0 peaks)

Format control code⁽¹⁾

Title

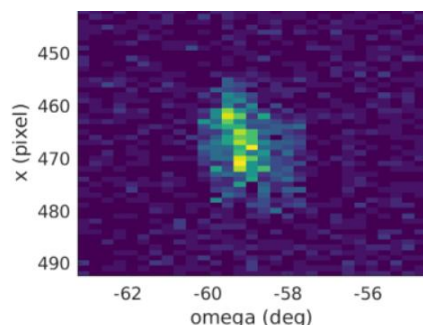
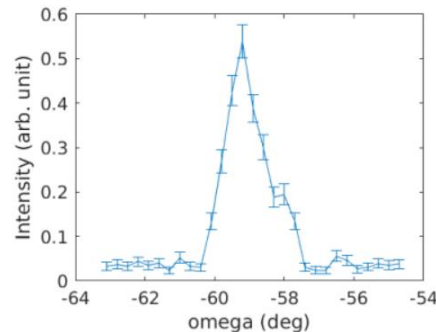
No. 1 reason of the “non reflection found” error

header

body

Wavelength, ltyp⁽²⁾, lpow⁽³⁾

Each intensity is an integration of a 3-D peak

	H	K	L	Int	$\sigma(\text{Int})$	$n^{(4)}$
1	Single crystal data of MnWO4-17pCo (hb3a)					
2	(3i5,2f8.2,i4,3f8.2)					
3	1.53600	0	0			
4	-0	1	-0	244.02	13.24	1
5	-1	-0	-0	1009.99	57.60	1
6	1	0	-0	1006.03	54.50	1
7	-0	1	-1	856.64	46.40	1
8	-0	1	1	906.26	58.99	1
9	-1	1	-0	176.37	10.25	1
10	1	1	-0	177.44	9.66	1
11	-1	-0	1	57.03	2.35	1
12	1	0	-1	57.60	3.37	1
13	-1	-0	-1	20.82	1.72	1
14	1	0	1	18.90	1.82	1
15	-1	1	1	37.60	2.13	1
16	1	1	-1	31.34	2.57	1
17	-1	1	-1	24.64	1.67	1
18	1	1	1	28.80	2.37	1
19	-0	2	-0	144.77	9.90	1
20	-0	2	-1	1035.63	58.27	1
21	-0	2	1	1044.62	64.79	1

1 i-integer, f-float. 3i5 = 3 integer each occupies 5 spaces. 2f8.2 = 2 floats each occupies 8 spaces, 2 digits after decimal.

2 ltyp - always use 0 (for integrated intensity), see Fullprof Manual, page 138

3 lpow - use 0 for normal single crystal data, 1 for twinned single crystal data, 2 for integrated powder data, see FP manual, Page 138.

4 Number of crystal domains. Use >1 if the peak belongs to a different domain. See FP manual, Page 139 for twinned crystals.

5 Direction cosines - The incident and diffraction beam orientation, (not used in current data), often used in absorption correction.

Explanation to Fullprof single crystal data file (k ≠ 0 peaks)

Number of k-vectors

$k_1 = (0.217, 1/2, -0.46)$

$k_2 = (-0.271, -1.2, 0.46)$

MnWO4_magneticAF2_5K.int								
Single crystal data of MnWO4-17pCo (hb3a)								
(4i4,2f8.2,i4,3f8.2)								
1.536 0 0								
2								
1 0.217 .5 -0.46								
2 -0.217 -.5 0.46								
7	-0	0	-0	1	103.78	3.58	1	
8	-0	0	1	1	164.93	6.66	1	
9	-1	0	-0	1	51.55	2.40	1	
10	-1	0	1	1	225.85	9.26	1	
11	-0	1	-0	1	174.34	7.73	1	
12	1	0	-0	1	72.95	3.04	1	
13	-0	1	1	1	5.04	0.58	1	
14	1	0	1	1	101.87	4.62	1	
15	-0	0	-1	1	155.64	7.05	1	
16	-1	1	-0	1	130.48	6.54	1	
17	-1	1	1	1	3.58	0.54	1	
18	-1	0	2	1	63.37	3.54	1	
19	1	1	-0	1	150.43	5.95	1	
20	1	1	1	1	2.79	0.58	1	
21	-0	1	-1	1	5.84	0.69	1	

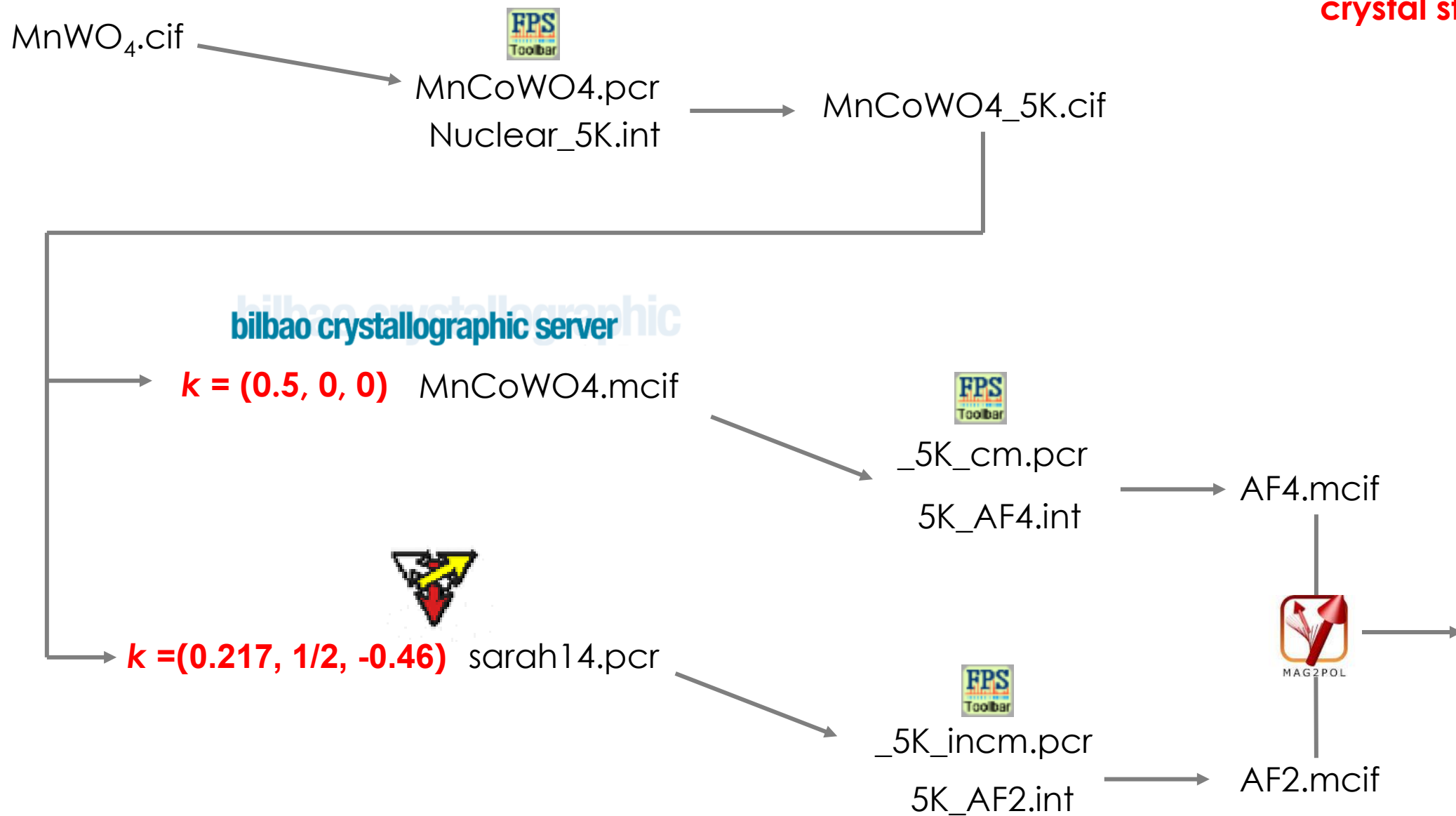
H, K, L $\mathbf{n}_k$ Int $\sigma(\text{Int})$ n

header

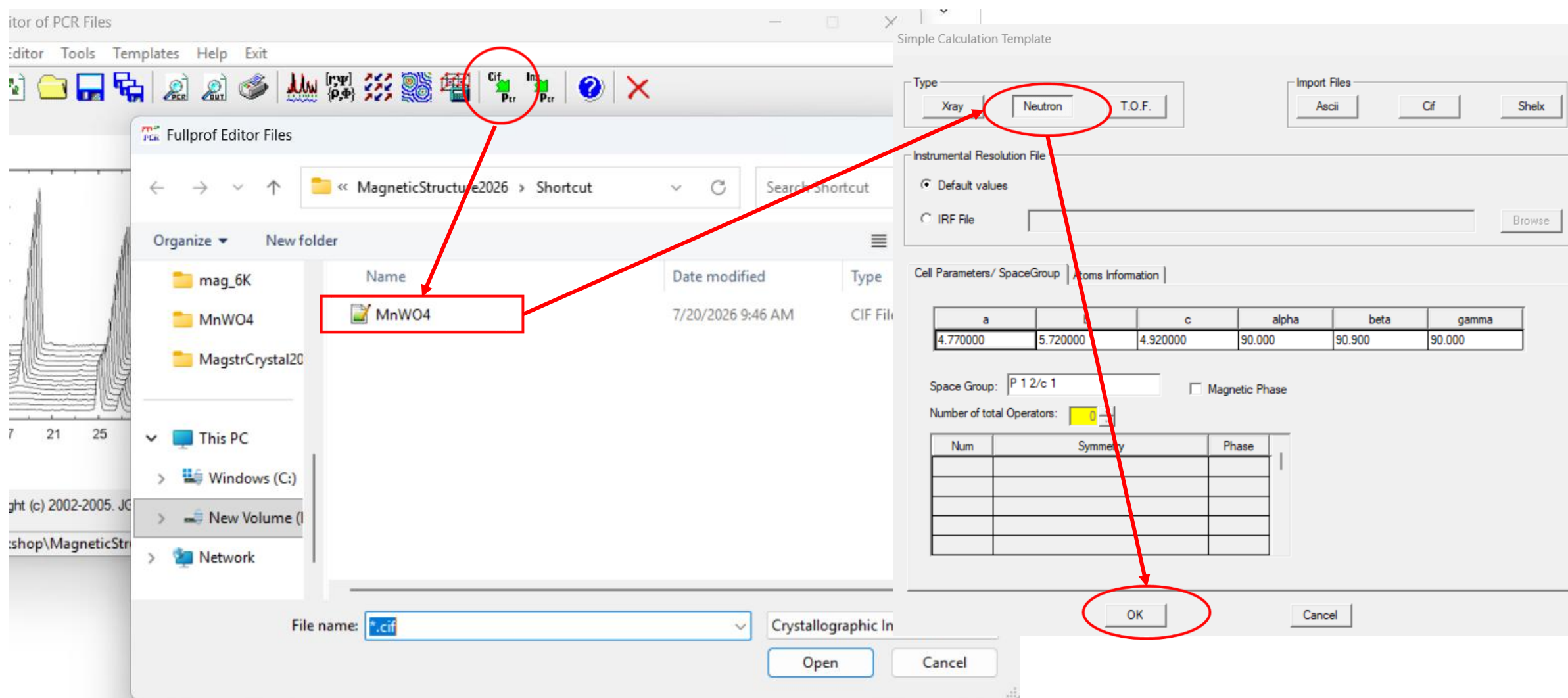
body

$\mathbf{Q} = (H, K, L) + k(\mathbf{n}_k)$. E.g., $(H, K, L) = [-1 \ 0 \ 0]$ and $\mathbf{n}_k = 1$ means $\mathbf{Q} = (-1, 0, 0) + (0.217, 0.5, -0.46) = (-0.783, 0.5, -0.46)$

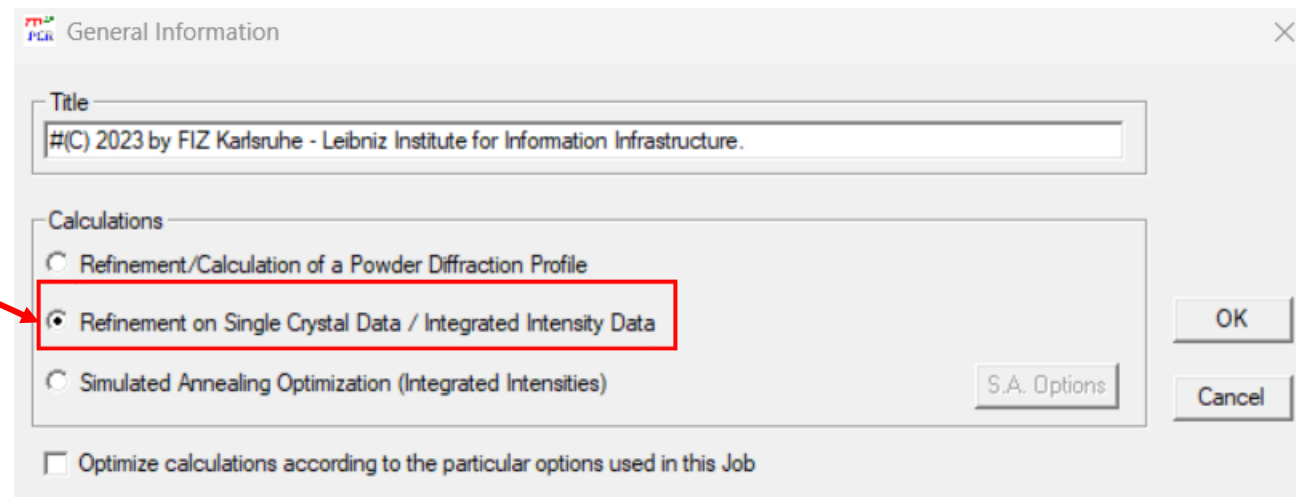
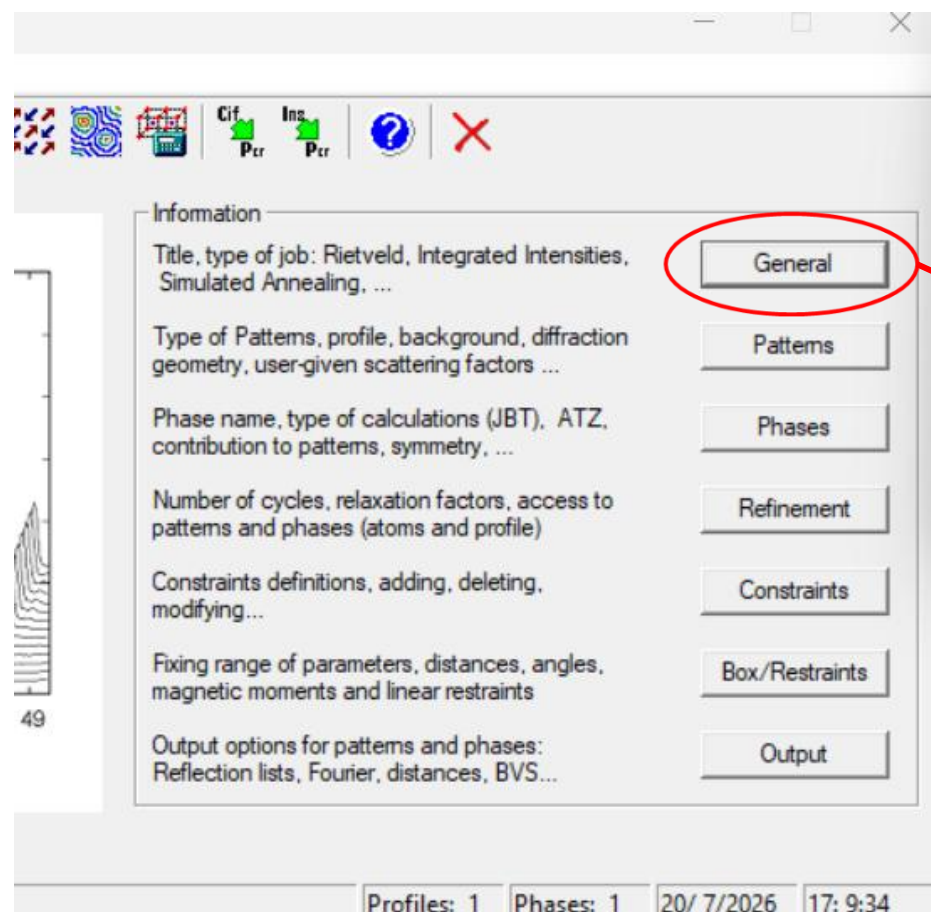
Always start from the
crystal structure!



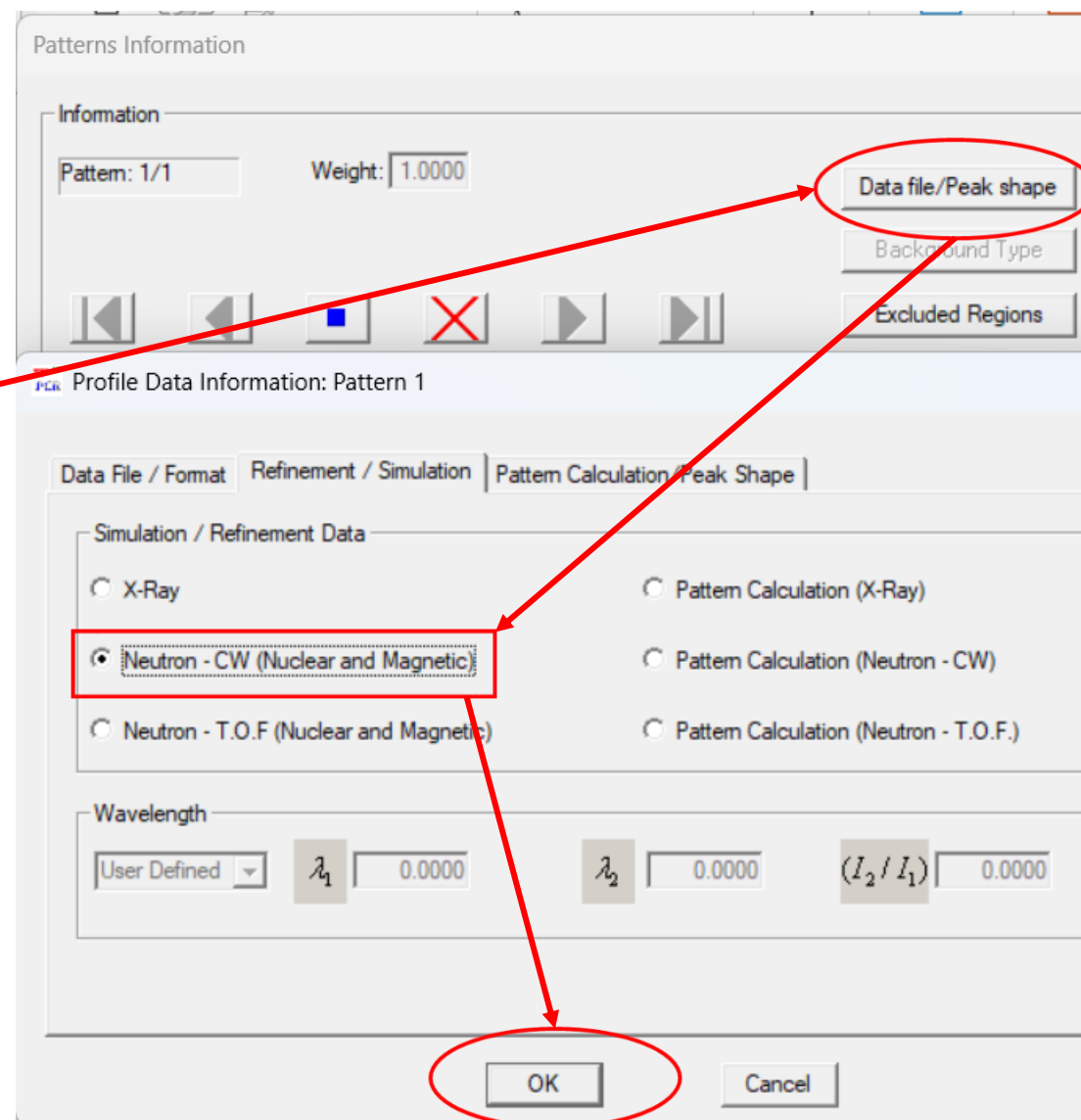
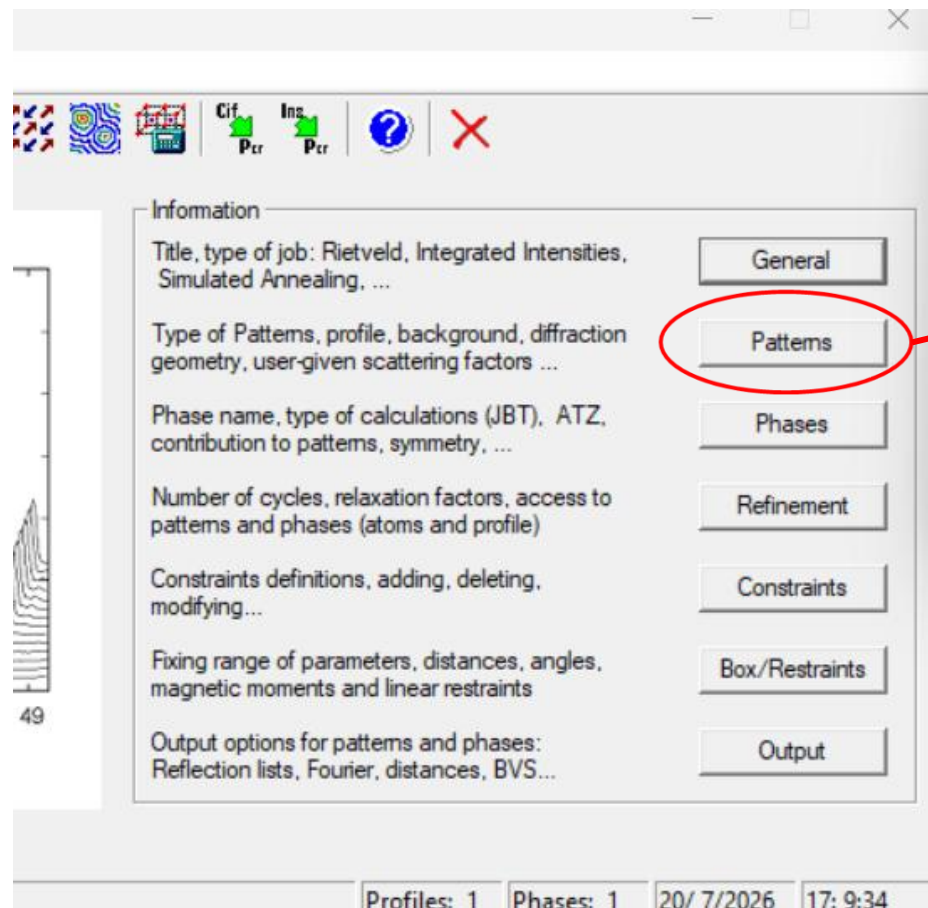
Step 0.1, Load .cif file into EdPCR



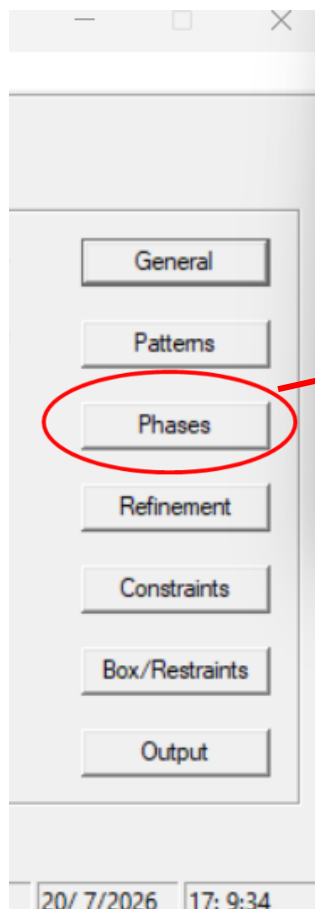
Step 0.2.1, Changing the .pcr into single crystal format



Step 0.2.2, Changing the.pcr into single crystal format



Step 0.2.3, Changing the .pcr into single crystal format



Phase Information: Phase 1

General Information on Phases

Name of Phase :

Calculation:

Coefficient to calculate the weight percentage of the Phase: ☐ Calculated automatically ☒ Provided by user

Contribution to patterns, preferred orientation direction, reflection list, ...

Space Group symbol/number, symmetry operators, basis functions, etc

Pattern Contribution Information for Phase 1

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

☒ Current Phase contributes to the pattern

Type of Pattern

☐ X-Ray ☐ Pattern Calculation (X-Ray)

☒ Neutron (Constant Wavelength) ☐ Pattern Calculation (Neutron - Constant Wavelength)

Nuclear and Magnetic

☐ Neutron (T.O.F.) ☐ Pattern Calculation (Neutron - T.O.F.)

Nuclear and Magnetic

Peak Shape

☒ Codefil.shp ☐ Global.shp

Intensities

Reflection list:

☐ Use special control of parameters for peak overlap, rejected reflections for current phase

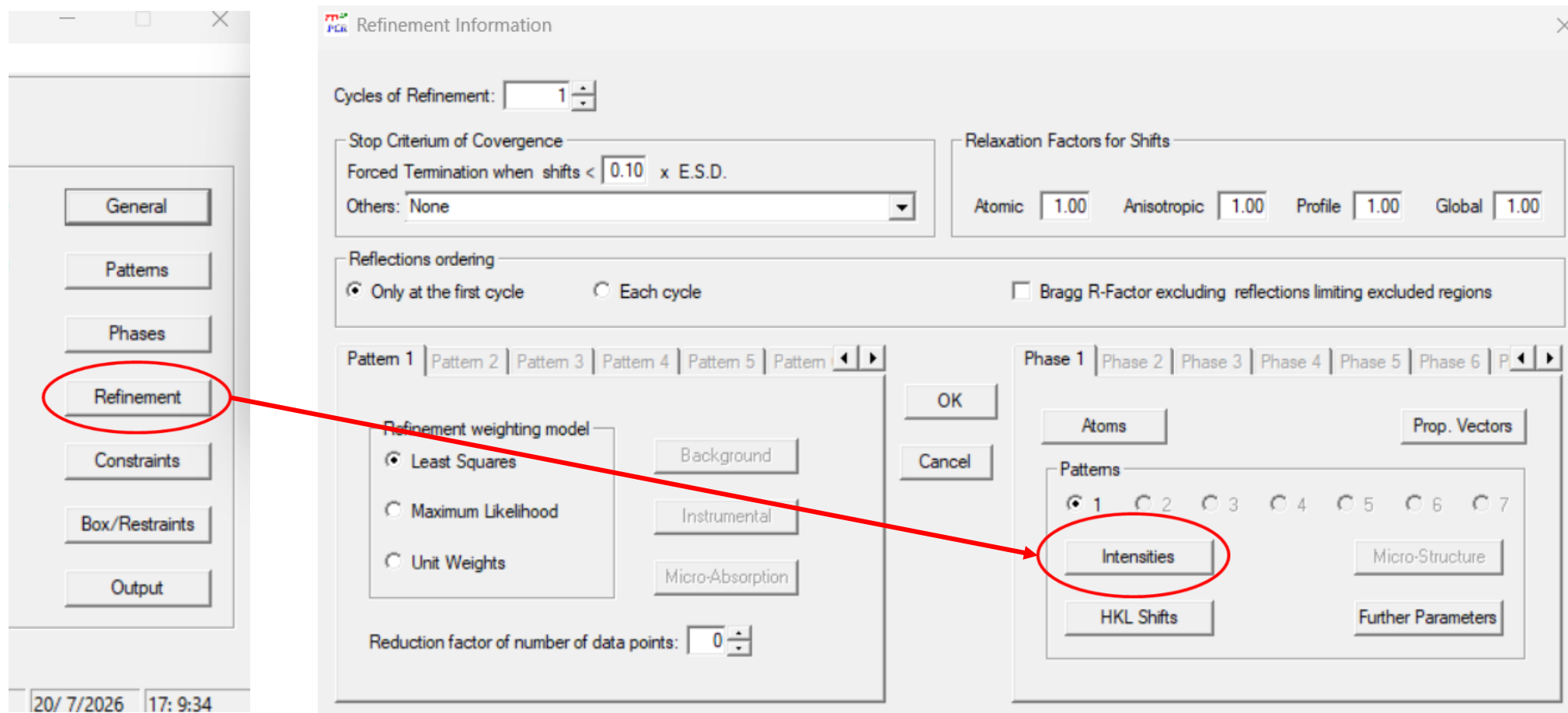
Brindley coefficient:

Global weight of the integrated intensity data vs profile data:

Factor for excluding reflections [< Factor * Sigma(I)]:

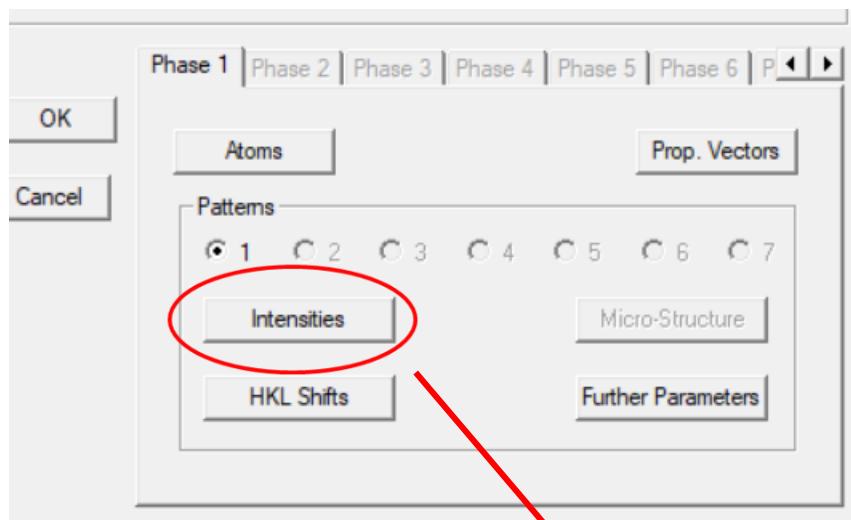
Weights are divide by reduced Chi**2 of precedent cycle:

Step 0.3.0, Integrity check



Single crystal pcr shows "Intensity" rather than "Profile"

Step 1.0, Refine the scale factor



Integrate Intensities: Phase 1 Pattern 1

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	4.77000	5.72000	4.92000	90.00	90.90	90.00

Scale Factors

	1	2	3	4	5	6
Coefficients	.10000E-02 ☒	0.0000 ☐	0.0000 ☐	0.0000 ☐	0.0000 ☐	0.0000 ☐

Extinction Parameters

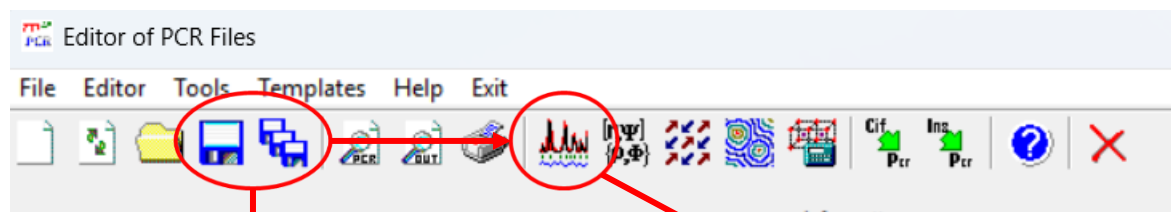
	1	2	3	4	5	6
Coefficients	0.0000 ☐	0.0000 ☐	0.0000 ☐	0.0000 ☐	0.0000 ☐	0.0000 ☐

Buttons: Refine All, Fix All, Cancel, OK

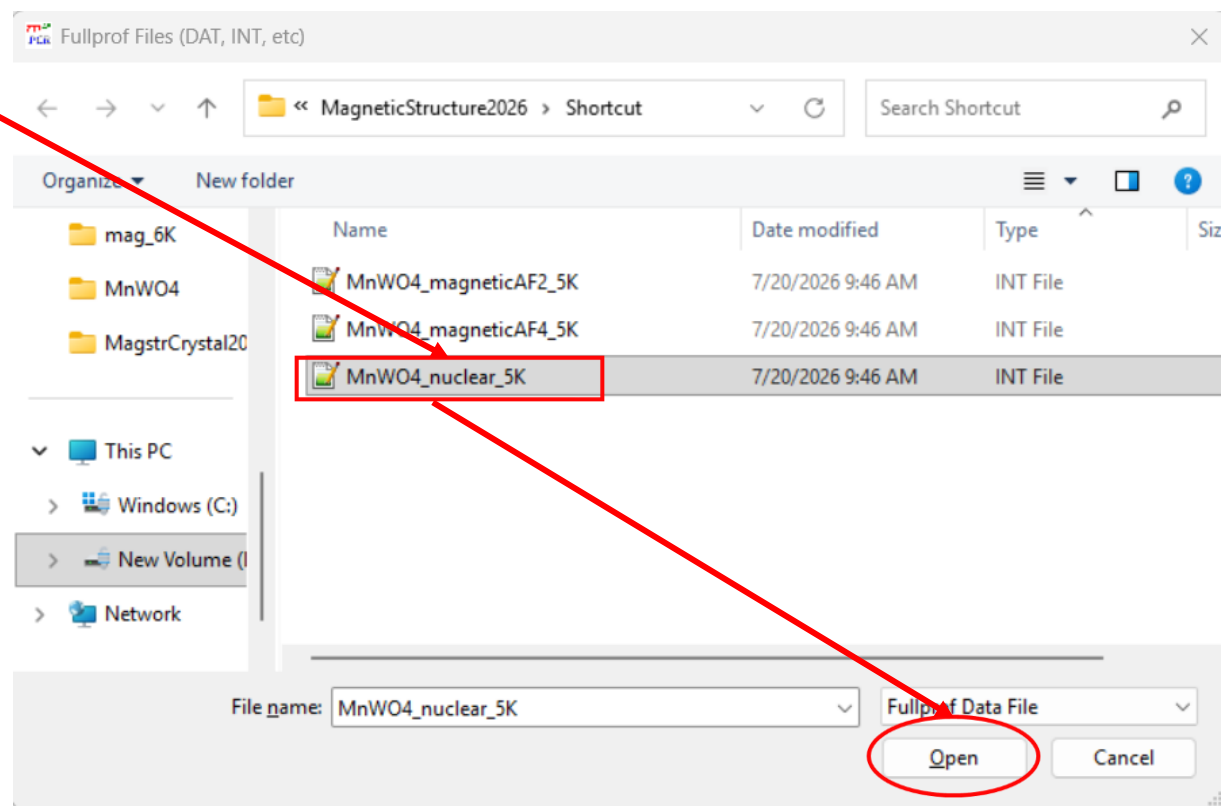
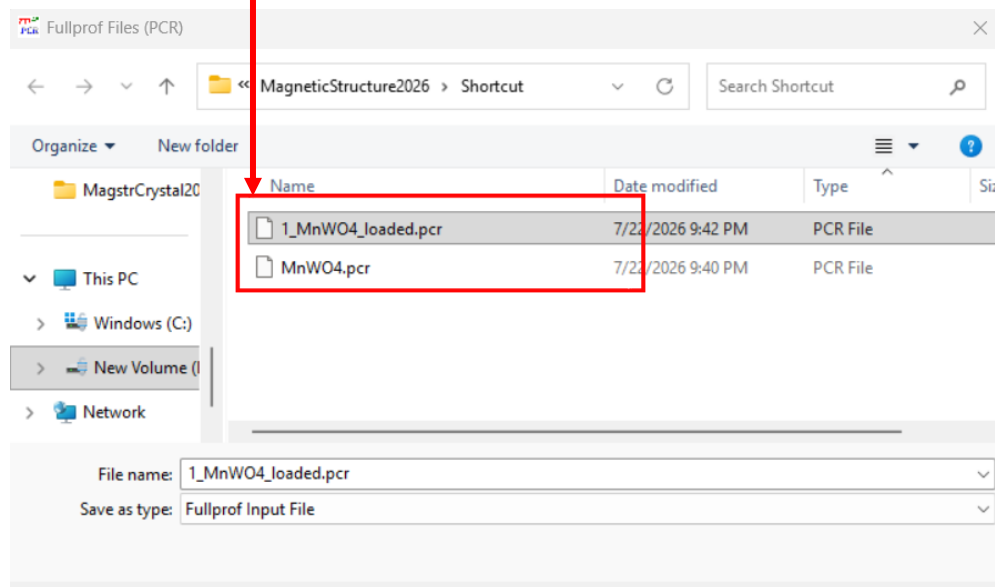
Refine the 1st Scale factor, Set all remaining parameters to 0

2nd, 3rd, .. Scale factors are used for multiple crystal domains

Step 1.1, Save .pcr and Run Fullprof



Always save
Constantly backup



Step 1.2, Validation of the crystal structure

```
FullProf Program
Load Edit PCR Mode Run Exit
Repeat "Run" till converge

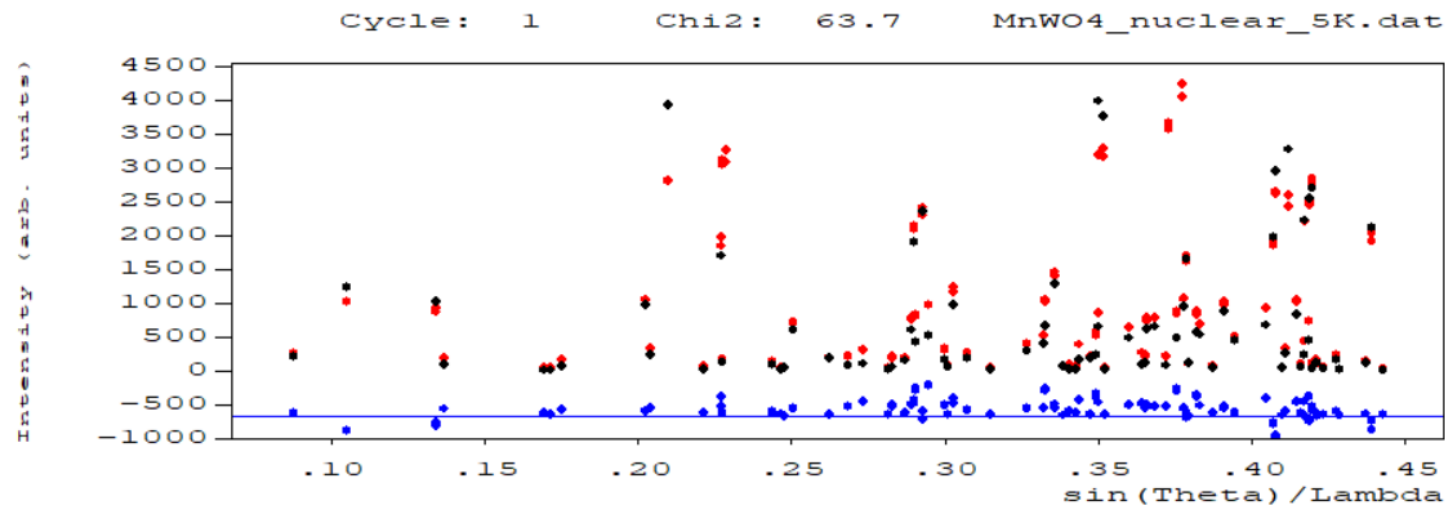
=> Convergence reached at this CYCLE !!!!!: CYCLE No.      1
=> Global user-weighted Chi2 (Bragg contrib.):    63.71
=> -----> Pattern#      1
=> Phase:      1
=> RF2 -factor :    30.45
=> RF2w-factor :    42.21
=> RF -factor :    16.78
=> Chi2(Intens):    63.71
=> N_eff Reflect.:    168 and    0.000    * sigma < Int
=> Normal end, final calculations and writing...

=> CPU Time:      0.441 seconds
=> 0.007 minutes

=> END   Date:22/07/2026   Time => 21:48:49.716
```

R-factors

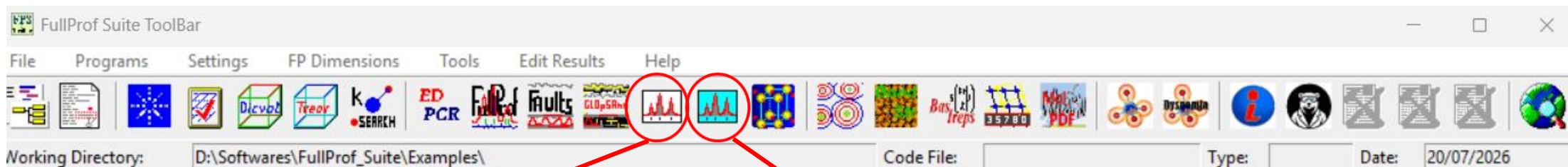
Recommend read: Toby 2006,
R-factors in Rietveld: How good is good enough?



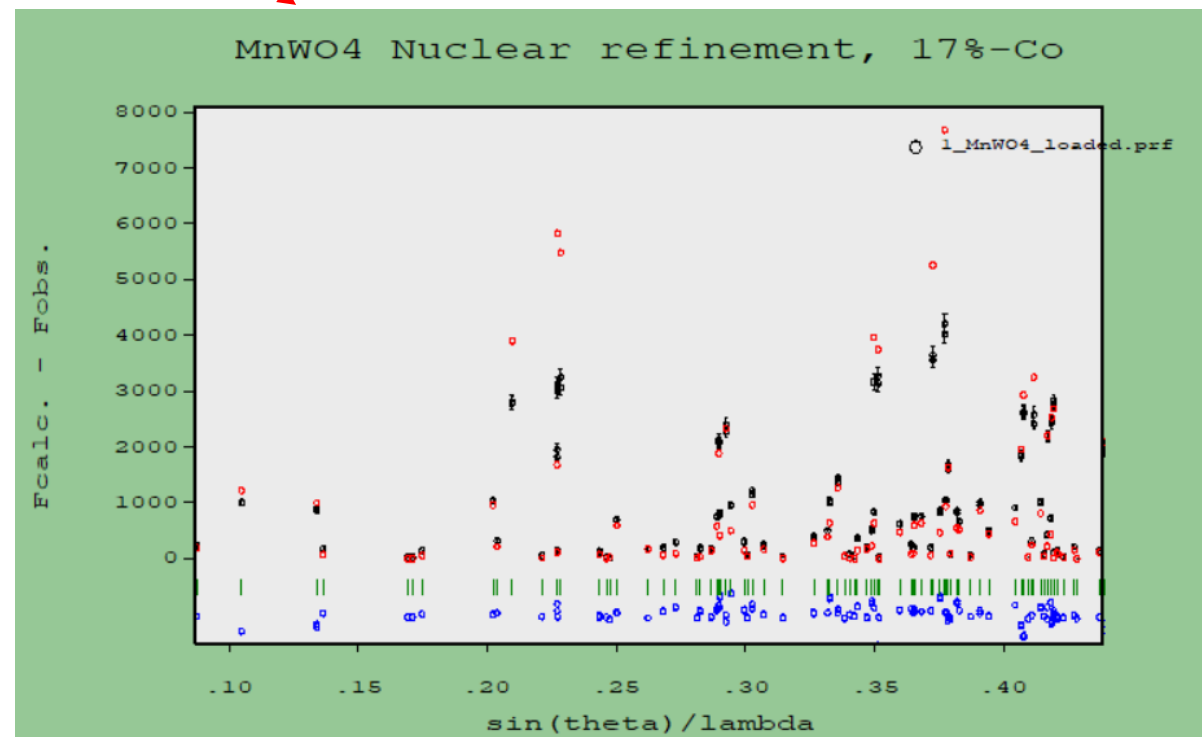
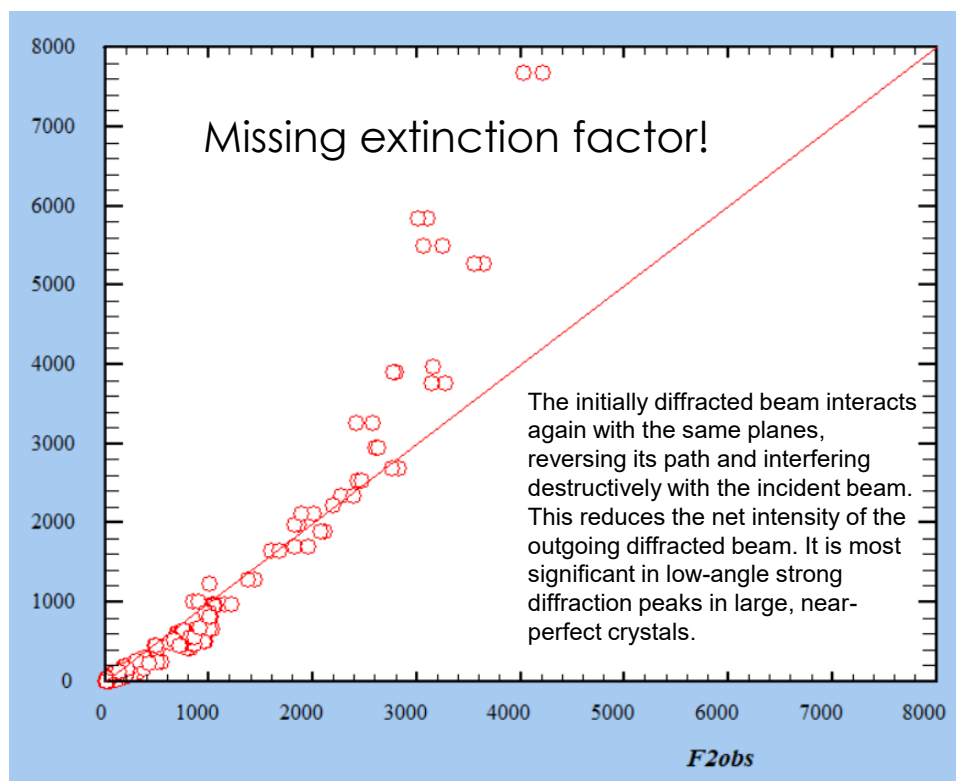
Calculated peak Intensity
Measured
Difference

$$2d\sin\theta = \lambda \rightarrow \frac{\sin\theta}{\lambda} = \frac{1}{2d} = 4\pi Q$$

Step 1.3, View refinement results in Winplotr



Open the .prf file in either version of Winplotr



Observed vs calculated (more often used)

Q vs Intensity



Step 1.4, Refine the extinction factor and atomic positions

Integrate Intensities: Phase 1 Pattern 1

Cell Parameters

	a	b	c
Coefficients	4.77000	5.72000	4.92000

Scale Factors

	1	2	3
Coefficients	242.90 ☒	0.0000 ☐	0.0000 ☐

Extinction Parameters

	1	2	3
Coefficients	1.0000 ☒	0.0000 ☐	0.0000 ☐

FullProf Program

Load Edit PCR Mode **Run** Exit

```
=> Convergence reached at this CYCLE !!!!!: CYCLE No.      1
=> Global user-weighted Chi2 (Bragg contrib.):    31.84
=> -----> Pattern#      1
=> Phase:      1
=> RF2 -factor :    10.43
=> RF2w-factor :    29.84
=> RF -factor :     8.331
=> Chi2(Intens):    31.84
=> N_eff Reflect.:    168 and    0.000    * sigma < Int
=> Normal end, final calculations and writing...

=> CPU Time:      0.610 seconds
=> 0.010 minutes

=> END    Date:22/07/2026    Time => 22:21:21.489
```

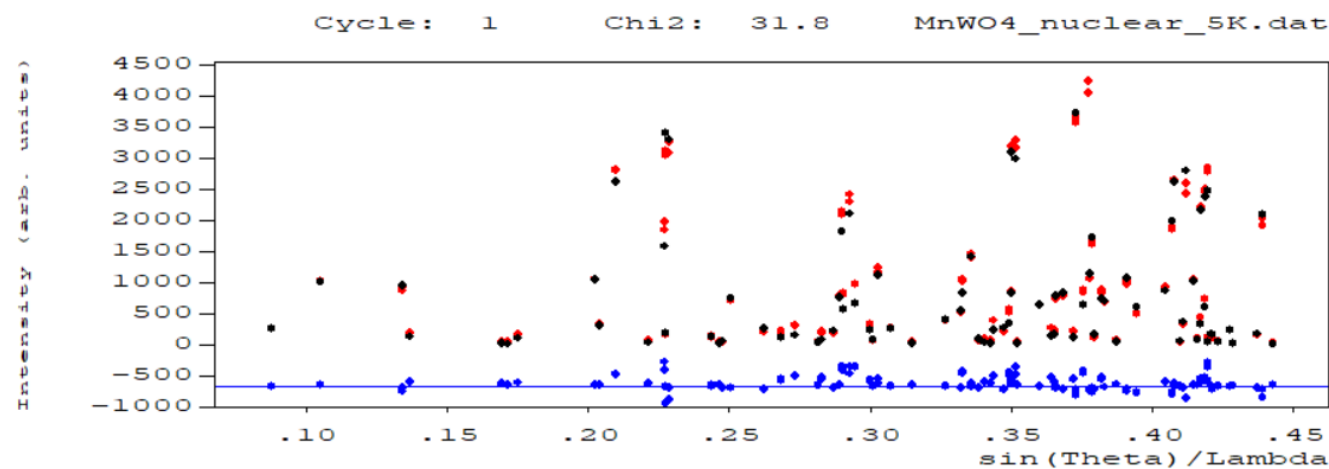
Refine both the SF and the extinction parameter

Scale Factors

	1	2
Coefficients	374.70 ☒	0.0000 ☐

Extinction Parameters

	1	2
Coefficients	45.460 ☒	0.0000 ☐



Step 1.4, Refine the atomic positions and B-factors

Atoms Information: Phase 1

List of Atoms

Number of Atoms: 4

	Label	Ntyp	X		Y		Z		B		Occ		Them. Fact.
Atom # 1	Mn1	MN	0.50000	☒	0.68480	☒	0.25000	☒	0.70272	☒	0.50000	☒	Isotropic
Atom # 2	W1	W	0.00000	☒	0.18010	☒	0.25000	☒	0.83694	☒	0.50000	☒	Isotropic
Atom # 3	O1	O	0.21090	☒	0.10362	☒	0.94030	☒	0.74219	☒	1.00000	☒	Isotropic
Atom # 4	O2	O	0.25110	☒	0.37542	☒	0.39380	☒	0.79746	☒	1.00000	☒	Isotropic

Anisotropic Thermal Factors / Form Factors

	B11/F1		B22/F2		B33/F3		B12/F4		B13/F5		B23/F6		F7	
#		☐		☐		☐		☐		☐		☐		☐
#		☐		☐		☐		☐		☐		☐		☐
#		☐		☐		☐		☐		☐		☐		☐
#		☐		☐		☐		☐		☐		☐		☐

Special Form Factors

	SASH-Type	Matrix	j=1	j=2	j=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
#	Spherical												
	Spherical												
	Spherical												

Refine Positions

Refine B_iso

Refine B_aniso

Fix All

Cancel

OK

B_{aniso} and atomic occupancies can be refined based on need of study and confidence in data quality. For this example, refining only B_{iso} is suffice

Step 1.4, Refine the atomic positions and B-factors

FullProf Program

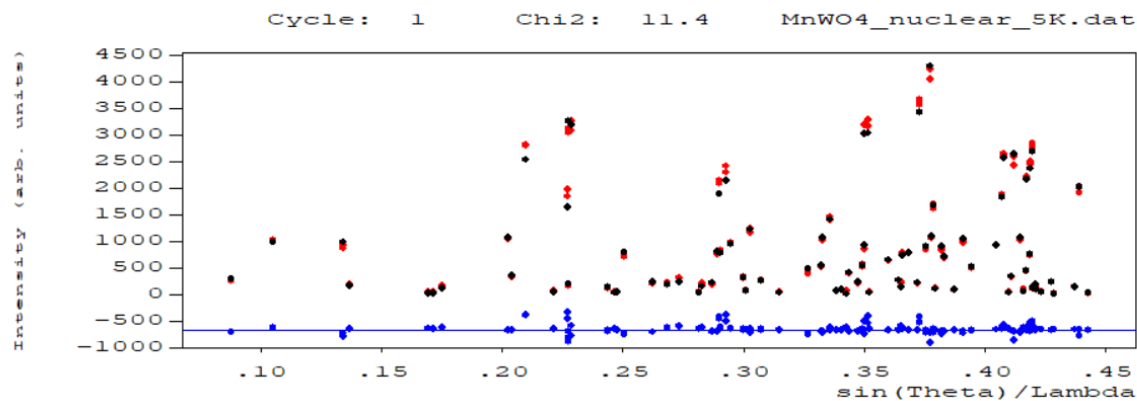
Load Edit PCR Mode Run Exit

```
=> Writing results for cycle 1
=> Global user-weighted Chi2 (Bragg contrib.): 11.37
=> -----> Pattern# 1
=> Phase: 1
=> RF2 -factor : 5.758
=> RF2w-factor : 17.18
=> RF -factor : 4.185
=> Chi2(Intens): 11.37
=> N_eff Reflect.: 168 and 0.000 * sigma < Int
=> Conv. not yet reached -> [Max] Shift( X_O2)/(eps*Sigma)= -1.27 abs> 1
=> Normal end, final calculations and writing...
```

=> CPU Time: 0.426 seconds

=> 0.007 minutes

=> END Date:22/07/2026 Time => 22:30:00.767



Number of Atoms: 4

	Label	Ntyp	X	Y	Z	B	Occ	Them. Fact.
Atom # 1	Mn1	MN	0.50000	0.68511	0.25000	2.98730	0.50000	Isotropic
Atom # 2	W1	W	0.00000	0.18058	0.25000	0.82779	0.50000	Isotropic
Atom # 3	O1	O	0.21140	0.10285	0.94092	0.99620	1.00000	Isotropic
Atom # 4	O2	O	0.25434	0.37546	0.39358	0.93564	1.00000	Isotropic

Almost there but something feels off..
Because we forgot the Co-doping!

Refine Positions

Refine B_iso

Refine B_aniso

Fix All

Step 1.5, Adding Co atoms

List of Atoms

Number of Atoms: **5** **Add a new atom**

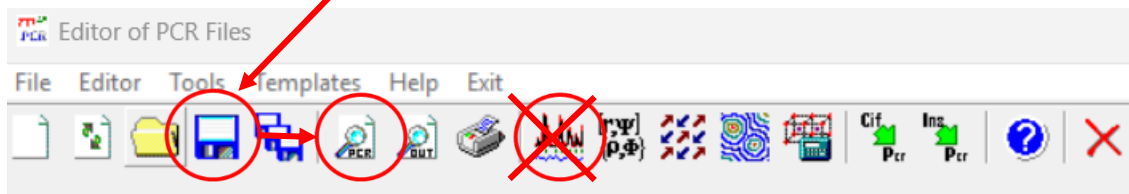
Copy whole line of Mn, change Occ to 0.4 (80%)

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Mn1	MN	0.50000	0.68509	0.25000	2.99266	0.40000	Isotropic
Atom # 2	W1	W	0.00000	0.18056	0.25000	0.83062	0.50000	Isotropic
Atom # 3	O1	O	0.21144	0.10279	0.94092	1.00150	1.00000	Isotropic
Atom # 4	O2	O	0.25430	0.37545	0.39361	0.94421	1.00000	Isotropic

Atom # 2	W1	W	0.00000	0.18056	0.25000	0.83062	0.50000	Isotropic
Atom # 3	O1	O	0.21144	0.10279	0.94092	1.00150	1.00000	Isotropic
Atom # 4	O2	O	0.25430	0.37545	0.39361	0.94421	1.00000	Isotropic
Atom # 5	Co1	Co	0.50000	0.68509	0.25000	2.99266	0.10000	Isotropic

Paste to new atom, change new atom to Co and set Occ = 0.1 (20%), refine Occ

Save and edit .pcr (or open .pcr in any text editor). DO NOT RUN REFINEMENT!



Nominal is 83% Mn and 17% Co

We want to replace some Mn by Co without changing the total occupancy

Occupancy in Fullprof is defined related to the SG symmetry and Wyckoff positions. In this case, P 2/c has 4 symmetry operations. Mn1 and W1 are at 2e and 2f Wyckoff positions. Hence their occ in Fullprof are $2(\text{atom})/4(\text{symmetry operations}) = 0.5$

It probably is written this way because someone wanted to simply loop through all symmetries and duplicate all atoms when generating a unit cell..

Step 1.6, Constraining Mn and Co

```
15 !Number of refined parameters
-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 0.0000
-----
MnWO4 Nuclear refinement, 17%-Co
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
  5  0  0  0.0 0.0 1.0  0  4  0  0  0      605.571    0  0  0
!
!
P 1 2/c 1
!Atom Typ      X      Y      Z      Biso      Occ      In Fin N_t Spc /Codes
Mn1  MN      0.50000 0.68509 0.25000 2.99266 0.40000  0  0  0  0
      0.00      41.00      0.00      21.00 -151.00
W1   W      0.00000 0.18056 0.25000 0.83062 0.50000  0  0  0  0
      0.00      81.00      0.00      61.00 0.00
O1   O      0.21144 0.10279 0.94092 1.00150 1.00000  0  0  0  0
      111.00 121.00 131.00 101.00 0.00
O2   O      0.25430 0.37545 0.39361 0.94421 1.00000  0  0  0  0
      91.00  71.00  51.00 141.00 0.00
Co1  Co      0.50000 0.68509 0.25000 2.99266 0.10000  0  0  0  0
      0.00      41.00      0.00      21.00 151.00
```

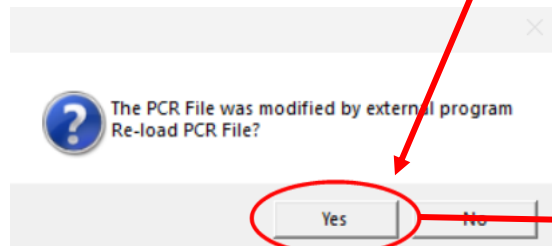
Copy the control code of Co occ (151.00 in this case),
paste it to Mn, change it to negative

Control code defines the refining parameters
and the constraints among them.

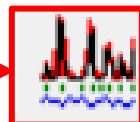
In this case, 151.00 means Co occ. is constrained to the
15th parameter in refinement and will iterate by the
relative speed of 1.00; -151.00 means Mn occ. is
constrained to the same parameter but will iterate by
the relative speed of -1.00.

Note: Y and Biso of Mn and Co are also constrained.

Multiplicity and decimal are allowed. E.g., it is possible
to constrain a parameter by using control code 150.50
or 152.00, which will cause the parameter to move by
half or twice much compared to another parameter
using 151.00



Save, reload, run

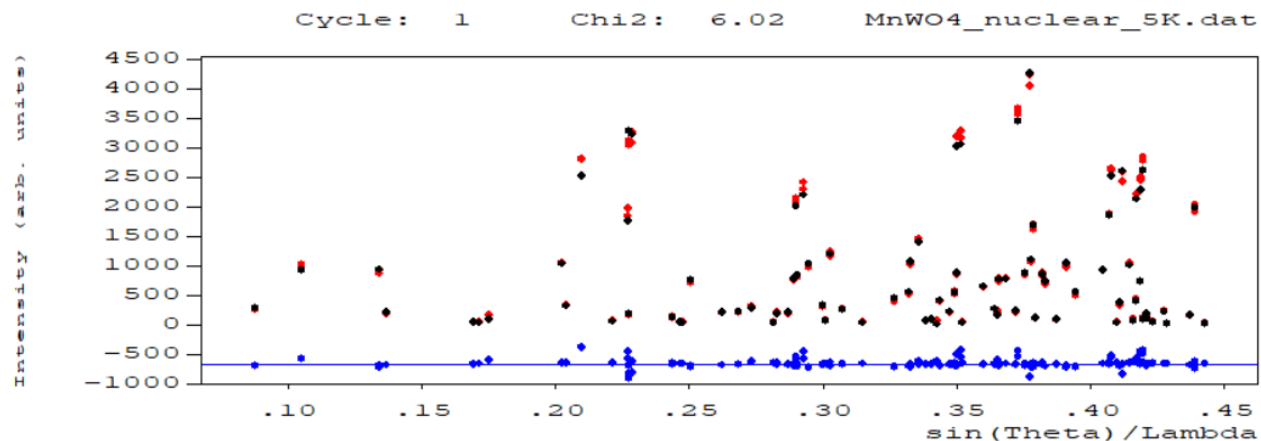


Step 1.7, Refine the Mn and Co occupancy

```
=> Convergence reached at this CYCLE !!!!!: CYCLE No.      1
=> Global user-weighted Chi2 (Bragg contrib.):    6.016
=> -----> Pattern#      1
=> Phase:      1
=>   RF2 -factor :    5.188
=>   RF2w-factor :   12.46
=>   RF  -factor :    3.468
=>   Chi2(Intens):    6.016
=>   N_eff Reflect.:   168 and    0.000    * sigma < Int
=> Normal end, final calculations and writing...
```

```
=> CPU Time:      1.209 seconds
=> 0.020 minutes
```

```
=> END   Date:22/07/2026   Time => 23:38:43.072
```



List of Atoms

Number of Atoms: 5

	Label	Ntyp	X	Y	Z	B	Occ
Atom # 1	Mn1	MN	0.50000	0.68449	0.25000	0.85033	0.41882
Atom # 2	W1	W	0.00000	0.18021	0.25000	1.12237	0.50000
Atom # 3	O1	O	0.21233	0.10301	0.94049	1.36822	1.00000
Atom # 4	O2	O	0.25370	0.37546	0.39455	1.33879	1.00000
Atom # 5	Co1	Co	0.50000	0.68449	0.25000	0.85033	0.08118

Note the constrained parameters are showing red

Step 1.8, half lambda refinement

Check numbers of parameter here

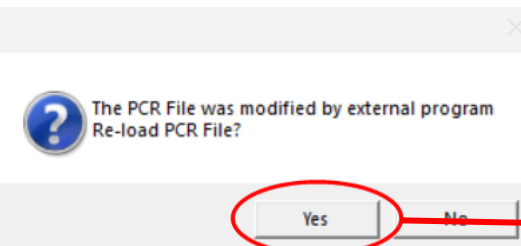
```
15 !Number of refined parameters
-----
Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 0.0000
-----
MnWO4 Nuclear refinement, 17%-Co
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
5 0 0 0.0 0.0 1.0 0 4 0 0 0 606.869 0 0 0
!
P 1 2/c 1 <--Space group symbol
!Atom Typ X Y Z Biso Occ In Fin N_t spc /Codes
Mn1 MN 0.50000 0.68449 0.25000 0.85033 0.41882 0 0 0 0
0.00 41.00 0.00 21.00 -151.00
w1 w 0.00000 0.18021 0.25000 1.12237 0.50000 0 0 0 0
0.00 81.00 0.00 61.00 0.00
o1 o 0.21233 0.10301 0.94049 1.36822 1.00000 0 0 0 0
111.00 121.00 131.00 101.00 0.00
o2 o 0.25370 0.37546 0.39455 1.33879 1.00000 0 0 0 0
91.00 71.00 51.00 141.00 0.00
Co1 Co 0.50000 0.68449 0.25000 0.85033 0.08118 0 0 0 0
0.00 41.00 0.00 21.00 151.00
!-----> scale, Extinction and cell Parameters for Pattern # 1
! Scale Factors
! Sc1 Sc2 Sc3 Sc4 Sc5 Sc6
544.3 0.000 0.000 0.000 0.000 0.000 0.000
11.00 0.00 0.00 0.00 0.00 0.00
! Extinction Parameters
! Ext1 Ext2 Ext3 Ext4 Ext5 Ext6 Ext7 Ext-Model
98.15 0.000 0.000 0.000 0.000 0.000 0.000 0.000 1
31.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma # Cell Info
4.770000 5.719997 4.920001 90.000000 90.900047 90.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! x-Lambda/2
0.01000
161.00
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
0.087 150.000 1
```

set lambda/2 to 0.01 and give an unused control code

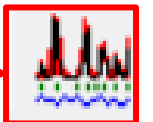
Lambda/2 contamination comes from the higher order reflection of the Si (220) monochromator. It only exist for the ~1.54 Å wavelength and can be drastically reduced using a PG-filter.

Without PG filter: ~1% to 2% in flux

With PG filter: ~0.05% to 0.1% in flux



Save, reload, run



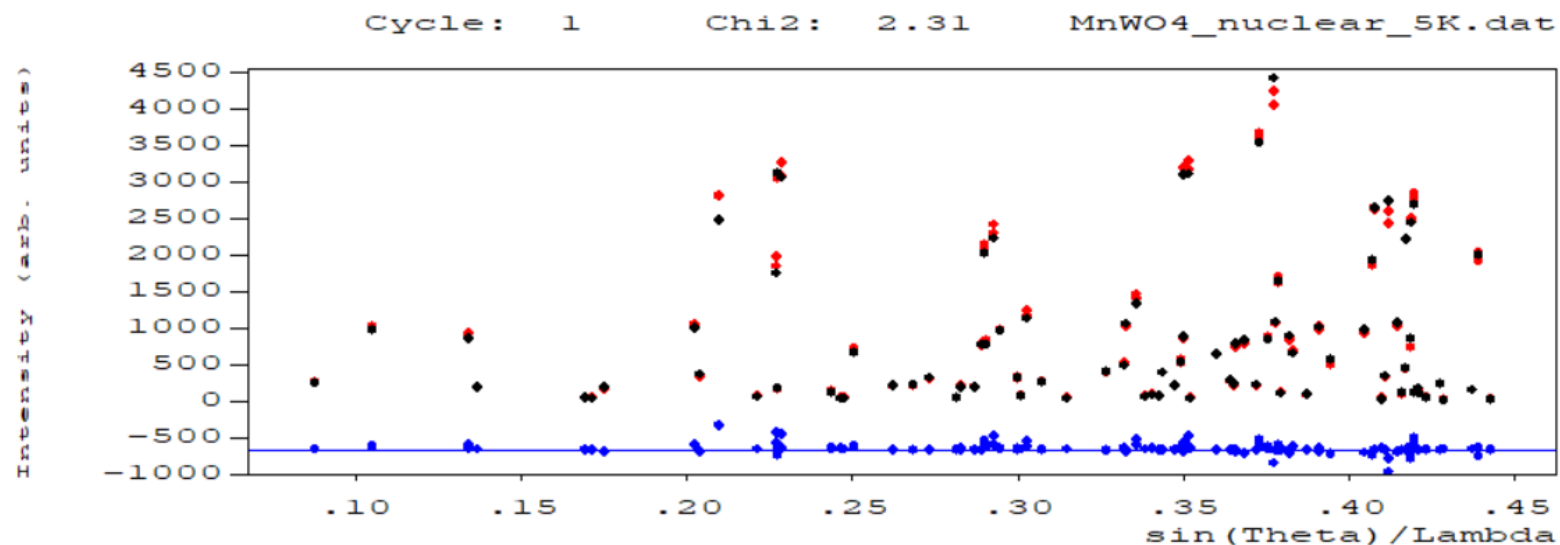
Step 1.9, Finalize the refinement

```
=> Convergence reached at this CYCLE !!!!!: CYCLE No.      1
=> Global user-weighted Chi2 (Bragg contrib.):    2.309
=> -----> Pattern#      1
=> Phase:      1
=>   RF2 -factor :    4.419
=>   RF2w-factor :    7.718
=>   RF  -factor :    2.495
=>   Chi2(Intens):    2.309
=>   N_eff Reflect.:    168 and    0.000    * sigma < Int
=> Normal end, final calculations and writing...
```

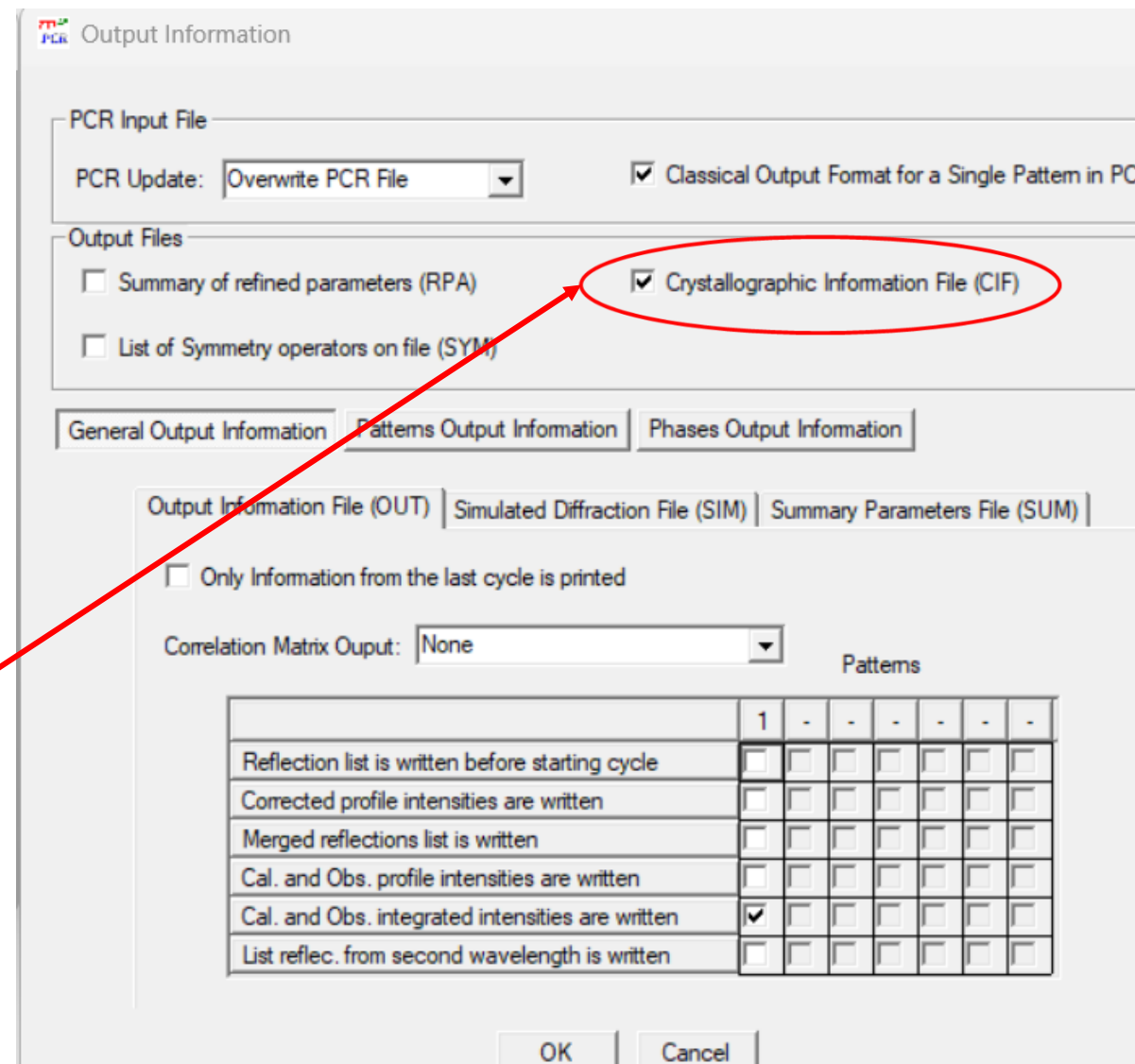
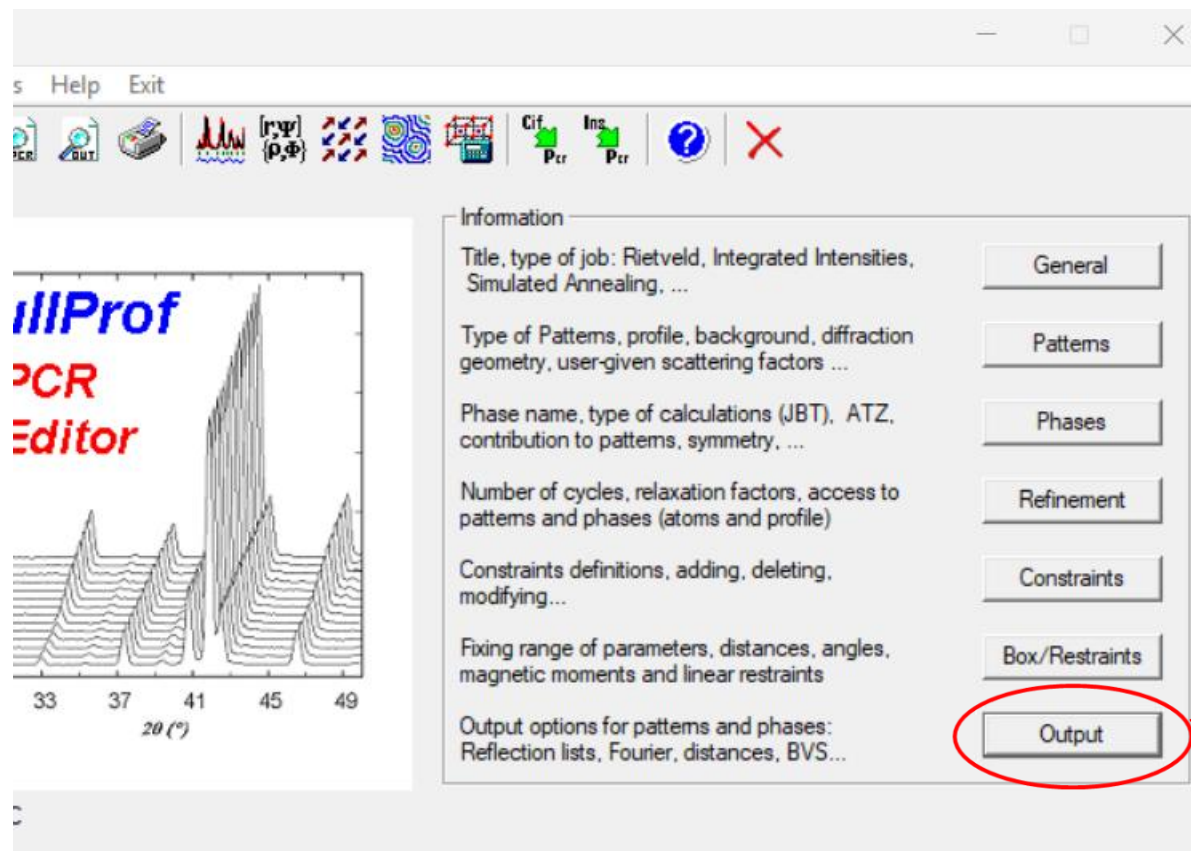
```
=> CPU Time:      0.945 seconds
```

```
=> 0.016 minutes
```

```
=> END   Date:22/07/2026   Time => 23:53:14.757
```



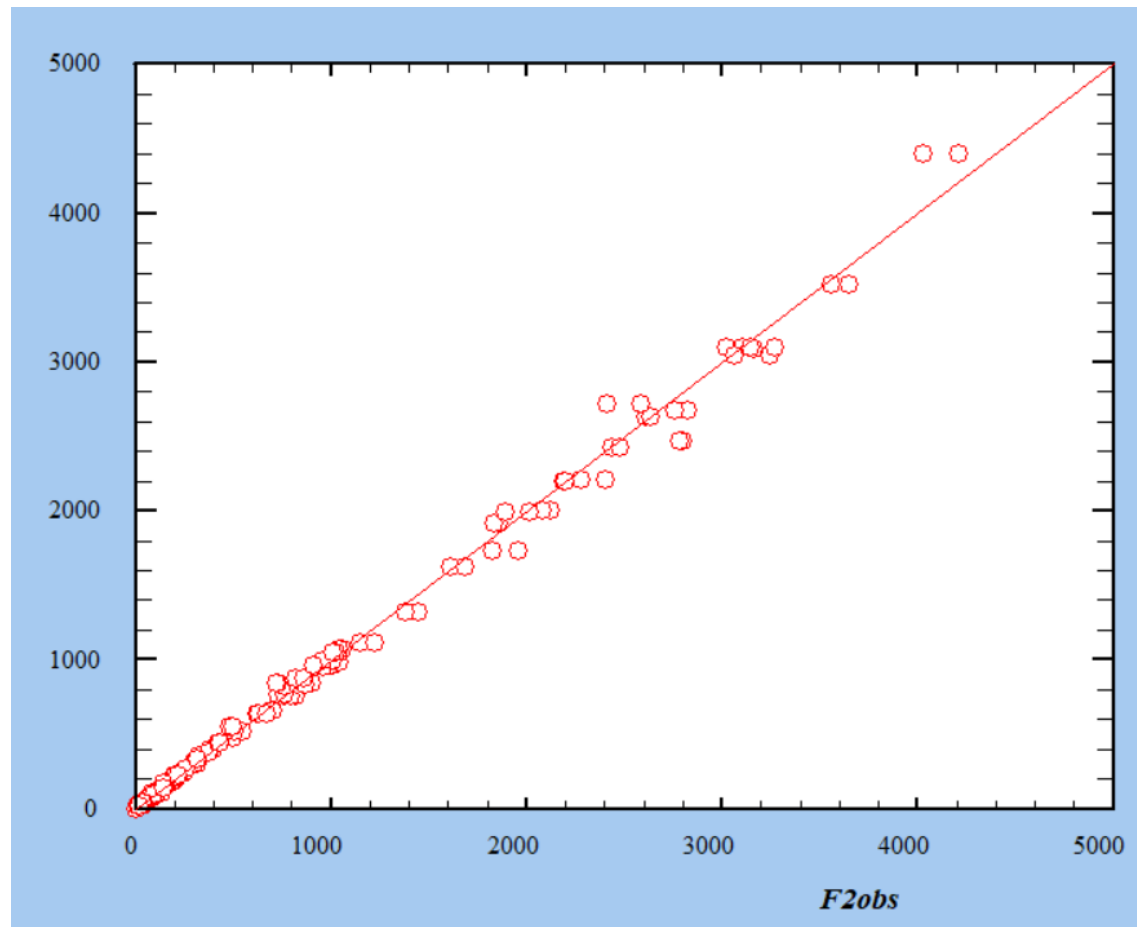
Step 1.10, Output the .cif file



Step 1.11, Visualize the Results



MnCoWO4_5K.prf



MnCoWO4_5K.sum

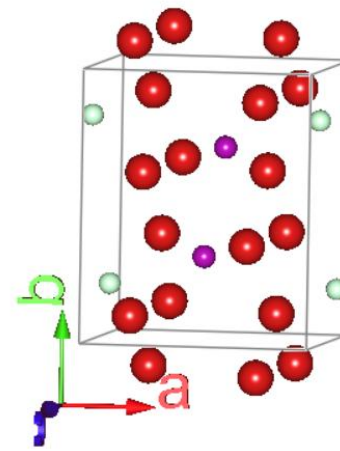
=> Phase No. 1 MnWO4 Nuclear refinement, 17%-Co P 1 2/c 1

=> No. of reflections for pattern#: 1: 168

==> ATOM PARAMETERS:

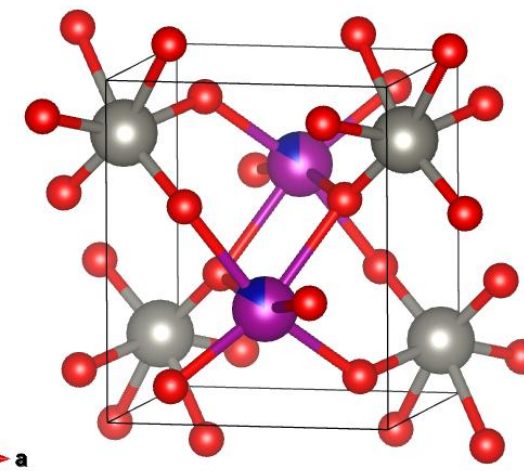
Name	x	sx	y	sy	z	sz	B	SB	occ.	socc.	Mult
Mn1	0.50000(0)		0.68488(57)		0.25000(0)		0.629(123)		0.417(2)		2
W1	0.00000(0)		0.18006(33)		0.25000(0)		0.758(63)		0.500(0)		2
O1	0.21100(23)		0.10360(20)		0.94038(26)		0.670(44)		1.000(0)		4
O2	0.25102(30)		0.37544(14)		0.39396(27)		0.726(45)		1.000(0)		4
Co1	0.50000(0)		0.68488(57)		0.25000(0)		0.629(123)		0.083(2)		2

MnCoWO4_5K.fst



(FPStudio)

MnCoWO4_5K.cif



(VESTA)

Step 2.1.0, Generate a magnetic phase for $k = (0.5, 0, 0)$.

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Space-group symmetry

Magnetic Symmetry and Applications

Magnetic groups

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones 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 2.1.1, Generate a magnetic .mcif for $k = (0.5, 0, 0)$

Enter the serial number of the space group of the parent paramagnetic phase:

choose it 13

[Choose an alternative magnetic group](#)

Space group P 2/c (No. 13)

Introduce the magnetic wave vector(s)

[Alternatively give the basis vectors of the supercell](#)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} 0.5 k_{1y} 0 k_{1z} 0

[Show the independent vectors of the star](#)

☐ Choose the whole star of the propagation vector

[More wave-vectors needed](#)

$k = (0.5, 0, 0)$

•
•
•

☒ List of subgroups

☐ Graph of subgroups

Submit

Scroll to bottom and “Submit”

Step 2.1.2, Generate a magnetic .mcif for k = (0.5, 0, 0)

Input data

Subgroups of the paramagnetic space group :
Lowest magnetic space group to consider:
Magnetic propagation wave-vectors

$P2/c1'$ (N. 13)
 $P1$ (N. 1.1)
(0.5,0,0)

List of subgroups that fulfill the given conditions

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P_a2/c (No. 13.70)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps	☒
2	P_a2/c (No. 13.70)	$\begin{pmatrix} 2 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -2 & 0 & -1 & 0 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps	☒
3	P_a2/c (No. 13.70)	$\begin{pmatrix} 2 & 0 & 2 & 1/2 \\ 0 & 1 & 0 & 0 \\ -2 & 0 & -1 & 0 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps	☒
4	P_a2/c (No. 13.70)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps	☒
5	$P_a c$ (No. 7.27)	$\begin{pmatrix} 2 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -2 & 0 & -1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐
6	$P_a c$ (No. 7.27)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps	☐

•
•
•

Select/Deselect all subgroups
☒ Include structure data of the parent phase

Submit selected subgroups to MAGMODELIZE: Submit

Start by selecting the maximum Magnetic Space Groups (MSGs)

Note they are the same MSG but of different super cell selection. This is because the parent SG is monoclinic, hence a- and c- axis can have multiple choices.

Do “Include structure data” and Submit

Step 2.1.3, Generate a magnetic .mcif for $k = (0.5, 0, 0)$

Parent paramagnetic structure cif file

Option 1: Please submit a structure file (CIF format):

2_MnCoWO4_5K.cif

Note: The space group of the cif file will supersede any previous one.

Select the refinement output .cif file and Upload

Parent phase structure data: Magnetic Atoms

Parent space group: *P2/c* (No. 13)

Unit cell parameters (Angstroms and degrees): $a=4.77000$, $b=5.72000$, $c=4.92000$, $\alpha=90.0000$, $\beta=90.9000$, $\gamma=90.0000$

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Occupancies	Magnetic?
1	Mn1	Mn	2f	0.50000 0.68490 0.25000	0.833	☒
2	W1	W	2e	0.00000 0.18010 0.25000	1	☐
3	O1	O	4g	0.21100 0.10360 0.94040	1	☐
4	O2	O	4g	0.25100 0.37544 0.39400	1	☐
5	Co1	Co	2f	0.50000 0.68490 0.25000	0.167	☐

Choose Mn as the magnetic atom

Step 2.1.4, Generate a magnetic .mcif for $k = (0.5, 0, 0)$

Selected magnetic space subgroup for the parent space group $P2/c$ (No. 13)

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	P_a2/c (#13.70) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	P_a2/c (#13.70) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 \\ -2 & 0 & -1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	P_a2/c (#13.70) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 2 & 1/2 \\ 0 & 1 & 0 & 0 \\ -2 & 0 & -1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	P_a2/c (#13.70) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

mCIFs of the transformed structure in the selected subgroups ('ksubgroupsmag_mCIFs_3411932.zip')

Download the whole .zip file

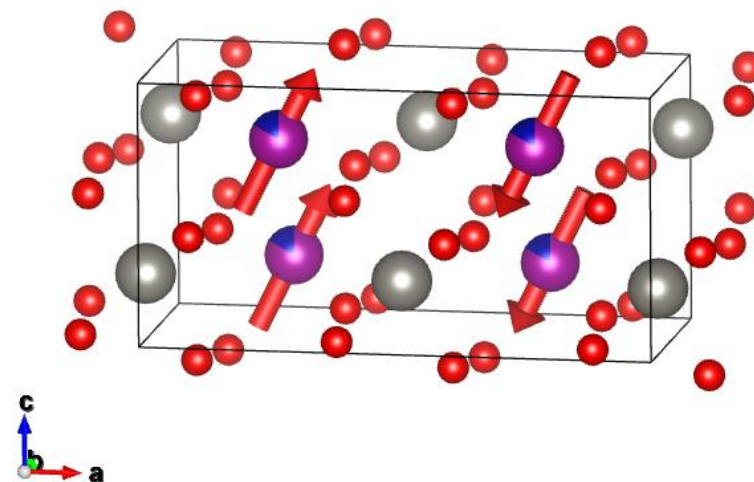
Step 2.1.4.1, How to fast examine a .mcif file

```
3.mcif
84 loop_
85   _atom_site_label
86   _atom_site_type_symbol
87   _atom_site_fract_x
88   _atom_site_fract_y
89   _atom_site_fract_z
90   _atom_site_occupancy
91 Mn1 Mn 0.25000 0.68490 0.25000 0.833
92 W1 W 0.00000 0.18010 0.25000 1.
93 O1 O 0.10550 0.10360 0.94040 1.
94 O2 O 0.12550 0.37544 0.39400 1.
95 Co1 Co 0.25000 0.68490 0.25000 0.167
96
97 loop_
98   _atom_site_moment.label
99   _atom_site_moment.crystalaxis_x
100  _atom_site_moment.crystalaxis_y
101  _atom_site_moment.crystalaxis_z
102  _atom_site_moment.symmform
103 Mn1 1.00000 0.00000 2.00000 mx,0,mz
```

Open the .mcif file using a text editor, scroll to bottom, change the symmetry allowed magnetic moments to non-zero numbers.



Save and Open the edited .mcif file in Vesta:



Step 2.2, Convert an .mcif into .pcr

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Space-group symmetry

Magnetic Symmetry and Applications

Magnetic groups	
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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

mCIF2PCR: Transformation from mCIF to PCR format (FullProf).

it can be used as (rof) is used). By tion. The file can

Choose a structure file (mCIF format):

Choose File 2.mcif Convert

The file has been successfully converted.

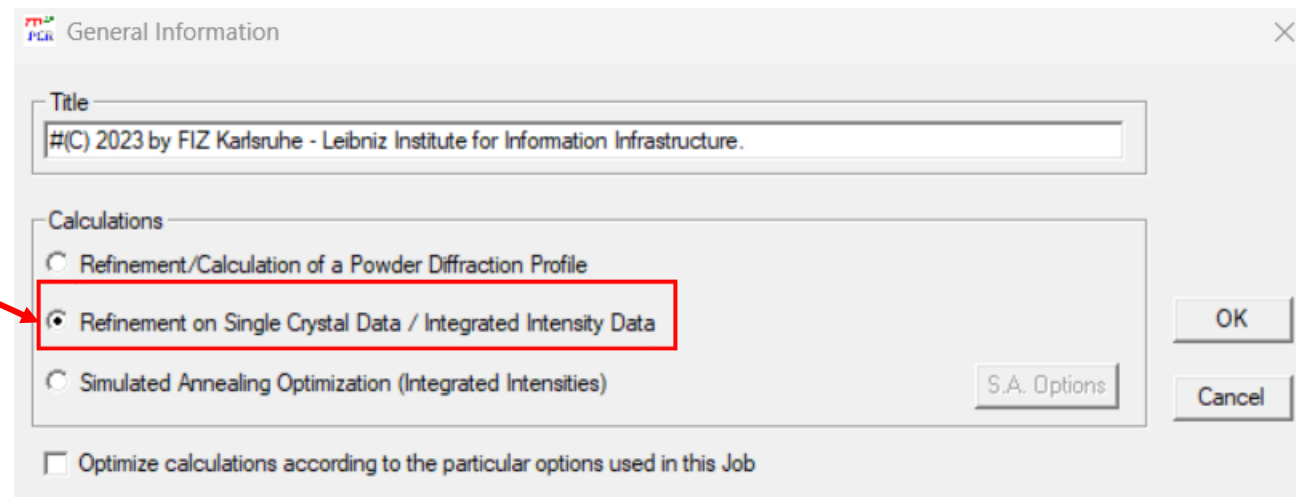
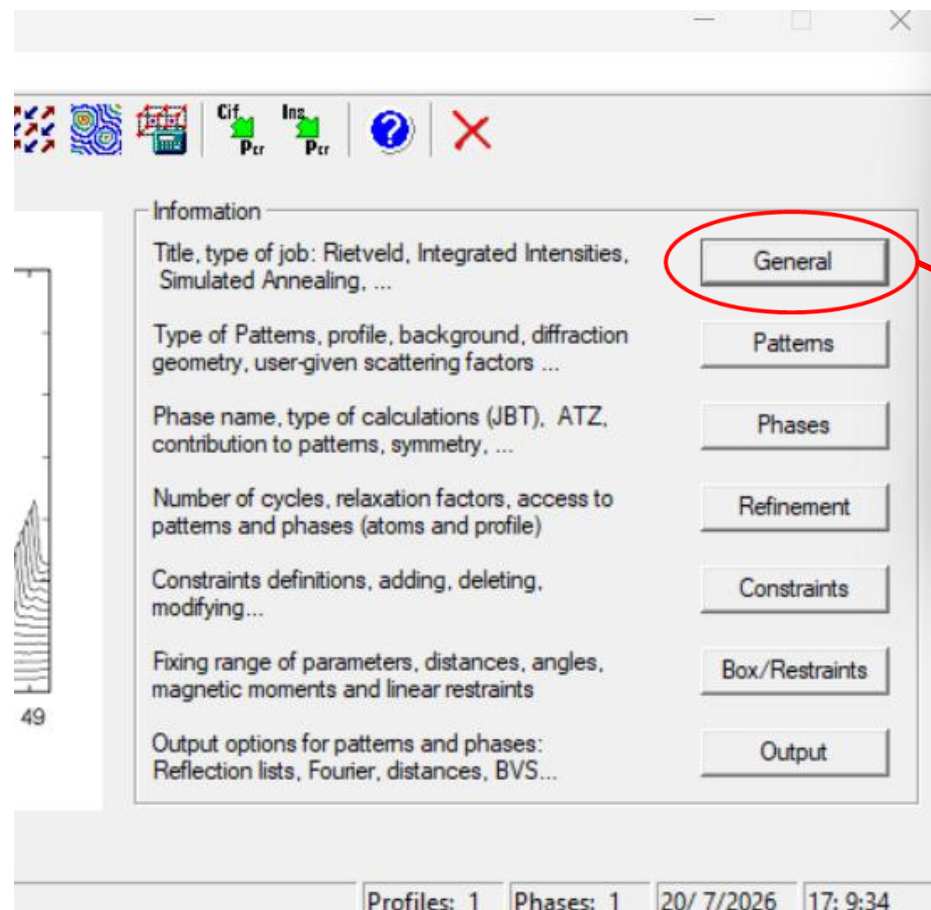
[Click to download it](#)

```
Windows PowerShell
PS D:\Softwares> cd..
PS D:\> cd .\Softwares\FullProf_Suite\
PS D:\Softwares\FullProf_Suite> .\mCIF_to_PCR.exe d:\3.mcif
d:\3.mcif

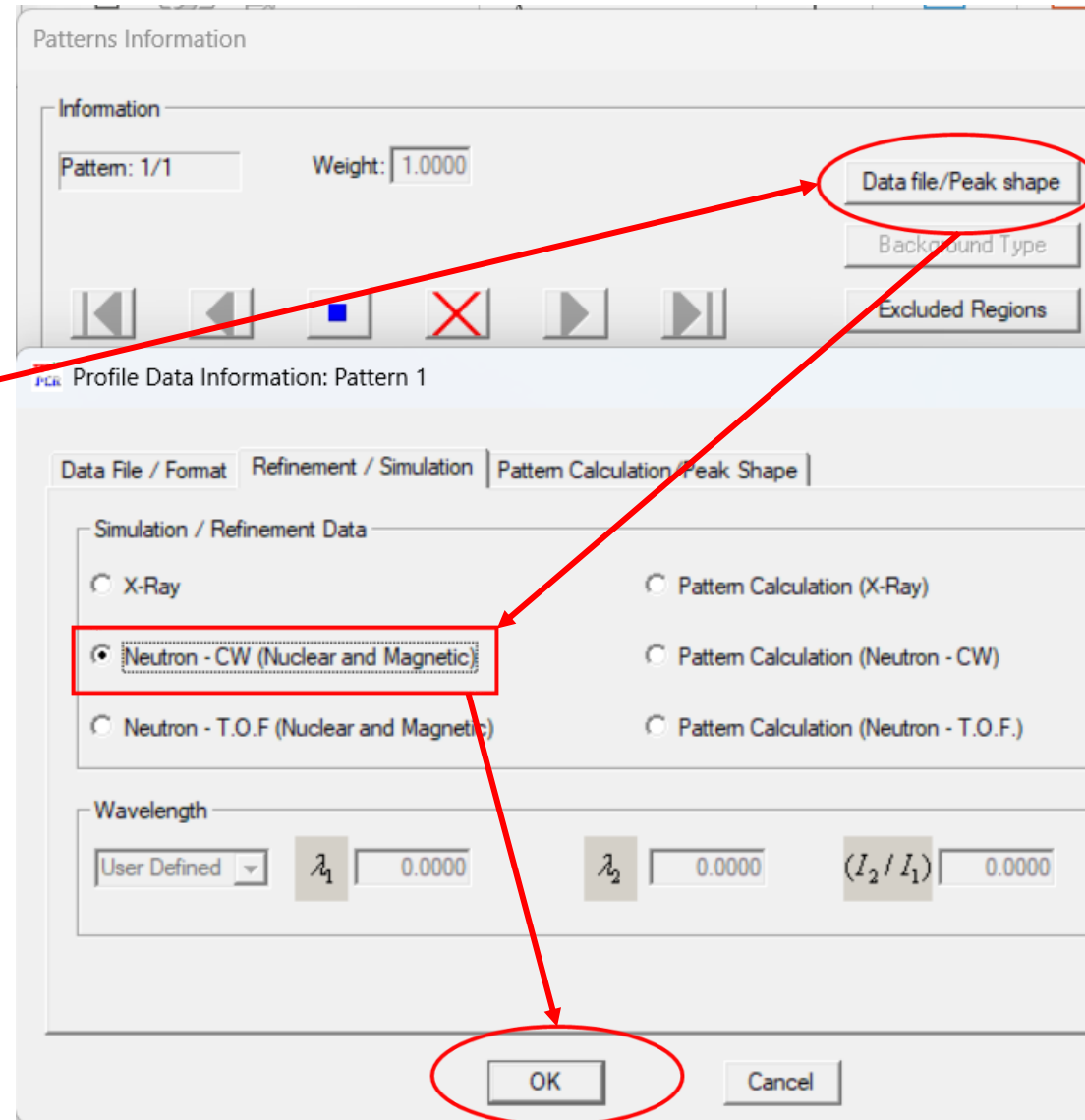
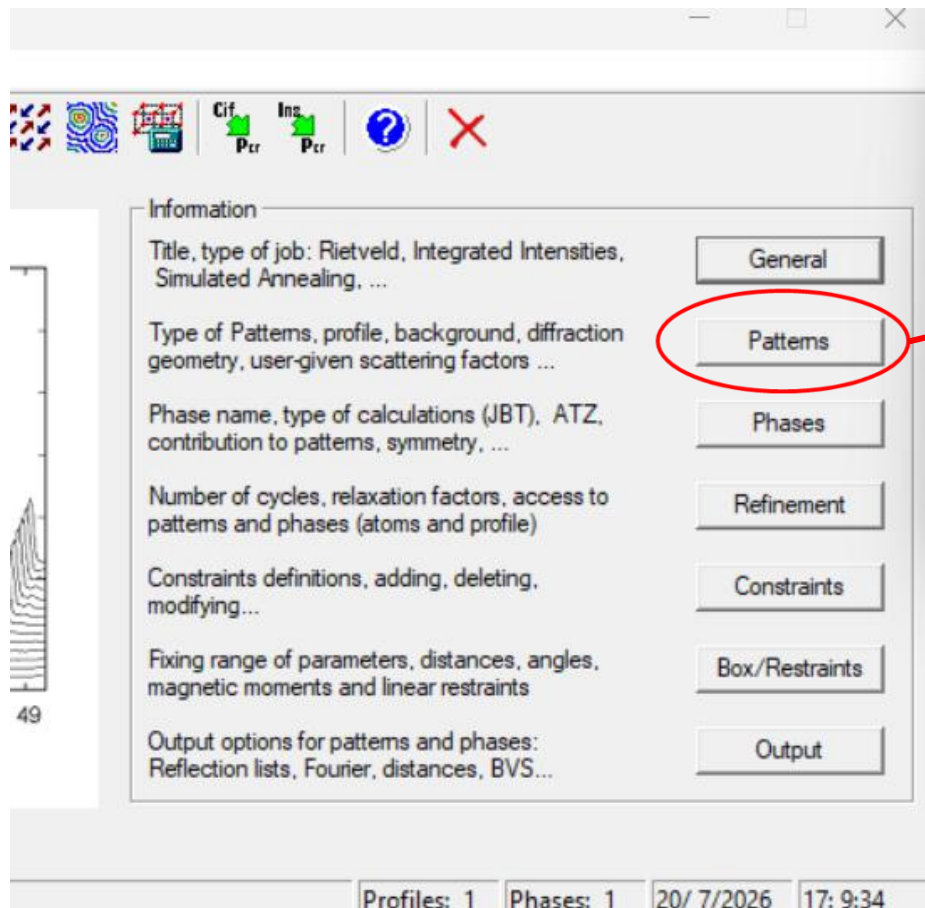
=> Reading Input mCIF file: d:\3.mcif
=> Input mCIF file: d:\3.mcif treated correctly!

Information on Magnetic Space Group:
-----
=> Shubnikov Number: 0
=> BNS Number: 13.70
=> OG Number:
=> BNS Symbol: P_a2/c
=> OG Symbol:
=> UNIFIED Symbol:
=> Type of Magnetic group: 4
=> Parent group number: 13
=> Parent group Symbol: P 2/c
=> Magnetic point group Symbol:
=> Laue Class for Cell constr.:
=> Transformation to parent: a,b,c;0,0,0
=> Transformation from parent: 2a,b,c;0,0,0
=> Transformation to standard: a-2c,b,a-c;1/4,0,0
=> Transformation from standard:
=> Crystal system:
=> Lattice type:
=> Lattice type Symbol:
=> Number of centring vectors: 0
=> Number of anti-translations: 1
=> Number of reduced set of S.O.: 4
=> General Multiplicity: 8
=> Centred: 0
=> Centre at: (1/4,0,0)
=> Centrosymmetry: Centric (-1 not at origin)
=> Generators (exc. -1&L): 0
```

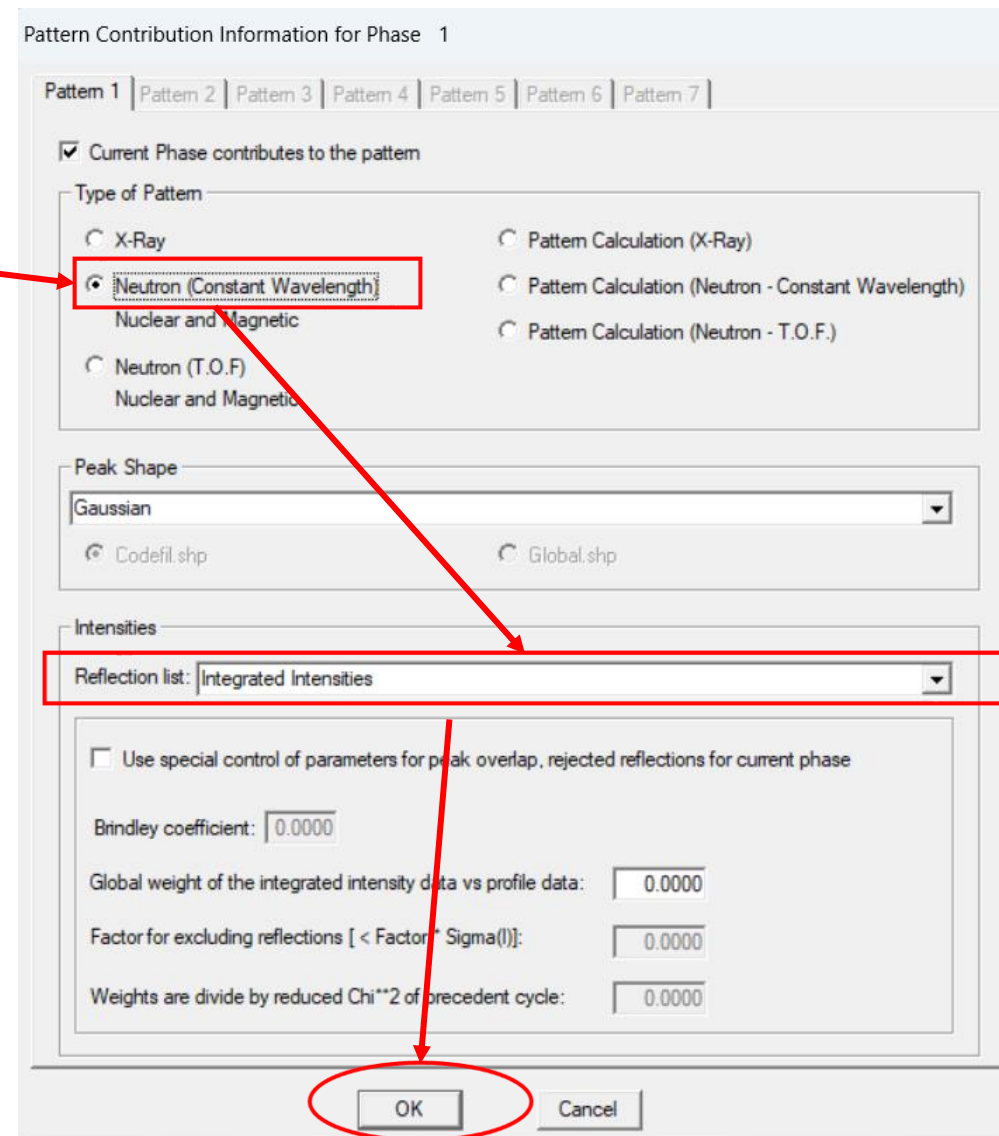
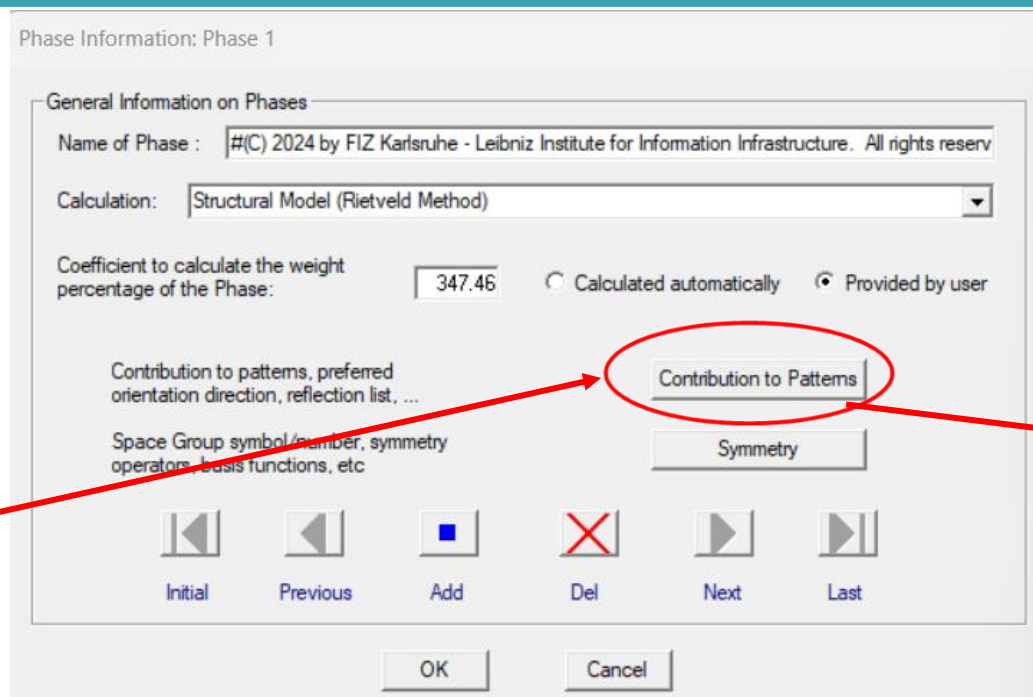
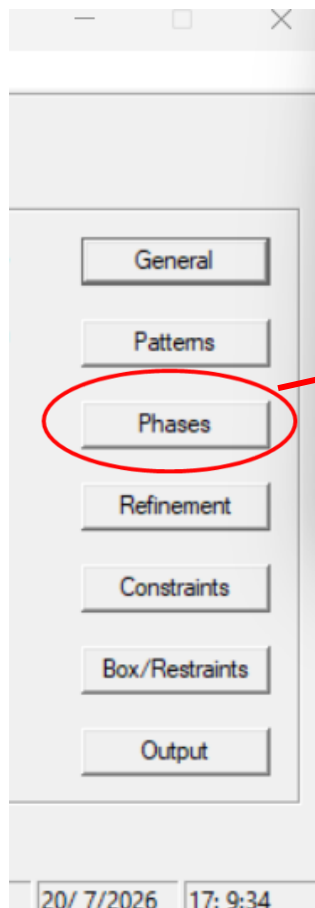
Step 2.3.1, Changing the .pcr into single crystal format



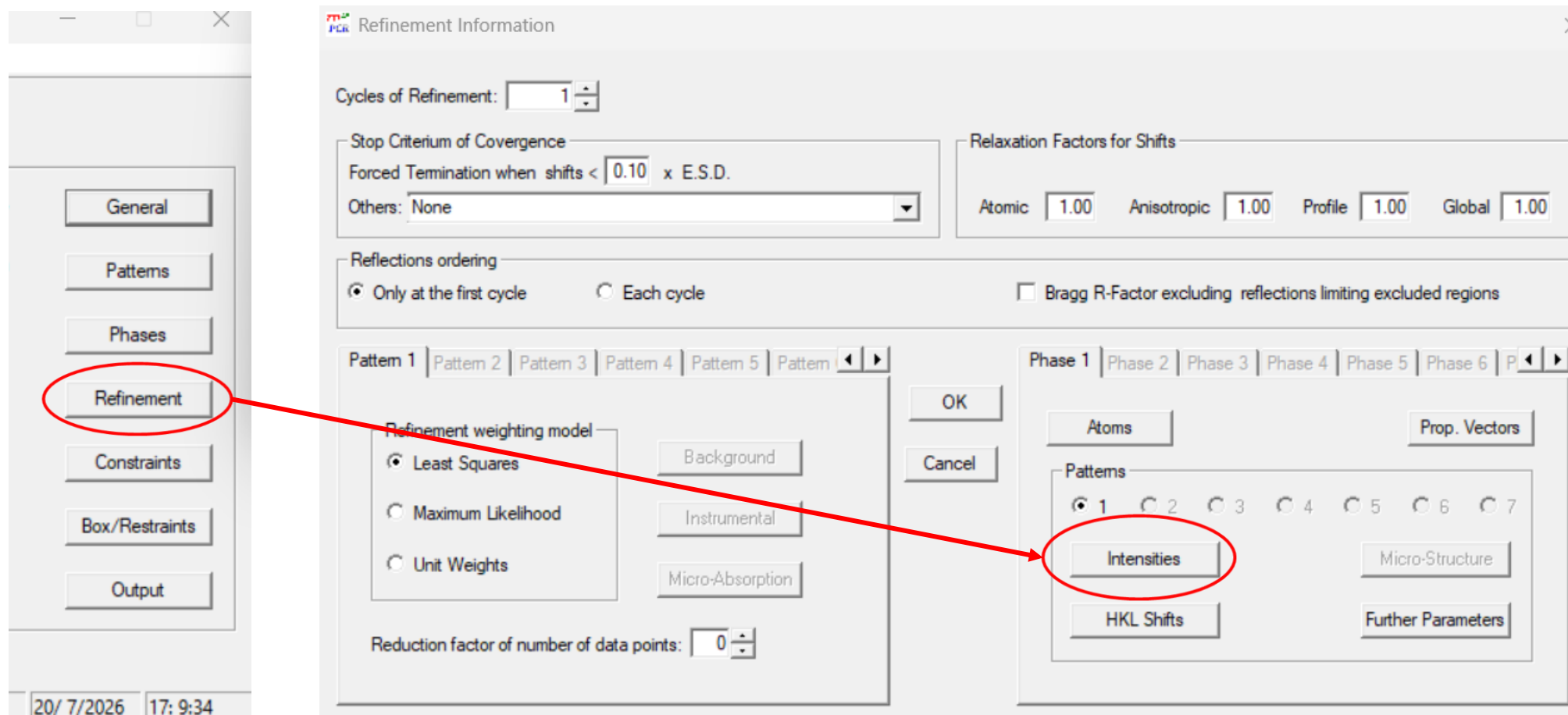
Step 2.3.2, Changing the.pcr into single crystal format



Step 2.3.3, Changing the .pcr into single crystal format



Step 2.4.0, Integrity check



Single crystal pcr shows "Intensity" rather than "Profile"

Step 2.4.1, Setting the SF and extinction parameters

Relaxation Factors for Shifts

Atomic Anisotropic Profile Global

☐ Bragg R-Factor excluding reflections limiting excluded regions

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5 | Phase 6 | P < >

OK Cancel

Atoms Prop. Vectors

Patterns

☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7

Intensities Micro-Structure

HKL Shifts Further Parameters

Integrate Intensities: Phase 1 Pattern 1

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	9.54000	5.72000	4.92000	90.00	90.90	90.00

Use nuclear refinement's SF/4 (2² because unit cell doubled)

Scale Factors

	1	2	3	4	5	6
Coefficients	113.78	0.0000	0.0000	0.0000	0.0000	0.0000

Extinction Parameters

	1	2	3	4	5	6
Coefficients	19.735	0.0000	0.0000	0.0000	0.0000	0.0000

Cancel OK

Note the MSG .pcr is now using a 2*1*1 super cell (a = 9.54)
double unit cell → double numbers of atoms → 4 times F²
Extinction correction parameter was also multiplied by F²:

$$F'_c = kF_c \left[1 + 0.001 \cdot x \cdot F_c^2 \cdot \frac{\lambda^3}{\sin(2\theta)} \right]^{-\frac{1}{4}}$$

(Fullprof manual did not mention which “empirical formula in SHELX” was used, but they all make use of the xFc² term, where x is the extinction parameter)

Scale Factors

	1
Coefficients	455.12

Extinction Parameters

	1
Coefficients	78.940

(From nuclear refinement)

Step 2.4.2, Setting the magnetic atoms

Change atom type to MMN3

Copy B-factors from nuclear refinement

Relaxation Factors for Shifts

Atomic Anisotropic Profile Global

☐ Bragg R-Factor excluding reflections limiting excluded regions

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5 | Phase 6 | P < >

OK Cancel

Atoms Prop. Vectors

Patterns

☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7

Intensities Micro-Structure

HKL Shifts Further Parameters

List of Atoms

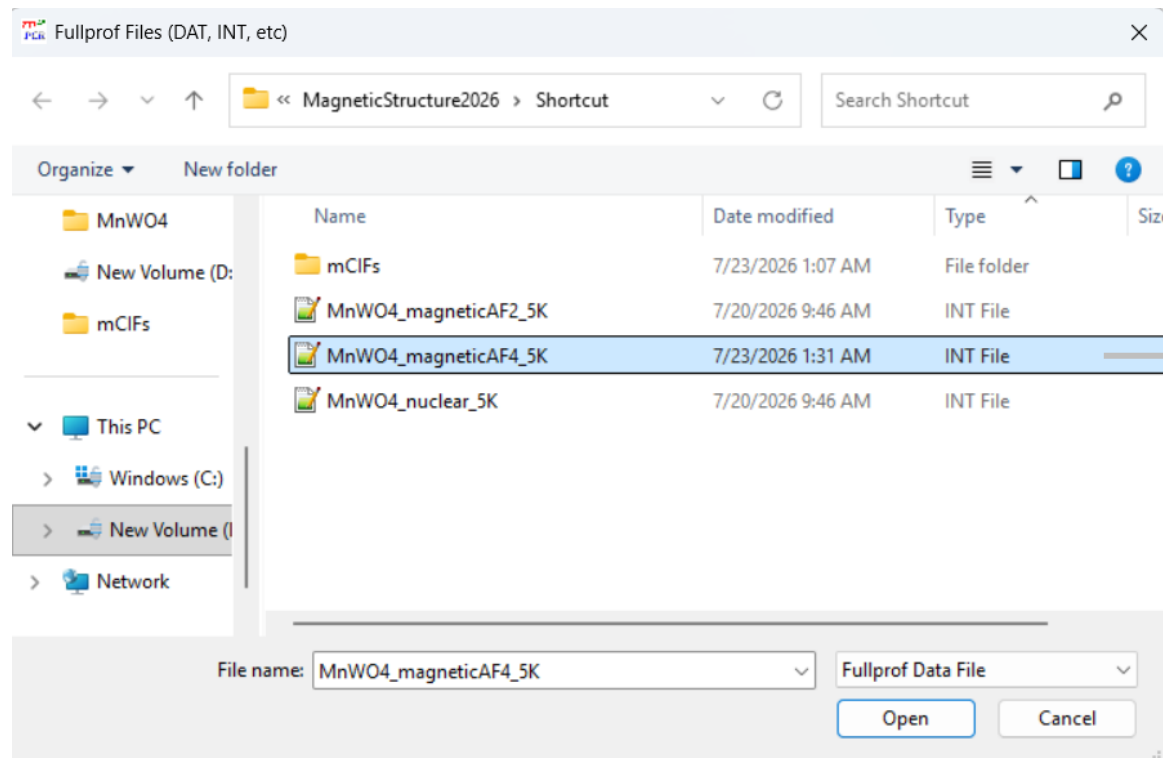
Number of Atoms:

	Label	Ntyp	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Mn1	MMN3	1	0	0.25000	0.68480	0.25000	0.63231	0.50000
Atom # 2	W1	W	1	0	0.00000	0.18010	0.25000	0.76178	0.50000
Atom # 3	O1	O	1	0	0.10545	0.10362	0.94030	0.66906	1.00000
Atom # 4	O2	O	1	0	0.12555	0.37542	0.39380	0.72573	1.00000

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

Refine magnetic moment sizes

Step 2.4.3, Run refinement



magneticAF4_5K.int is indexed using the 2x1x1 MSG supercell

A screenshot of a text editor window showing the content of the file 'MnWO4_magneticAF4_5K.int'. The file contains a list of indexed magnetic peaks. The first line is a title, followed by single crystal data, data format, wavelength, and a table of indexed peaks. The table has columns for h, k, l, F^2, sigma(F^2), and code. The first row is highlighted in blue.

h	k	l	F ²	sigma(F ²)	code
-5	-0	-0	110.39	12.01	1
-3	-0	-1	3.38	14.47	1
-3	-0	-0	241.57	13.11	1
-3	-0	1	2.12	1.67	1
-3	-0	2	0.00	0.00	1
-3	1	-2	33.77	4.20	1
-3	1	-1	238.44	11.91	1
-3	1	-0	44.39	4.43	1
-3	1	1	74.11	5.28	1
-3	1	2	4.39	0.87	1
-3	2	-1	105.88	15.81	1
-3	2	-0	83.88	6.50	1
-3	2	1	60.03	6.61	1
-1	-0	-0	315.36	17.39	1
-1	-0	1	0.00	0.00	1
-1	-0	2	50.36	4.57	1
-1	1	-1	287.53	20.73	1
-1	1	-0	88.50	5.81	1
-1	1	1	148.06	8.93	1

H are doubled in this datafile. E.g. (-5 0 0) here is (-2.5 0 0) magnetic peak in the original cell

Step 2.4.4, Refinement results

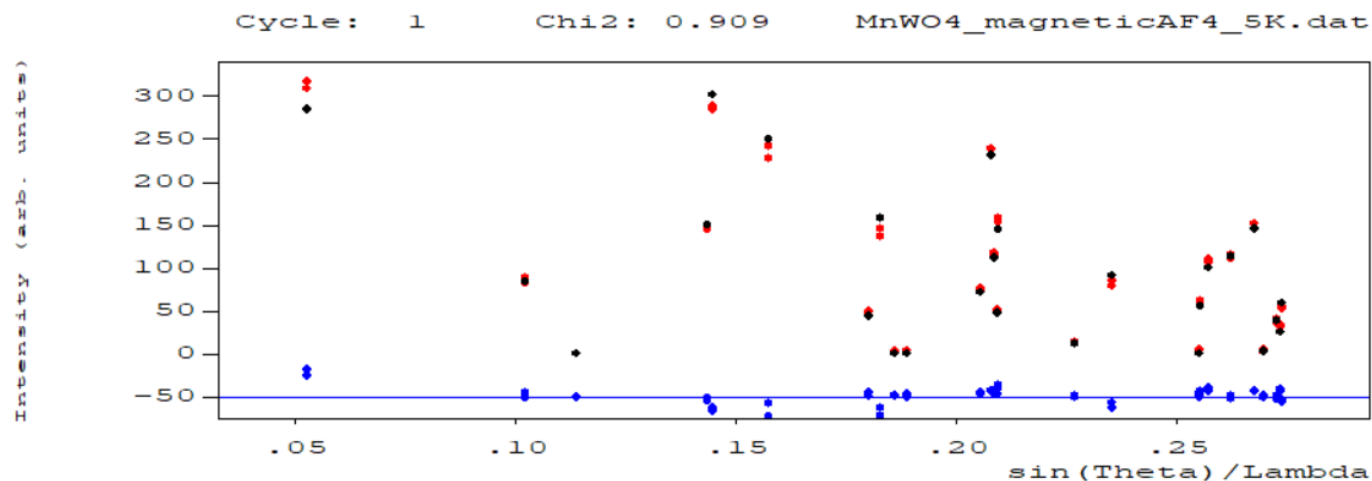
	Label	Ntyp	Mag. Rot.	Prog. V...	X		Y		Z		B		Occ	
Atom # 1	Mn1	MMN2	1	0	0.25000	☐	0.68480	☐	0.25000	☐	0.63231	☐	0.50000	☐
Atom # 2	W1	W	1	0	0.00000	☐	0.18010	☐	0.25000	☐	0.76178	☐	0.50000	☐
Atom # 3	O1	O	1	0	0.10545	☐	0.10362	☐	0.94030	☐	0.66906	☐	1.00000	☐
Atom # 4	O2	O	1	0	0.12555	☐	0.37542	☐	0.39380	☐	0.72573	☐	1.00000	☐

	Re[x]		Re[y]		Re[z]		Im[x]		Im[y]		Im[z]		MPhase	
Atom #1	-1.48484	☒	0.00000	☐	1.94915	☒	0.00000	☐	0.00000	☐	0.00000	☐	0.00000	☐

```
=> Phase: 1
=> RF2 -factor : 6.661
=> RF2w-factor : 8.385
=> RF -factor : 4.989
=> Chi2(Intens): 0.9093
=> N_eff Reflect.: 52 and 0.000 * sigma < Int
=> RF2-pure magnetic : 6.661
=> RF -pure magnetic : 4.989
=> Conv. not yet reached -> [Max] Shift( Rx_Mn1)/(eps*Sigma)= -1.83 abs> 1
=> Normal end, final calculations and writing...
=> Contribution to Yi for phase: 1

=> CPU Time: 0.355 seconds
=> 0.006 minutes

=> END Date:23/07/2026 Time => 06:53:22.883
```



Step 2.5.1, Add Co atom back

To add the Co atom back, we need to again edit the .pcr file:

```
2      !Number of refined parameters
-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 0.0000 Magnetic R-Factor: 0.0000
-----
Nuclear and Magnetic Structure -> 3 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 4 2 0 0 605.571 0 7 0
!
P_a2/c number:13.70 <--Magnetic Space group symbol (BNS/UNI symbol & number)
Transform to standard: a-2c,b,a-c;1/4,0,0
Parent Space Group: P2/c IT_number: 13
Transform from Parent: 2a,b,c;0,0,0
! Nsym Cen N_Clat N_Ant
! 4 0 0 1
!
! Anti-Centring vectors
! 0.50000 0.00000 0.00000
! Symmetry operators
! 1 x,y,z,+1
! 2 -x,-y,-z,-1
! 3 x,-y,z+1/2,-1
! 4 -x,y,-z+1/2,+1
!
! Atom Typ Mag vek X Y Z Biso Occ N_type Spc/Fftype /Line below:Codes
! RX Ry Rz Ix Iy Iz beta23 / Line below:Codes
! beta11 beta22 beta33 beta12 beta13 beta23
Mn1 MMN2 1 0 0.25000 0.68480 0.25000 0.63231 0.41657 1 0 #
-1.48868 0.00000 1.74167 0.00000 0.00000 0.00000 0.00000 <--MagPar
21.00 0.00 11.00 0.00 0.00 0.00 0.00
Co1 MCO2 1 0 0.25000 0.68480 0.25000 0.63231 0.08343 1 0 #
-1.48868 0.00000 1.74167 0.00000 0.00000 0.00000 0.00000 <--MagPar
21.00 0.00 11.00 0.00 0.00 0.00 0.00
w1 w 1 0 0.00000 0.18010 0.25000 0.76178 0.50000 0 0 #
0.00 0.00 0.00 0.00 0.00
o1 o 1 0 0.10545 0.10362 0.94030 0.66906 1.00000 0 0 #
0.00 0.00 0.00 0.00 0.00
o2 o 1 0 0.12555 0.37542 0.39380 0.72573 1.00000 0 0 #
0.00 0.00 0.00 0.00 0.00
!-----> Scale, Extinction and Cell Parameters for Pattern # 1
```

Delete VARY mxmymz

Change Nat to 5

VARY mxmymz: This keyword auto refines all symmetry-allowed magnetic moments And override any manual set constrains

Another often used keyword: mag_only, only calculate magnetic intensities

Nat: number of atoms

Copy whole block of Mn atom to below, change Mn into Co, MMN3 into MCO3

Copy Mn occ and Co occ from nuclear refinement

Step 2.5.2, Save, Reload, Run

```
=> -----> Pattern#      1
=> Phase:      1
=>   RF2 -factor :    6.381
=>   RF2w-factor :    8.322
=>   RF  -factor :    4.845
=>   Chi2(Intens):  0.8957
=>   N_eff Reflect.:   52 and   0.000  *
=>   RF2-pure magnetic :    6.381
=>   RF -pure magnetic :    4.845
=> Normal end, final calculations and writing...
=> Contribution to Yi for phase:      1
```

```
=> CPU Time:      0.578 seconds
=> 0.010 minutes
```

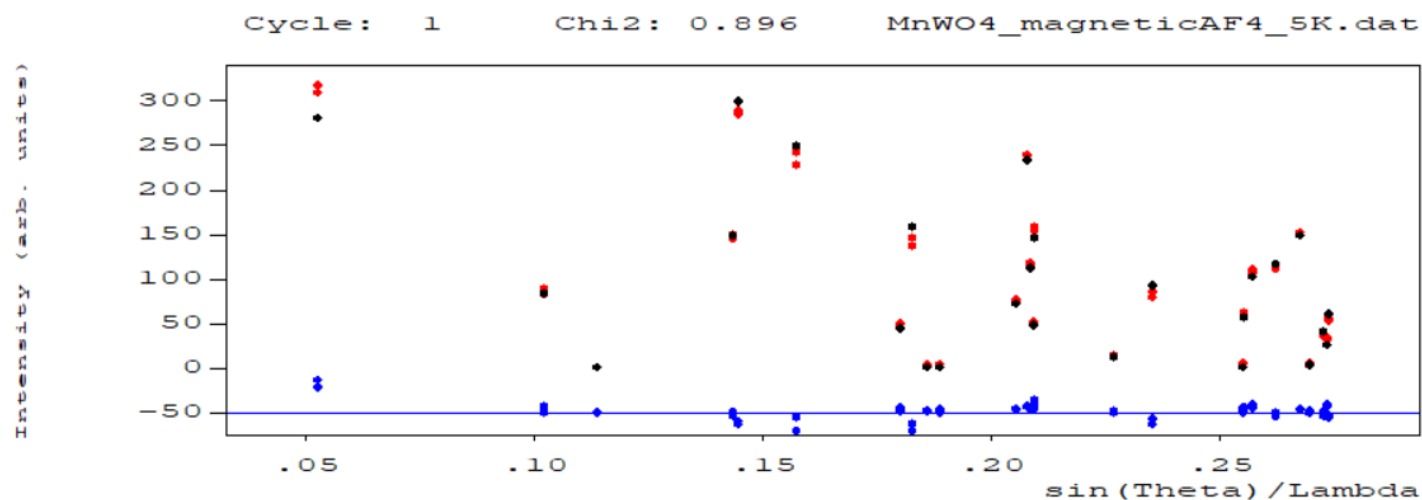
```
=> END   Date:23/07/2026   Time => 03:15:36.574
```

List of Atoms

Number of Atoms:

	Label	Ntyp	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Mn1	MMN2	1	0	0.25000	0.68480	0.25000	0.63231	0.41657
Atom # 2	Co1	MCO2	1	0	0.25000	0.68480	0.25000	0.63231	0.08343
Atom # 3	W1	W	1	0	0.00000	0.18010	0.25000	0.76178	0.50000
Atom # 4	O1	O	1	0	0.10545	0.10362	0.94030	0.66906	1.00000

	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom #1	-1.46425	0.00000	1.92700	0.00000	0.00000	0.00000	0.00000
Atom #2	-1.46425	0.00000	1.92700	0.00000	0.00000	0.00000	0.00000

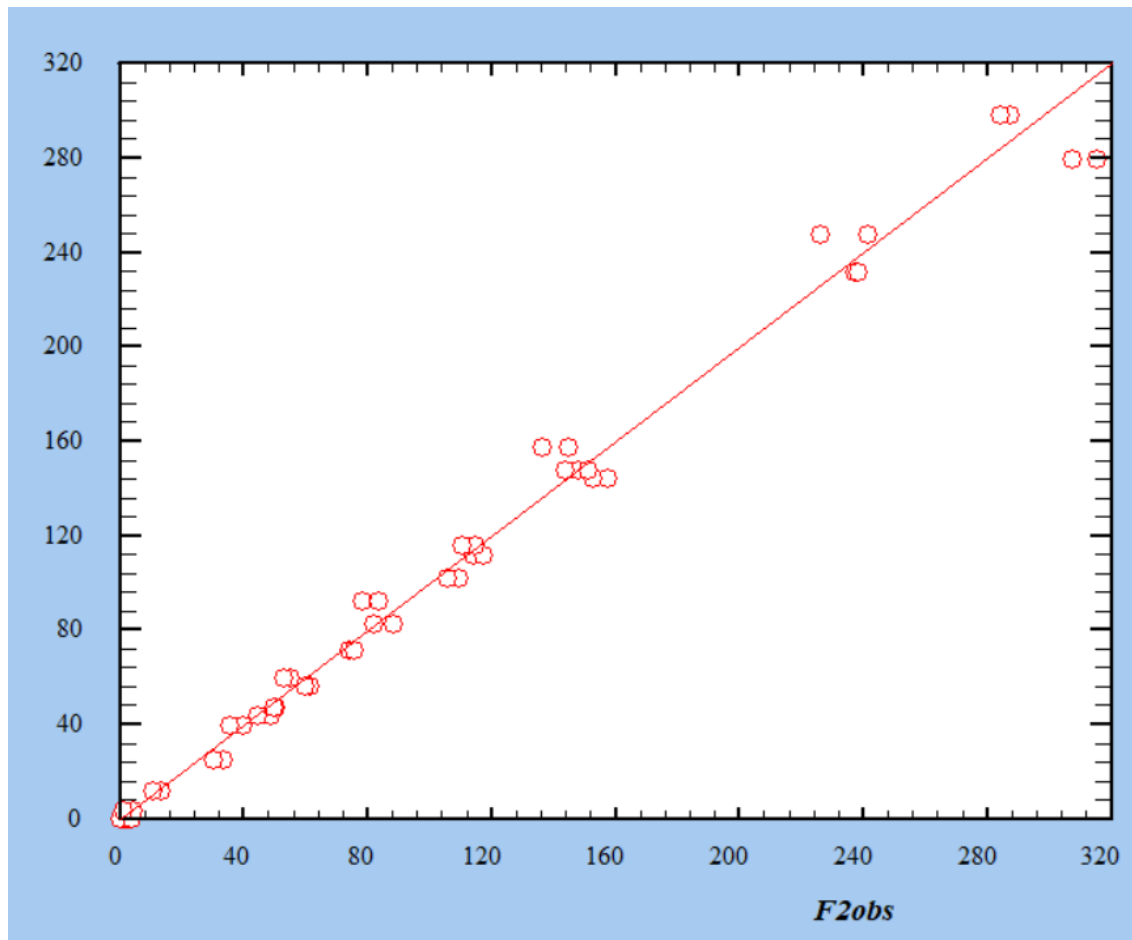


Only marginal change in the results because Co and Mn have very similar magnetic form factors.

Step 2.6, Visualize the results



MnCoWO₄_5K_cm.prf



MnCoWO₄_5K_cm.sum

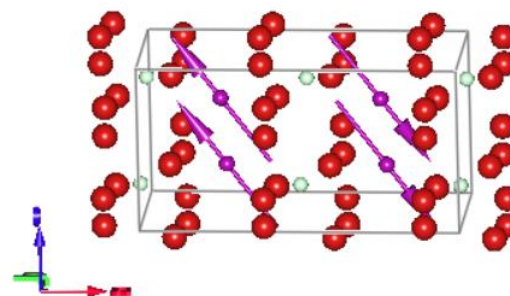
==> ATOM PARAMETERS:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
Mn1	0.25000(0)		0.68480(0)		0.25000(0)		0.632(0)		0.417(0)		8
Co1	0.25000(0)		0.68480(0)		0.25000(0)		0.632(0)		0.083(0)		8
W1	0.00000(0)		0.18010(0)		0.25000(0)		0.762(0)		0.500(0)		8
O1	0.10545(0)		0.10362(0)		0.94030(0)		0.669(0)		1.000(0)		16
O2	0.12555(0)		0.37542(0)		0.39380(0)		0.726(0)		1.000(0)		16

==> MAGNETIC MOMENT PARAMETERS:

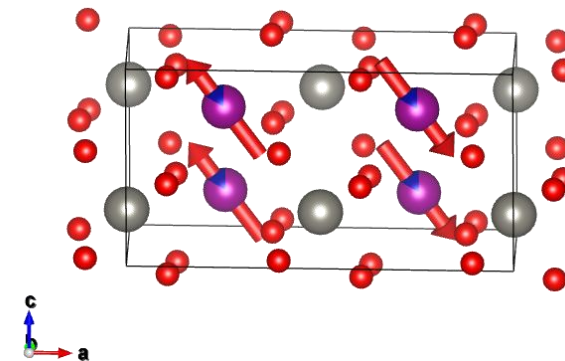
Name	Mx	sMx	My	sMy	Mz	sMz	M	sM	MPhas	sMPhas
Mn1	-1.464(25)		0.000(0)		1.927(18)		2.4384(156)		0.0000(0)	
Co1	-1.464(25)		0.000(0)		1.927(18)		2.4384(156)		0.0000(0)	

..._5K_cm.fst



(FPStudio)

..._5K_cm.mcif



(VESTA)

Step 3.1.1, IR analysis for the $k = (0.217, 1/2, -0.46)$ phase using SARAh

Wills Group

Magnetism and magnetic materials

HOME

WINDOWS SOFTWARE

WEB SOFTWARE- NEW APPS!

VIDEO LE

<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>

SARAh webRefine – FullProf

Three pieces of advice for using SARAh webRefine : **1.** change your browser settings to allow you <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and ! your file so that its path contains no special characters: special characters and those with PHP c

-Andrew (February 2022)



Space group :

{13:b1, P 1 2/c 1, C 2h 4} ▾

Select the correct convention of Space group No.13 (P 1 2/c 1)

Propagation vector :

0.217 0.5 -0.46

Input incommensurate wave vector

Crystallographic coordinates with each **moment carrying atom** on a separate line :

e.g. Cu2 1/2 1/2 -1/2

Mn1 0.5 0.68488 0.25

Use atom coordinates from the structure unit cell

Submit



Step 3.1.2, IR analysis for the $k = (0.217, 1/2, -0.46)$ phase using SARAh

Method 1. Conventional analysis - as projected basis vectors

Select command (generate template for magnetic phase for pcr; edit pcr with magnetic phase present):

2. single crystal 2. make template pcr

Select "single crystal"

☒ Mn1 $\Gamma_1 \psi_1$	☒ Mn1 $\Gamma_2 \psi_3$
☒ Mn1 $\Gamma_1 \psi_2$	
☒ Mn1 $\Gamma_1 \psi_3$	
☒ Mn1 $\Gamma_2 \psi_1$	
☒ Mn1 $\Gamma_2 \psi_2$	

Select all basis vectors and output a pcr

(Your browser should be set to ask for the download location so the pcr file can be overwritten. Please look in '4.')

Submit

Table. The basis vectors projected from the different IRs :

$\left\{ \begin{array}{l} \Gamma_1 \psi_1 \\ \text{Mn1 } 1) \quad 1. \ 0. \ 0., \\ \quad 2) \ 0.125333 - 0.992115 i \ 0. \ 0. \end{array} \right\},$	$\left\{ \begin{array}{l} \Gamma_1 \psi_2 \\ \text{Mn1 } 1) \ 0., \\ \quad 2) \ 0. \ -0.125333 + 0.992115 i \ 0. \end{array} \right\},$	$\left\{ \begin{array}{l} \Gamma_1 \psi_3 \\ \text{Mn1 } 1) \ 0. \ 0. \\ \quad 2) \ 0. \ 0. \ 0.125333 - 0.992115 i \end{array} \right\}$
$\left\{ \begin{array}{l} \Gamma_2 \psi_1 \\ \text{Mn1 } 1) \quad 1. \ 0. \ 0., \\ \quad 2) \ -0.125333 + 0.992115 i \ 0. \ 0. \end{array} \right\},$	$\left\{ \begin{array}{l} \Gamma_2 \psi_2 \\ \text{Mn1 } 1) \ 0., \\ \quad 2) \ 0. \ 0.125333 - 0.992115 i \ 0. \end{array} \right\},$	$\left\{ \begin{array}{l} \Gamma_2 \psi_3 \\ \text{Mn1 } 1) \ 0. \ 0. \\ \quad 2) \ 0. \ 0. \ -0.125333 + 0.992115 i \end{array} \right\}$

2 IRs, each has 3 basis vector

$$0.125333 - 0.992115i = e^{-0.23 \cdot 2\pi i}$$

Step 3.1.3, IR analysis for the $\mathbf{k} = (0.217, 1/2, -0.46)$ phase using SARAh

$$G_0: \{(x, y, z), (-x, y, -z+1/2), (-x, -y, -z), (x, -y, z+1/2)\}$$

Symmetries in the P 2/c SG

$$G_{\mathbf{k}}: \{(x, y, z), (x, -y, z+1/2)\}$$

Little group $G_{\mathbf{k}}$: the rotation matrix keeps the $\mathbf{k}$ invariant - Symmetry operations of the magnetic structure

Table 7. Symmetry related positions for the basis listing basis vectors):

Mn1	1:	0.5	0.68448	0.25
	2:	0.5	0.31552	0.75

$$\text{Mn1 } (0.5 \ 0.68 \ 0.25) \quad \mathbf{M}$$



$$(x, -y, z+1/2)$$

$$\text{Mn2}_{\text{b-}} (0.5 \ -0.68 \ 0.75) \quad \mathbf{M}\alpha$$



$$(x, -y, z+1/2)$$

$$\text{Mn1}_{\text{c+}} (0.5 \ 0.68 \ 1.25) \quad \mathbf{M}\alpha^2 = \mathbf{M}e^{-0.46*2\pi i}$$

Two magnetic atoms in a unit cell.

The two atoms are connected by $(x, -y, z+1/2)$ – an element in $G_{\mathbf{k}}$, means they are restrained by magnetic symmetry related to this operation.

By applying $(x, -y, z+1/2)$ twice, Mn1 translates one unit cell along c. By the definition of propagation vector, it gains a phase factor of $e^{-0.46*2\pi i}$

$$\alpha^2 = e^{-0.46*2\pi i} \rightarrow \alpha = e^{-0.23*2\pi i} \text{ or } -e^{-0.23*2\pi i}$$

Which are the two 1-D IRs of the little group $G_{\mathbf{k}}$

Table 8. The final IRs :

$$\begin{pmatrix} g1 & g28 \\ (1) & (0.125333 - 0.992115 i) \\ (1) & (-0.125333 + 0.992115 i) \end{pmatrix}$$

52

- 
- OAK RIDGE
National Laboratory

The image shows a side-by-side comparison of two Notepad++ windows. The left window displays the file 'SARAh_sg13_magnetic_phase_template.pcr' and the right window displays '5_MnCoWO4_5K_sarah.pcr'. Both files contain crystallographic data in a structured format. In the left file, a red box highlights the 'Nat Dis Mom' section (lines 6-10) and the 'Scale Factors' section (lines 27-30). In the right file, a red box highlights the 'Nat Dis Ang' section (lines 19-23) and the 'Scale Factors' section (lines 35-38). An arrow points from the 'Scale Factors' section of the left file to the 'Scale Factors' section of the right file, indicating a comparison or transfer of information.

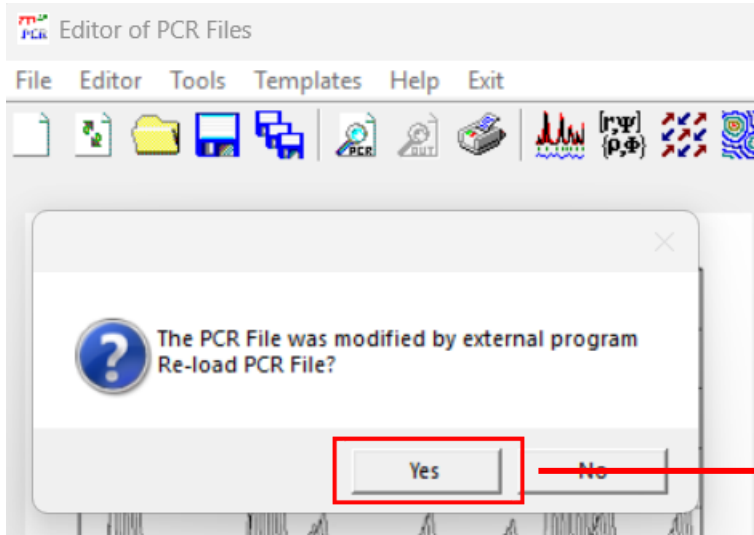
Step 3.2.2, Making an incommensurate .pcr for refinement

- Leave the Scale Factor, Extinction Parameters and Lattice parameters untouched
- **Ensure the wave vector is (0.217, 0.5 -0.46) – consistent with the data file**
- Copy the lines below the lattice parameters into the refinement pcr before the x-lambda/2 line.

```
SARAh_sg13_magnetic_phase_template.pcr
10 ! Nsym Cen Laue Ireps N_Bas
11 | 2 1 1 -1 6
12 ! Real(0)-Imaginary(1) indicator for Ci
13 0 0 0 0 0 0
14 !
15 SYMM X , Y , Z
16 BASR 1. 0 0 0 1. 0 0 0 1. 1. 0 0 0 1. 0 0 0 1.
17 BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18 SYMM X , 1 - Y , 1/2 + Z
19 BASR 0.1253 0 0 0 -0.1253 0 0 0 0.1253 -0.1253 0 0 0 0.1253
20 BASI 0.9921 0 0 0 -0.9921 0 0 0 0.9921 -0.9921 0 0 0 0.9921
21 !Atom Typ Mag Vek X Y Z Bis0 Occ C1 C2
22 ! C4 C5 C6 C7 C8 C9 MagPh
23 Mn1 MMN5 1 0 0.50000 0.68488 0.25000 .30000 1.00000 0.000 0.00
24 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
25 0.000 0.000 0.000 0.000 0.000 0.000 0.00000
26 0.00 0.00 0.00 0.00 0.00 0.00 0.00
27 ! Scale Factors
28 ! Sc1 Sc2 Sc3 Sc4 Sc5 Sc6
29 100.0 0.000 0.000 0.000 0.000 0.000
30 .00 0.00 0.00 0.00 0.00 0.00
31 ! Extinction Parameters
32 ! Ext1 Ext2 Ext3 Ext4 Ext5 Ext6 Ext7
33 0.000 0.000 0.000 0.000 0.000 0.000 0.000
34 0.00 0.00 0.00 0.00 0.00 0.00 0.00
35 ! a b c alpha beta gamma
36 7 7 17 90 90 120
37 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
38 ! Not yet used parameters
39 0.00000 0.00000 0.00000 0.00000 0.00000
40 0.00 0.00 0.00 0.00 0.00
41 ! Propagation vectors:
42 0.217 0.5 -0.46 Propagation Vector 1
43 0.000000 0.000000 0.000000

5_MnCoWO4_5K_sarah.pcr
25 ! Real(0)-Imaginary(1) indicator for Ci
26 0 0 0 0 0 0
27 !
28 SYMM X , Y , Z
29 BASR 1. 0 0 0 1. 0 0 0 1. 1. 0 0 0 1. 0 0 0 1.
30 BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31 SYMM X , 1 - Y , 1/2 + Z
32 BASR 0.1253 0 0 0 -0.1253 0 0 0 0.1253 -0.1253 0 0 0 0.1253
33 BASI 0.9921 0 0 0 -0.9921 0 0 0 0.9921 -0.9921 0 0 0 0.9921
34 !Atom Typ Mag Vek X Y Z Bis0 Occ C1 C2
35 ! C4 C5 C6 C7 C8 C9 MagPh
36 Mn1 MMN5 1 0 0.50000 0.68488 0.25000 .30000 1.00000 0.000 0.00
37 0.000 0.000 0.00 0.00 0.00 0.00 0.00 0.00
38 0.000 0.000 0.000 0.000 0.000 0.000 0.00000
39 0.00 0.00 0.00 0.00 0.00 0.00 0.00
40 !-----> Scale, Extinction and Cell Parameters for Pattern # 1
41 ! Scale Factors
42 ! Sc1 Sc2 Sc3 Sc4 Sc5 Sc6
43 455.2 0.000 0.000 0.000 0.000 0.000
44 11.00 0.00 0.00 0.00 0.00 0.00
45 ! Extinction Parameters
46 ! Ext1 Ext2 Ext3 Ext4 Ext5 Ext6
47 78.98 0.000 0.000 0.000 0.000 0.000
48 31.00 0.00 0.00 0.00 0.00 0.00
49 ! a b c alpha beta gamma # Cel
50 4.770000 5.719997 4.920001 90.000000 90.900047 90.000000
51 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
52
53 ! x-Lambda/2
54 0.02137
55 161.00
56 ! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
57 0.087 150.000 1
58
```

Step 3.2.3, Making an incommensurate .pcr for refinement



- Refinements → Intensities
- Fix the scale factor and extinction Parameters. They should be same with the nuclear refinement

Integrate Intensities: Phase 1 Pattern 1

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	4.77000	5.72000	4.92000	90.00	90.90	90.00

Scale Factors

	1	2	3	4	5	6
Coefficients	455.20	0.0000	0.0000	0.0000	0.0000	0.0000

Extinction Parameters

	1	2	3	4	5	6
Coefficients	78.980	0.0000	0.0000	0.0000	0.0000	0.0000

Refine All

Fix All

Cancel

OK

Step 3.2.4, Making an incommensurate .pcr for refinement

- Refinements → Atoms
- Change atom type to MMN2
- copy Mn's B-factor from the nuclear refinement
- Refine C1, C2, C3. Save pcr, save as a new file, run

List of Atoms

Number of Atoms:

	Label	Ntyp	Mag. Rot.	Prog. Vec.	X	Y	Z	B	Occ
Atom # 1	Mn1	MMN2	1	0	0.50000	0.68488	0.25000	0.63200	1.00000

	Rx	Ry	Rz	lx	ly	lz	MPhase
Atom #1							

Basis Functions Coefficients

	C1	C2	C3	C4	C5	C6	C7
Atom # 1	1.00000 ✓	1.00000 ✓	1.00000 ✓	0.00000	0.00000	0.00000	0.00000

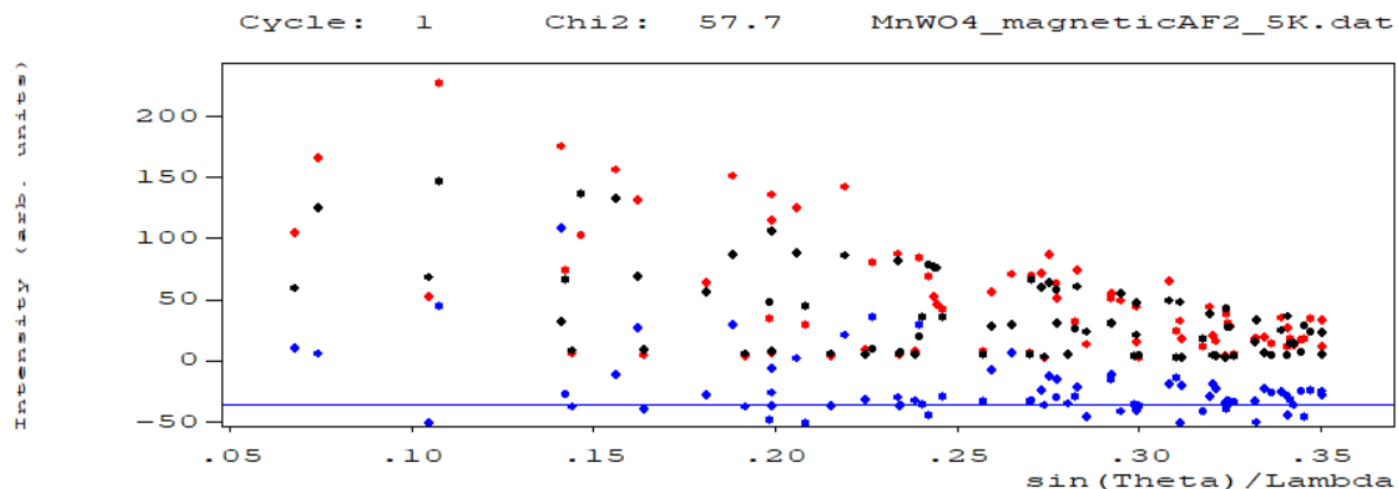
Step 3.3.1, Refining the incommensurate magnetic structure

- Refine Bravely

```
Load Edit PCR Mode Run Exit
=> Global user-weighted Chi2 (Bragg contrib.): 57.69
=> -----> Pattern# 1
=> Phase: 1
=> RF2 -factor : 35.24
=> RF2w-factor : 42.73
=> RF -factor : 20.83
=> Chi2(Intens): 57.69
=> N_eff Reflect.: 82 and 0.000 * sigma < Int
=> RF2-satellites : 35.24
=> RF -satellites : 20.83
=> Normal end, final calculations and writing...

=> CPU Time: 0.463 seconds
=> 0.008 minutes

=> END Date:23/07/2026 Time => 05:35:07.287
```



Step 3.3.2, Refining the incommensurate magnetic structure

- It looks like only C2 has a significant moment.
- fix C1 and C3 to 0 for now, choose C4 and C6 instead:

List of Atoms

Number of Atoms:

	Label	Ntyp	Mag. Rot.	Prog. Vec.	X	Y	Z	B	Occ
Atom # 1	MN1	MMN2	1	0	0.50000	0.68488	0.25000	0.63200	1.00000

	Rx	Ry	Rz	lx	ly	lz	MPhase
Atom #1							

Basis Functions Coefficients

	C1	C2	C3	C4	C5	C6	C7
Atom # 1	0.48800	3.56100	0.27000	0.00000	0.00000	0.00000	0.00000



Basis Functions Coefficients

	C1	C2	C3	C4	C5	C6	C7
Atom # 1	0.48800	3.56100	0.27000	1.00000	0.00000	1.00000	0.00000

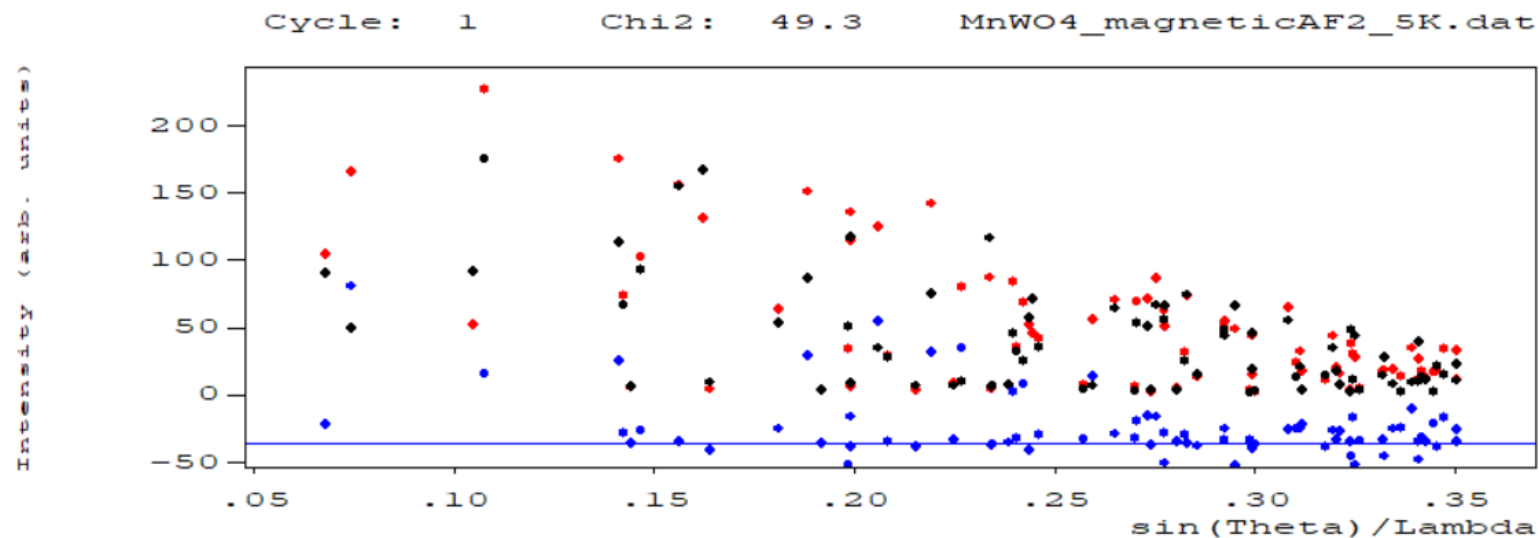
Step 3.3.3, Refining the incommensurate magnetic structure

- Again, refine bravely:

```
=> -----> Pattern#      1
=> Phase:      1
=> RF2 -factor :   32.56
=> RF2w-factor :   39.49
=> RF  -factor :   19.25
=> Chi2(Intens):   49.27
=> N_eff Reflect.:   82 and   0.000   * sigma < Int
=> RF2-satellites :   32.56
=> RF -satellites :   19.25
=> Conv. not yet reached -> [Max] Shift( C2_MN1)/(eps*Sigma)=  -2.54 abs> 1
=> Normal end, final calculations and writing...

=> CPU Time:      0.406 seconds
=> 0.007 minutes

=> END   Date:23/07/2026   Time => 06:57:02.551
```



Step 3.3.5, Refining the incommensurate magnetic structure

- Refine bravely till it converge:

```
=> Global user-weigthed Chi2 (Bragg contrib.): 1.989
=> -----> Pattern# 1
=> Phase: 1
=> RF2 -factor : 5.028
=> RF2w-factor : 7.934
=> RF -factor : 3.343
=> Chi2(Intens): 1.989
=> N_eff Reflect.: 82 and 0.000 * sigma < Int
=> RF2-satellites : 5.028
=> RF -satellites : 3.343
=> Normal end, final calculations and writing...
```

```
=> CPU Time: 0.488 seconds
```

```
=> 0.008 minutes
```

```
=> END Date:23/07/2026 Time => 07:02:53.817
```

List of Atoms

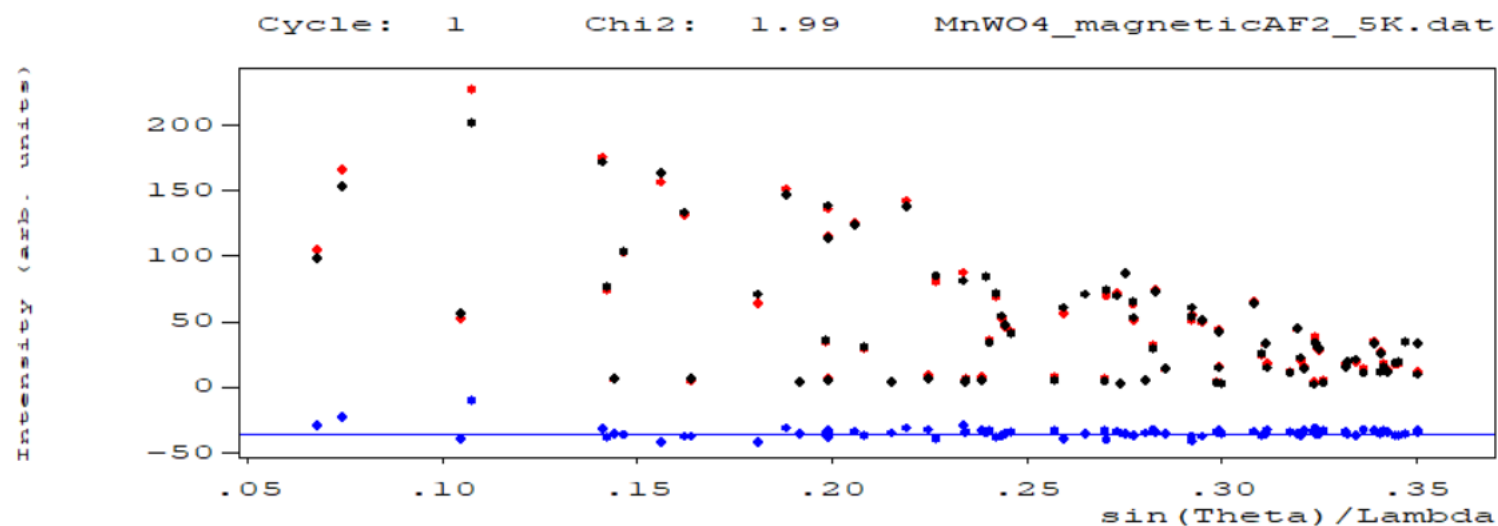
Number of Atoms: 1

	Label	Ntyp	Mag. Rot.	Prog. Vec.	X	Y	Z	B	Occ
Atom # 1	Mn1	MMN2	1	0	0.50000	0.68488	0.25000	0.63200	1.00000

	Rx	Ry	Rz	lx	ly	lz	MPhase
Atom #1							

Basis Functions Coefficients

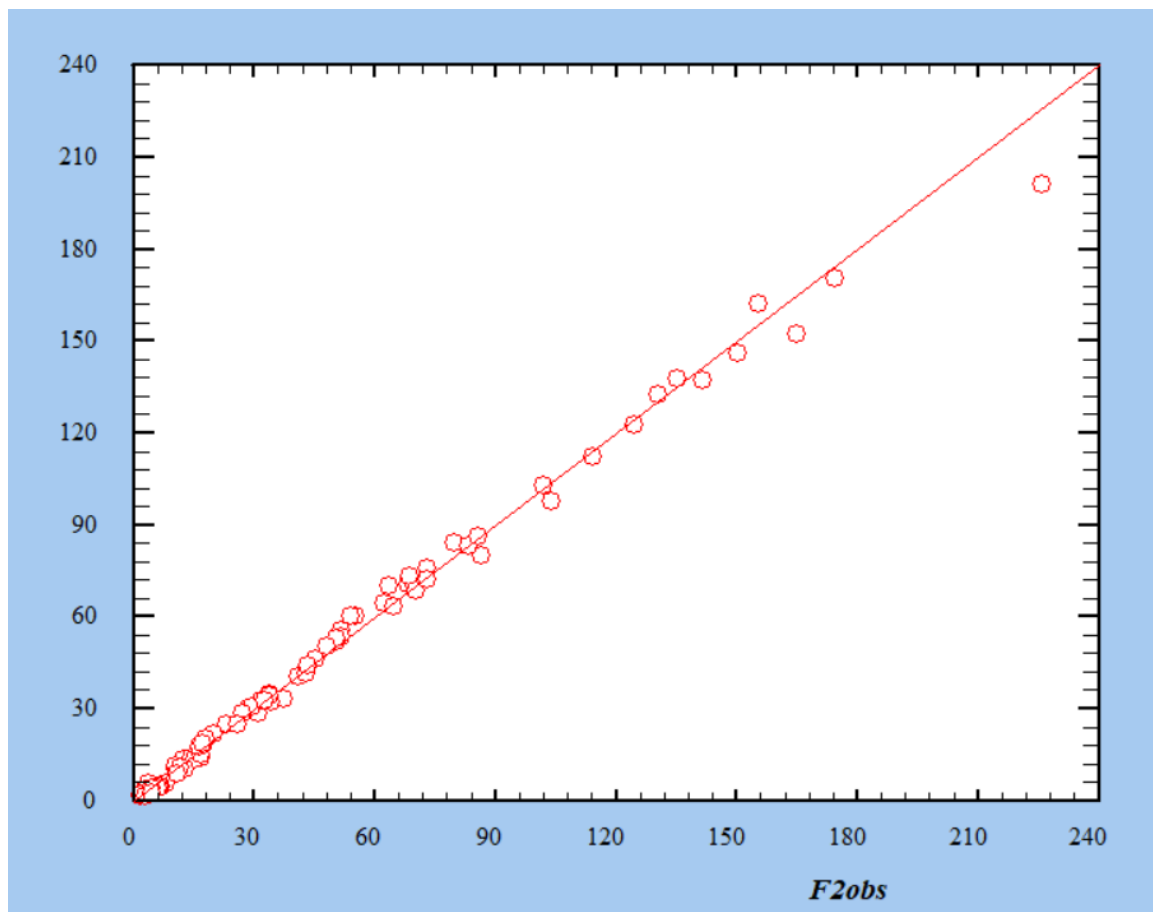
	C1	C2	C3	C4	C5	C6	C7
Atom # 1	0.00000	2.70800	0.00000	2.38100	0.00000	1.73000	0.00000



Step 3.4, Illustrate the result



MnCoWO₄_5K_incm.prf

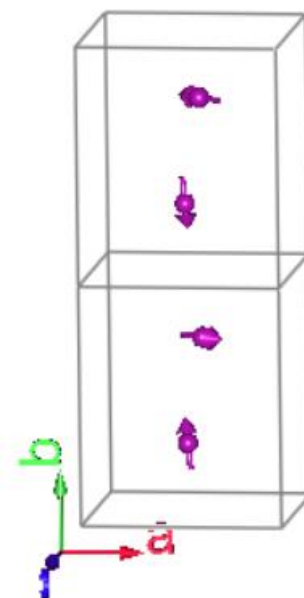


MnCoWO₄_5K_incm.sum

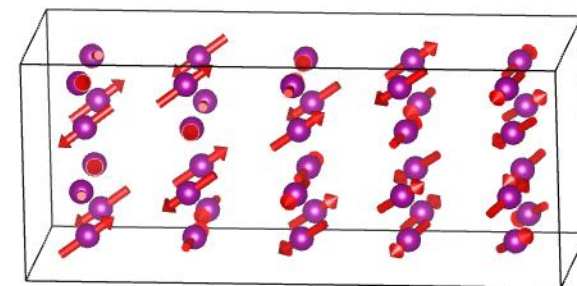
```
=> Real(0)-Imaginary(1) indicators of basis functions coefficients
      C1:0    C2:1    C3:0    C4:0    C5:0    C6:0

Mn1    C1=  0.0000(  0) C2=  2.7081( 326) C3=  0.0000(  0)
      C4=  2.3812( 476) C5=  0.0000(  0) C6=  1.7297( 643)
      C7=  0.0000(  0) C8=  0.0000(  0) C9=  0.0000(  0)
Phase/2pi=  0.0000(  0)
```

..._5K_incm.fst



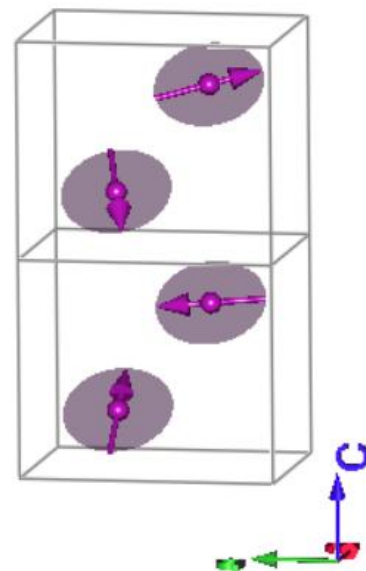
..._5K_incm.mcif



Step 3.5, Plot incommensurate magnetic structure in FPStudio

- Open the .fst file using text editor, add Keyword: ENVELOPE at the highlighted position

```
6_MnCoWO4_5K_incm.out 6_MnCoWO4_5K_incm1.fst
1 FILE for FullProf Studio: generated automatically by FullProf
2 tle: MnWO4 Nuclear refinement, 17%-Co
3 CEG P 1
4 L 4.770000 5.719997 4.920001 90.0000 90.9000 90.0000 DISPLAY MULTIPLE
5 -0.15 1.15 -0.15 1.15 -0.15 1.15
6
7
8 TICE P
9 0.21700 0.50000 -0.46000
10 M x,y,z
11 M u,v,w,0.0
12 OM Mn1_1 Mn 0.50000 0.68488 0.25000 SCALE 1.0 GROUP ENVELOPE
13 1 1 2.38121 0.00000 1.72974 0.00000 2.70807 0.00000 0.00000
14 OM Mn1_2 Mn 0.50000 0.31512 0.75000 SCALE 1.0 GROUP ENVELOPE
15 1 1 -0.29837 2.68668 -0.21674 -2.36240 -0.33932 -1.71608 0.00000
16
```



Step 3.6, Plot incommensurate magnetic structure in Mag2Pol

Symmetry

Space group:

Cell: a = b = c =
 α = β = γ =

Number of symmetry operators: Number of irreps:

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000
2	x	-y	z+1/2	u	v	w	-0.230

Atoms

Number of sites:

	Atom	x	y	z	B	occ	plot	color	R	S
1	MMN3	0.50000	0.68490	0.25000	0.008	0.833	☒	blue	10	1.0
2	W	0.00000	0.18010	0.25000	0.010	1.000	☒	red	10	1.0
3	O	0.21100	0.10360	0.94040	0.009	1.000	☒	green	10	1.0
4	O	0.25100	0.37544	0.39400	0.009	1.000	☒	green	10	1.0
5	Co	0.50000	0.68490	0.25000	0.008	0.167	☒	yellow	10	1.0

Spins

Propagation vector: q = ☒ +q $\neq$ -q

	Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
1	MMN3	2.381	0.000	1.730	0.000	2.708	0.000	0.000

Box: a: - b: - c: - Domain

View along: Rotation axis: direct

Mn

W

O

Co

Step 3.7, Plot incommensurate magnetic structure in Mag2Pol

Symmetry

Space group:

Cell: a = b = c =

α = β = γ =

Number of symmetry operators: Number of irreps:

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000
2	x	-y	z+1/2	u	v	w	0.000

Atoms

Number of sites:

	Atom	x	y	z	B	occ	plot	color	R	S
1	MMN3	0.50000	0.68490	0.25000	0.008	0.833	☒	☐	10	1.0
2	W	0.00000	0.18010	0.25000	0.010	1.000	☒	☐	10	1.0
3	O	0.21100	0.10360	0.94040	0.009	1.000	☒	☐	10	1.0
4	O	0.25100	0.37544	0.39400	0.009	1.000	☒	☐	10	1.0
5	CO	0.50000	0.68490	0.25000	0.008	0.167	☒	☐	10	1.0

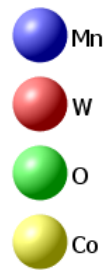
Spins

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

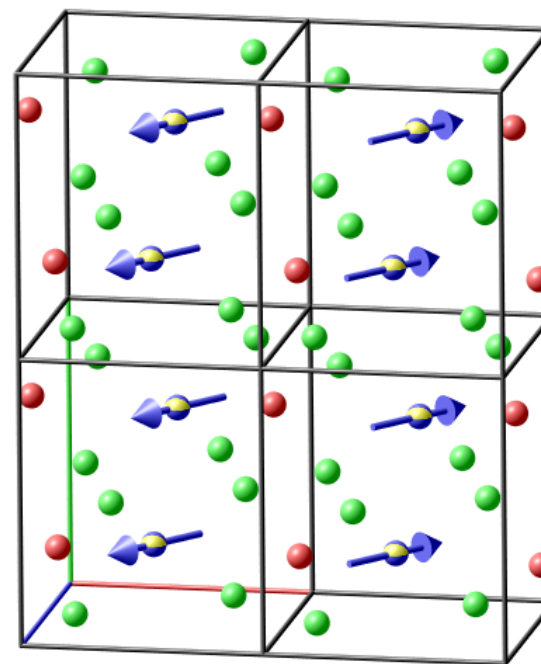
	Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
1	MMN3	-1.464	0.000	1.927	0.000	0.000	0.000	0.000

Box: a: - b: - c: - Domain: Phase:

View along: Rotation axis: direct Step (°): Zoom:



Right click to add another phase



Step 3.8, Plot incommensurate magnetic structure in Mag2Pol

File Generate Structure Fit Geometry Form factors Tools View Help



Multi-Q structure

Box: a: 0.00 - 2.00 b: 0.00 - 1.00 c: 0.00 - 2.00 Domain number: 1

View along: custom Rotation: 0 0 1 direct Step: 5 Zoom: -60

Mn
W
O
Co

