

Determination of incommensurate magnetic structures using FullProf Suite

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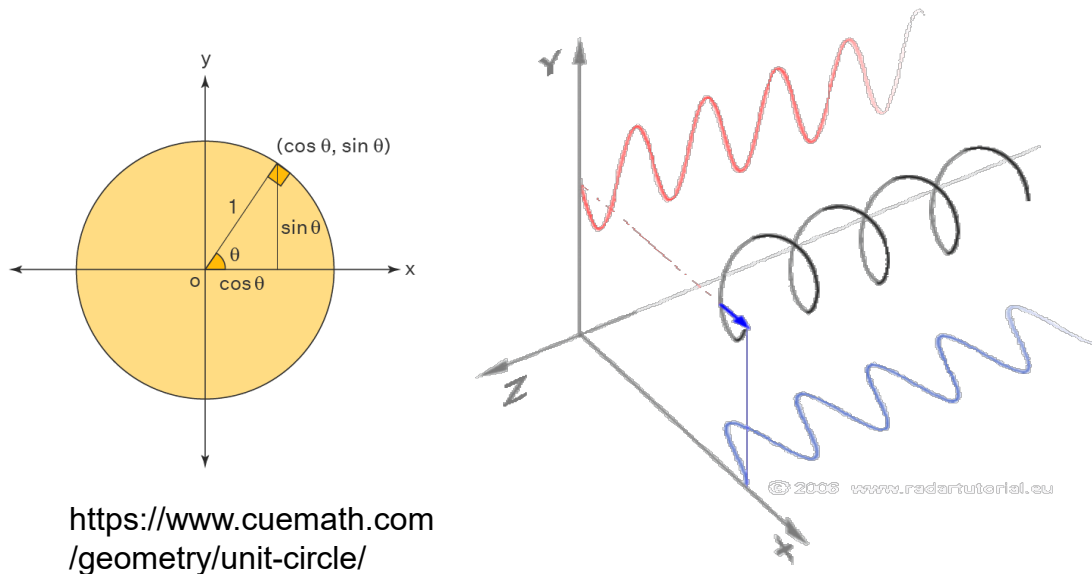


Incommensurate = wavevector $\mathbf{k}$ has irrational components

Description of modulated structures

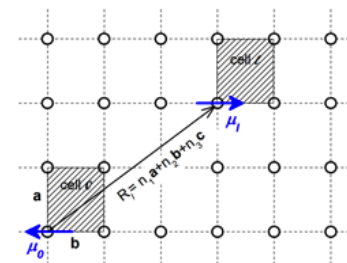
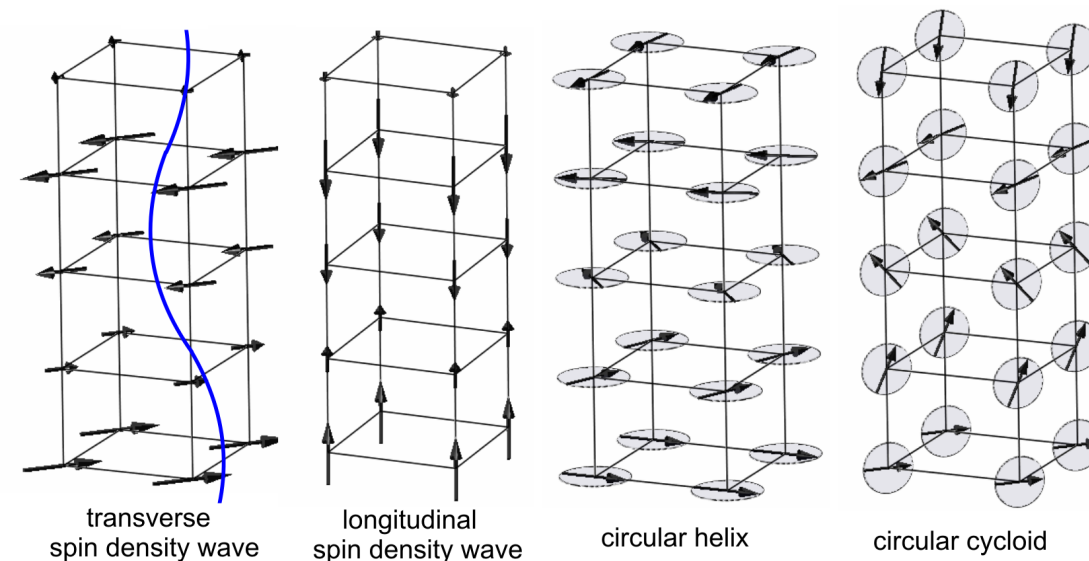
$$\boldsymbol{\mu}_{lj} = \mathbf{S}_{oj} [\cos(\mathbf{k}\mathbf{R}_l) \hat{\mathbf{u}}_j + p \sin(\mathbf{k}\mathbf{R}_l) \hat{\mathbf{v}}_j]$$

- Amplitude modulated (spin density wave)
- Spiral structures (helix or cycloid)



$\mathbf{k}$ is not kept invariant ($-\mathbf{k} \neq \mathbf{k} + \mathbf{H}$)

$$\begin{aligned} \boldsymbol{\mu}_{lj} &= \mathbf{S}_{\mathbf{k}j} e^{-2\pi i \mathbf{k}\mathbf{R}_l} + \mathbf{S}_{-\mathbf{k}j} e^{2\pi i \mathbf{k}\mathbf{R}_l} & \mathbf{S}_{\mathbf{k}j} &= \sum_{\lambda n} C_v^{\lambda n} \psi_v^{j\lambda n} \\ &= \text{Re}(\mathbf{S}_{\mathbf{k}j}) \cos(2\pi \mathbf{k}\mathbf{R}_l) + \text{Im}(\mathbf{S}_{\mathbf{k}j}) \sin(2\pi \mathbf{k}\mathbf{R}_l) \end{aligned}$$



Types of incommensurate magnetic structures

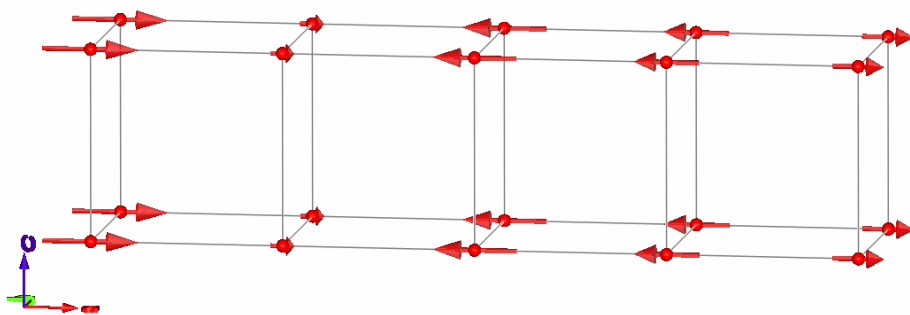
$$\mu_{lj} = \mathbf{S}_{\mathbf{k}j} e^{-2\pi i \mathbf{k} \mathbf{R}_l} + \mathbf{S}_{-\mathbf{k}j} e^{2\pi i \mathbf{k} \mathbf{R}_l} = \text{Re}(\mathbf{S}_{\mathbf{k}j}) \cos(2\pi \mathbf{k} \mathbf{R}_l) + \text{Im}(\mathbf{S}_{\mathbf{k}j}) \sin(2\pi \mathbf{k} \mathbf{R}_l)$$

➤ case of $\mathbf{S}_{\mathbf{k}j} = \text{Real}; \text{Im}(\mathbf{S}_{\mathbf{k}j}) = 0 \rightarrow \mu_{lj} = S_{oj} \cos 2\pi(\mathbf{k} \mathbf{R}_l + \varphi_j) \hat{\mathbf{u}}_j$

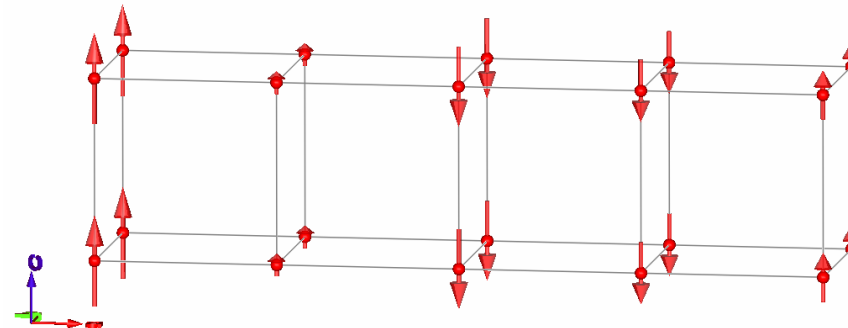
$\hat{\mathbf{u}}_j$ is a unit vector giving the moment direction, and φ_j is a phase factor

Amplitude modulated structure or sine-wave

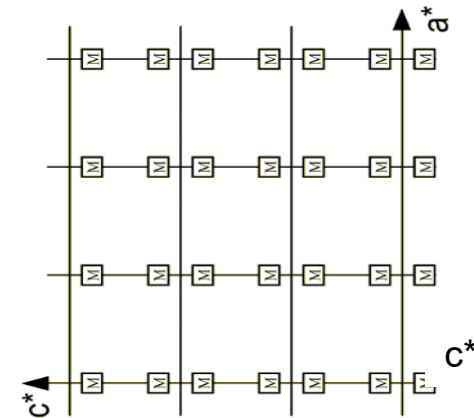
$\hat{\mathbf{u}}_j \parallel \mathbf{k} \rightarrow$ Longitudinal spin-density waves (SDW)



$\hat{\mathbf{u}}_j \perp \mathbf{k} \rightarrow$ Transverse spin-density waves



incommensurate $\mathbf{k} = (0.21, 0, 0)$



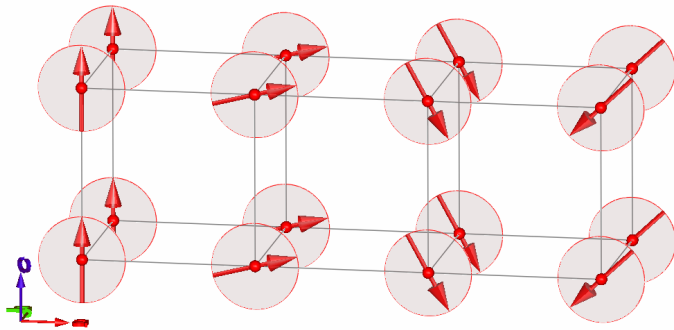
Types of incommensurate magnetic structures

$$\boldsymbol{\mu}_{lj} = \text{Re}(\mathbf{S}_{\mathbf{k}j}) \cos(2\pi \mathbf{k} \mathbf{R}_l) + \text{Im}(\mathbf{S}_{\mathbf{k}j}) \sin(2\pi \mathbf{k} \mathbf{R}_l)$$

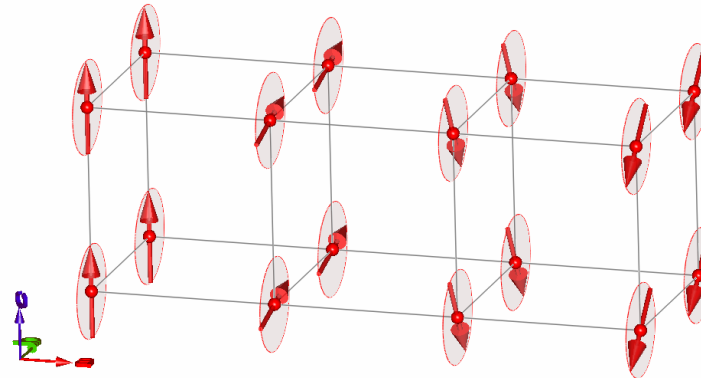
➤ case of complex $\mathbf{S}_{\mathbf{k}j} = \mathbf{S}_{oj}(\hat{\mathbf{u}}_j + i p_j \cdot \hat{\mathbf{v}}_j) e^{i\varphi_j} \quad (\hat{\mathbf{u}}_j \cdot \hat{\mathbf{v}}_j = \mathbf{0}; |\hat{\mathbf{u}}| = |\hat{\mathbf{v}}| = 1),$

→ $\boldsymbol{\mu}_{lj} = \mathbf{S}_{oj} [\cos(2\pi \mathbf{k} \mathbf{R}_l + \varphi_j) \hat{\mathbf{u}}_j + p \sin(2\pi \mathbf{k} \mathbf{R}_l + \varphi_j) \hat{\mathbf{v}}_j]$ *helical structure*

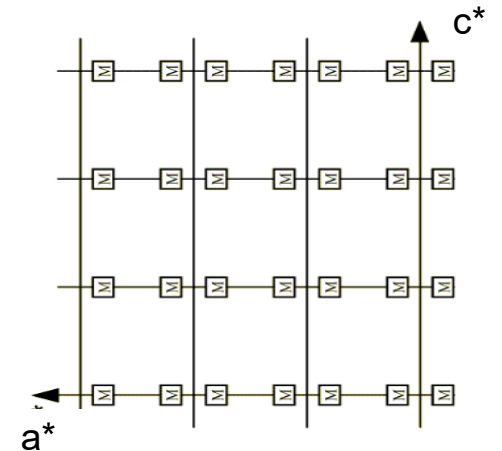
$\mathbf{k} \parallel (\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j) \rightarrow \text{cycloid}$



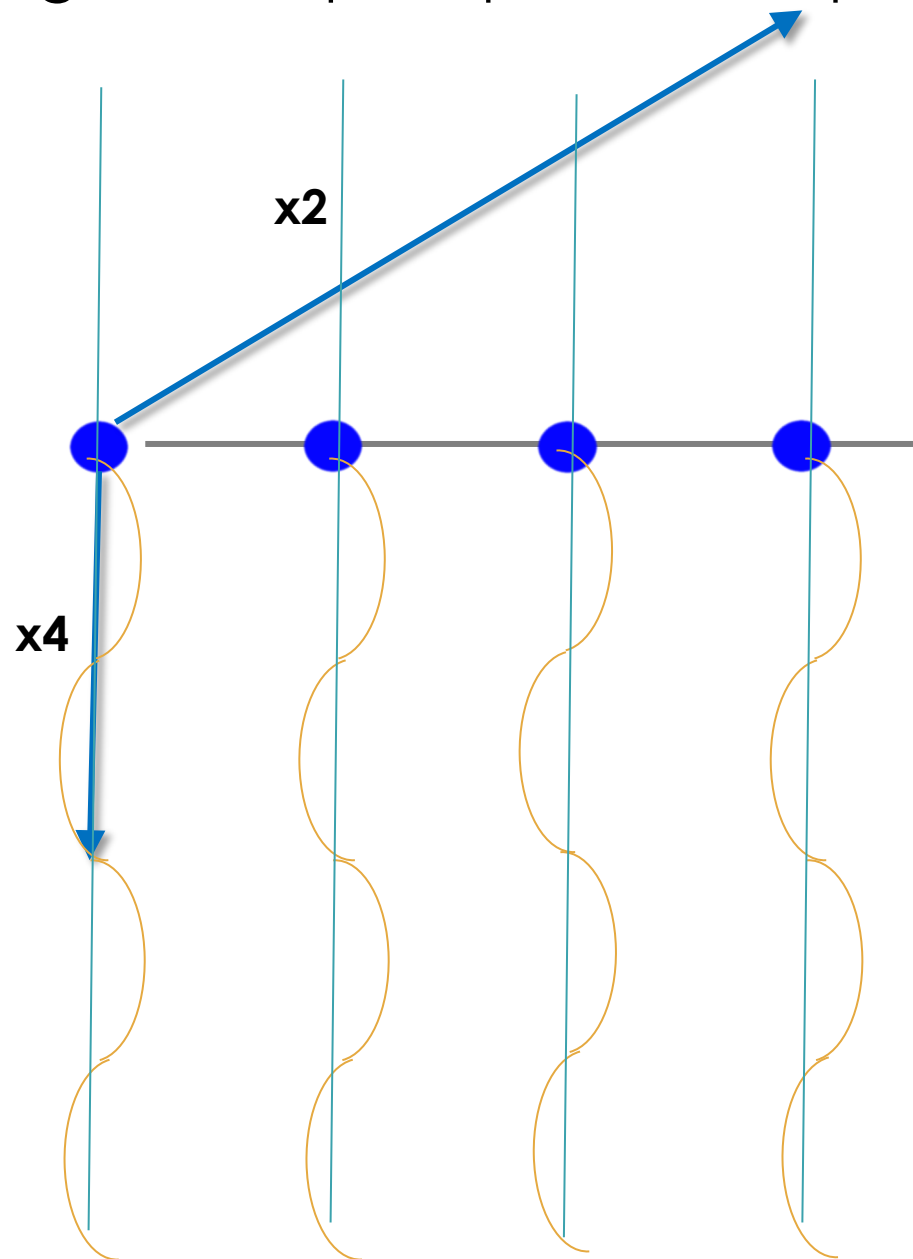
$\mathbf{k} \perp (\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j) \rightarrow \text{helix or spiral}$



incommensurate $\mathbf{k} = (0.21, 0, 0)$



Magnetic Super-Space-Groups (MSSG)



- Implemented by de Wolff (*Acta Cryst. A*, 30, 777, 1974) to describe periodic perturbations
- Incommensurate modulations destroy translational periodicity
- Treat each atom in the 1D unit cell as a wave along a new “phase” dimension (x_4).
- Translational periodicity is recovered by performing an additional translation along the internal coordinate $x_4 = \mathbf{k}(\mathbf{R}_l + \mathbf{r}_j)$.
- we get one extra phase dimension for each of the d independent modulation waves
We call the result $(3+d)$ -dimensional superspace.

$$\mu_j(x_4) = \mathbf{M}_j e^{ix_4} + \mathbf{M}_j^* e^{-ix_4}$$

$$\mathbf{S}_{\mathbf{k}j} = \mathbf{M}_{\mathbf{k}j} \exp(i\mathbf{k} \cdot \mathbf{r}_j)$$

Branton Campbell presentation:

<https://www.youtube.com/watch?v=4c9QXyax4Qg>

research papers



ISSN 2053-2733

Enumeration and tabulation of magnetic (3+d)-dimensional superspace groups

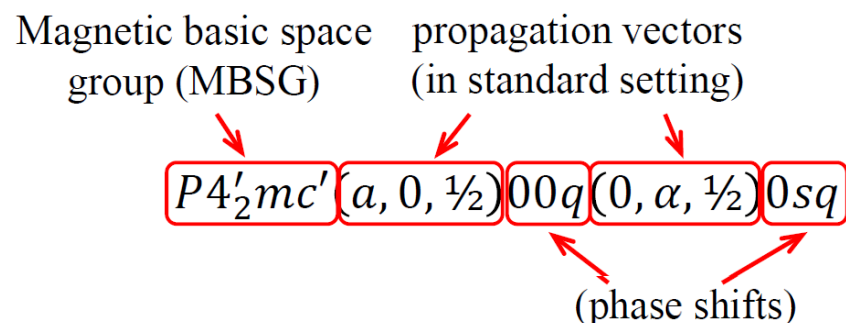
Harold T. Stokes and Branton J. Campbell*

Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA. *Correspondence e-mail: branton_campbell@byu.edu

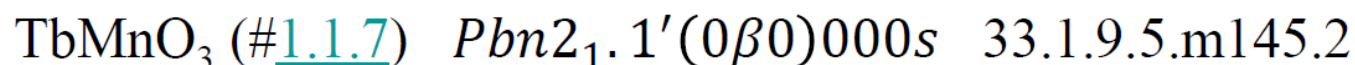
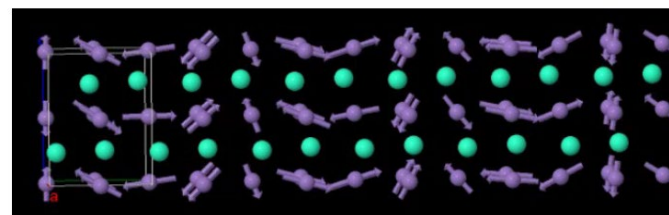
Received 14 January 2022
Accepted 10 April 2022

A magnetic superspace group (MSSG) simultaneously constrains both the magnetic and non-magnetic (e.g. displacive, occupational, rotation and strain)

	MPG	MSG (d=0)	MSSG (d=1)	MSSG (d=2)	MSSG (d=3)
Type 1	32	230	775	3338	12584
Type 2	32	230	775	3338	12584
Type 3	58	674	3100	15218	60799
Type 4	--	517	4653	31862	176101
Total	122	1651	9303	53756	262068



Example:

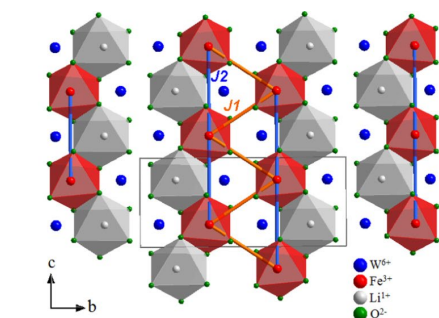


For more information :

J. M. Perez-Mato, J. L. Ribeiro, V. Petříček and M. I. Aroyo, “Magnetic superspace groups and symmetry constraints in incommensurate magnetic phases “J. Phys. Condens. Matter, 24, 163201, 2012.

LiFe(WO₄)₂: Multiferroic with cycloidal magnetic structure

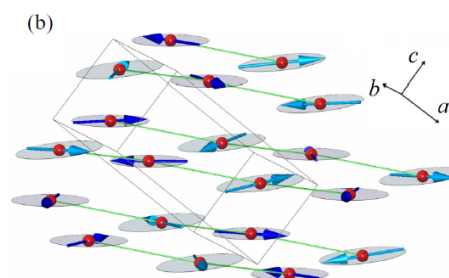
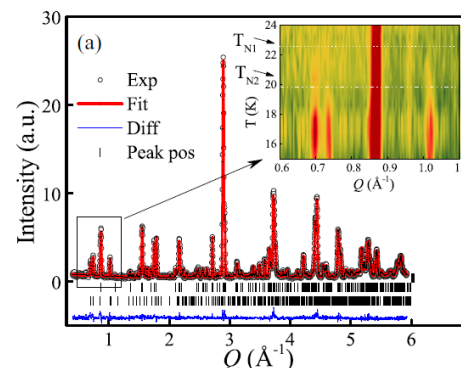
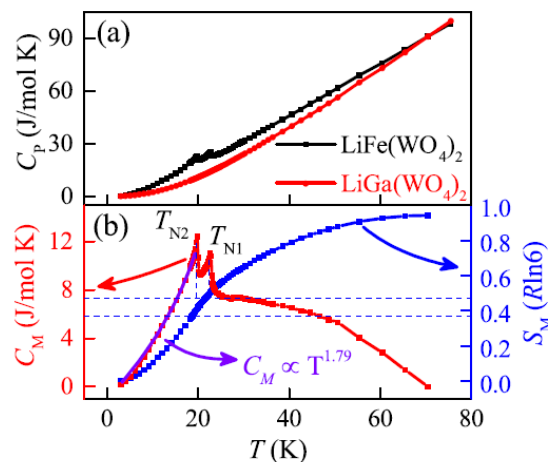
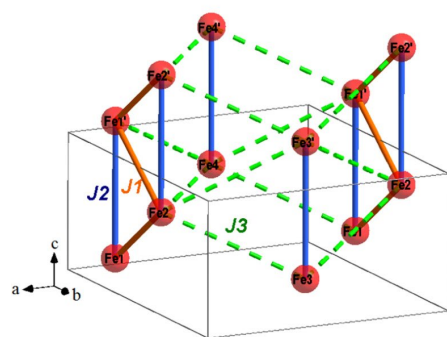
monoclinic C2/c structure consisting of stacked (100)-layers of mixed [LiO6] and [FeO6] edge-sharing octahedra arranged in frustrated two-leg spin ladders, separated by layers composed of tungstate [WO6] octahedra.



$$a = 9.2997 \text{ \AA}, b = 11.4302 \text{ \AA}$$

$$c = 4.9072 \text{ \AA}, \beta = 90.65^\circ$$

Two successive magnetic transitions are observed at $T_{N1} = 22.6 \text{ K}$ and $T_{N2} = 19.7 \text{ K}$



Meifeng Liu *et al.*, "Cycloidal magnetism driven ferroelectricity in double tungstate LiFe(WO₄)₂", *Phys. Rev. B* 95, 195134 (2017)

Single crystal study
S. Biesenkamp *et al.*
PRB 103 134412 (2021)
confirmed the powder results



LiFe(WO₄)₂ (#1.1.129)

[view in Jmol](#)
[Download mcif file](#)

Files provided for this tutorial:

- Neutron powder diffraction data (BT1) data files measured at 30 K and 5 K (in XYSigma format):
[LiFeW2O8-5K.dat](#); [LiFeW2O8-30K.dat](#)
- Instrument resolution file: [bt1_fp.irf](#)
- CIF files for crystal structure: [LiFeW2O8.cif](#)
- Supporting information: [LiFe\(WO4\)_PhysRevB.95.195134](#)
- PCR Solutions (backup files)
“LiFeW2O8_nuc.pcr”

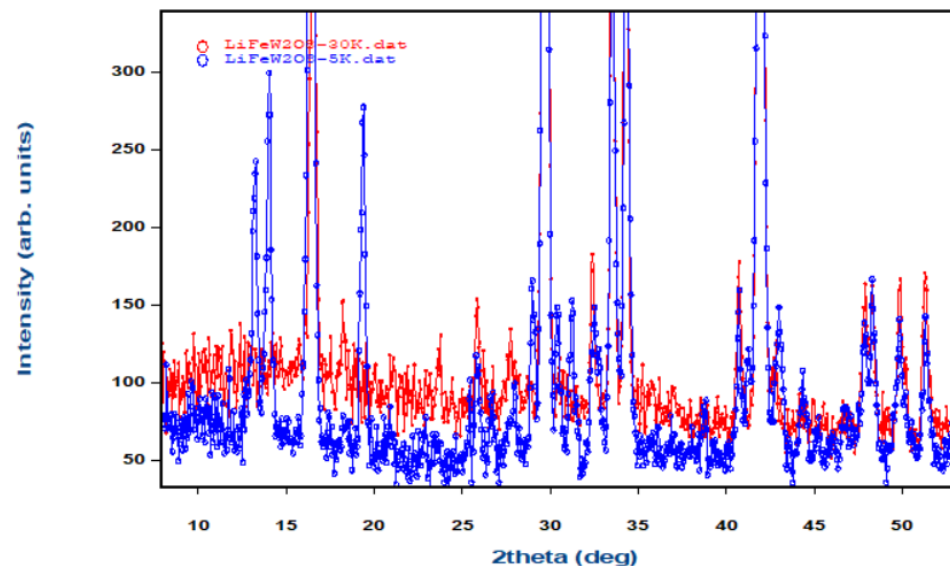
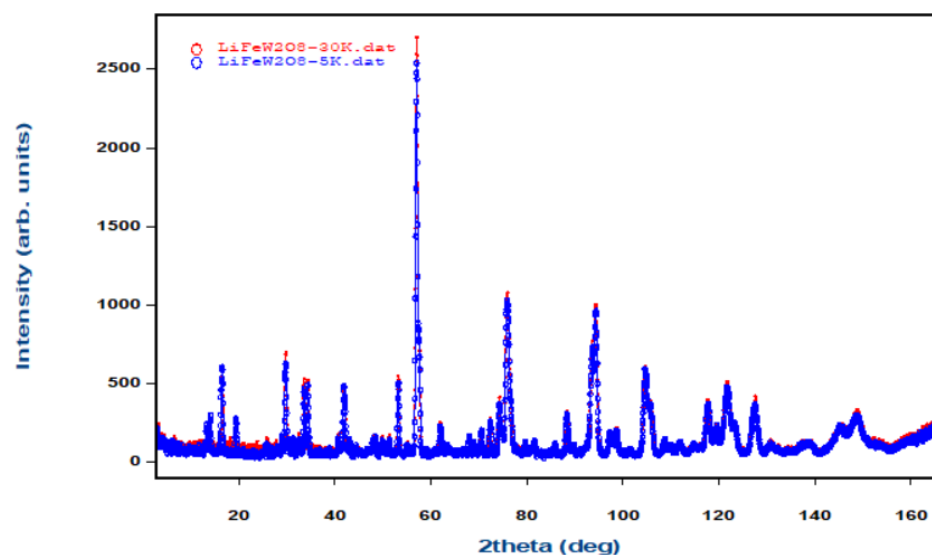
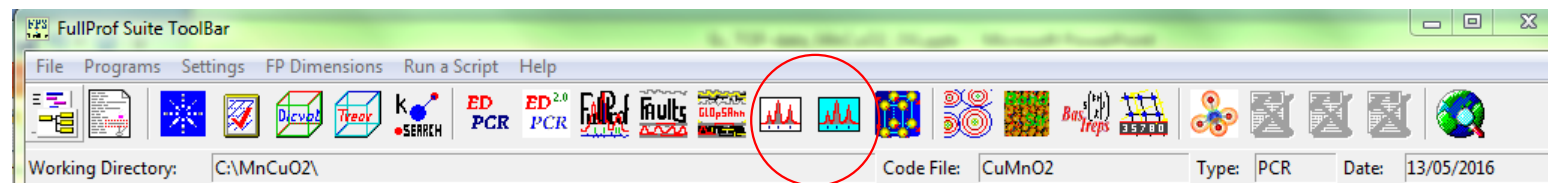
Exercise Steps:

- I. Import the known crystal structure/instrument parameters to create a PCR file
- II. Refine the structural model and the profile parameters
- III. Identify the magnetic reflections and determine the propagation vector (k-search in Winplotr)
- IV. Perform symmetry analysis to obtain IRs and Basis vectors
- V. Select a magnetic model and add it as a second phase in the PCR file
- VI. Perform refinement for the magnetic phase
- VII. Display the magnetic structure using *FPStudio*
- VIII. Identify possible magnetic models using ISODISTORT
- IX. Select a magnetic model (mcif) and convert it to PCR format
- X. Configure the new PCR file and perform refinement
- XI. Display the magnetic structure using MVISUALIZE or Vesta

Irrep approach
(SARAh or BasIreps)

Super-space group
approach
(ISODISTORT)

Observe the differences in the data measured at 30 K and 5 K



The 5 K data contains additional Bragg peaks at low two-theta angles.

The crystal structure needs to be well determined before attempting to model the magnetic peaks. Check the presence of impurities in the sample (this is especially important when dealing with incommensurate orders).

Import the known crystal structure/instrument parameters to create a PCR file

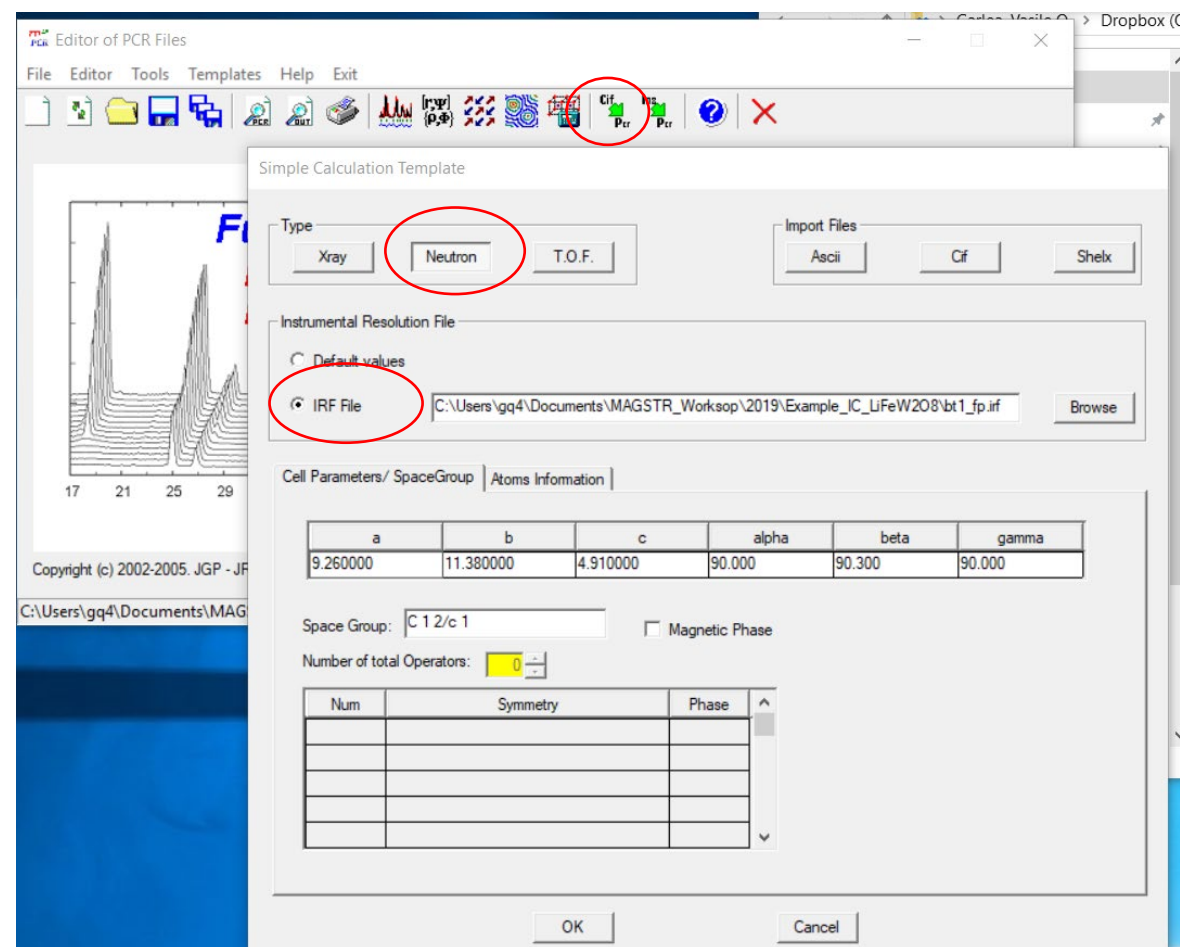
- use “**Cif → Pcr**” button in **EdPCR** to import the crystallographic information file CIF (**LiFeW2O8.cif**) and create the FullProf input file (*.PCR)

Atom (Wyck.)	x	y	z	B
W (8f)	0.2468(2)	0.0910(4)	0.250(1)	0.34(7)
Fe (4e)	0	0.3359(3)	0.25	0.1(1)
Li (4e)	0.5	0.342(1)	0.25	0.7(2)
O1 (8f)	0.3634(4)	0.0586(3)	0.9225(6)	0.12(2)
O2 (8f)	0.3806(3)	0.1821(3)	0.4127(6)	0.12(2)
O3 (8f)	0.3559(3)	0.5483(3)	0.9451(6)	0.12(2)
O4 (8f)	0.3773(4)	0.6946(2)	0.3936(6)	0.12(2)

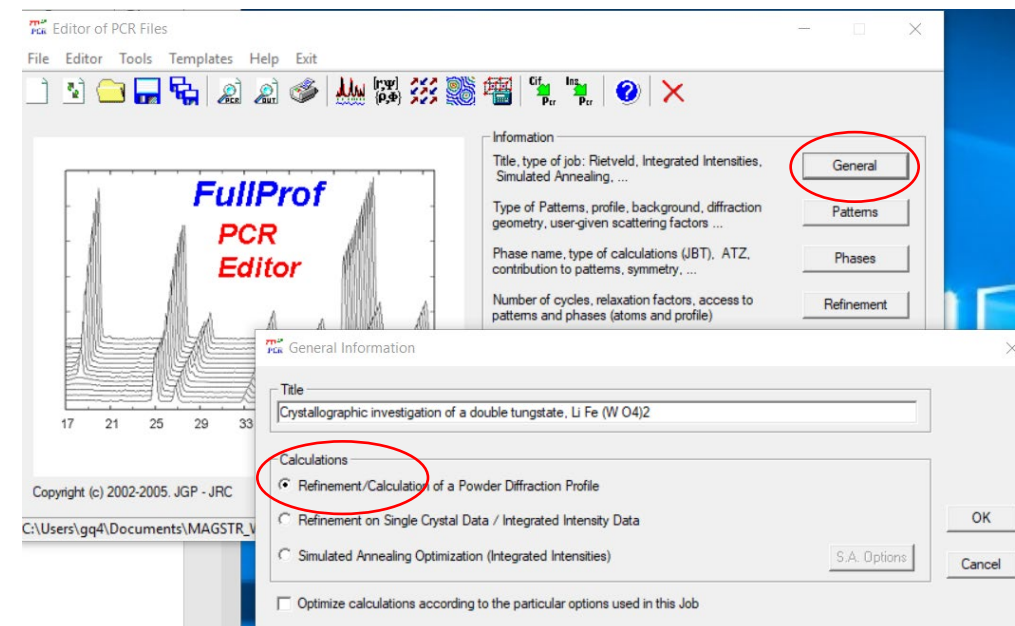
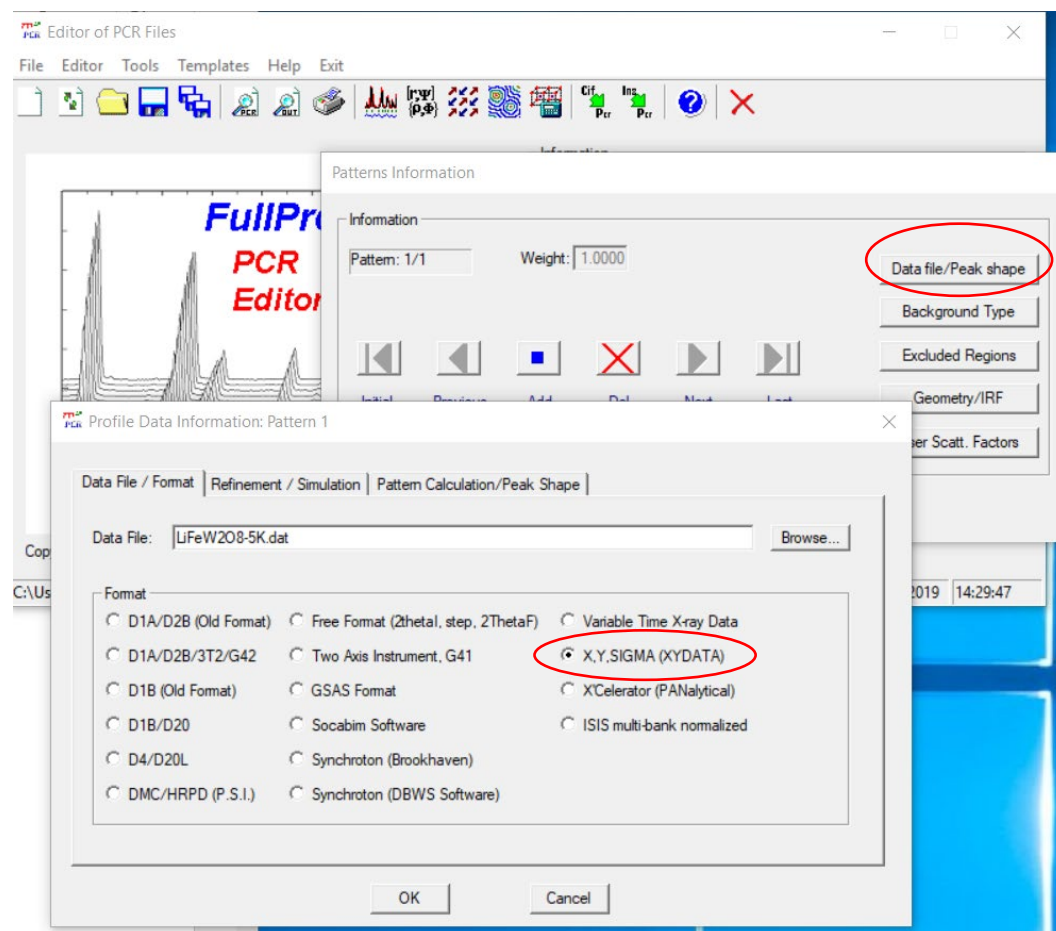
SP: $C2/c$, $a = 9.2687(1) \text{ \AA}$, $b = 11.3964(1) \text{ \AA}$,
 $c = 4.89368(6) \text{ \AA}$, $\beta = 90.564(1) \text{ deg.}$, $\chi^2 = 1.1$

Note: occ = site multip./general multip.
 Always check if this has been correctly
 calculated after importing the .cif file.

- in the new window, select the “**Neutron**” tab for the type of calculations
- use the “Browse” button to upload the instrument resolution file “**IRF**” : **bt1_fp.irf**



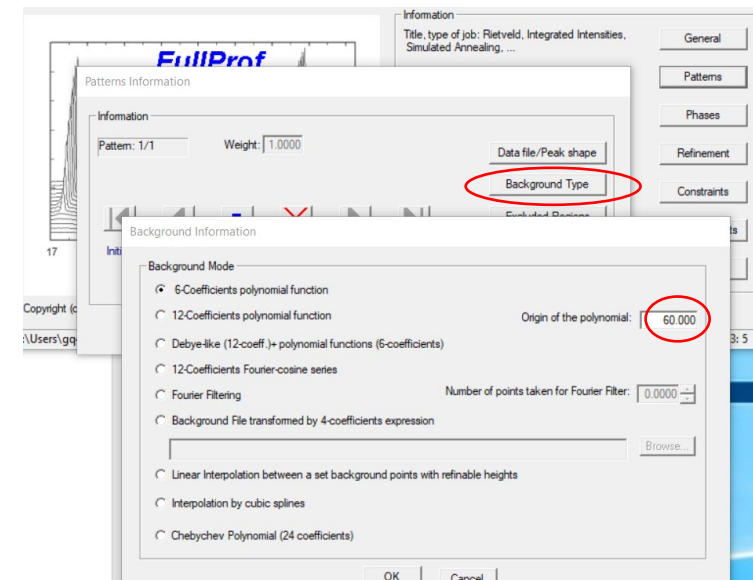
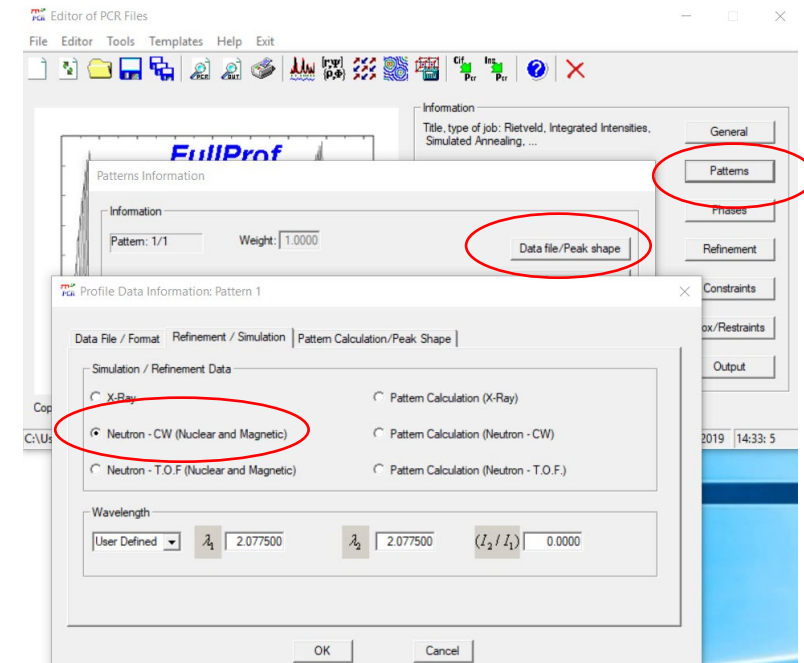
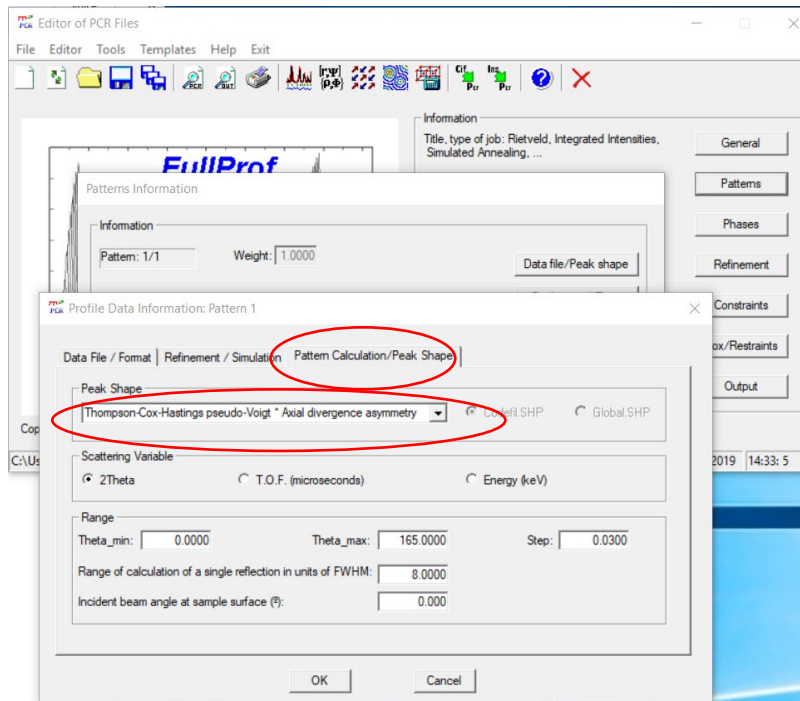
- In “**General**” tab, you’ll see the first option “**Refinement of Powder diffraction**” as the default selection



- Open the “**Patterns**” Tab, and then the “**Data file/ peak shape**” and select the “**XYSIGMA**” for the data file format

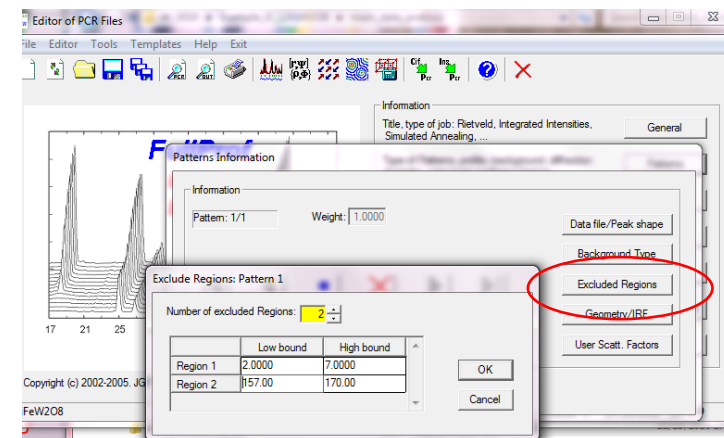
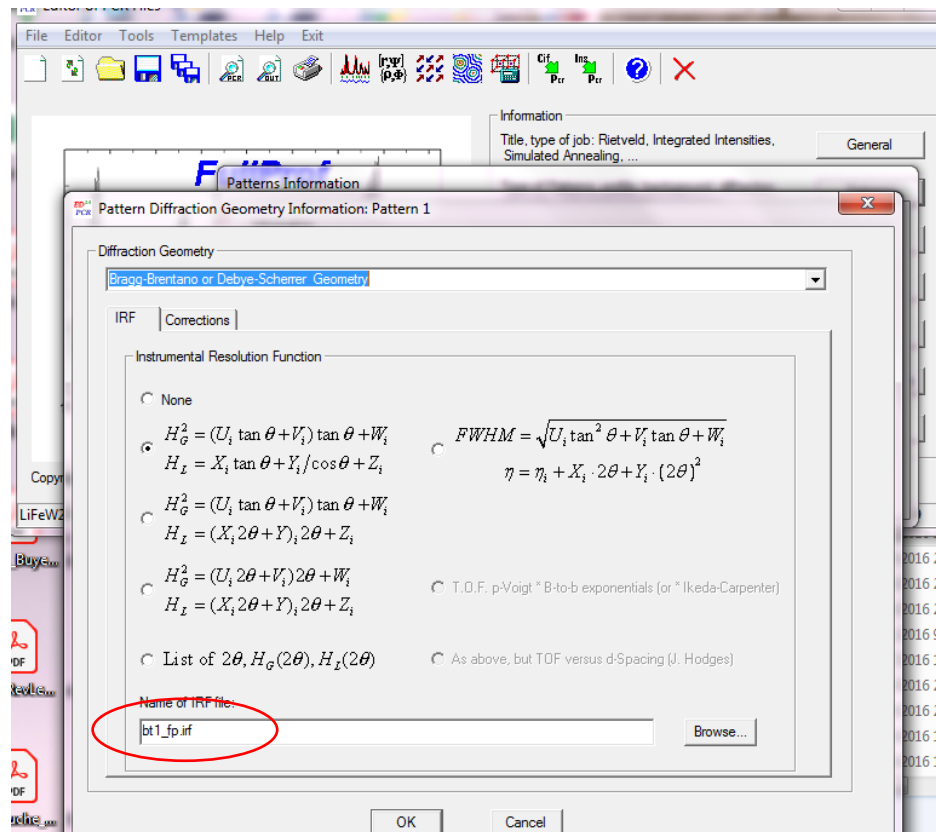
In the “*Patterns*” & “*Data file/ peak shape*” tabs, select the “Refinement/Simulation”, and make sure to select “*Neutron-CW*”

In “*Data file/ peak shape*” - “Pattern calculation/Peak Shape” tab, select the “Thompson-Cox-Hastings pseudo-Voigt * Axial divergence asymmetry” for the peak shape type

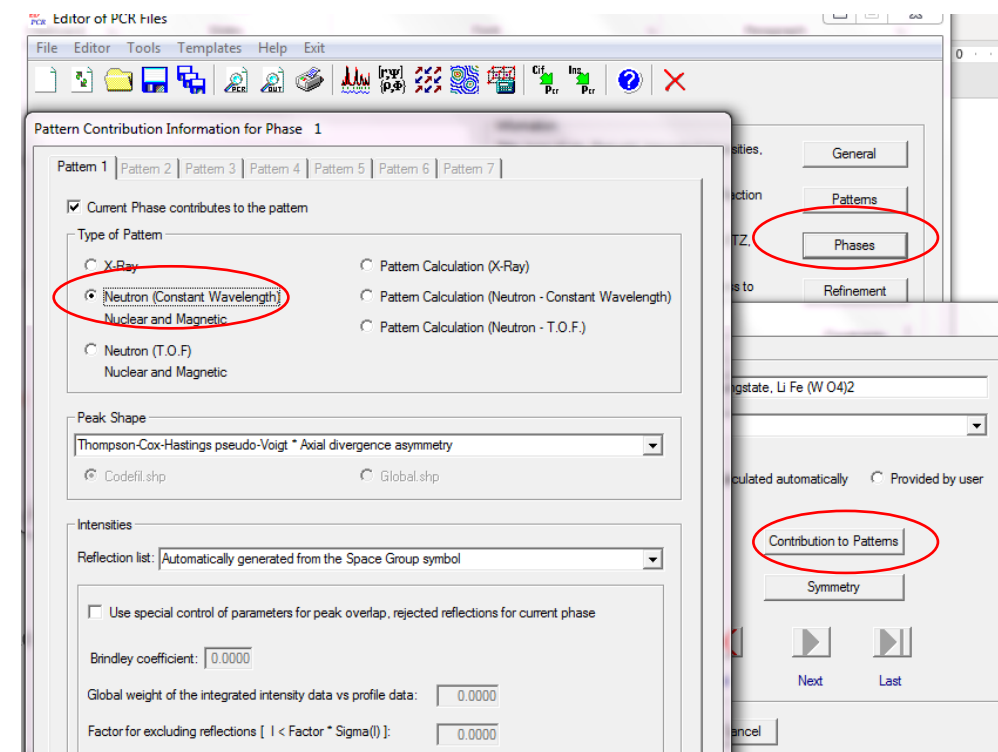


For the background information, select the “*6-coefficients polynomial function*”

Add two **excluded regions** with the scattering ranges 2 to 7 deg , and 157 to 170 deg



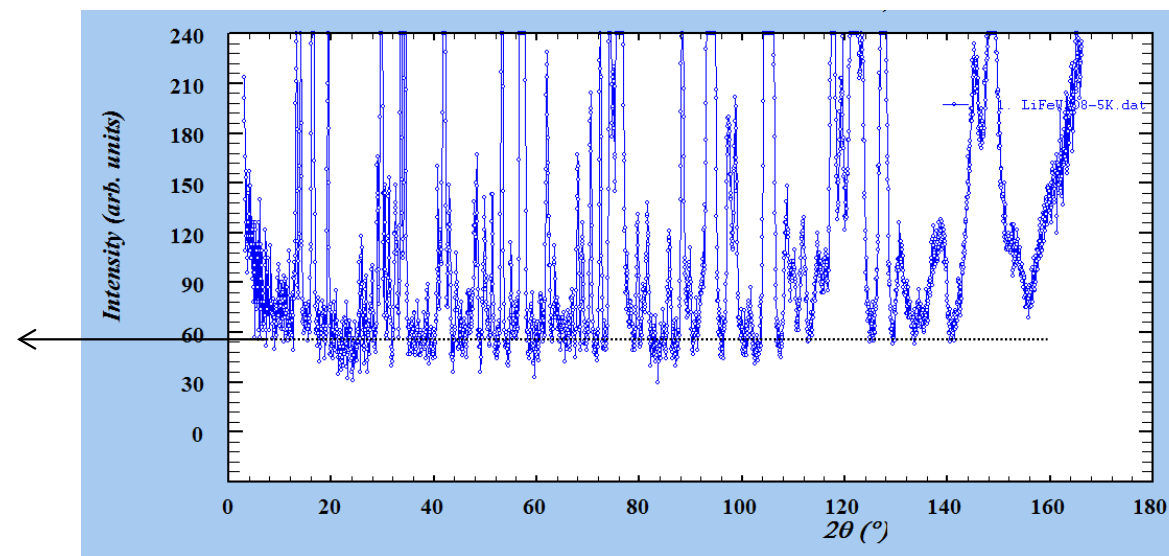
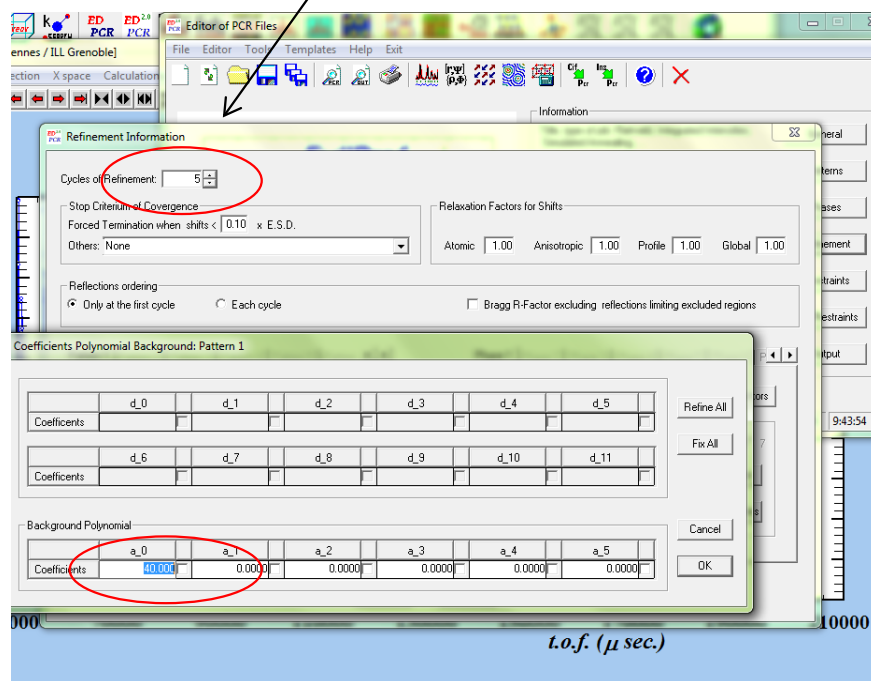
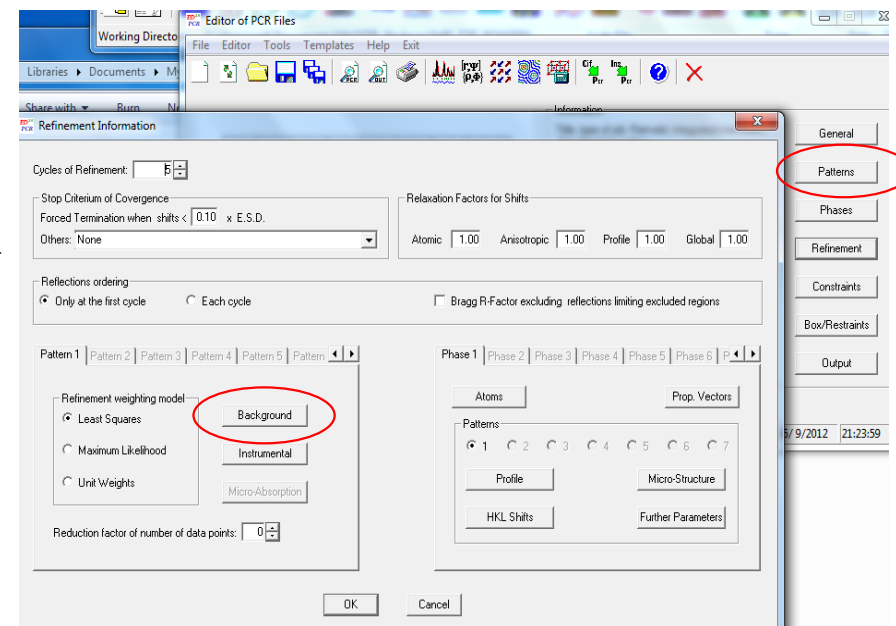
In the "**Geometry/IRF**" tab, you should see the IRF file that you previously assigned to the BT1 data



Open the "**Phases**" tab (1) and then click on the "Contribution to patterns" and select the "current phase contributes to the pattern " and "**Neutron CW**" and "**Thompson-Cox-Hastings pseudo-Voigt** " for the peak shape

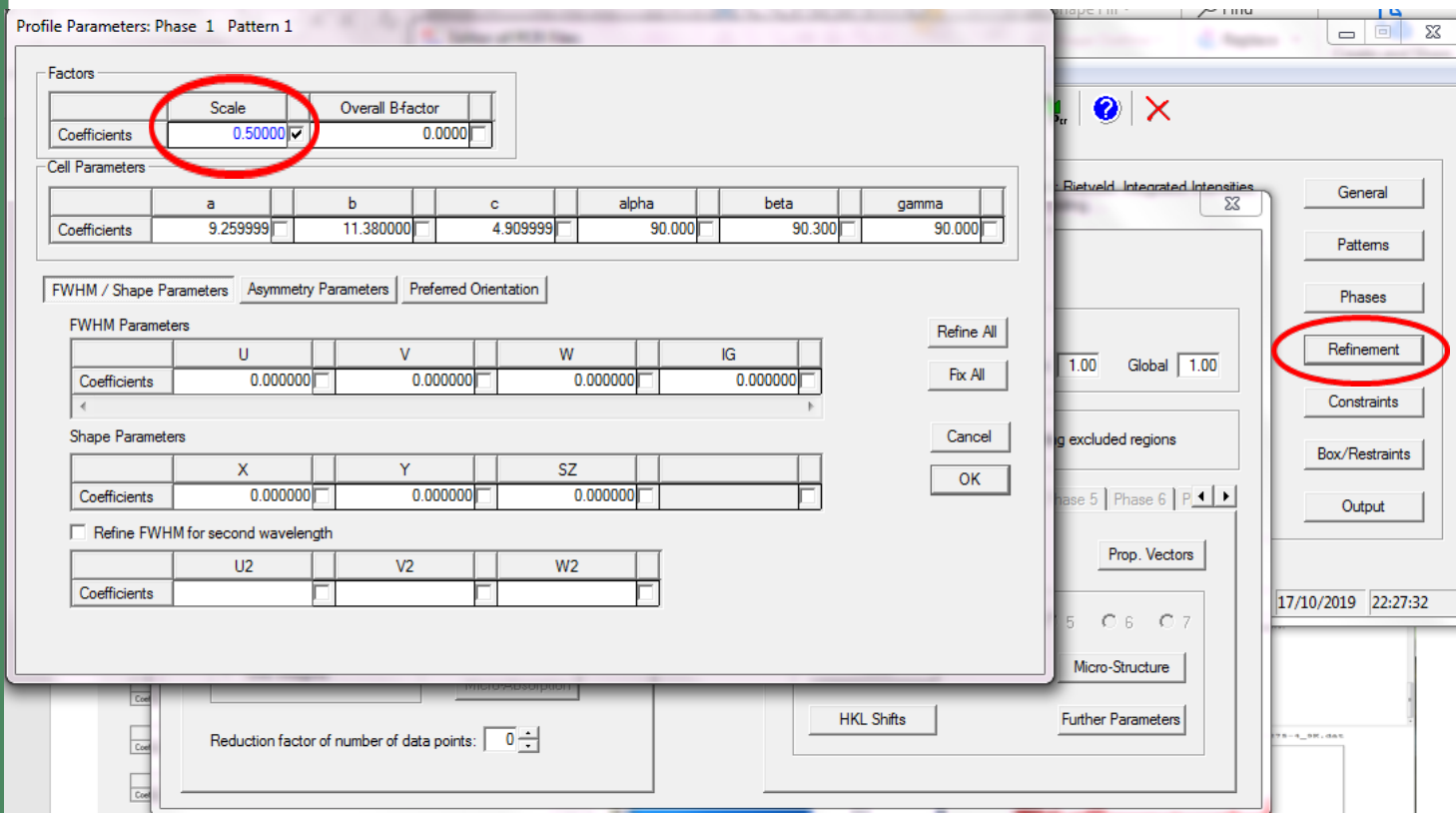
Open the “**Refinement**” tab and then the “**Background**” and add a value for the “a₀” coefficient that will give a first flat line approximation for the background (~ 50, read it from the data file)

One can also increase the number in the “**Cycles of refinement**” box, to 5 or higher. This only becomes important when we are setting some parameters for being refined.

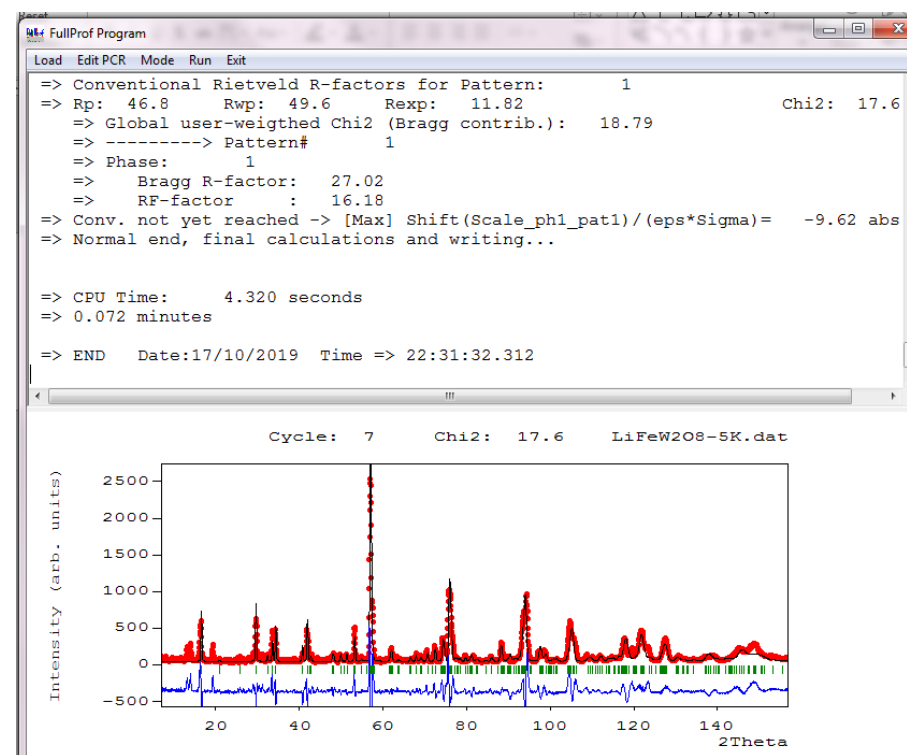


Refine the structural and profile parameters

In the same “*Refinement*” window, click on the “*Profile*” tab and set the number for the “*Scale factor*” to (use 0.5 for this example). Remember to SAVE the PCR file by clicking the “Save” button, every time a change has been made

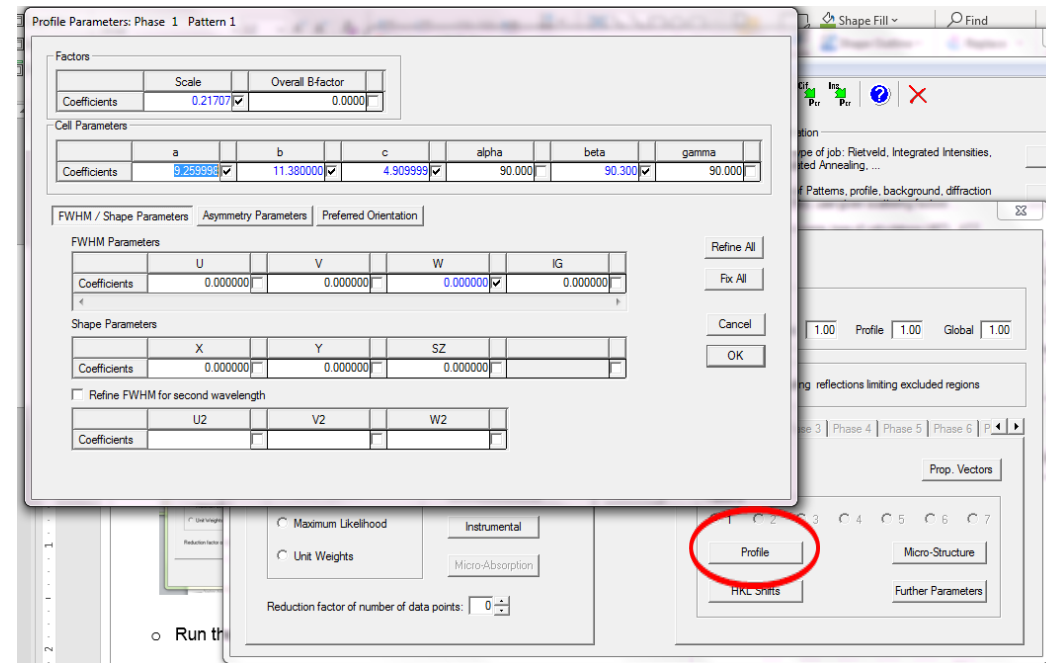
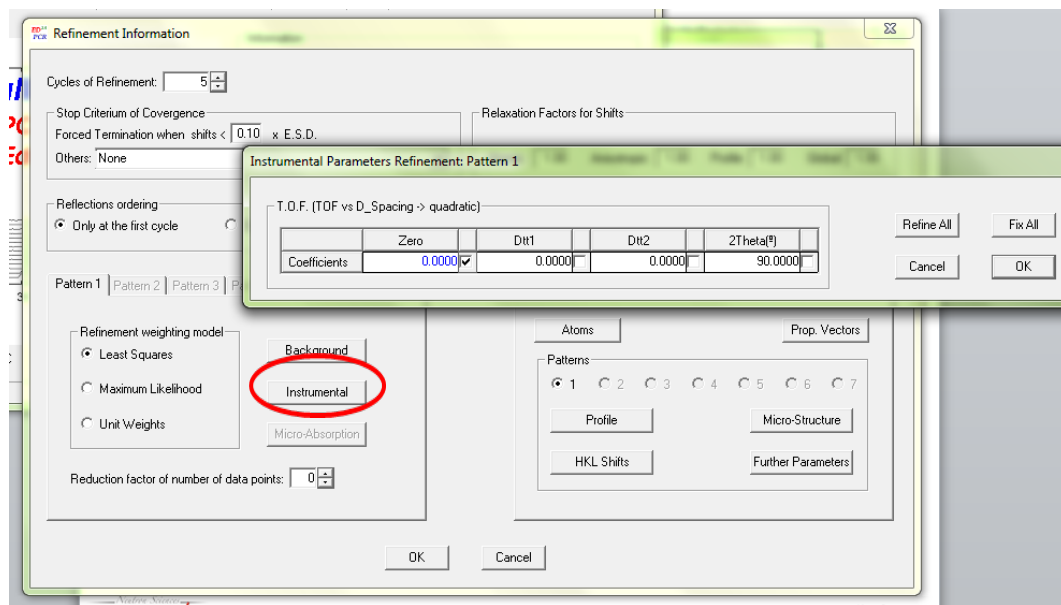


Run the Fullprof program and select the “*LiFeW2O8-5K.dat*” file for data.



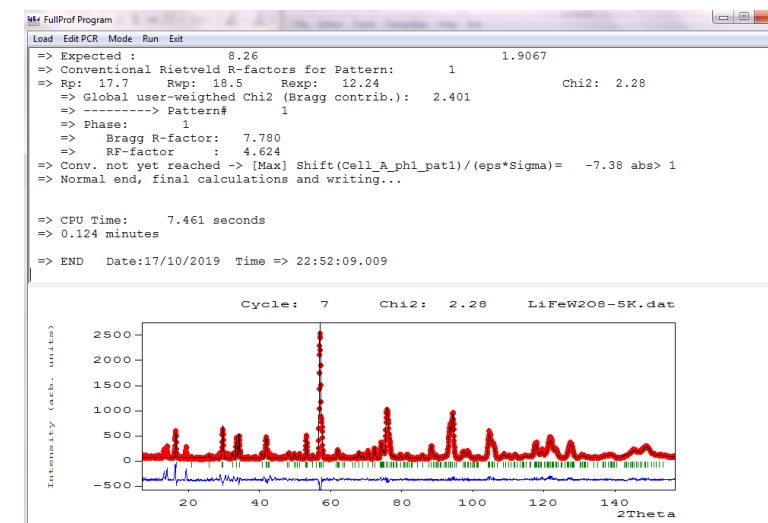
Refine a number of parameters (e.g.: scale factor, lattice parameters, profile parameters, background coefficients, zero shift, as well as atomic positions) to improve the fit.

Note: The profile parameters will only show the deviations of the U, V, W X, Y parameters from those defined in the IRF file.



Run the Fullprof program again to fit the data

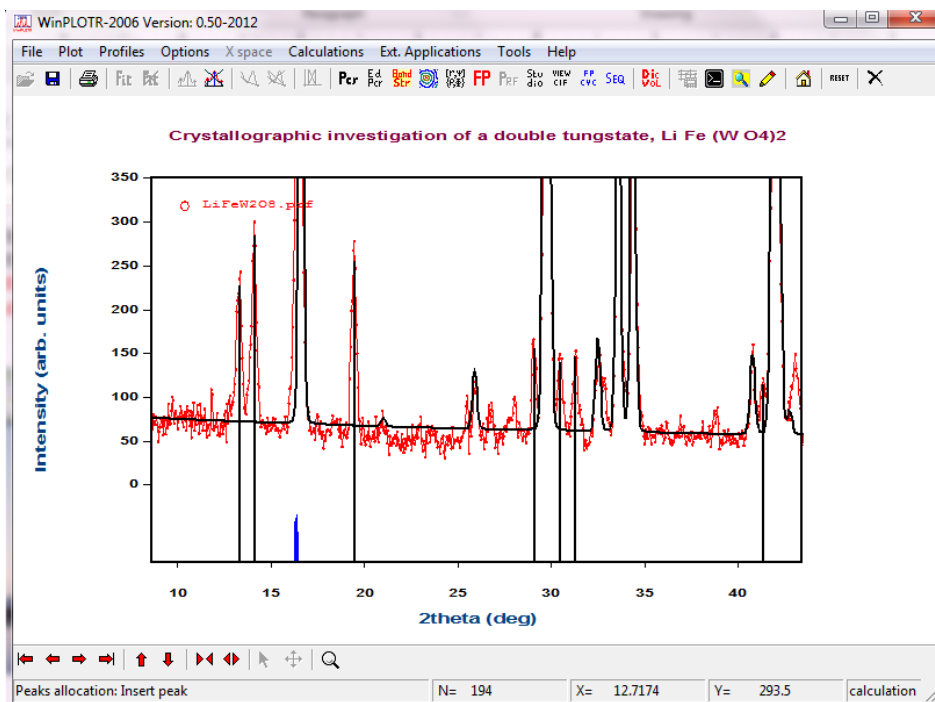
In case you couldn't follow these steps, a PCR file for fitting the nuclear contribution is provided "**LiFeW2O8_nuc.pcr**"



Determine the propagation vector ($\mathbf{k}$)

Open the PFR file (Rietveld plot) with the WINPLOTR-2006 and select the magnetic reflections. Go to “*Calculations – Peak detection – Enable*”, followed by “*Calculations – Peak detection – Insert peak*”

Select the peaks at $2\theta \sim 13.33, \sim 14.14, \sim 29.12, \sim 30.47$ and 31.29 deg, and save them into the “*k-search format*” by doing “*Calculations*” – “*Peak detection*” – “*Save peaks*”



The “*k-search*” window will display the input parameters that are automatically initialized. The restriction to commensurate wavevectors (“*special k-vectors*”) will not give any solution. One must test incommensurate $\mathbf{k}$ by testing different high symmetry direction. Since the structure is C-centered the $\mathbf{k}$ -search needs to be extended from 0.5 to 1 values.

- A suggested incommensurate solution is $\mathbf{k} = (0.89, 0.0, 0.33)$

=> List of the best 10 solutions for 6 satellites

Kx	Ky	Kz	R-factor
0.890000	0.000000	0.330000	1.382324
0.900000	0.000000	0.330000	1.440757
0.880000	0.000000	0.330000	2.709579
0.910000	0.000000	0.330000	2.931234
0.890000	0.000000	0.340000	3.230400
0.880000	0.000000	0.340000	3.262982
0.890000	0.000000	0.670000	3.482375
0.890000	0.000000	0.660000	3.625372
0.900000	0.000000	0.340000	3.633707
0.880000	0.000000	0.660000	4.076433

Perform symmetry analysis to obtain IRs and Basis vectors

Irrep approach

using the SARAh program at

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

Select the SARAh webRefine from the web-software tab and introduce the paramagnetic space group (#15), the *k*-vector and the Fe atom position



SARAh webRefine – FullProf

Two pieces of advice for using SARAh webRefine : 1. change your browser settings to allow you to select where you save downloads (and overwrite files), 2. when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information.

-Andrew (February 2022)



Space group :

Propagation vector :

Crystallographic coordinates with each atom on a separate line :

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

Fe 0.00000 0.33421 0.25000

There are 2 possible irreducible representation (IRs) allowed for the Fe ion at the 4e position, as summarized in the Table.

TABLE II. Basis vectors for the space group $C12/c1$ with $\mathbf{k} = (0.89, 0, 0.332)$. The decomposition of the magnetic representation for the Fe site $(0, 0.335, 0.25)$ is $\Gamma_{\text{Mag}} = 3\Gamma_1^1 + 3\Gamma_2^1$. The atoms of the nonprimitive basis are defined according to 1: $(0, 0.335, 0.25)$, 2: $(0, 0.665, 0.75)$. The ζ parameter is $\exp(-2\pi i \mathbf{k} \cdot \mathbf{t})$.

IR	BV	Fe1 (0, 0.335, 0.25)	Fe2 (0, 0.665, 0.75)
Γ_1	ψ_1	(1, 0, 0)	$(-\zeta, 0, 0)$
	ψ_2	(0, 1, 0)	(0, ζ , 0)
	ψ_3	(0, 0, 1)	(0, 0, $-\zeta$)
Γ_2	ψ_4	(1, 0, 0)	(ζ , 0, 0)
	ψ_5	(0, 1, 0)	(0, $-\zeta$, 0)
	ψ_6	(0, 0, 1)	(0, 0, ζ)

Select a magnetic model and add it as a second phase

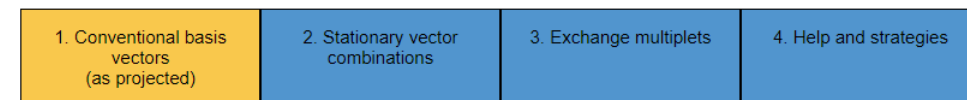
Irrep approach

- Select powder format and the option “add new phase to pcr”. Choose the pcr you want to modify for magnetic refinement.

Note: you need to set the browser to ask for download location

- Select all BV of the two available IRs

- Save the new pcr file under different name
Ex: **lifew2o8_irrep.pcr**



Method 1. Conventional analysis - as projected basis vectors

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

1. powder format 1. add new phase to pcr Choose File lifew2o8_irrep.pcr

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

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

Submit

Table. The basis vectors projected from the different IRs :

$\Gamma_1 \psi_1$	$\Gamma_1 \psi_2$	$\Gamma_1 \psi_3$
$\begin{pmatrix} \text{Fe } 1 \\ 2 \end{pmatrix} \begin{pmatrix} 1.0 & 0. \\ -0.509041 & -0.860742 i \end{pmatrix}$	$\begin{pmatrix} \text{Fe } 1 \\ 2 \end{pmatrix} \begin{pmatrix} 0. & 1.0 \\ 0.509041 & +0.860742 i \end{pmatrix}$	$\begin{pmatrix} \text{Fe } 1 \\ 2 \end{pmatrix} \begin{pmatrix} 0.0 & 1. \\ 0. & -0.509041 - 0.860742 i \end{pmatrix}$

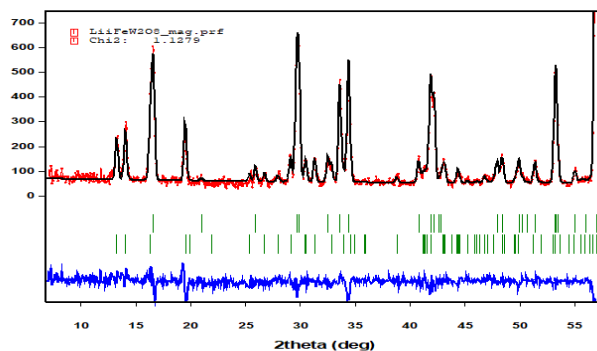
```
!-----
! Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 46.66
!-----
Template magnetic phase by SARAH - web Representational Analysis
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt IrF Isy Str Furth ATZ Nvk Npr More
! 1 0 0 0.0 0.0 1.0 1 0 -2 0 0 2233.933 1 7 0
!
!
C -1
! Nsym Cen Laue Ireps N_Bas
! 2 1 1 -1 6
! Real(0)-Imaginary(1) indicator for C1
! 0 0 0 0 0
!
SYMM X, Y, Z
BASR 1. 0 0 0 1. 0 0 0 1. 1. 0 0 0 1. 0 0 0 1.
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM X, 1 - Y, 1/2 + Z
BASR -0.509 0 0 0 0.509 0 0 0 -0.509 0.509 0 0 0 -0.509 0 0 0 0.509
BASR 0.8607 0 0 0 -0.8607 0 0 0 0.8607 -0.8607 0 0 0 0.8607 0 0 0 -0.8607
!Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
Fe MFE3 1 0 0 0.33421 0.25000 .30000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
0.2369683 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00000 0.000 0.000 0.000 0.000 0.000
! U V W X Y GauSiz LorSiz Size-Model
0.000000 0.000000 0.009051 0.000000 0.000044 0.000000 0.000000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma #Cell Info
9.268055 11.394946 4.893242 90.000000 90.569206 90.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
0.89 0. 0.33 Propagation Vector 1
0.000000 0.000000 0.000000
```

Edit the PCR file and refine the magnetic phase

Irrep approach

$$\mu_{lj} = 2\text{Re}(\mathbf{S}_{kj}) \cos(2\pi \mathbf{kR}_l) + 2\text{Im}(\mathbf{S}_{kj}) \sin(2\pi \mathbf{kR}_l)$$

- The section dedicated to the “profile parameters” of the magnetic phase should remain unchanged. The scale factor and lattice parameters have to be the same as for the nuclear phase. The profile parameters could be allowed to change after finding a good model.
- Combination of different BVs could be tested to get the best fit.
- The c2, c4 and c6 coefficients need to be initiated to some non-zero values. To describe a spiral structure, c2 (0 1 0) must be set as imaginary (1)
- Run the Fullprof fit and examine the calculated magnetic intensities.



```

!-----
! Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 46.66
!-----
Template magnetic phase by SARAh - web Representational Analysis
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
1 0 0 0.0 0.0 1.0 1 0 -2 0 0 2233.933 -1 7 0
!
!
C -1 <--Space group symbol
! Nsym Cen Laue Ireps N_Bas
2 1 1 -1 6
! Real(0)-Imaginary(1) indicator for Ci
0 1 0 0 0
!
SYMM X , Y , Z
BASR 1. 0 0 0 1. 0 0 0 1. 1. 0 0 0 1. 0 0 0 1.
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM X , 1 - Y , 1/2 + Z
BASR -0.509 0 0 0 0.509 0 0 0 -0.509 0.509 0 0 0 -0.509 0 0 0 0.509
BASI 0.8607 0 0 0 -0.8607 0 0 0 0.8607 -0.8607 0 0 0 0.8607 0 0 0 -0.8607
!Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
Fe MFE3 1 0 0 0.33421 0.25000 .30000 1.00000 0.000 2.000 0.000
2.000 0.000 2.000 0.000 0.000 0.000 0.00000
21.00 0.00 31.00 0.00 0.00 0.00 0.00

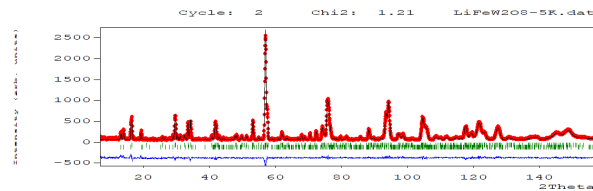
```

- You can also refine the k vector value and the peaks profile for improving the fit.

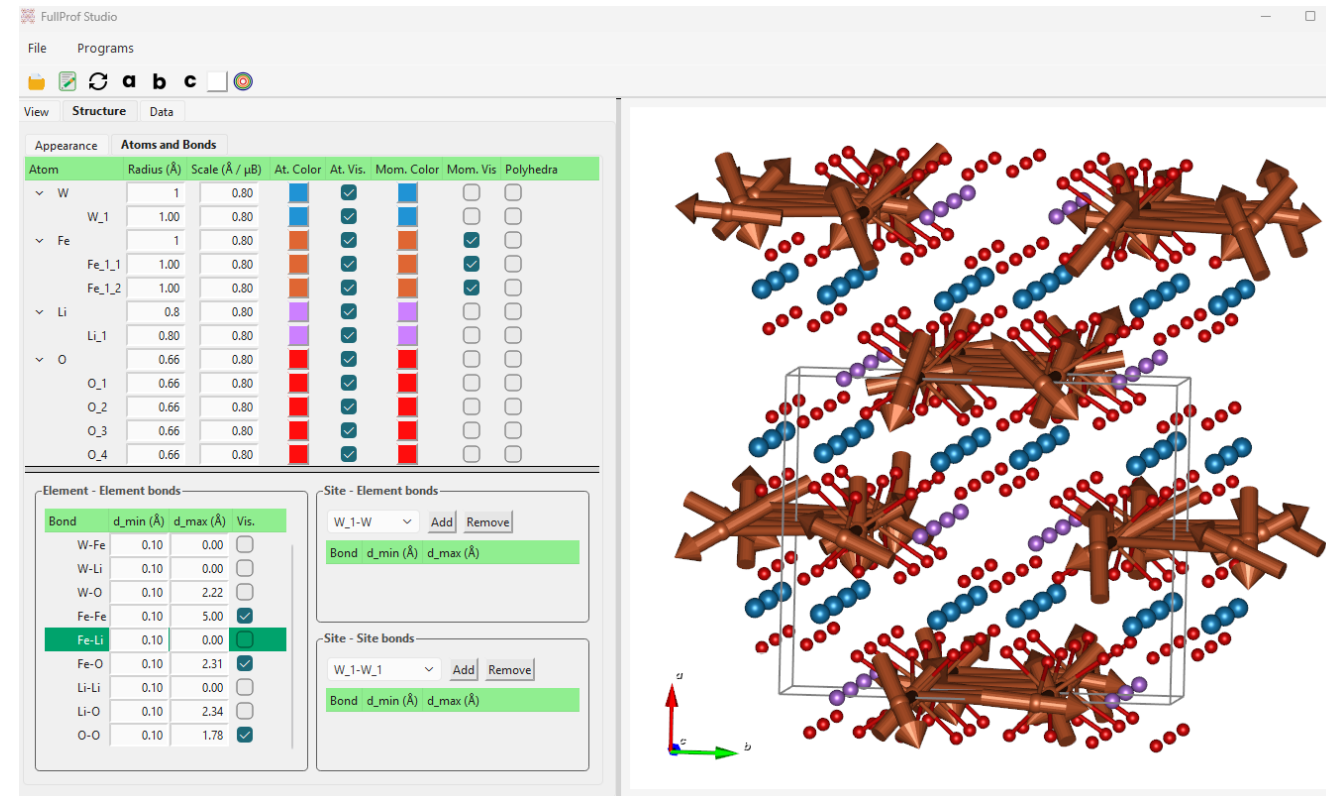
Display the magnetic structure using *FPStudio*

Irrep approach

```
FullProf Program
=> Convergence reached at this CYCLE (!!!!) CYCLE No. 2
=> R-Factors: 7.28 9.12 Chi2: 1.21 DW-Stat.: 1.0204 Patt#: 1
=> Expected: 8.29 1.8905
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 12.9 Rwp: 13.5 Ragg: 12.25 Chi2: 1.21
=> Global user-weighted Chi2 (Bragg contrib.): 1.245
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 5.368
=> RP-factor: 3.329
=> Phase: 2
=> Magnetic R-factor: 26.15
=> Normal end, final calculations and writing...
=> CPU Time: 1.691 seconds
=> 0.032 minutes
=> END Date:21/07/2024 Time => 14:29:22.346
```



- to visualize the magnetic structure, use **FPStudio** program, which reads the *.fst file, generated automatically by Fullprof.
- A different *.fst file will get created for each phase in the pcr file. To merge the magnetic and the nuclear phases into a single *.fst file, one must add in the title line for the nuclear phase the code “magph 2”



Note, VESTA will not work for mcif files created from Irrep approach, because the program does not use the *k*-vector concept.

Identify possible magnetic models using ISODISTORT

Super-space group approach

(<https://stokes.byu.edu/iso/isodistortform.php>)

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of crystal structures.

How to cite: To cite a tool from the ISOTROPY Software Suite, see the citation instructions on the tool's individual home page: H. T. Stokes, D. M. Hatch, and B. J. Campbell, ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- **ISODISTORT:** Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, rotations, and site occupancies.
- **ISOSUBGROUP:** Interactive program using user-friendly interface to list isotropy subgroups.
- **ISOTROPY:** Interactive program using command lines to explore isotropy subgroups and their associated distortion modes.
- **S.MODES:** Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the displacement modes.
- **FROZSL:** Calculate phonon frequencies and displacement modes using the method of frozen phonons.
- **ISOVIZ:** Stand-alone utility for viewing interactive distortions created by ISODISTORT (installers only, alpha version).

Space groups and irreducible representations

- **ISOCIF:** Create or modify CIF files.
- **FINDSYM:** Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **ISO-IR:** Tables of Irreducible Representations. The 2011 version of IR matrices.
- **ISO-MAG:** Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

- **ISO(3+d)D:** (3+d)-Dimensional Superspace Groups for d=1,2,3
- **ISO(3+1)D:** Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List
- **FINDSSG:** Identify the superspace group symmetry given a list of symmetry operators.
- **TRANSFORMSSG:** Transform a superspace group to a new setting.

ISODISTORT

Version 6.7.2, Sep 2020

Harold T. Stokes, Branton J. Campbell, and Dorian M. Hatch, Department of Physics and Astronomy, Brigham Young University, Provo, UT

Description: ISODISTORT is a user-friendly internet-based tool for exploring the structural distortion modes of crystalline materials. The application further allows one to visualize and interactively manipulate the modes generated in ISODISTORT.

NOTE: Interactive visualizations must now be saved to disk and opened with the standalone **ISOVIZ** app

[Help](#), [Tutorials](#), [Version History](#)

[Legacy copy of ISODISTORT version 5.6.1, August 2013](#)

Begin by entering the structure of parent phase: ?

[Get started quickly with a cubic perovskite parent.](#)

Import parent structure from a CIF structure file: dymn6ge6_...lear.cif

If you don't have a parent CIF, create one using **ISOCIF**.

Upload the cif file
LiFeW2O8.cif

ISODISTORT: search

Space Group: 15 C2/c C2h-6, Lattice parameters: a= 9.26000, b= 11.38000, c= 4.91000, alpha= 90.00000, beta= 90.30000, gamma= 90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
W1 8f (x,y,z), x= 0.24600, y= 0.09140, z= 0.24700, Fe1 4e (0,y,1/4), y= 0.33600, Li1 4e (0,y,1/4), y= -0.17300, O1 8f (x,y,z), x= 0.38700, y= 0.06200, z= -0.06000, O2 8f (x,y,z), x= -0.12200, y= 0.19700, z= 0.38900
Include magnetic Fe3+ distortions

Types of distortions to be considered ?

strain: ☐
Displacive: all ☐ none ☐ W6+ ☐ Fe3+ ☐ Li1+ ☐ O2- ☐
Occupational: all ☐ none ☐ W6+ ☐ Fe3+ ☐ Li1+ ☐ O2- ☐
Magnetic: all ☐ none ☐ W6+ ☐ Fe3+ ☒ Li1+ ☐ O2- ☐
Rotational: all ☐ none ☐ W6+ ☐ Fe3+ ☐ Li1+ ☐ O2- ☐

Important: You must click on Change to implement any changes in the above type of distortions to be considered.

Method 1: Search over all special k points ?

Crystal system(s): triclinic ☐ monoclinic ☐ orthorhombic ☐ tetragonal ☐ trigonal ☐ hexagonal ☐ cubic ☐
Space-group symmetry: no choice ☐ Conventional lattice: no choice ☐ Primitive lattice: no choice ☐

Method 2: General method - search over specific k points ?

k vector 1: B, k1 (a,0,g) a= 0.89 b= g= 0.33 # of independent incommensurate modulations= 1
k vector 2: B, k1 (a,0,g) a= 0.89 b= g= 0.33 # of independent incommensurate modulations= 1
Change number of superposed IRs: 2 ?

Important: You must click on Change to implement any changes in the number of superposed IRs.

Select the magnetic “distortions” on Fe
(click on “change” to save the setting)

Use “method 2” to select the two Ireps
corresponding to the k1 (a,0,g)

Select the two possible Irreducible representations, and then the superspace group B2.1'(a,b,0)0s

ISODISTORT: irreducible representation

Space Group: 15 C2/c C2h-6, Lattice parameters: a= 9.26000, b= 11.38000, c= 4.91000, alpha= 90.00000, beta= 90.30000, gamma= 90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
W1 8f (x,y,z), x= 0.24600, y= 0.09140, z= 0.24700, Fe1 4e (0,y,1/4), y= 0.33600, Li1 4e (0,y,1/4), y= -0.17300, O1 8f (x,y,z), x= 0.38700, y= 0.06200, z= -0.06000, O2 8f (x,y,z), x= -0.12200, y= 0.19700, z= 0.38900
Include magnetic Fe3+ distortions
k point: B, k1 (a,0,g), a=0.89000, g=0.33000 (1 incommensurate modulation/1 arm)
k point: B, k1 (a,0,g), a=0.89000, g=0.33000 (1 incommensurate modulation/1 arm)

Choose each superposed IR and OPD (optional):

IR 1: mB1, mk1t2 OPD: ?
IR 2: mB2, mk1t1 OPD: OK

Initialize the amplitudes to some initial values and save the magnetic distortion file to CIF

P-P (a,0|b,0) 5.1.4.1.m14.2 B2.1'(a,b,0)0s, basis={ (1,0,0,0), (0,0,1,0), (0,-1,0,0), (0,0,0,1) }, parent-like basis={ (1/8,0,0,0), (0,1/8,0,0), (0,0,1/8,0), (0,0,0,1/8) }, origin=(0,0,1/4,0), s=1, i=2, k-active= (0.89000,0,0.33000)
Lattice parameters of undistorted supercell: a=9.26000, b=4.91000, c=11.38000, alpha=90.00000, beta=90.00000, gamma=90.30000
Lattice parameters of undistorted supercell with parent-like basis: a=9.26000, b=11.38000, c=4.91000, alpha=90.00000, beta=90.30000, gamma=90.00000

☐ Save interactive distortion ☒ CIF file ? ☐ Distortion file ? ☐ Domains ? ☐ Modes details ☐ Complete modes details ? ☐ IR matrices OK

Enter mode and strain amplitudes: ?

C2/c[0.89000,0,0.33000]mB1 (a,0) 15.1.4.1.m86.2 B2/b.1'(a,b,0)0s, basis={ (0,0,1,0), (1/2,1/2,0,0), (-1/2,1/2,0,0), (0,0,0,1) }, parent-like basis={ (1/2,0,0,0), (0,1/2,0,0), (0,0,1/2,0), (0,0,0,1/2) }, origin=(0,0,0,0)

1 [Fe1:e:mag]A(a)

1 [Fe1:e:mag]B_1(a)

1 [Fe1:e:mag]B_2(a)

C2/c[0.89000,0,0.33000]mB2 (a,0) 15.1.4.1.m86.2 B2/b.1'(a,b,0)0s, basis={ (0,0,1,1), (1/2,1/2,0,0), (-1/2,1/2,0,0), (0,0,0,1) }, parent-like basis={ (1/8,0,0,0), (0,1/8,0,0), (0,0,1/8,0), (0,0,0,1/8) }, origin=(0,0,0,3/4)

1 [Fe1:e:mag]A(a)

1 [Fe1:e:mag]B_1(a)

1 [Fe1:e:mag]B_2(a)

ISODISTORT: order parameter direction

Space Group: 15 C2/c C2h-6, Lattice parameters: a= 9.26000, b= 11.38000, c= 4.91000, alpha= 90.00000, beta= 90.30000, gamma= 90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting, parent-like basis vectors of the subgroup lattice displayed
W1 8f (x,y,z), x= 0.24600, y= 0.09140, z= 0.24700, Fe1 4e (0,y,1/4), y= 0.33600, Li1 4e (0,y,1/4), y= -0.17300, O1 8f (x,y,z), x= 0.38700, y= 0.06200, z= -0.06000, O2 8f (x,y,z), x= 0.39200, y= 0.17800, z= 0.42000, O3 8f (x,y,z), x= -0.12200, y= 0.19700, z= 0.38900
Include magnetic Fe3+ distortions
k point: B, k1 (a,0,g), a=0.89000, g=0.33000 (1 incommensurate modulation/1 arm)
IR: mB1, mk1t2
k point: B, k1 (a,0,g), a=0.89000, g=0.33000 (1 incommensurate modulation/1 arm)
IR: mB2, mk1t1

Finish selecting the distortion mode by choosing an order parameter direction ?

☒ P-P (a,0|b,0) 5.1.4.1.m14.2 B2.1'(a,b,0)0s, basis={ (1,0,0,0), (0,0,1,0), (0,-1,0,0), (0,0,0,1) }, parent-like basis={ (1/8,0,0,0), (0,1/8,0,0), (0,0,1/8,0), (0,0,0,1/8) }, origin=(0,0,1/4,0), s=1, i=2, k-active= (0.89000,0,0.33000)
☐ P-P (a,0|b,0) 2.1.1.1.m5.2 P-1.1'(a,b,g)0s, basis={ (0,0,1,0), (1/2,1/2,0,0), (-1/2,1/2,0,0), (0,0,0,1) }, parent-like basis={ (1/2,0,0,0), (0,1/2,0,0), (0,0,1/2,0), (0,0,0,1/2) }, origin=(0,0,0,0), s=1, i=2, k-active= (0.89000,0,0.33000)
☐ C-C (a,b|c,d) 1.1.1.1.m2.2 P1.1'(a,b,g)0s, basis={ (0,0,1,0), (1/2,1/2,0,0), (-1/2,1/2,0,0), (0,0,0,1) }, parent-like basis={ (1/2,0,0,0), (0,1/2,0,0), (0,0,1/2,0), (0,0,0,1/2) }, origin=(0,0,0,0), s=1, i=4, k-active= (0.89000,0,0.33000)

OK

Lower in the webpage you can select the option to save the model into parent like basis

☒ Use alternate (possibly nonstandard) setting in CIF, Topas, Fullprof, or modes details output (matrix S⁻¹)

Relative to ☒ parent ☐ subgroup

Basis vectors of subgroup lattice (rational numbers):

a_{s1} = a_{s1} + a_{s2} + a_{s3} + a_{s4}

a_{s2} = a_{s1} + a_{s2} + a_{s3} + a_{s4}

a_{s3} = a_{s1} + a_{s2} + a_{s3} + a_{s4}

a_{s4} = a_{s1} + a_{s2} + a_{s3} + a_{s4}

Origin of subgroup (either rational or decimal numbers):

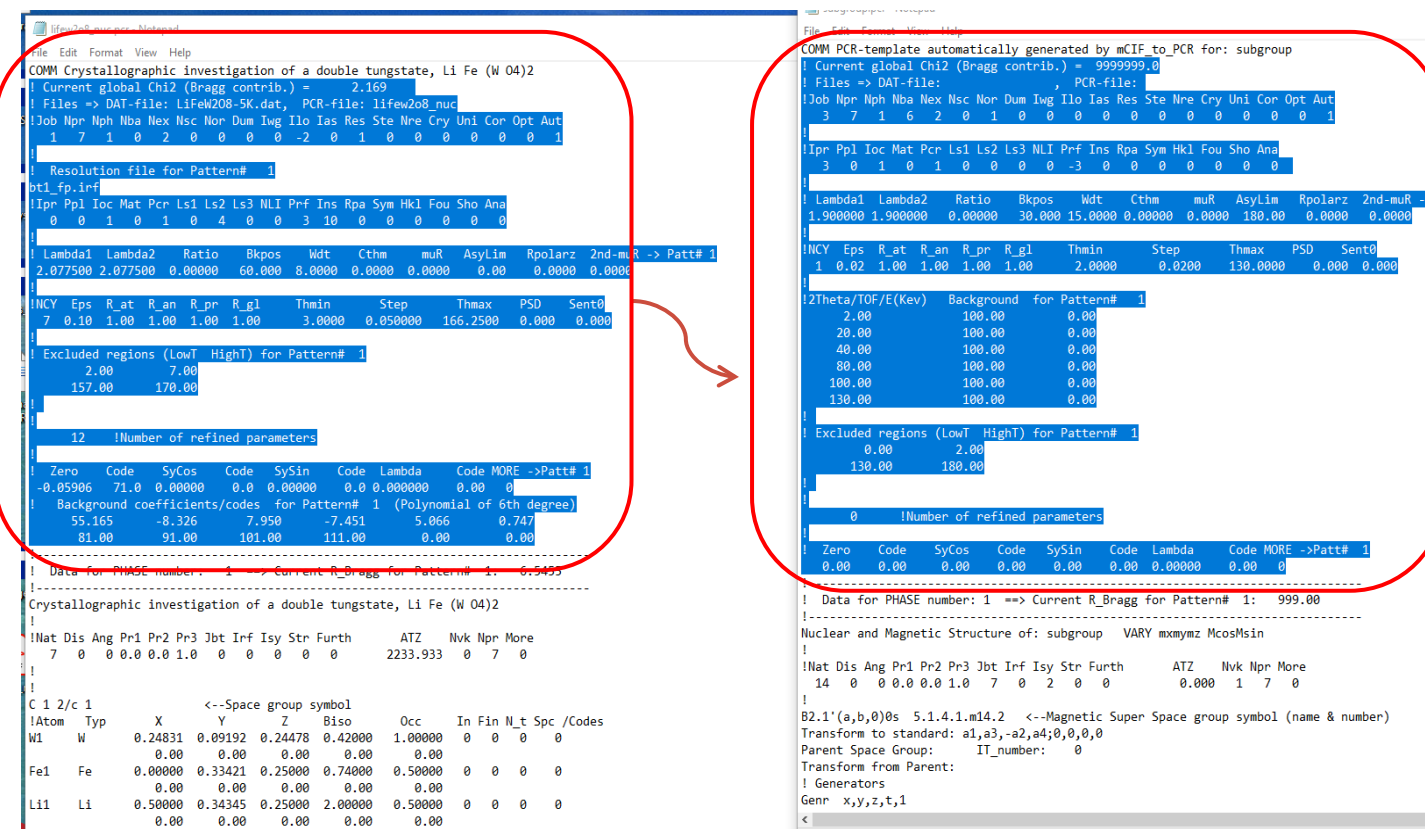
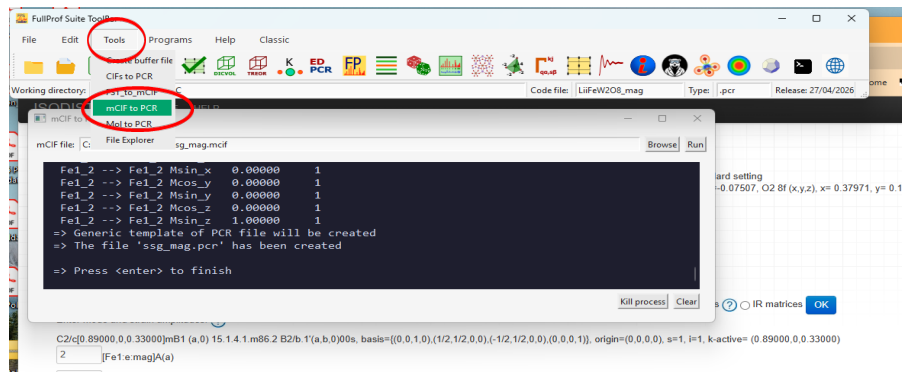
r' = a_{s1} + a_{s2} + a_{s3} + a_{s4}

A file "name.mcif" has to be saved to your computer.
(If you accidentally save it as *.cif, rename the extensions to *.mcif)

Convert the MCIF to PCR format

SSG approach

Load the newly created mcif file into the FullProf Toolbar and use the mcif-to-pcr tool to create the PCR file.
Note: you need to select in the toolbar the correct working directory where you saved the mcif



Load the PCR file in the toolbar and open it with the text editor. The PCR will need to be modified by copying the instrument & data description from the PCR created for the “nuclear” refinement

Copy the section describing scale factor and profile parameters. Copy the lattice parameters , but only if the lattice definition is the same with the parent phase.

Important : Do not remove the k-vector information at the end of the phase description.

```

12      !Number of refined parameters
!
! Zero   Code  SyCos   Code  SySin   Code  Lambda   Code MORE ->Patt# 1
-0.05906 71.0  0.00000  0.0  0.00000  0.0  0.000000  0.00  0
! Background coefficients/codes for Pattern# 1 (Polynomial of 6th degree)
55.165   -8.326   7.950   -7.451   5.066   0.747
81.00    91.00   101.00   111.00   0.00    0.00
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 6.5455
!-----
Crystallographic investigation of a double tungstate, Li Fe (W O4)2
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
7  0  0 0.0 0.0 1.0  0  0  0  0  0      2233.933  0  7  0
!
!
C 1 2/c 1
!Atom  Typ      X      Y      Z      Occ      In Fin N_t Spc /Codes
W1     W      0.24831 0.09192 0.24478 0.42000 1.00000 0  0  0  0
Fe1    Fe      0.00000 0.33421 0.25000 0.74000 0.50000 0  0  0  0
Li1    Li      0.50000 0.34345 0.25000 2.00000 0.50000 0  0  0  0
O1     O      0.36480 0.05924 0.92493 0.45422 1.00000 0  0  0  0
O2     O      0.37971 0.18197 0.41116 0.45422 1.00000 0  0  0  0
O3     O      0.35709 0.54854 0.94233 0.45422 1.00000 0  0  0  0
O4     O      0.37763 0.69357 0.39354 0.45422 1.00000 0  0  0  0
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
0.2369683 0.00000 0.00000 0.00000 0.00000 0.00000 0
121.00000 0.00 0.00 0.00 0.00 0.00
! U V W X Y GauSiz LorSiz Size-Model
0.000000 0.000000 0.009051 0.000000 0.000044 0.000000 0.000000 0.00
0.00 0.00 51.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma #Cell Info
9.268055 11.394946 4.893242 90.000000 90.569206 90.000000
61.00000 41.00000 31.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
7.000 157.000 1

```

```

File Edit Format View Help
Fe1_2 MFE3 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00000 0.66400 0.50000 0.00000 0.25000 1 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MagM0-Moment: 0.00000 0.00000 0.00000 <- Homogeneous magnetic moment
0.00000 0.00000 0.00000
Mcos-Msin-1: 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 <-Amplitudes
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
Li1_1 Li1+ 0 0.00000 0.82700 0.00000 0.00000 0.25000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
Li1_2 Li1+ 0 0.00000 0.17300 0.50000 0.00000 0.25000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O1_1 O2- 0 0.88700 0.56200 0.69000 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O1_2 O2- 0 0.61300 -0.06200 0.81000 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O2_1 O2- 0 0.89200 0.67800 0.17000 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O2_2 O2- 0 0.60800 0.82200 0.33000 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O3_1 O2- 0 0.35600 0.55200 0.67900 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O3_2 O2- 0 0.14400 -0.05200 0.82100 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O4_1 O2- 0 0.37800 0.69700 0.13900 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O4_2 O2- 0 0.12200 0.80300 0.36100 0.00000 0.50000 0 0 #
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
!-----> Profile Parameters for Pattern # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
1.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00000 0.00 0.00 0.00 0.00 0.00
! U V W X Y GauSiz LorSiz Size-Model
0.176002 -0.197806 0.091452 0.000000 0.030076 0.000000 0.000000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma #Cell Info
9.260000 11.380000 4.910000 90.000000 90.300003 90.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
0.890000 0.000000 0.330000 1 1.0000 <- Propagation Vector, nharm, sint1_lim
0.00000 0.00000 0.00000
! 2Th1/TOF1 2Th2/TOF2 Pattern # 1
2.000 130.000 1

```

```

! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00
!-----
Nuclear and Magnetic Structure of: subgroup VARY mxmymz McosMsin
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Inf Isy Str Furth ATZ Nvk Npr More
  14  0  0 0.0 0.0 1.0  7  0  2  0  0      0.000  1  7  0
!
B2.1'(a,b,0)0s 5.1.4.1.m14.2 <--Magnetic Super Space group symbol (name & number)
Transform to standard: a1,a3,-a2,a4;0,0,0
Parent Space Group:      IT_number:  0
Transform from Parent:
! Generators
Genr  x,y,z,t,1
Genr -x,y,-z,-t,1
Genr  x,y,z,t+1/2,-1
Genr -x,y,-z,-t+1/2,-1
Genr  x+1/2,y+1/2,z,t,1
Genr -x+1/2,y+1/2,-z,-t,1
Genr  x+1/2,y+1/2,z,t+1/2,-1
Genr -x+1/2,y+1/2,-z,-t+1/2,-1
N_qc  1
Q_coeff
  1
!
!Atom  Typ  Max_Qcoeff      X      Y      Z      Biso      Occ  N_type Spc
!
!      Mcosx      Mcosy      Mcosz      Msinx      Msiny      Msinz
!      beta11      beta22      beta33      beta12      beta13      beta23
W1_1   W      0      0.74600  0.59140  -0.00300  0.420  0.50000  0  0  #
      0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
W1_2   W      0      0.75400  -0.09140  0.50300  0.420  0.50000  0  0  #
      0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
Fe1_1  MFE3    1      0.00000  0.33600  0.00000  0.00000  0.70000  0.25000  1  0
      0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
Mag10-Moment:  0.00000  0.00000  0.00000  <- Homogeneous magnetic moment
      0.00000  0.00000  0.00000
Mcos-Msin-1:  0.00000  2.00000  0.00000  2.00003  0.00000  2.01047  <-Amp
      0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
Fe1_2  MFE3    1      0.00000  0.66400  0.50000  0.70000  0.25000  1  0
      0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
Mag10-Moment:  0.00000  0.00000  0.00000  <- Homogeneous magnetic moment
      0.00000  0.00000  0.00000
Mcos-Msin-1:  0.00000  2.00000  0.00000  2.00003  0.00000  2.01047  <-Amp
      0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
Li1_1  Li      0      0.00000  0.82700  0.00000  2.00000  0.25000  0  0
      0.00000  0.00000  0.00000  0.00000  0.00000
Li1_2  Li      0      0.00000  0.17300  0.50000  2.00000  0.25000  0  0
      0.00000  0.00000  0.00000  0.00000  0.00000
O1_1   O      0      0.88700  0.56200  0.69000  0.454  0.50000  0  0  #
      0.00000  0.00000  0.00000  0.00000  0.00000
O1_2   O      0      0.61300  -0.06200  0.81000  0.454  0.50000  0  0  #
      0.00000  0.00000  0.00000  0.00000  0.00000

```

The command line VARY mxmymz McosMsin is varying all allowed magnetic moment projections for all sites.

Make sure that the atoms identifiers are correct. They have to be MFE3, and no valence value for nuclear atoms

If you used non-zero thermal parameters (B) , then you need to update their values to those obtained from the structural refinement.

It is a good practice to fix all parameters (including scale factor) when you run the refinement for the first time.

Just leave VARY mxmymz McosMsin to see if they converge to a reasonable solution

use the Fullprof Suite tool to run the refinement

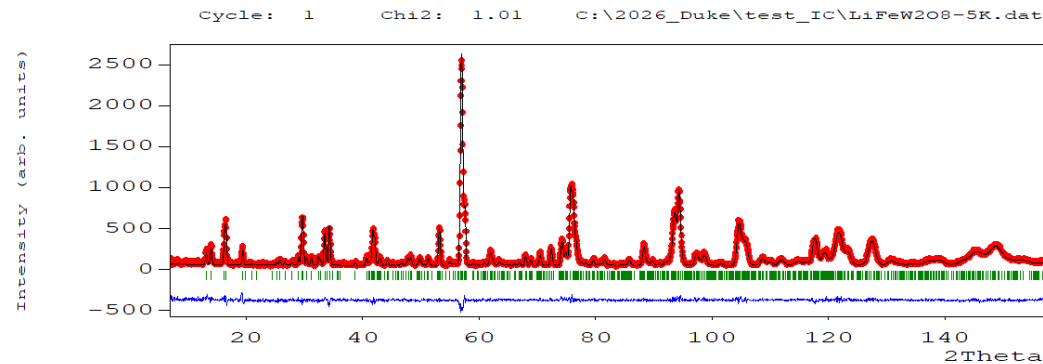
```

FullProf Program
Load Edit PCR Mode Run Exit

=> Convergence reached at this CYCLE !!!!!: CYCLE No.      1
=> R-Factors:      6.76      8.34      Chi2: 1.01      DW-Stat.: 1.1762      Patt#: 1
=> Expected :      8.29
=> Conventional Rietveld R-factors for Pattern:      1
=> Rp: 11.3      Rwp: 12.1      Rexp: 12.04      Chi2: 1.01
=> Global user-weighted Chi2 (Bragg contrib.): 1.037
=> -----> Pattern#      1
=> Phase:      1
=> Bragg R-factor: 4.796
=> RF-factor : 3.586
=> Nuclear R-factor: 3.761
=> Magnetic R-factor: 17.60
=> Pure Magnetic R-factor: 17.60
=> Normal end, final calculations and writing...

=> CPU Time:      0.695 seconds
=> 0.012 minutes
=> END      Date:18/07/2026      Time => 21:20:57.954

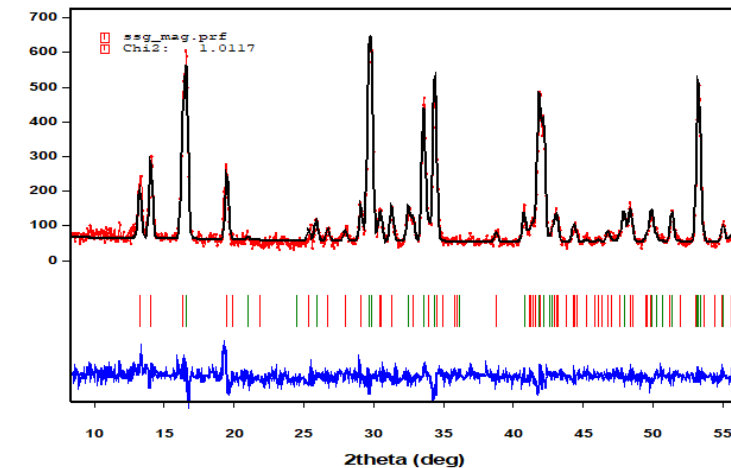
```



- the fit can be further improved by refining the scale factor, k-vector, lattice parameters, profile parameter, background and zero offset.

Consider constraining the Fe1 and Fe2 to have the same moments. Set identical flags for refinement and remove the command line “VARY mxmymz McosMsin”

Atom	Typ	Max_Qcoeff	X	Y	Z	Biso	Occ	N_type	Spc	/ Line
below:Codes										
			Mcosx	Mcosy	Mcosz	Msinx	Msiny	Msinz	/ Line	
below:Codes										
			beta11	beta22	beta33	beta12	beta13	beta23	/ Line	
below:Codes										
W1_1	W	0	0.74831	0.59192	-0.00522	0.40000	0.50000	0	0	#
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
W1_2	W	0	0.75169	-0.09192	0.50522	0.40000	0.50000	0	0	#
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
Fe1_1	MFE3	1	0.00000	0.33421	0.00000	0.40000	0.25000	1	0	#
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
MagM0-Moment:			0.00000	0.00000	0.00000	<- Homogeneous magnetic moment				
			0.00000	0.00000	0.00000					
Mcos-Msin-1:			0.00000	3.95662	0.00000	2.43643	0.00000	3.32282	<-Amplitudes of	
Modulated moments			0.00000	31.00000	0.00000	21.00000	0.00000	11.00000		
Fe1_2	MFE3	1	0.00000	0.66579	0.50000	0.40000	0.25000	1	0	#
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
MagM0-Moment:			0.00000	0.00000	0.00000	<- Homogeneous magnetic moment				
			0.00000	0.00000	0.00000					
Mcos-Msin-1:			0.00000	3.95662	0.00000	2.43643	0.00000	3.32282	<-Amplitudes of	
Modulated moments			0.00000	31.00000	0.00000	21.00000	0.00000	11.00000		
Li1_1	Li	0	0.00000	0.84345	0.00000	2.00000	0.25000	0	0	#
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
Li1_2	Li	0	0.00000	0.15655	0.50000	2.00000	0.25000	0	0	#



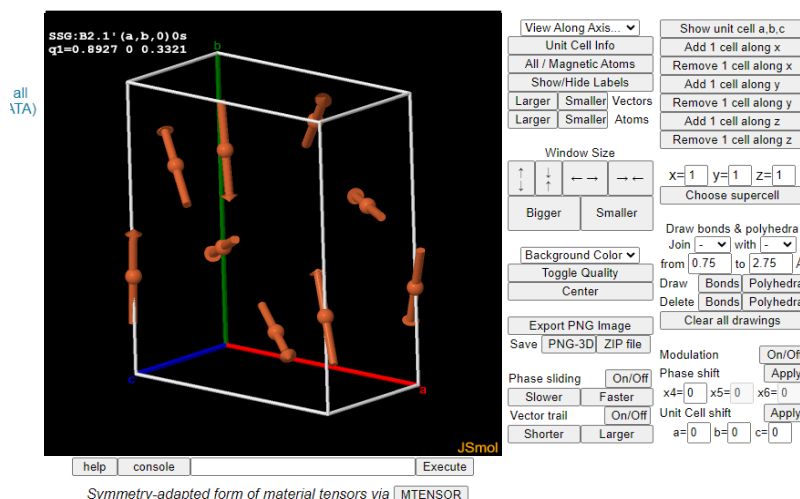
Display the magnetic structure using *MVISUALIZE* or *Vesta*

SSG approach

to visualize the magnetic structure from SSG approach, the best tool is **MVISUALIZE** (using the k-vector information)

- Look for the file "pcr-file-name_ssg1.mcif"

MVISUALIZE: 3D Visualization of magnetic structures with Jmol



Commands for saving animated gifs:
animation MODE LOOP
capture "test.gif" 25.0

VESTA program, reads the pcr-file-name1.mcif file, generated automatically by Fullprof in a P1 description and using the supercell defined by command MULTCELL (to substitute the k-vector in generating the moment modulation across multiple unit cells)

```
!      a      b      c      alpha      beta      gamma      #Cell Info
      9.268054 11.394943 4.893241 90.000000 90.569206 90.000000 #MULTCELL 3 1 5
      81.00000 91.00000 101.00000 0.00000 111.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
0.8922502 0.0000000 0.3319647 1 1.0000 <-- Propagation Vector, nharm, sint1_lim
21 0000000 0 0000000 31 0000000
```

