OAK RIDGE National Laboratory

Determination of the incommensurate magnetic structure of $Fe_{1.16}Te$ using FullProf and Sarah (Basis vectors of Irreps)

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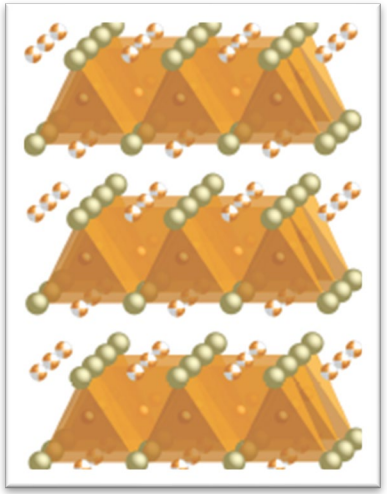
U.S. DEPARTMENT OF ENERGY

Magnetic phase diagram of $Fe_{1+x}Te$



E. E. Rodriguez *et al*, Phys. Rev. B 84, 064403 (2011)

- layers of edge- sharing $FeTe_4$ tetrahedra.
- extra interstitial Fe cations between the layers

Atom		x	y	z	occ.
Fe1	2a	0.75	0.25	0.00	1.0
Fe2	2c	0.25	0.25	0.69	x
Te	2c	0.25	0.25	0.280	1.0

T > 70K,

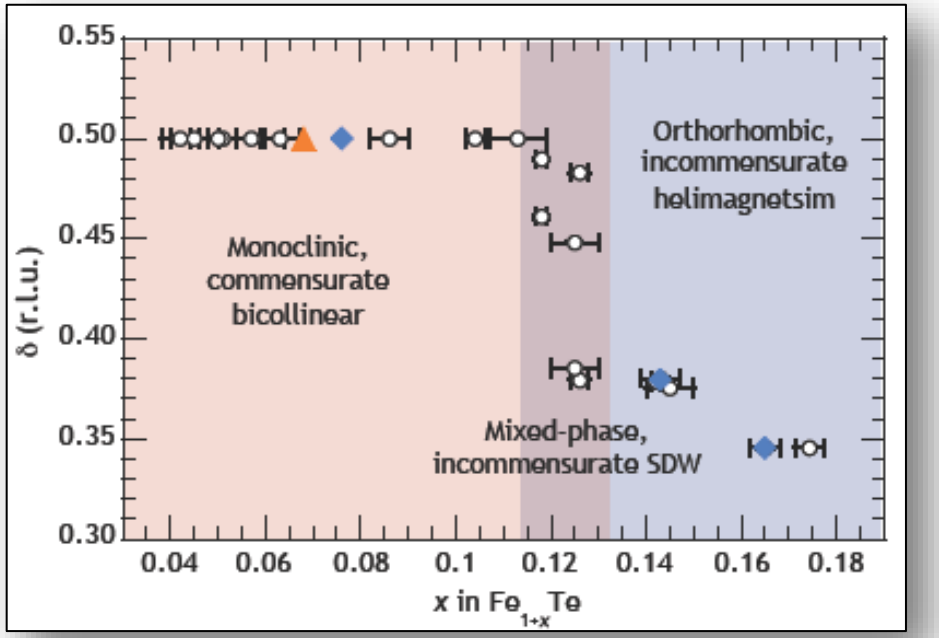
Paramagnetic phase:

P4/*n m m* , a ≈ 3.81A, c ≈ 6.24A

T < 70K,

x < 0.12 → P 2_1/*m*, *AFM Commensurate k*

x > 0.12 → P*mmn*, *AFM Incommensurate k*



Magnetic structure determination of $Fe_{1+x}Te$, with x= 0.16

- Neutron powder diffraction data collected using:
  HB2A –HFIR using λ = 2.41 Å
  Data files (in XYSIGMA format):
  Fe1p16Te_4K-2p41A.dat

- Instrument resolution file:
  hb2a_2p41A_resolution.irf

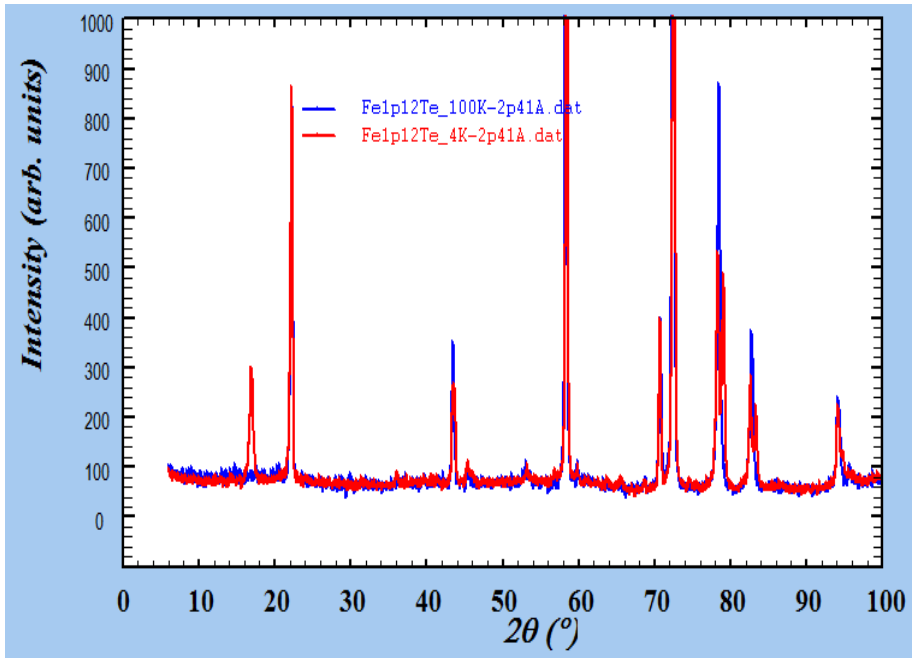
- CIF files for low-temp crystal structure:
  Fe1p16_4K.cif

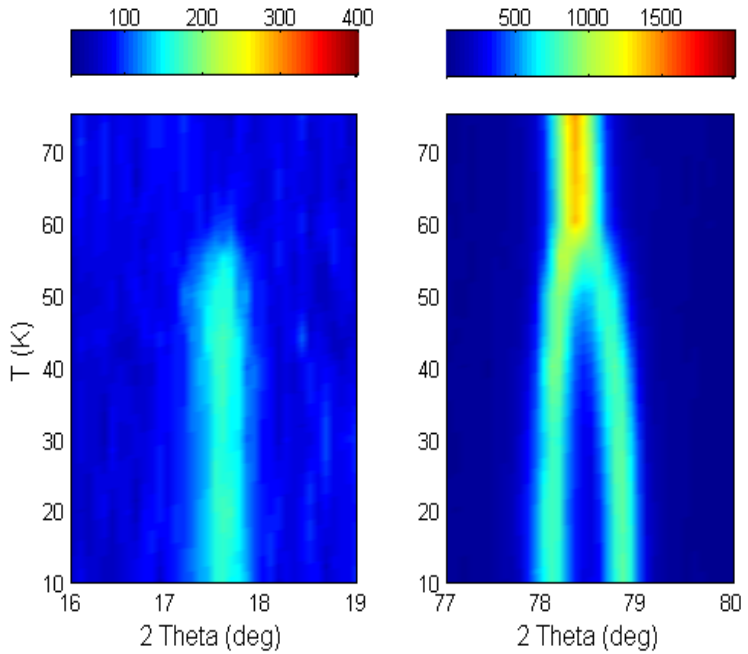
Steps for magnetic structure determination :

- Import the known crystal structure/instrument parameters to create a PCR file (*EdPcr, FullProf, Winplotr*)
- Refining the crystal structure for the paramagnetic state ($T > T_N$ or T_C) → obtain all the relevant structural and profile parameters. (not done in this example)
- Identify the magnetic reflections and determine the propagation vector (k-Search)
- Perform symmetry analysis (from the propagation vector, space group, atom positions) → IRs and Basis vectors (we will use web-based SARAh program)
- Select a magnetic model and add it as a second phase (magnetic phase) to the PCR file (using SARAh webRefine *)*
- Refine by LSQ the magnetic phase (FullProf)
- Visualize the magnetic structure model (FpStudio)

$Fe_{1.16}Te$: STEP1: Refine the crystal structure

Observe the differences in the data measured at different temperatures. In the case of Fe1.16Te, the magnetic order occurs at the same time with a structural transformation. In such situations, the crystal structure needs to be determined before attempting modeling the magnetic peaks,. This can be done using the high-Q (high-2theta angle) neutron data or from xray diffraction.





- use ***EdPCR*** to create the input file for FullProf (*.PCR)

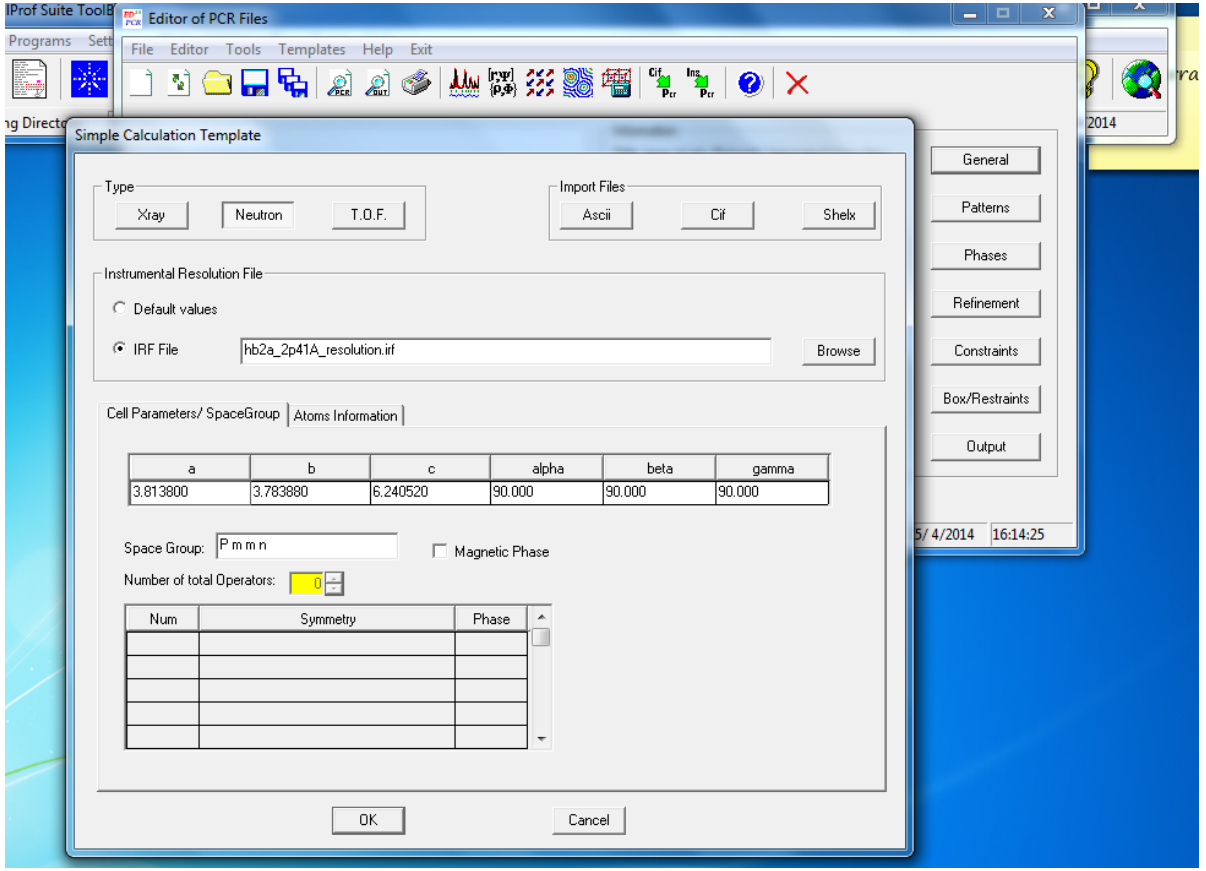
  - import the crystallographic information file CIF (Fe1p16_4K.cif))

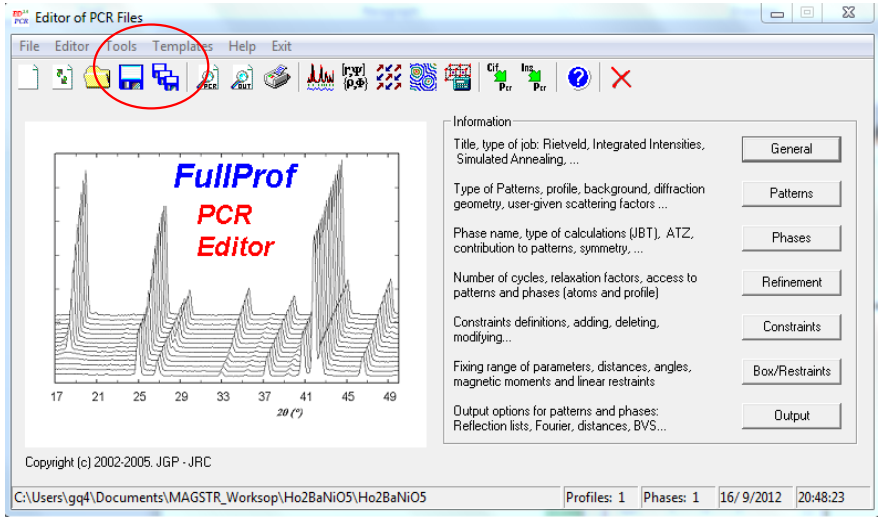
Low temperature structure: P*mmn*

Atom		x	y	z	occ.
Fe1	2b	0.75	0.25	0.003	1.0
Fe2	2a	0.25	0.25	0.72	0.16
Te	2a	0.25	0.25	0.286	1.0

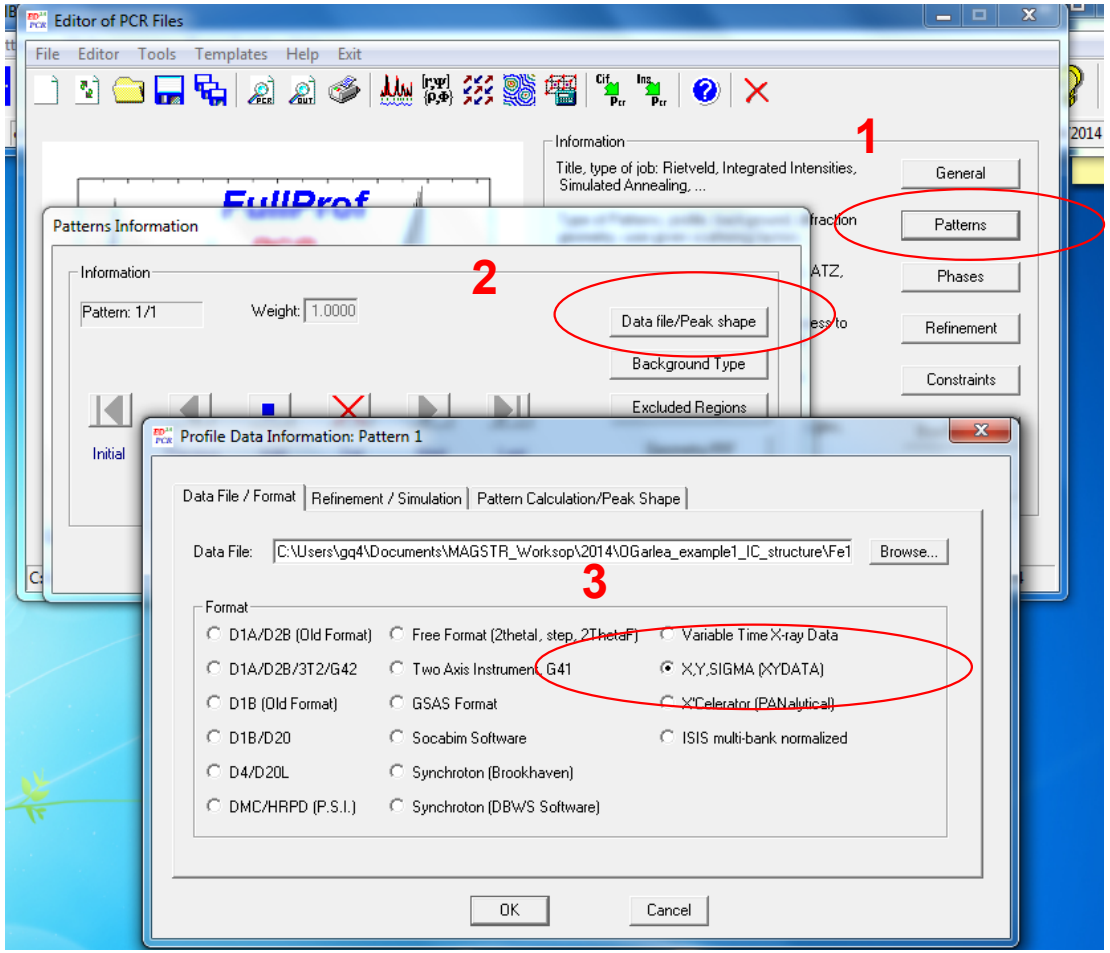
  - in the new window, select the “Neutron” tab for the type of calculations

  - use the “Browse” button to upload the instrument resolution file “IRF” hb2a_2p41A_resolution.irf



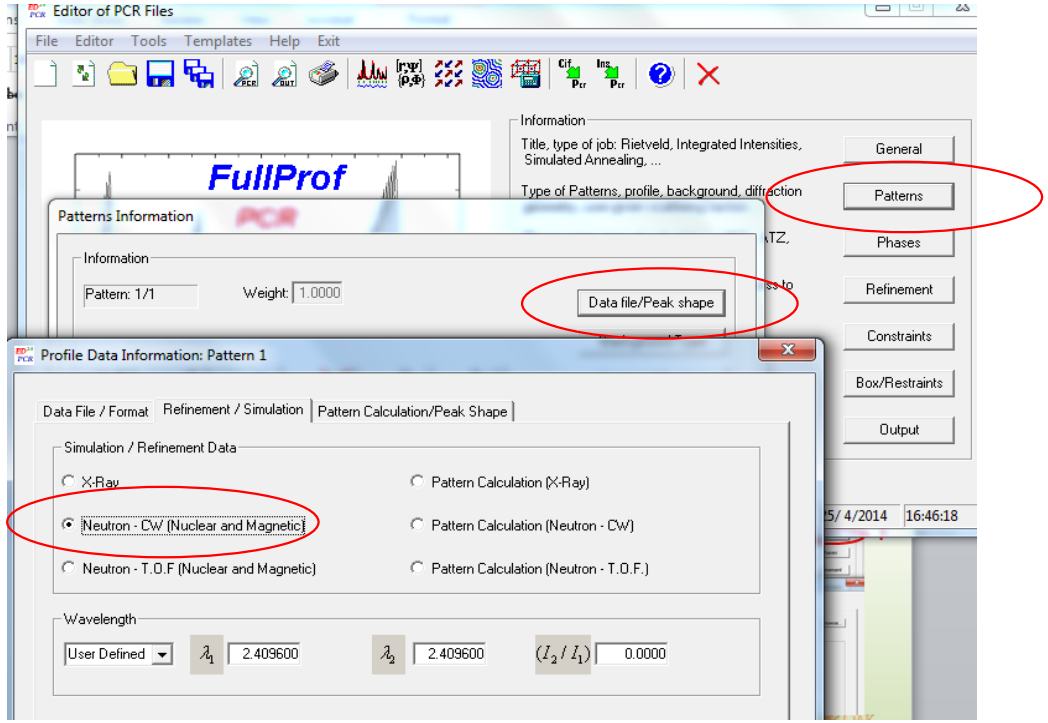


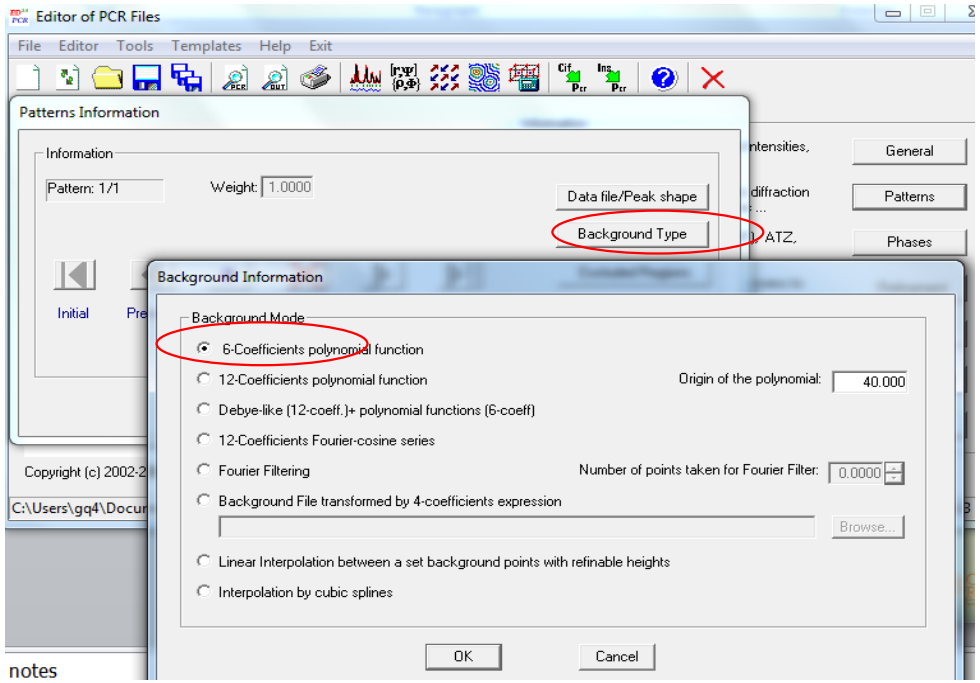
- save the PCR file by clicking the “Save” button



- open the “Patterns” tab (1) and then the “Data file/ peak shape” (2) and select the “XYSIGMA” for the data file format (3)

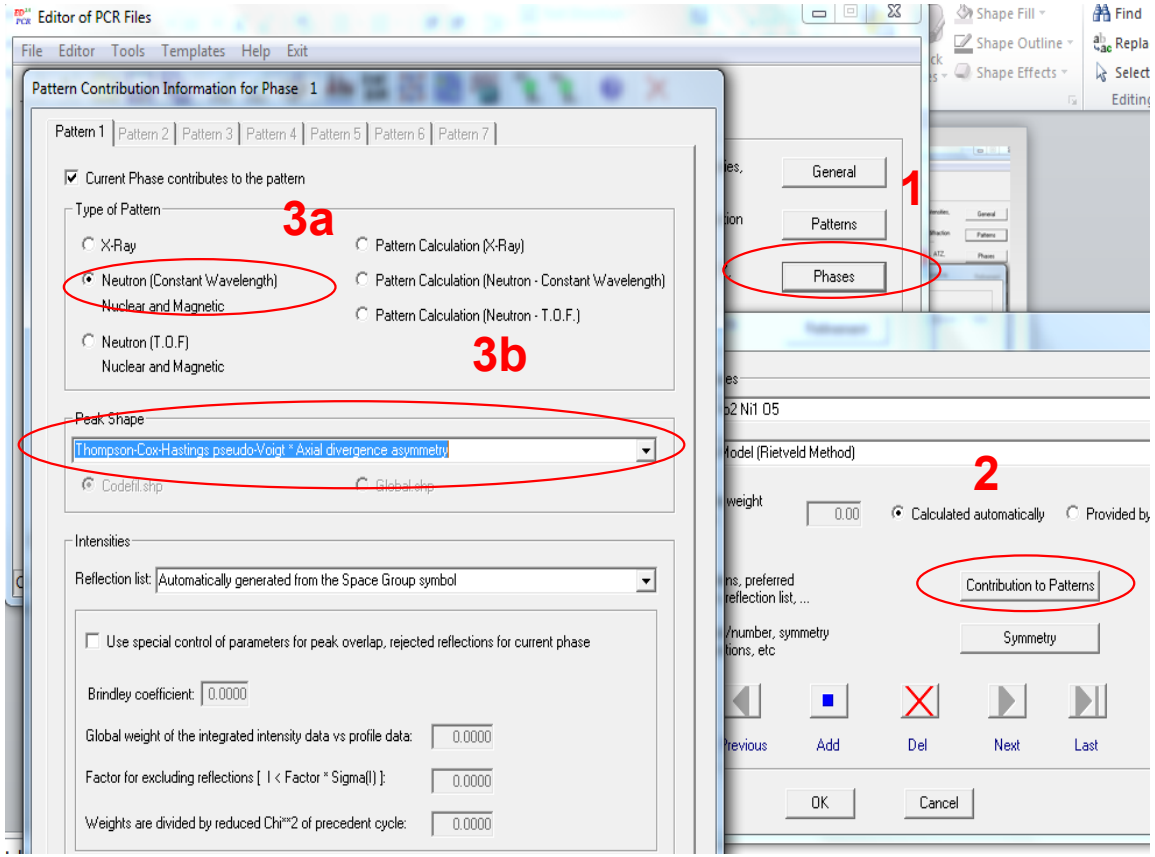
- In the “Patterns” tab , clock on the “Refinement/Simulation”, and make sure that “Neutron-CW” option is selected, and in the “Pattern calculation” the “Thompson-Cox-Hastings pseudo-Voigt” peak shape is chosen

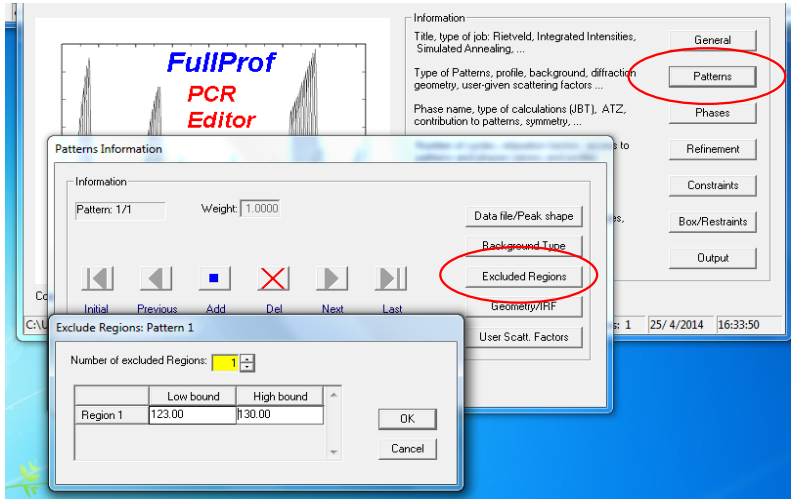




- For the background information, select the “6-coefficients polynomial function”

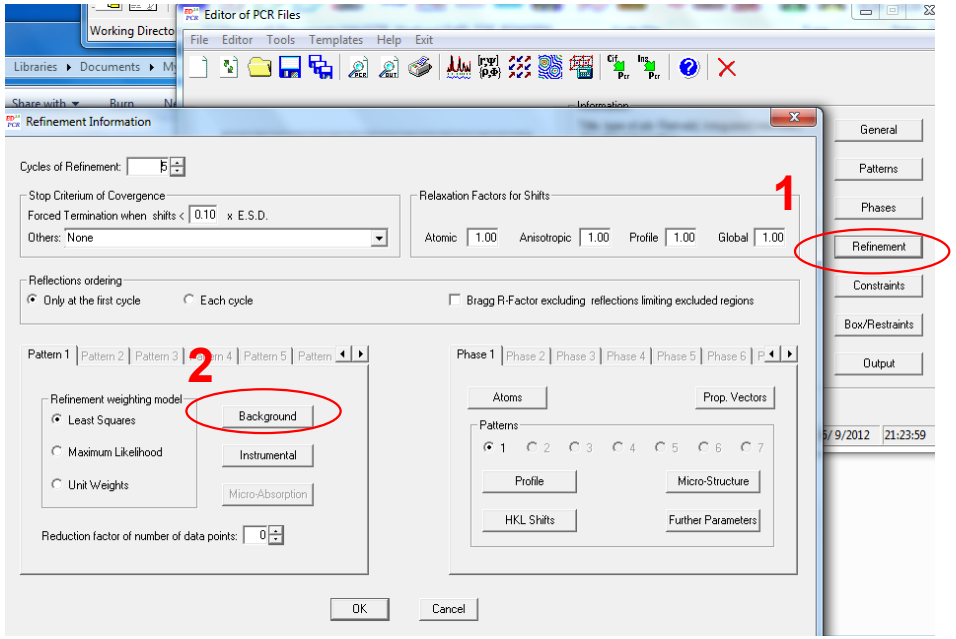
- Add one excluded region with the scattering range 123-130 deg

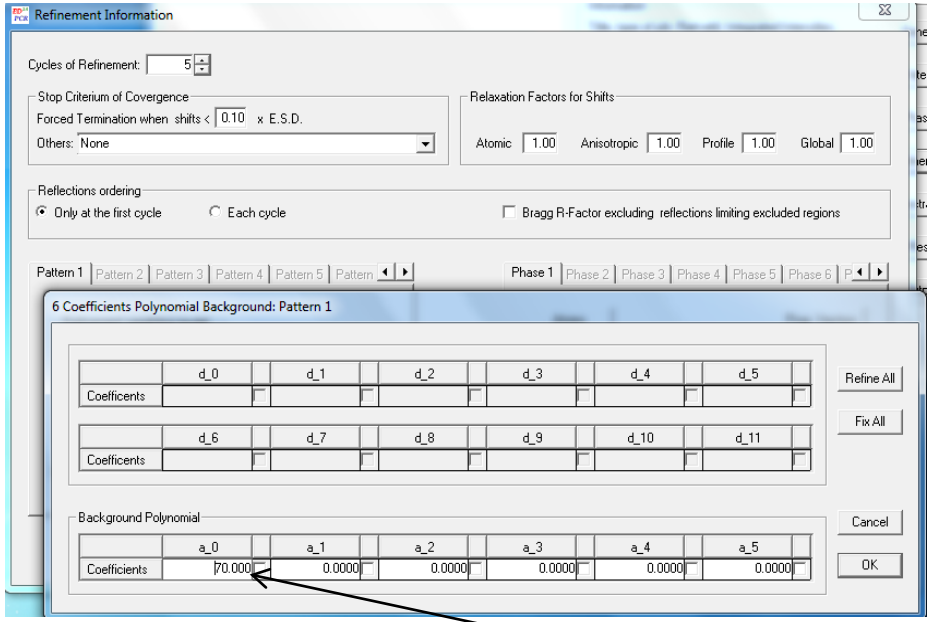


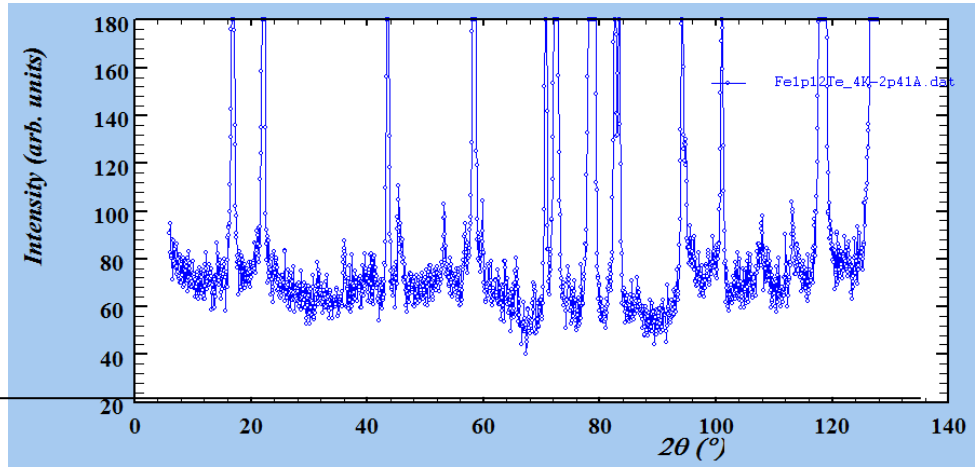


- From the main window of EdPcr, open the “Phases” tab (1) and then click on the “Contribution to patterns” (2) and then select the “current phase contributes to the pattern “ & “neutron (constant wavelength)“(3a) and “Thompson-Cox-Hastings pseudo-Voigt” for the peak shape (3b)

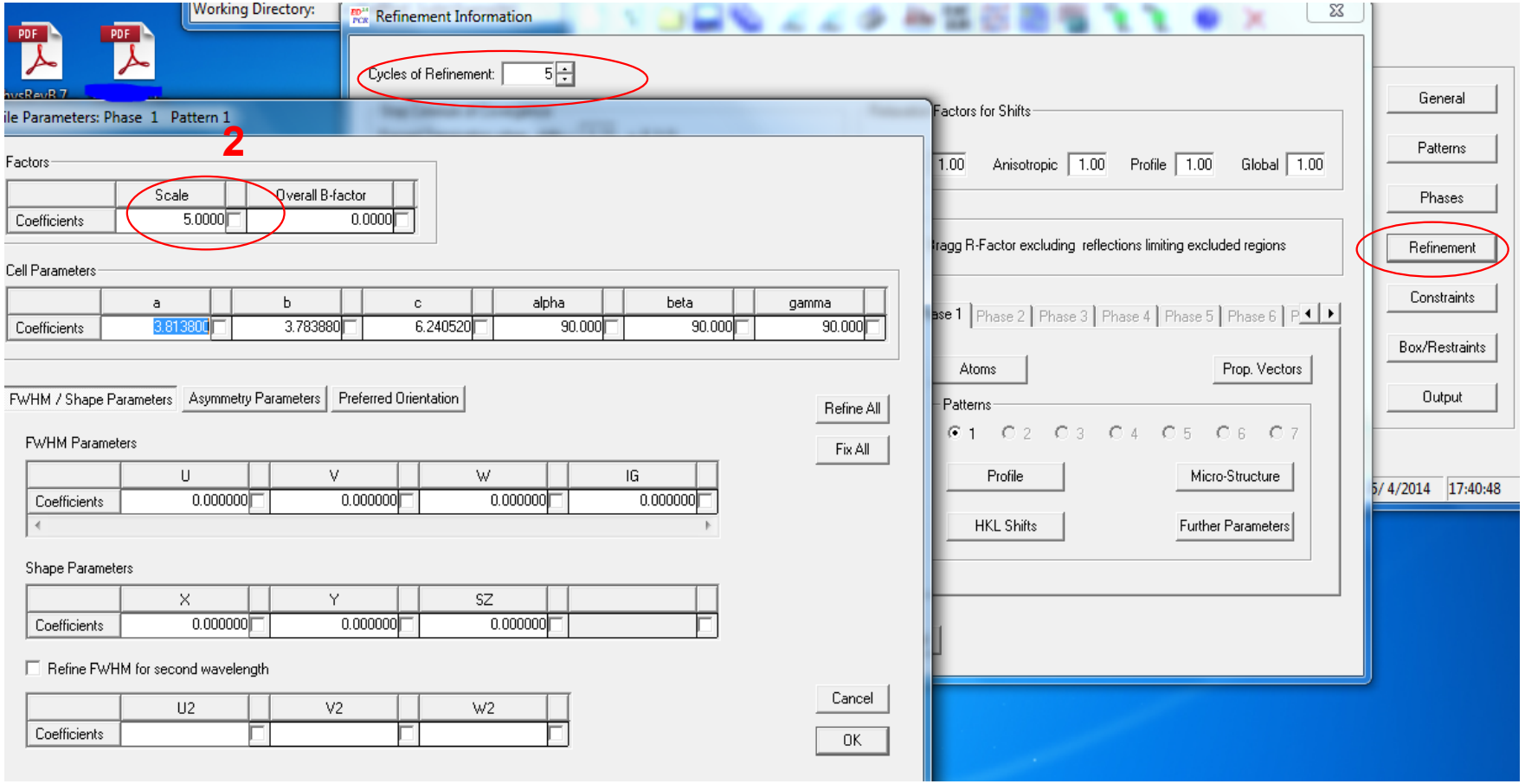
- Open the “Refinement” (1) and then the “Background” and add a value for the “a_o” coefficient that will give a first flat approximation for the background (~70, read it from the data file)



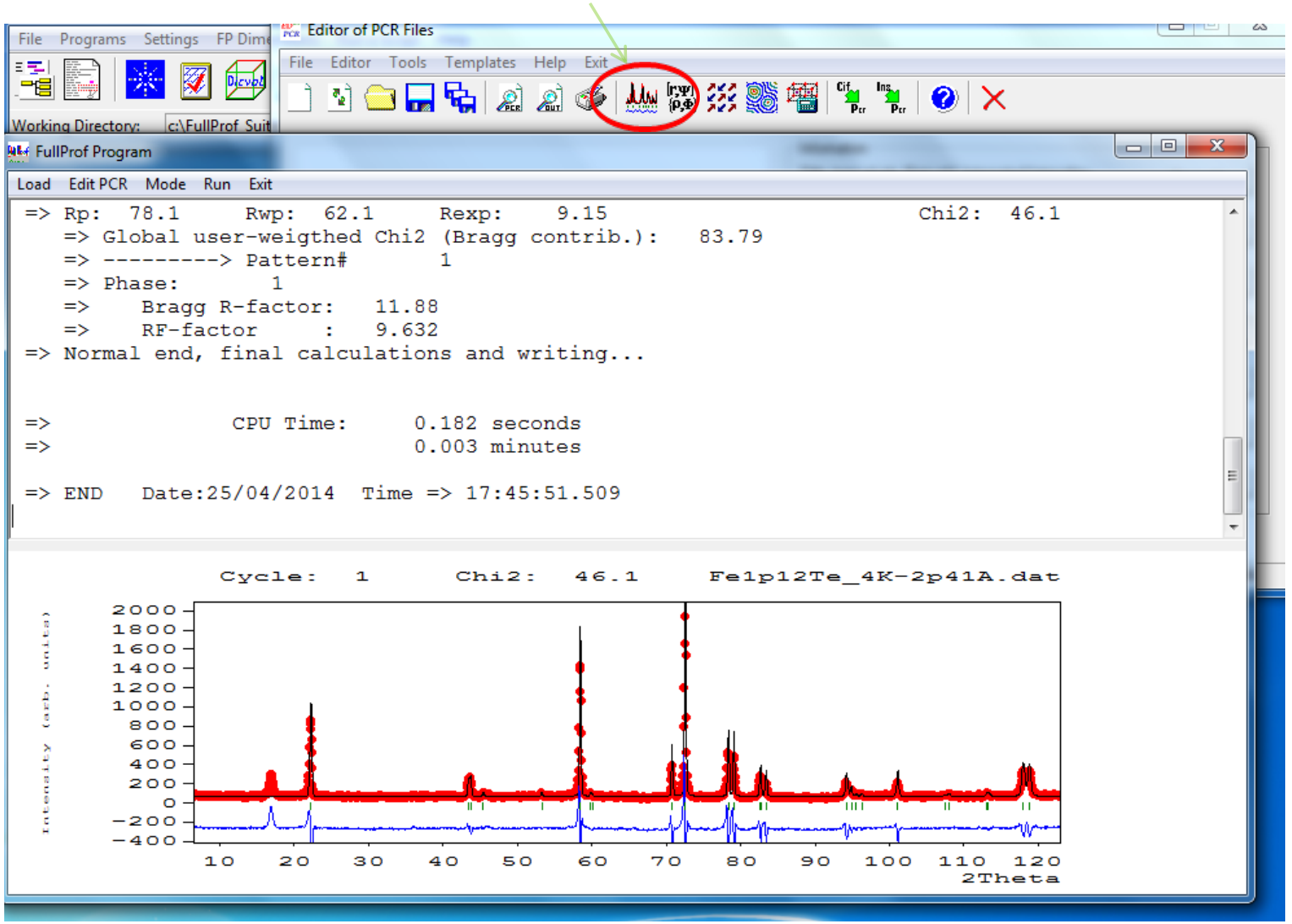




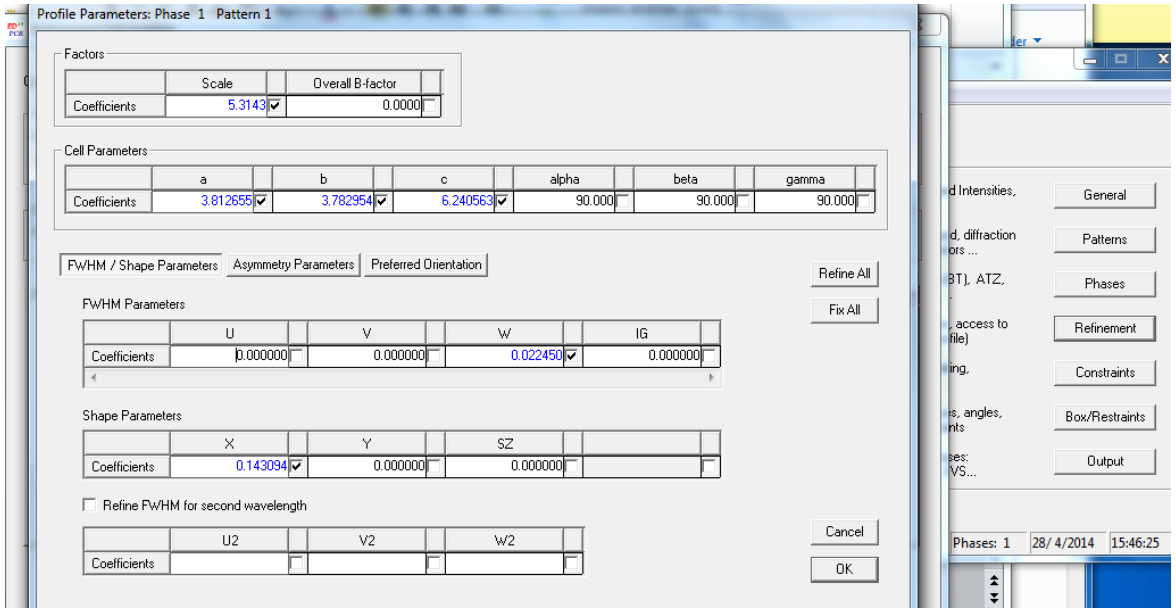
- From the same “Refinement” window (1) , click on the “Profile” tab and set a number for the “scale factor” (~ 5 for this example). The number of “cycles of refinement” can also be increased at this time
- save the PCR file by clicking the “Save” button, every time a change has been made

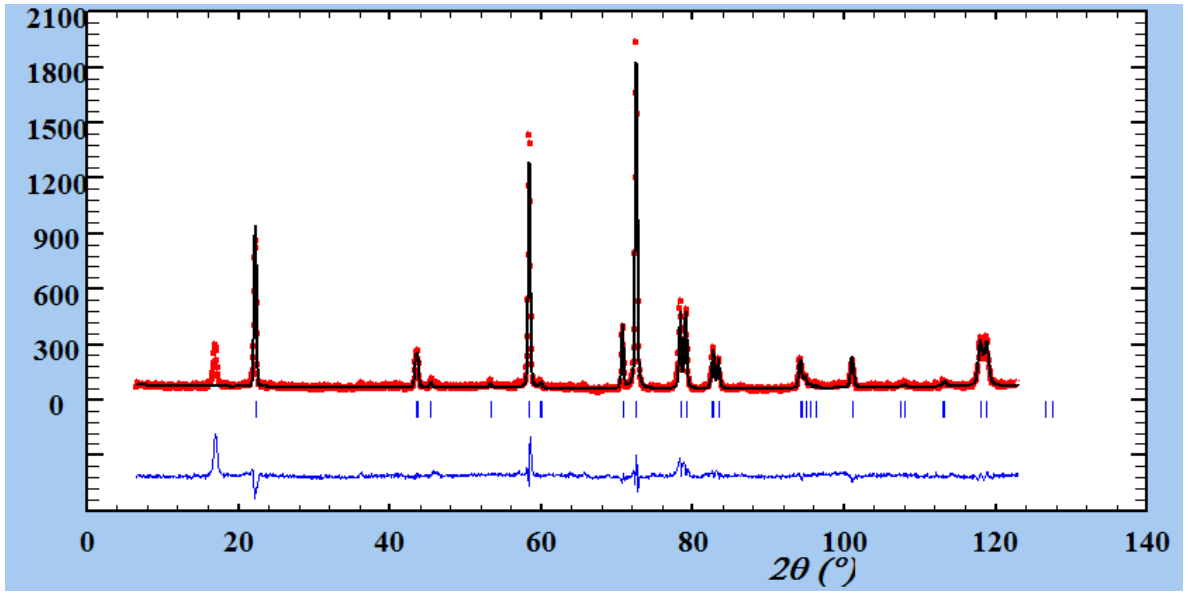


- Run the Fullprof program by click on button indicated below.
  All the parameters are fixed at this time.



- Refine a number of parameters (e.g: scale factor, lattice parameters, FWHM, coefficients of background polynomial, 2theta zero shift) to improve the fit.



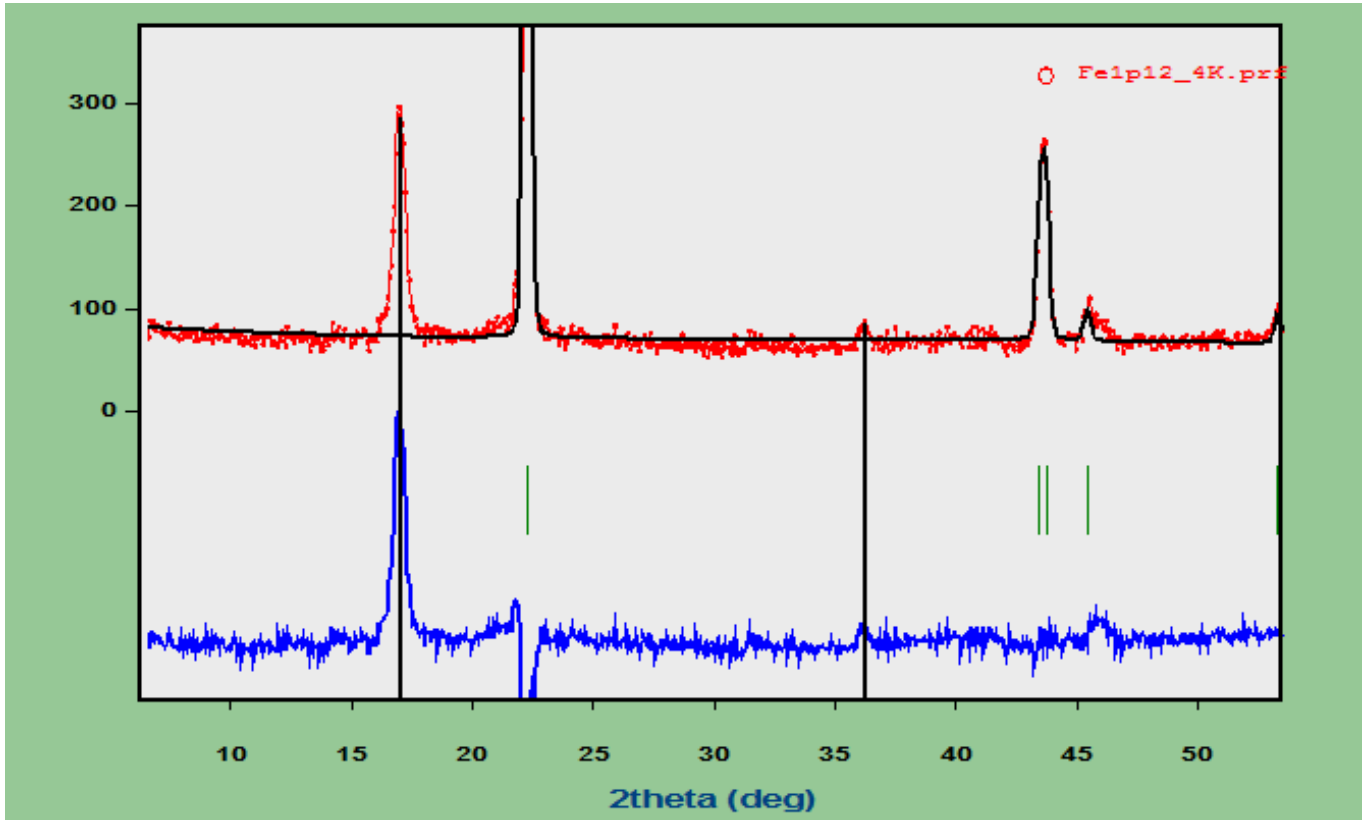


- Open the PRF file using WINPLOTR to observe the quality of the fit.
- Notice the un-indexed peaks that can be associated to the magnetic long range

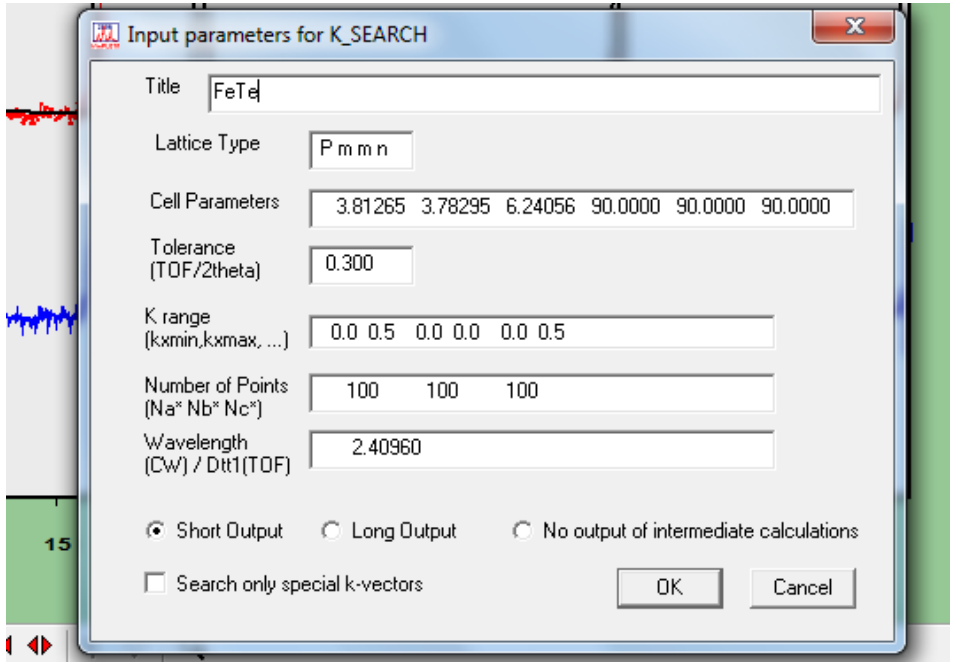
$Fe_{1.16}Te$: STEP2: Determine the k –wave vector

- 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 two peaks: at 2theta ~16.9 and ~ 36.3 deg and save them in a “K-search format” (“Calculations” – “Peak detection” –”Save peaks”)

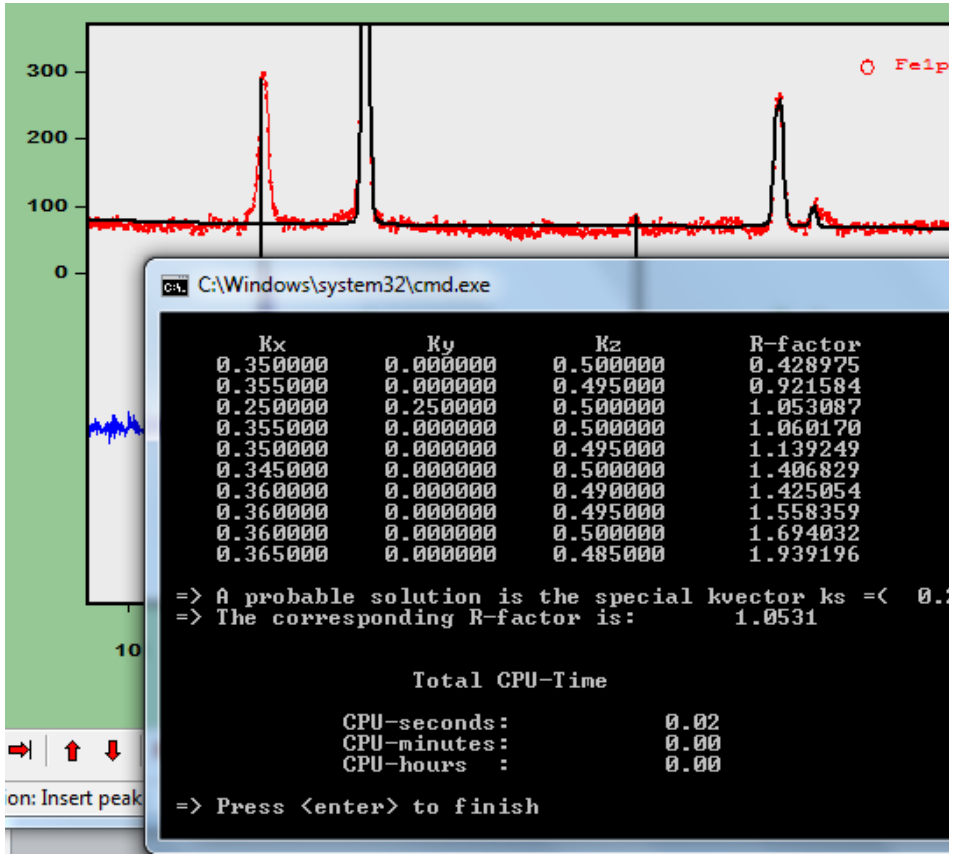


- Run the “k-search “ program to find the propagation vector and see the results listed in the file “k_search.kup”



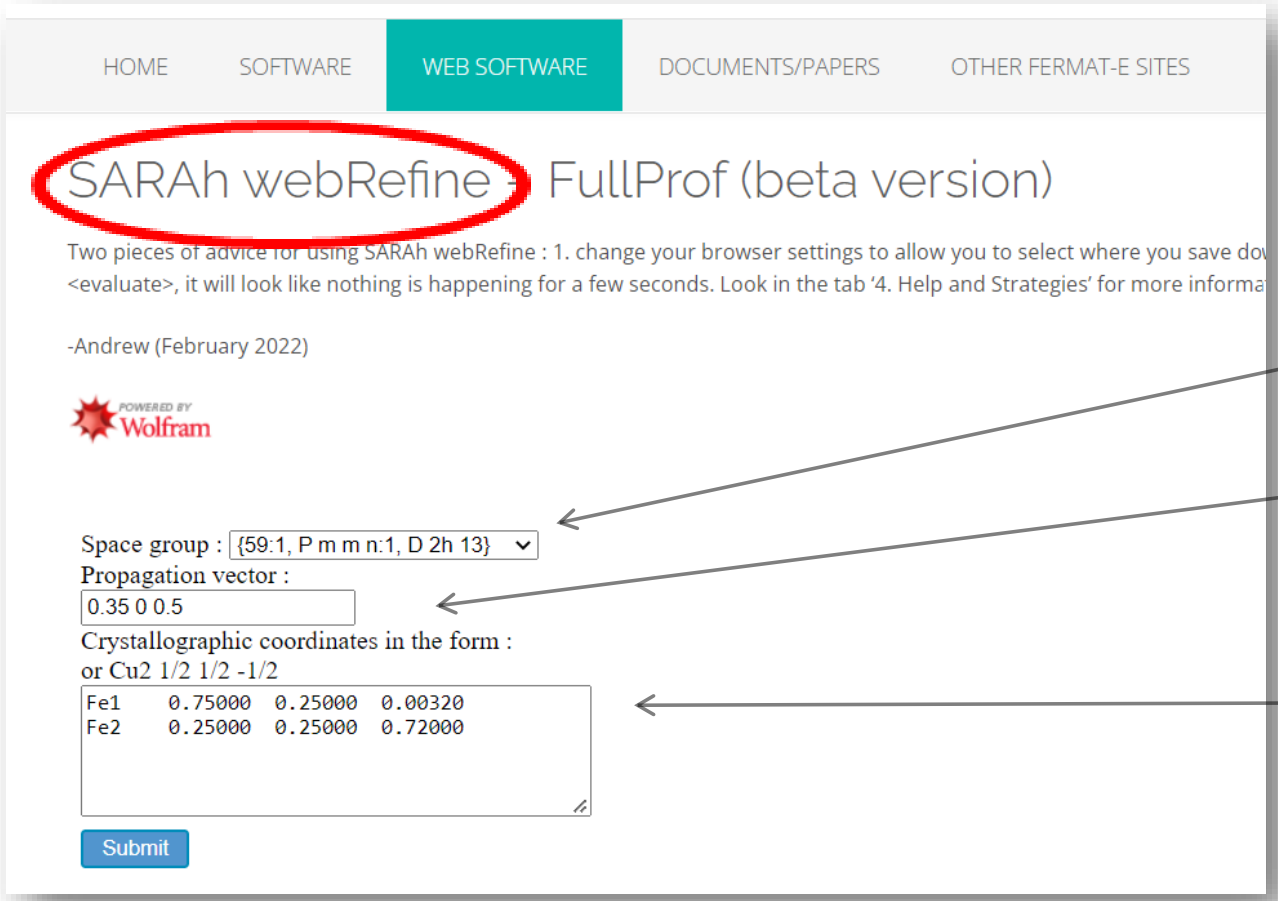
- A number of incommensurate solutions are suggested. Select the **k = (0.35 0 0.5)**

- Make sure to unselect the box “Search only special k-vector” and restrict K range for limiting number of solutions



$Fe_{1.16}Te$: STEP3: Symmetry analysis

- use the web-based SARAh program to generate the Irreducible representations and basis vectors associated with k= (0.35, 0, 0.5) and Pmmn (#59)



Space group: #59:2 / P m m n :2

Propagation vector

Positions of two Fe atoms

- The analysis performed with Sarah will give 4 IRs. as shown in the table:

1. Conventional basis vectors (as projected)	2. Stationary vector combinations	3. Exchange multiplets	4. Help and strategies

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 | 2. make template pcr

☐ Fe1 Γ_1 ψ_1	☐ Fe1 Γ_4 ψ_2	☐ Fe2 Γ_4 ψ_1
☐ Fe1 Γ_2 ψ_1	☐ Fe2 Γ_1 ψ_1	☐ Fe2 Γ_4 ψ_2
☐ Fe1 Γ_2 ψ_2	☐ Fe2 Γ_2 ψ_1	
☐ Fe1 Γ_3 ψ_1	☐ Fe2 Γ_2 ψ_2	
☐ Fe1 Γ_4 ψ_1	☐ Fe2 Γ_3 ψ_1	

(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' for an explanation/help.)

Table. The basis vectors projected from the different IRs :

$$\left\{\begin{array}{lll} & \Gamma_1 & \psi_1 \\ \text{Fe1} & 1) & 0. \qquad\qquad 2.\ \ 0. \\ & 2) & 0.\ \ 0.907981 - 1.78201\,i\ \ 0. \end{array}\right\}$$

$$\left\{\begin{array}{lll} & \Gamma_2 & \psi_1 \\ \text{Fe1} & 1) & 2.\ \ 0.\ \ 0. \\ & 2) & -0.907981 + 1.78201\,i\ \ 0.\ \ 0. \end{array}\right\},\ \left\{\begin{array}{lll} & \Gamma_2 & \psi_2 \\ \text{Fe1} & 1) & 0.\ \ 0. \qquad\qquad 2. \\ & 2) & 0.\ \ 0.\ \ 0.907981 - 1.78201\,i \end{array}\right\}$$

$$\left\{\begin{array}{lll} & \Gamma_3 & \psi_1 \\ \text{Fe1} & 1) & 0. \qquad\qquad 2.\ \ 0. \\ & 2) & 0.\ \ -0.907981 + 1.78201\,i\ \ 0. \end{array}\right\}$$

$$\left\{\begin{array}{lll} & \Gamma_4 & \psi_1 \\ \text{Fe1} & 1) & 2.\ \ 0.\ \ 0. \\ & 2) & 0.907981 - 1.78201\,i\ \ 0.\ \ 0. \end{array}\right\},\ \left\{\begin{array}{lll} & \Gamma_4 & \psi_2 \\ \text{Fe1} & 1) & 0.\ \ 0. \qquad\qquad 2. \\ & 2) & 0.\ \ 0.\ \ -0.907981 + 1.78201\,i \end{array}\right\}$$

	P mmn	
Irreps	Fe1_1	Fe1_ 2
Γ1	(0 1 0)	(0 ξ 0)
Γ2	(1 0 0)	(-ξ 0 0)
	(0 0 1)	(0 0 ξ)
Γ3	(0 1 0)	(0 -ξ 0)
Γ4	(1 0 0)	(ξ 0 0)
	(0 0 1)	(0 0 -ξ)

$\xi = \exp(-2i\pi kT)$,

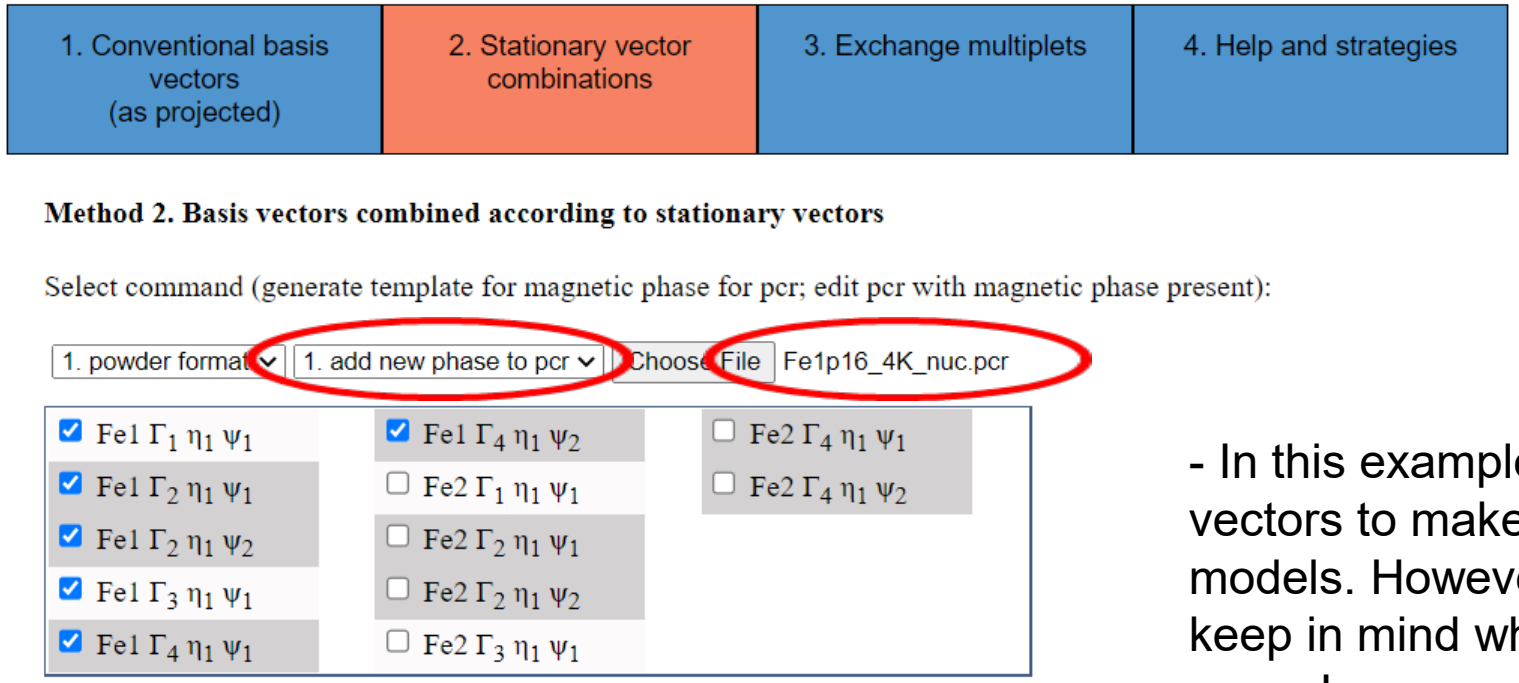
- Several models will successively be tested:

1) only the BV of Γ3 → SDW
2) Combining the BV of Γ3 and Γ4 → helix [bc-plane]
3) Combining the BV of Γ3 and Γ2 → cycloid [ab-plane]

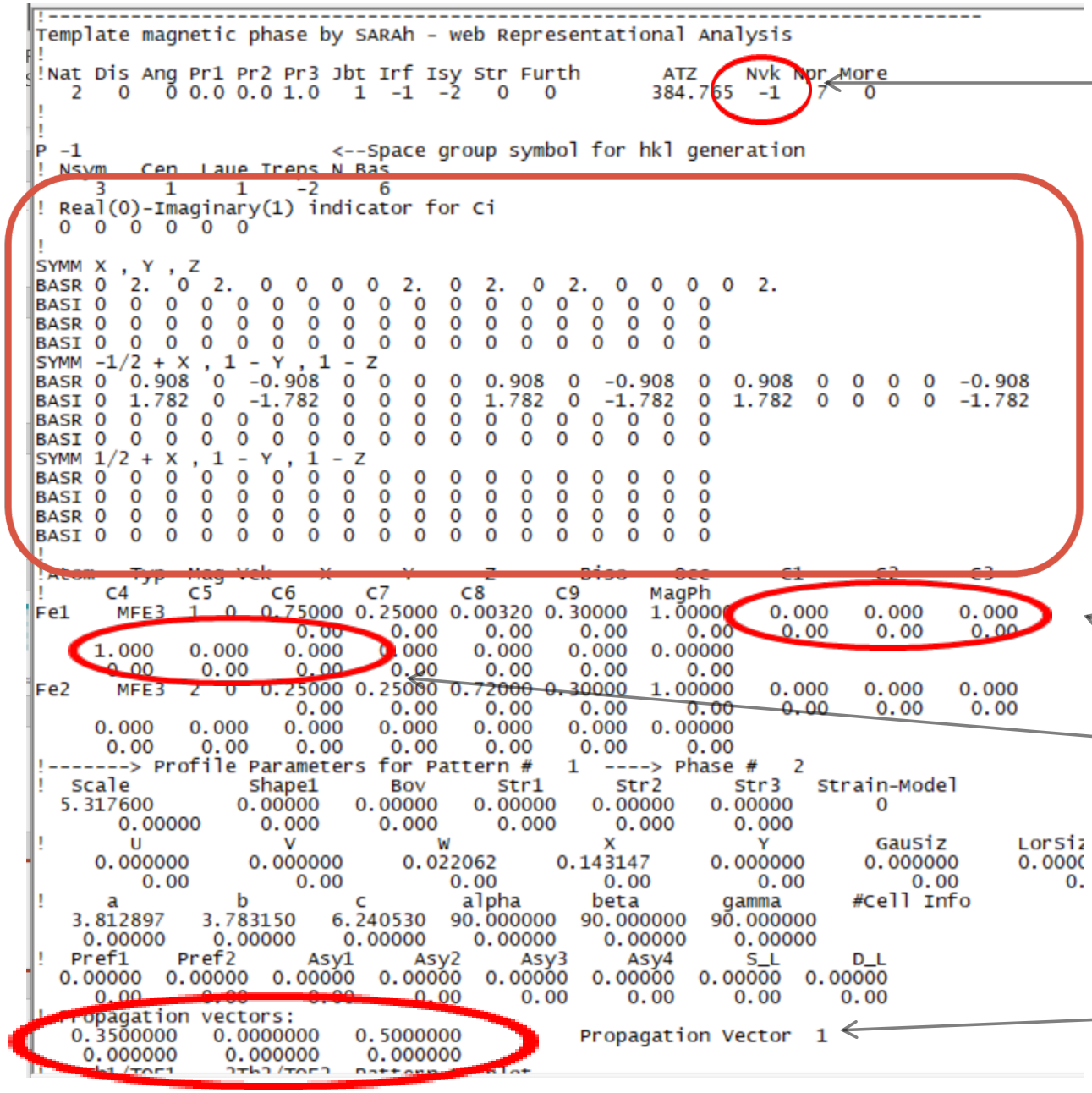
$Fe_{1.16}Te$: STEP4: Adding the magnetic phase as a second phase

- Sarah program can create a Fullprof-ready file (PCR) with the magnetic phase information or insert the magnetic phase into the original pcr file.

- Use the option “add new phase to pcr”, and choose the pcr file that you want to use, as shown below



- In this example, I am selecting all basis vectors to make it easier to test multiple models. However, it is good to always keep in mind what BVs belong to the same Irrep.



```
!-------------------------------------------------------------------------------
Template magnetic phase by SARAh - web Representational Analysis
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ     Nvk Npr More
   2   0   0 0.0 0.0 1.0   1  -1  -2   0   0       384.765  -1   7   0
!
!
P -1                       <--Space group symbol for hkl generation
! Nsym  Cen  Laue Ireps N_Bas
     3     1     1    -2     6
! Real(0)-Imaginary(1) indicator for Ci
  0  0  0  0  0  0
!
SYMM X , Y , Z
BASR 0  2.  0  2.  0  0  0  0  2.  0  2.  0  2.  0  0  0  0  2.
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM -1/2 + X , 1 - Y , 1 - Z
BASR 0  0.908  0  -0.908  0  0  0  0  0.908  0  -0.908  0  0.908  0  0  0  0  -0.908
BASI 0  1.782  0  -1.782  0  0  0  0  1.782  0  -1.782  0  1.782  0  0  0  0  -1.782
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM 1/2 + X , 1 - Y , 1 - Z
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
!
!Atom   Typ  Mag Vek    X       Y       Z       Biso     Occ      C1       C2       C3
!     C4      C5      C6      C7      C8      C9      MagPh
Fe1    MFE3  1  0  0.75000 0.25000 0.00320 0.30000  1.00000    0.000    0.000    0.000
                     0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
     1.000    0.000    0.000    0.000    0.000    0.000  0.00000
     0.00     0.00     0.00     0.00     0.00     0.00     0.00
Fe2    MFE3  2  0  0.25000 0.25000 0.72000 0.30000  1.00000    0.000    0.000    0.000
                     0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
     0.000    0.000    0.000    0.000    0.000    0.000  0.00000
     0.00     0.00     0.00     0.00     0.00     0.00     0.00
!-------> Profile Parameters for Pattern #   1  ----> Phase #   2
!  Scale          Shape1       Bov        Str1       Str2       Str3    Strain-Model
  5.317600       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
     0.000000    0.000000    0.022062    0.143147    0.000000    0.000000    0.0000
          0.00        0.00        0.00        0.00        0.00        0.00        0.
!      a          b          c        alpha       beta       gamma      #Cell Info
   3.812897   3.783150   6.240530  90.000000  90.000000  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:
   0.3500000   0.0000000   0.5000000        Propagation Vector  1
   0.000000    0.000000    0.000000
```

Number of k vectors (Nvk) needs to be changes to "-1" to account for the fact that k and –k are not equivalent.

The BV of all 4 Irreps

Coefficients of the basis vectors

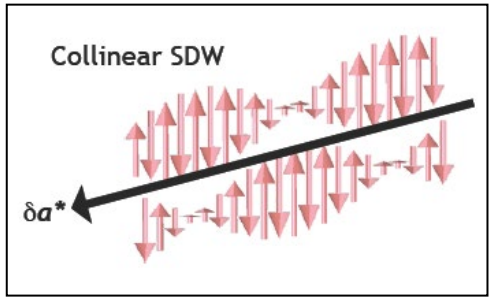
Propagation vector

```
!-------------------------------------------------------------------------------
Template magnetic phase by SARAh - web Representational Analysis
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ     Nvk Npr More
   2   0   0 0.0 0.0 1.0   1  -1  -2   0   0       384.765  -1   7   0
!
!
P -1                      <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
     3     1     1    -2     6
! Real(0)-Imaginary(1) indicator for Ci
  0  0  0  0  0  0
!
SYMM X , Y , Z
BASR 0  2.  0  2.  0  0  0  0  2.  0  2.  0  2.  0  0  0  0  2.
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM -1/2 + X , 1 - Y , 1 - Z
BASR 0  0.908  0  -0.908  0  0  0  0  0.908  0  -0.908  0  0.908  0  0  0  0  -0.908
BASI 0  1.782  0  -1.782  0  0  0  0  1.782  0  -1.782  0  1.782  0  0  0  0  -1.782
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM 1/2 + X , 1 - Y , 1 - Z
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
!
!Atom  Typ  Mag Vek    X       Y       Z       Biso    Occ      C1      C2      C3
!      C4      C5      C6      C7      C8      C9      MagPh
Fe1    MFE3  1  0  0.75000 0.25000 0.00320 0.30000  1.00000   0.000   0.000   0.000
                    0.00    0.00    0.00    0.00      0.00     0.00    0.00
       1.000   0.000  0.000   0.000   0.000   0.000   0.00000
        0.00    0.00    0.00    0.00    0.00    0.00      0.00
Fe2    MFE3  2  0  0.25000 0.25000 0.72000 0.30000  1.00000   0.000   0.000   0.000
                    0.00    0.00    0.00    0.00      0.00     0.00    0.00
       0.000   0.000   0.000   0.000   0.000   0.000   0.00000
        0.00    0.00    0.00    0.00    0.00    0.00      0.00
!-------> Profile Parameters for Pattern #   1  ----> Phase #   2
!  Scale          Shape1       Bov        Str1       Str2       Str3   Strain-Model
  5.317600       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      Lors
     0.000000    0.000000    0.022062    0.143147    0.000000    0.000000    0.00
          0.00        0.00        0.00        0.00        0.00        0.00
!      a          b          c        alpha       beta       gamma      #Cell Info
   3.812897   3.783150   6.240530  90.000000  90.000000  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:
   0.3500000   0.0000000   0.5000000          Propagation Vector  1
   0.000000    0.000000    0.000000
```

The BV of IR3

Use only the c4, for the IR3 (with a single basis vector to construct a spin density wave structure

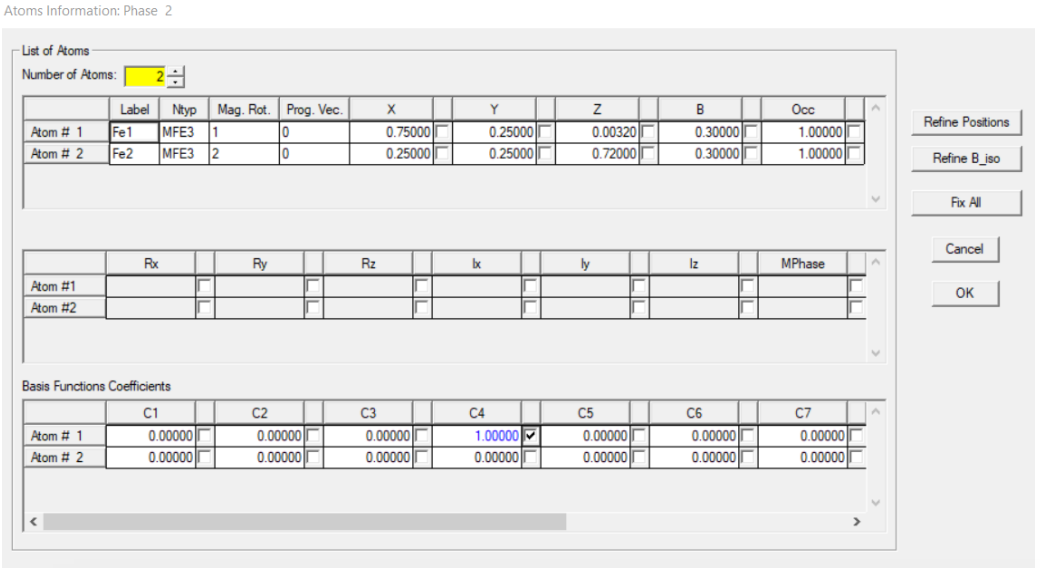
	P mmn	
Irreps	Fe1_1	Fe1_ 2
Γ1	(0 1 0)	(0 ξ 0)
Γ2	(1 0 0)	(-ξ 0 0)
	(0 0 1)	(0 0 ξ)
Γ3	(0 1 0)	(0 -ξ 0)
Γ4	(1 0 0)	(ξ 0 0)
	(0 0 1)	(0 0 -ξ)

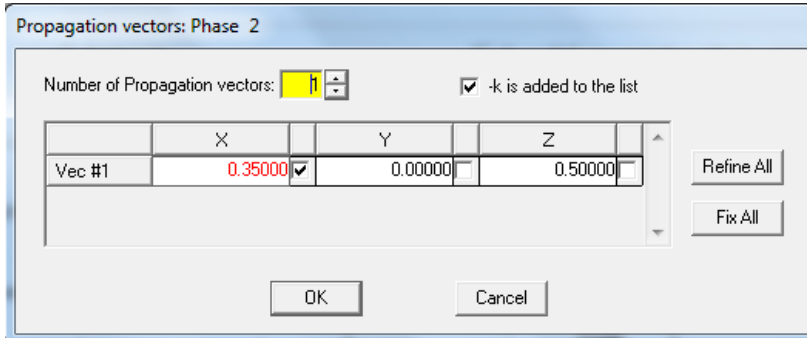


$Fe_{1.16}Te$: STEP5: Refine by LSQ the magnetic phase

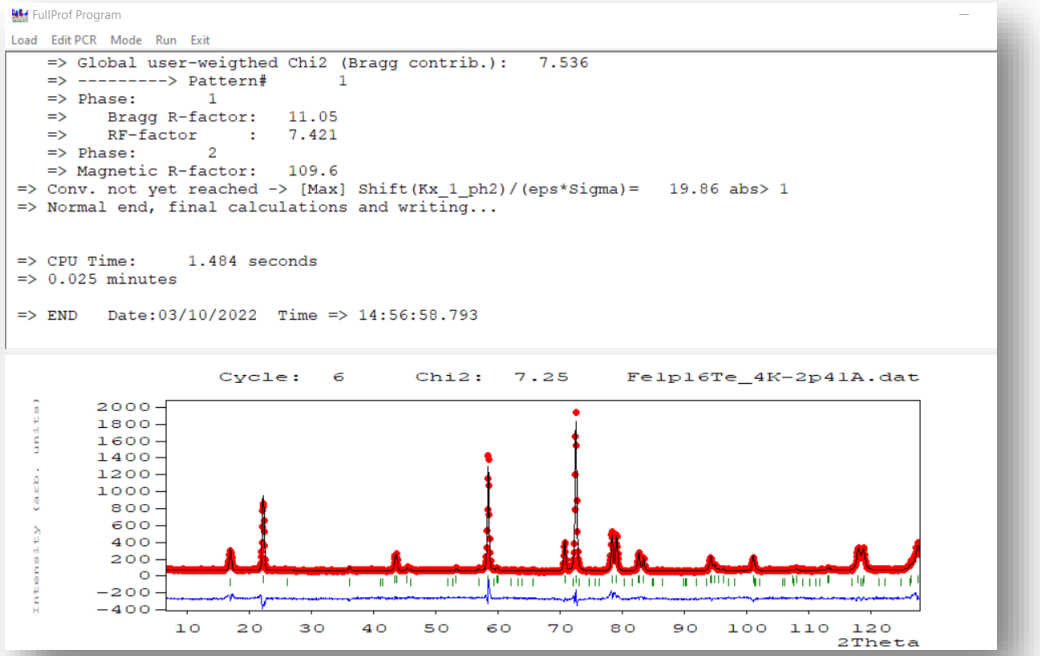
- In the EdPCR GUI go to the "atom information for phase two and initialize the c4 coefficient to 1 and mark it for refinement.

  - One can also refine the x component of the k- vector at this time:



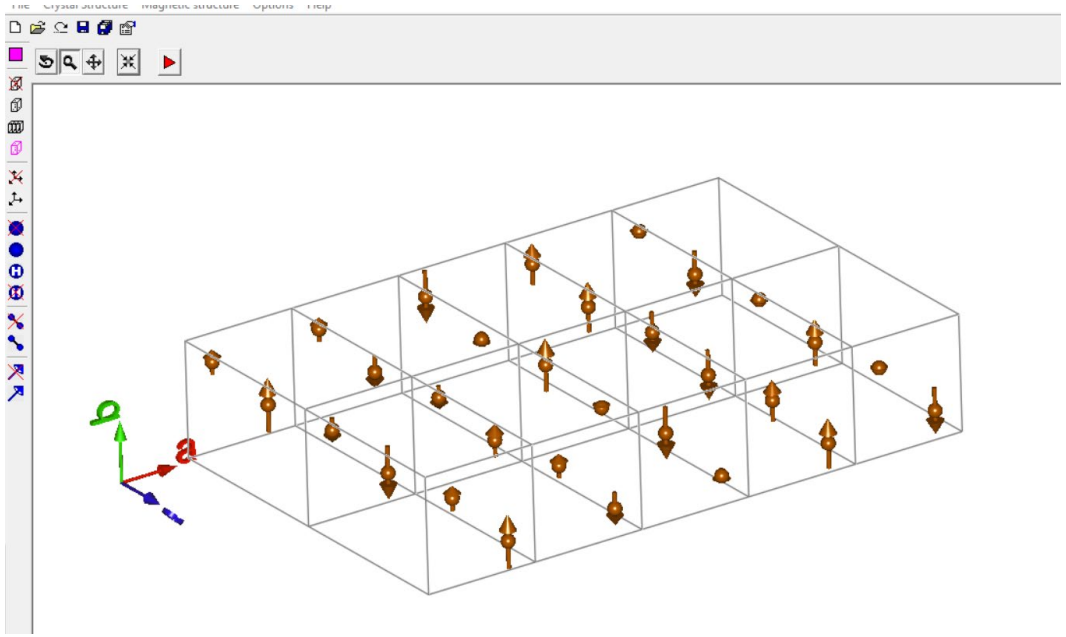


  - Run the Fullprof program and we'll obtain a satisfactory fitting of the magnetic peaks.



$Fe_{1.16}Te$: STEP6: Visualization of the magnetic structure

- to visualize the determined magnetic structure, you can use **FpStudio** program. It reads *.fst files, generated automatically by Fullprof



Edition of file: C:\Users\gq4\Documents\MAGSTR_Worksop\2014\OGarlea_example1_IC_structure\Fe12-HB2A\Fe1p12...

File Edit Search

```
!   FILE for FullProf Studio: generated automatically by FullProf
!Title: magnetic
SPACEG P -1
CELL      3.812646    3.782932    6.240587  90.0000  90.0000  90.0000   DISPLAY MULTIPLE
BOX    -0.15  4.15   -0.15  1.15    -0.15  1.15

{
LATTICE P
K      0.35372   0.00000   0.50000
SYMM  x,y,z
MSYM  u,v,w,0.0
MATOM Fe1_1       FE       0.75000  0.25000  0.00300  SCALE 1.0 GROUP
SKP            1  1  0.00000  1.77116  0.00000    0.00000  0.00000  0.00000    0.00000
MATOM Fe1_2       FE       0.25000  0.75000  0.99700  SCALE 1.0 GROUP
SKP            1  1  0.00000 -0.80411  0.00000    0.00000 -1.57811  0.00000    0.00000
}
```

Line:5 Col:18 NUM INS

- One can also use FpStudio to see the magnitude of the magnetic moment for any specific position, by selecting "Magnetic structure" – "List magnetic moments"

```
Magnetic lattice type : P
Unit Cell:       3.8129      3.7831      6.2405     90.0000     90.0000     90.0000

Current Box:    0   5   0   1   0   2

Magnetic k-vectors :
 0.35371  0.00000  0.50000

 Symmetry operations :
SYMM x,y,z
u,v,w,0.0

Atom : Fe1_1     Fe
-------------------------------------------------------------------------------
        x         y         z        Translation    k MSYM     m(a)      m(b)      m(c)      Mtot
  0.75000   0.25000   0.00320
                                  (  0,   0,   0)
                                                    1    1  0.00000  1.73424  0.00000
                                                       0.00000  1.73424  0.00000  1.73424
                                  (  0,   0,   1)
                                                    1    1  0.00000 -1.73424  0.00000
                                                       0.00000 -1.73424  0.00000  1.73424
                                  (  0,   0,   2)
                                                    1    1  0.00000  1.73424  0.00000
                                                       0.00000  1.73424  0.00000  1.73424
                                  (  1,   0,   0)
                                                    1    1  0.00000 -1.05178  0.00000
                                                       0.00000 -1.05178  0.00000  1.05178
                                  (  1,   0,   1)
                                                    1    1  0.00000  1.05178  0.00000
                                                       0.00000  1.05178  0.00000  1.05178
                                  (  1,   0,   2)
                                                    1    1  0.00000 -1.05178  0.00000
                                                       0.00000 -1.05178  0.00000  1.05178
                                  (  2,   0,   0)
                                                    1    1  0.00000 -0.45846  0.00000
                                                       0.00000 -0.45846  0.00000  0.45846
                                  (  2,   0,   1)
                                                    1    1  0.00000  0.45846  0.00000
                                                       0.00000  0.45846  0.00000  0.45846
```

$Fe_{1.16}Te$: back to STEP4 - Considering helical model

- Let's consider a helical structure given by the BV of Γ3 (*b*-component) and BV2 (*c*-component) of Γ4 .

```
P -1                          <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
    3     1     1    -2     6
! Real(0)-Imaginary(1) indicator for Ci
  0  0  0  0  0  1
!
SYMM X , Y , Z
BASR 0  2.  0  2.  0  0  0  0  2.  0  2.  0  2.  0  0  0  0  2.
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM -1/2 + X , 1 - Y , 1 - Z
BASR 0  0.908  0  -0.908  0  0  0  0  0.908  0  -0.908  0  0.908  0  0  0  0  -0.908
BASI 0  1.782  0  -1.782  0  0  0  0  1.782  0  -1.782  0  1.782  0  0  0  0  -1.782
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM 1/2 + X , 1 - Y , 1 - Z
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASR 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
BASI 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
!
!Atom  Typ  Mag Vek        X       Y       Z      Biso    Occ      C1      C2      C3
!     C4      C5      C6      C7      C8      C9      MagPh
Fe1    MFE3  1  0  0.75000 0.25000 0.00320 0.30000  1.00000   0.000   0.000   0.000
                    0.00    0.00    0.00    0.00     0.00     0.00    0.00    0.00
     0.867   0.000   0.867   0.000   0.000   0.000  0.00000
     21.00    0.00   21.00    0.00    0.00    0.00     0.00
Fe2    MFE3  2  0  0.25000 0.25000 0.72000 0.30000  1.00000   0.000   0.000   0.000
                    0.00    0.00    0.00    0.00     0.00     0.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
!-------> Profile Parameters for Pattern #   1  ----> Phase #   2
```

define the orthogonal BV as imaginary

Activate the BV of IR4 by non-zero C6

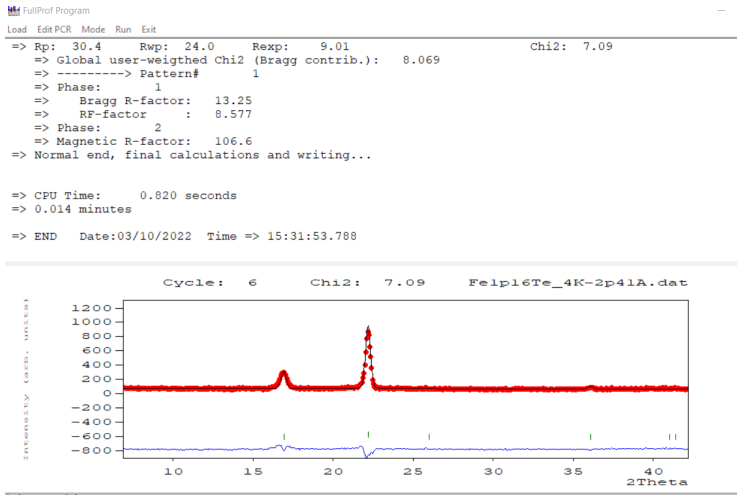
Use c4 and c6 , for constructing a helical structure

	P mmn	
Irreps	Fe1_1	Fe1_ 2
Γ1	(0 1 0)	(0 ξ 0)
Γ2	(1 0 0)	(-ξ 0 0)
	(0 0 1)	(0 0 ξ)
Γ3	(0 1 0)	(0 -ξ 0)
Γ4	(1 0 0)	(ξ 0 0)
	(0 0 1)	(0 0 -ξ)

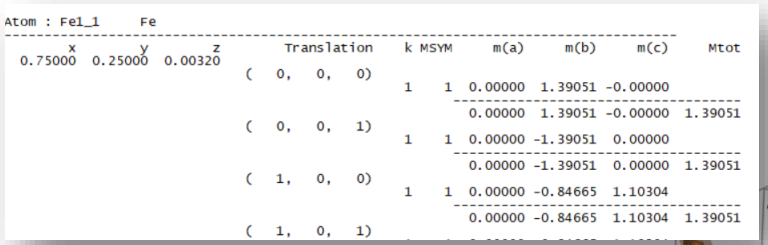
NOTE: helical structure consists of orthogonal components that are perpendicular to the incommensurate k vector.

- The C4 and C6 can be refined independently or constrained. Identical values of coefficients will produce a circular helix

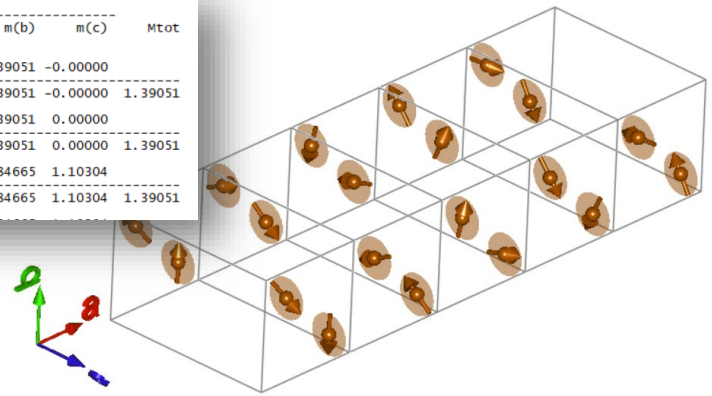
```
!
!Atom   Typ  Mag Vek     X        Y        Z        Biso     Occ      C1       C2       C3
!     C4       C5       C6       C7       C8       C9       MagPh
Fe1    MFE3  1   0   0.75000  0.25000  0.00320  0.30000  1.00000   0.000    0.000    0.000
                       0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
     0.695    0.000    0.695    0.000    0.000    0.000    0.00000
     21.00     0.00    21.00     0.00     0.00     0.00     0.00
Fe2    MFE3  2   0   0.25000  0.25000  0.72000  0.30000  1.00000   0.000    0.000    0.000
                       0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
     0.000    0.000    0.000    0.000    0.000    0.000    0.00000
      0.00     0.00     0.00     0.00     0.00     0.00     0.00
!-------> Profile Parameters for Pattern #   1  ----> Phase #   2
```



- run the Fullprof program and we'll obtain another satisfactory fitting of the magnetic peaks!
- visualize the helical magnetic structure



```
Atom : Fe1_1     Fe
------------------------------------------------------------------------------
      x        y        z          Translation    k MSYM     m(a)      m(b)      m(c)      Mtot
 0.75000  0.25000  0.00320   (  0,   0,   0)
                                                  1   1  0.00000  1.39051 -0.00000
                                                    ------------------------------------------
                                                    0.00000  1.39051 -0.00000  1.39051
                            (  0,   0,   1)
                                                  1   1  0.00000 -1.39051  0.00000
                                                    ------------------------------------------
                                                    0.00000 -1.39051  0.00000  1.39051
                            (  1,   0,   0)
                                                  1   1  0.00000 -0.84665  1.10304
                                                    ------------------------------------------
                                                    0.00000 -0.84665  1.10304  1.39051
                            (  1,   0,   1)
```



- You can edit the ".fst " file to display the envelope of the helical structure

```
File  Edit  Search
!   FILE for FullProf Studio: generated automatically by FullProf
!Title: Template magnetic phase by SARAh - web Representational Analysis
SPACEG P 1
CELL     3.812897    3.783150    6.240530  90.0000  90.0000  90.0000   DISPLAY MULTIPLE
BOX   -0.15  5.15   -0.15  1.15    -0.15  2.15

{
LATTICE P
K      0.35419    0.00000    0.50000
SYMM   x,y,z
MSYM   u,v,w,0.0
MATOM Fe1_1              Fe      0.75000  0.25000  0.00320  SCALE 1.0 GROUP Envelop 1 0 0 1
SKP            1  1    0.00000    1.39051    0.00000     0.00000   0.00000   1.39051     0.00000
MATOM Fe1_2              Fe      0.25000  0.75000  0.99680  SCALE 1.0 GROUP Envelop 1 0 0 1
SKP            1  1    0.00000   -0.63129    1.23895     0.00000  -1.23895  -0.63129     0.00000
}
```

$Fe_{1.16}Te$: back to STEP4 - Considering cycloid model

- Let's consider a cycloidal structure given by the BV of Γ3 (*b*-component) and BV1 (*a*-component) of Γ2 .

```
P -1                          <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
     3     1     1    -2     6
! Real(0)-Imaginary(1) indicator for Ci
  0  1  0  0  0  0
!
SYMM X , Y , Z
BASR 0  2.  0  2.  0  0  0  0  2.  0  2.  0  2.  0  0  0  0  2.
BASI 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
BASR 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
BASI 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
SYMM -1/2 + X , 1 - Y , 1 - Z
BASR 0  0.908  0  -0.908  0  0  0  0  0.908  0  -0.908  0  0.908  0  0  0  0  -0.908
BASI 0  1.782  0  -1.782  0  0  0  0  1.782  0  -1.782  0  1.782  0  0  0  0  -1.782
BASR 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
BASI 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
SYMM 1/2 + X , 1 - Y , 1 - Z
BASR 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
BASI 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
BASR 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
BASI 0  0   0  0   0  0  0  0  0   0  0   0  0   0  0  0  0  0
!
!Atom   Typ  Mag Vek    X        Y        Z        Biso     Occ      C1       C2       C3
!     C4       C5      C6       C7       C8       C9       MagPh
Fe1    MFE3  1  0  0.75000  0.25000  0.00320  0.30000  1.00000   0.000    0.695    0.000
                    0.00     0.00     0.00     0.00     0.00     0.00    21.00     0.00
     0.695    0.000    0.000    0.000    0.000    0.000  0.00000
     21.00     0.00     0.00     0.00     0.00     0.00     0.00
Fe2    MFE3  2  0  0.25000  0.25000  0.72000  0.30000  1.00000   0.000    0.000    0.000
                    0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
     0.000    0.000    0.000    0.000    0.000    0.000  0.00000
      0.00     0.00     0.00     0.00     0.00     0.00     0.00
```

define the orthogonal BV as imaginary

Activate the BV of IR2 by non-zero C2

Use c4 and c2 , for constructing a cycloid

	P mmn	
Irreps	Fe1_1	Fe1_ 2
Γ1	(0 1 0)	(0 ξ 0)
Γ2	(1 0 0)	(-ξ 0 0)
	(0 0 1)	(0 0 ξ)
Γ3	(0 1 0)	(0 -ξ 0)
Γ4	(1 0 0)	(ξ 0 0)
	(0 0 1)	(0 0 -ξ)

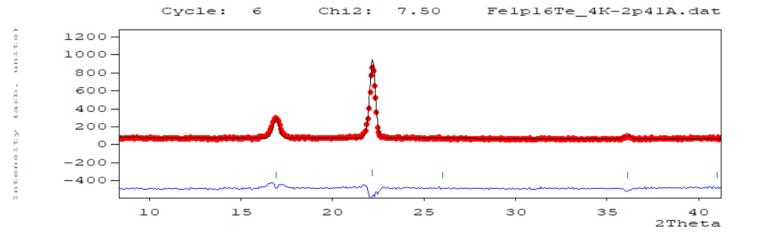
NOTE: cycloidal structure consists of orthogonal components, but one of component runs along the incommensurate k direction

- The C4 and C2 can be refined independently or constrained. Equal values will make a circular cycloid

```
=> Rp:  30.9     Rwp:  24.7     Rexp:    9.01                         Chi2:  7.50
   => Global user-weigthed Chi2 (Bragg contrib.):   8.385
   => ---------> Pattern#       1
   => Phase:       1
   =>    Bragg R-factor:   10.81
   =>    RF-factor     :   7.191
   => Phase:       2
   => Magnetic R-factor:   114.8
=> Normal end, final calculations and writing...


=> CPU Time:     1.250 seconds
=> 0.021 minutes

=> END   Date:03/10/2022  Time => 15:49:03.265
```



List of Atoms

Number of Atoms: 2

	Label	Ntyp	Mag. Rot.	Prog. Vec.	X	Y	Z	B	Occ
Atom # 1	Fe1	MFE3	1	0	0.75000	0.25000	0.00320	0.30000	1.00000
Atom # 2	Fe2	MFE3	2	0	0.25000	0.25000	0.72000	0.30000	1.00000

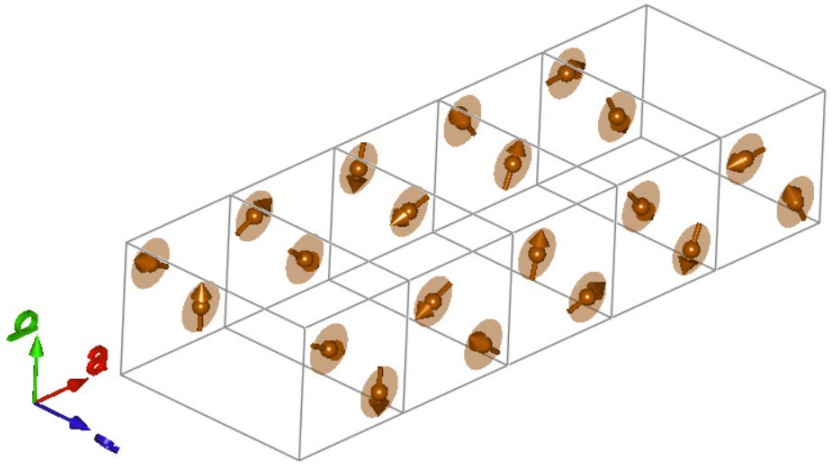
Refine Positions | Refine B_iso | Fix All | Cancel | OK

	Rx	Ry	Rz	Ix	Iy	Iz	MPhase
Atom #1							
Atom #2							

Basis Functions Coefficients

	C1	C2	C3	C4	C5	C6	C7
Atom # 1	0.00000	0.69400	0.00000	0.69400	0.00000	0.00000	0.00000
Atom # 2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

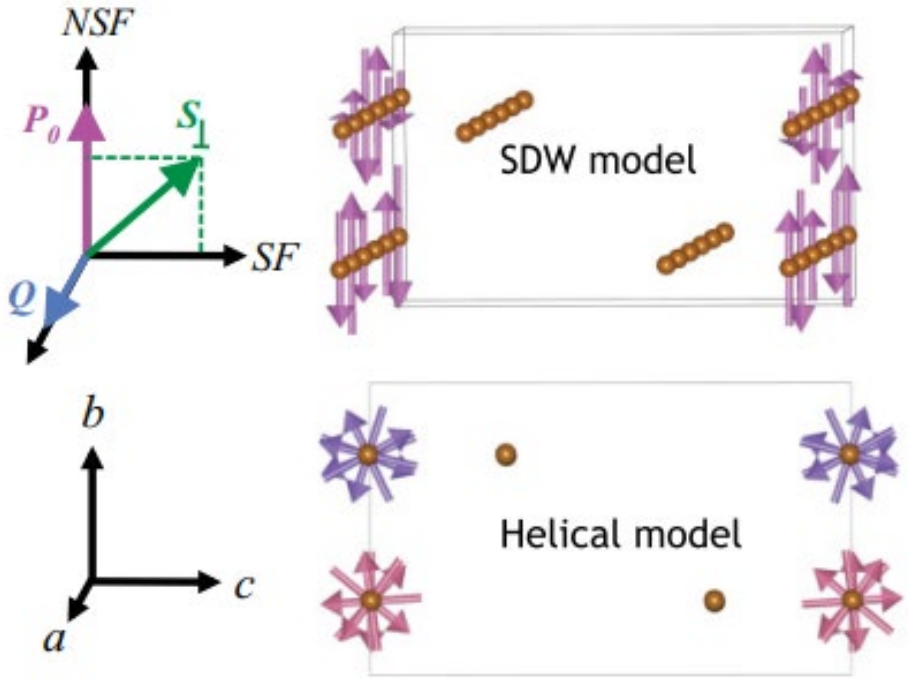
- run the Fullprof program and we'll obtain another satisfactory fitting of the magnetic peaks!
- visualize the cycloid structure



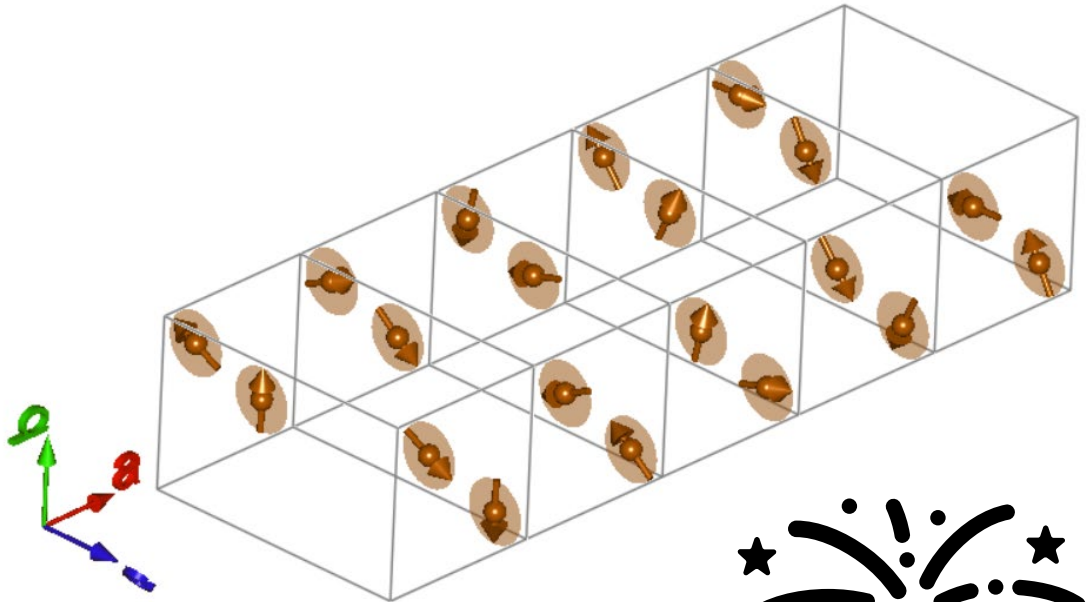

```
 Symmetry operations :
SYMM x,y,z
u,v,w,0.0

Atom : Fe1_1     Fe
------------------------------------------------------------------------------
      x       y       z        Translation    k MSYM     m(a)     m(b)     m(c)     Mtot
 0.75000 0.25000 0.00320
                                (  0,   0,   0)
                                                1    1 -0.00000  1.38890  0.00000
                                                      -0.00000  1.38890  0.00000  1.38890
                                (  0,   0,   1)
                                                1    1  0.00000 -1.38890  0.00000
                                                       0.00000 -1.38890  0.00000  1.38890
                                (  1,   0,   0)
                                                1    1  1.10129 -0.84629  0.00000
                                                       1.10129 -0.84629  0.00000  1.38890
                                (  1,   0,   1)
                                                1    1 -1.10129  0.84629  0.00000
```

Polarization analysis to determine the correct model



.. and the winner is ….



Helical magnetic structure