OAK RIDGE National Laboratory

Determination of the incommensurate magnetic structure of $Fe_{1.16}Te$ using Super SpaceGrup method

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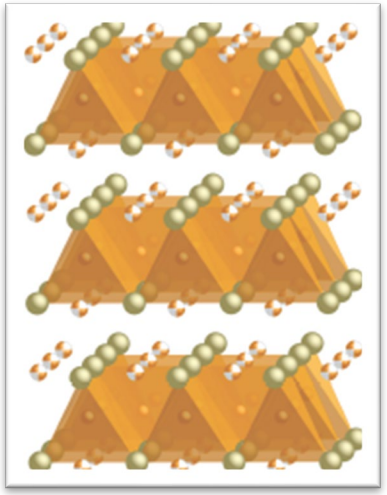
U.S. DEPARTMENT OF ENERGY

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,

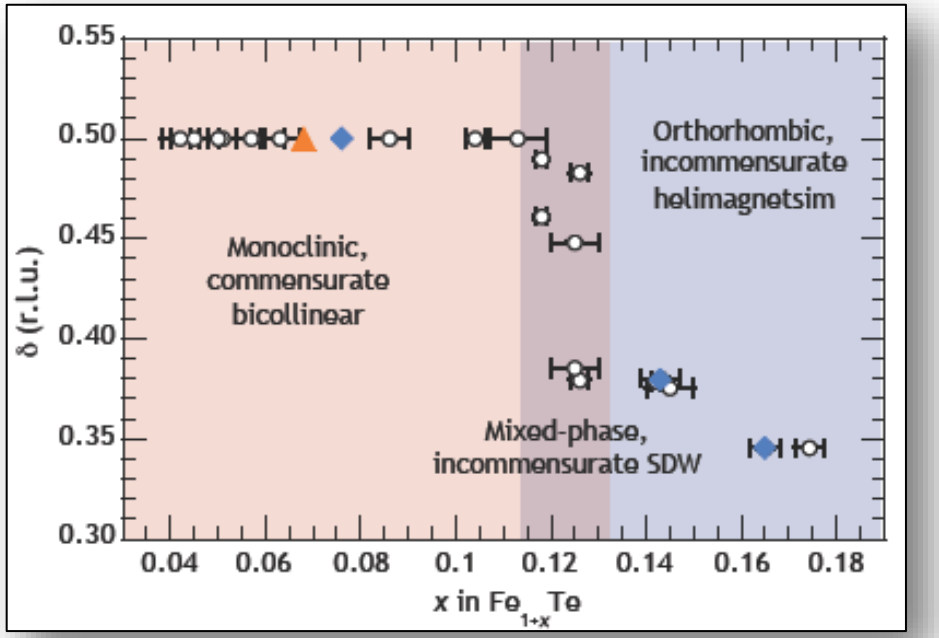
Paramagnetic phase:

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 :

I. Import the known crystal structure and input the instrument parameters to create a PCR file for nuclear phase refinement

II. Refine the structural model and the profile parameters for 4K data

III. Identify the magnetic reflections and determine the propagation vector (k-search in Winplotr)

IV. Identify possible magnetic models using ISODISTORT (described by superspace group symmetry)

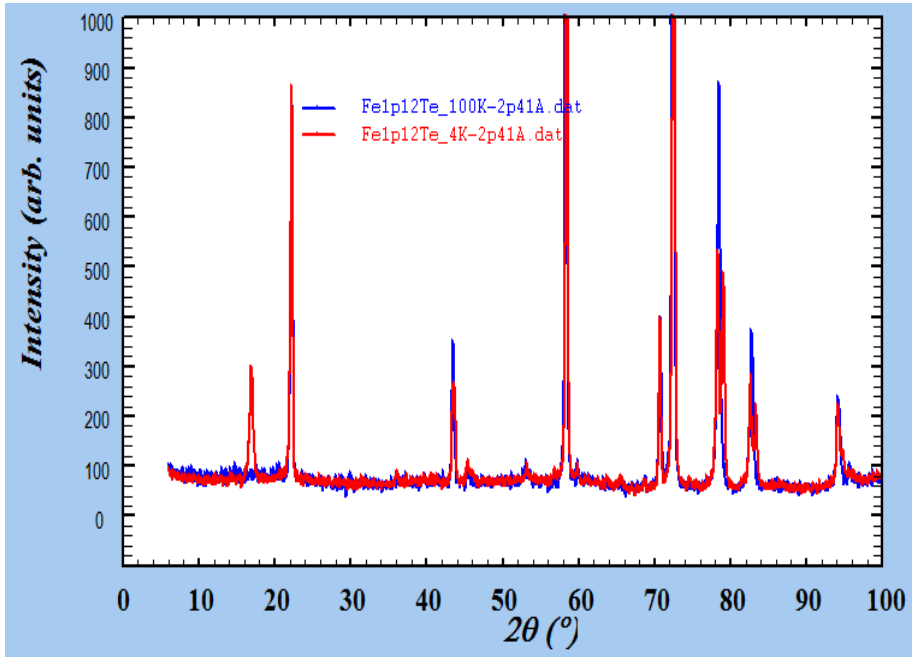
V. Select a magnetic model (mcif) and convert it to PCR format (single phase magnetic & nuclear)

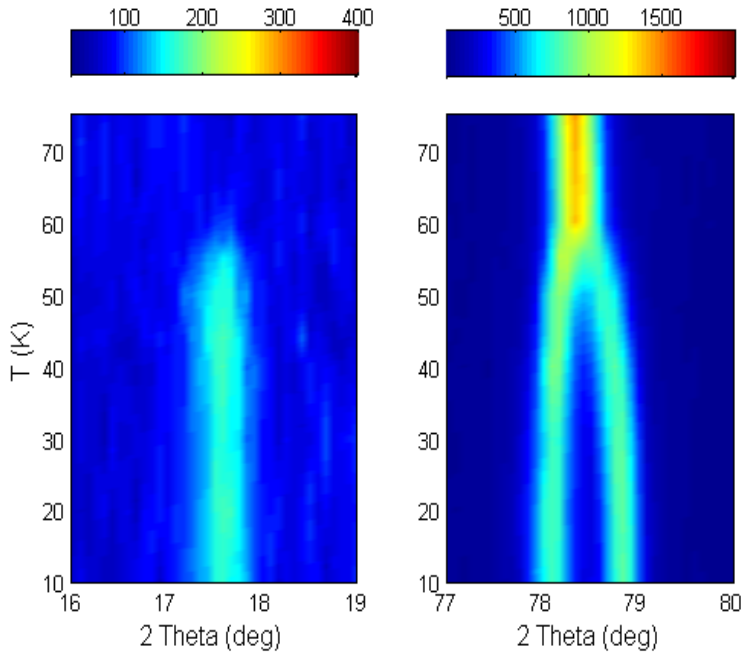
VI. Configure the new PCR file for the actual experimental setting and perform refinement

VII. Display the magnetic structure using *Vesta*

$Fe_{1.16}Te$: 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)

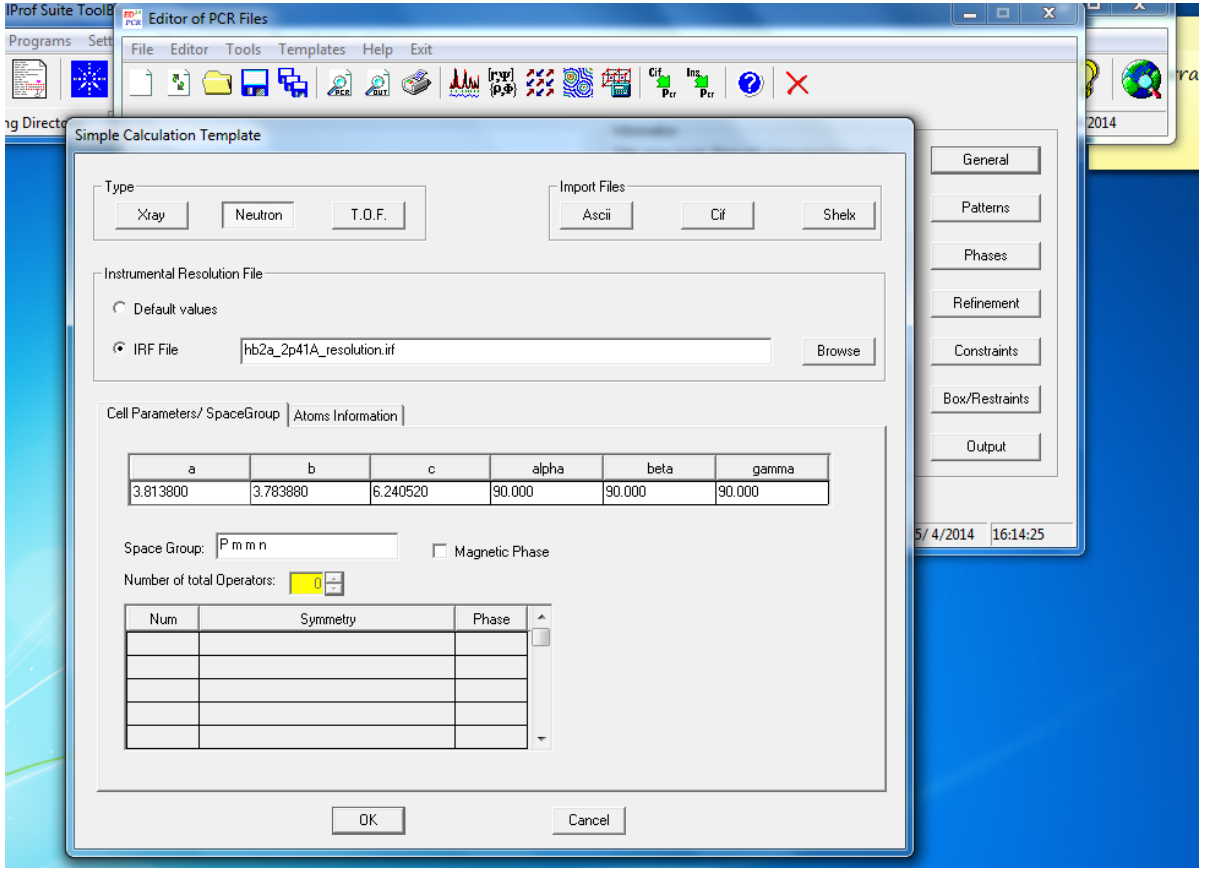
  - import the crystallographic information file CIF (Fe1p16_4K.cif))

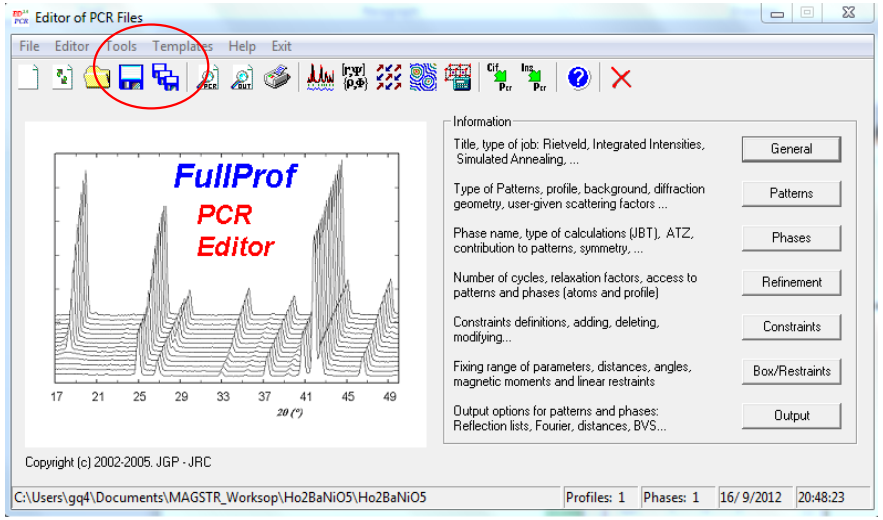
Low temperature structure: P*mmn*

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

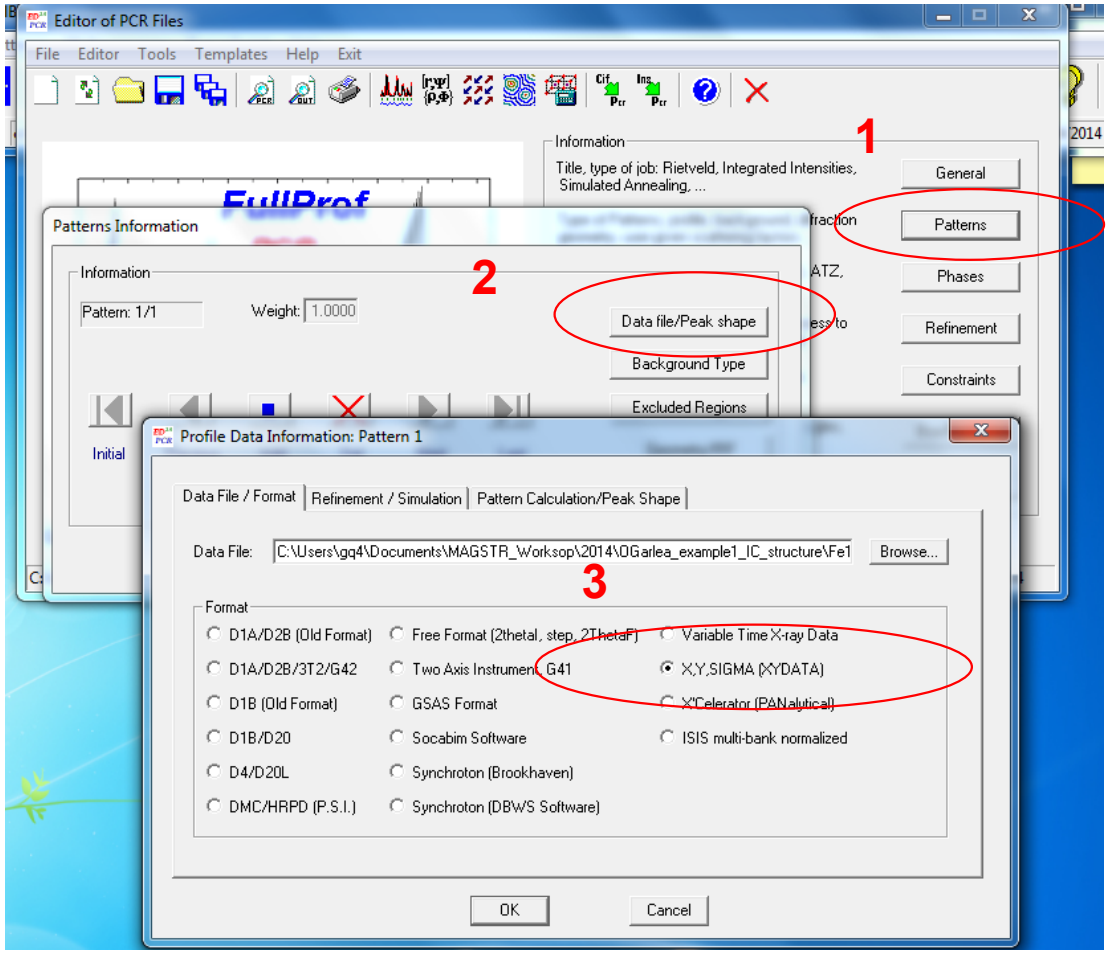
  - in the new window, select the “Neutron” tab for the type of calculations

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



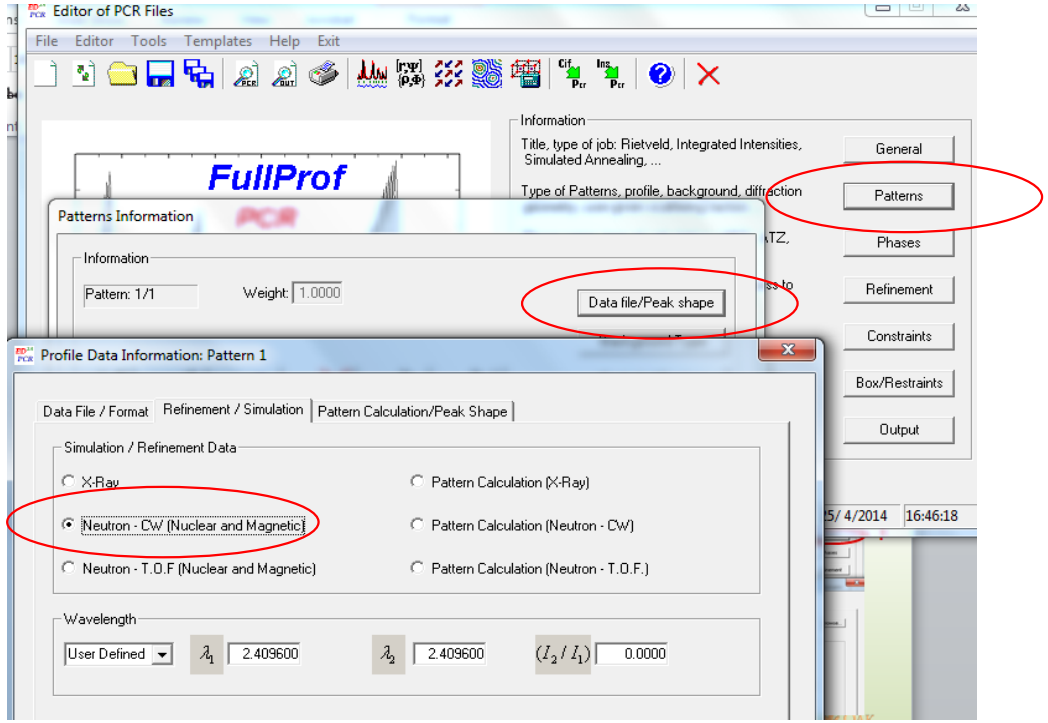


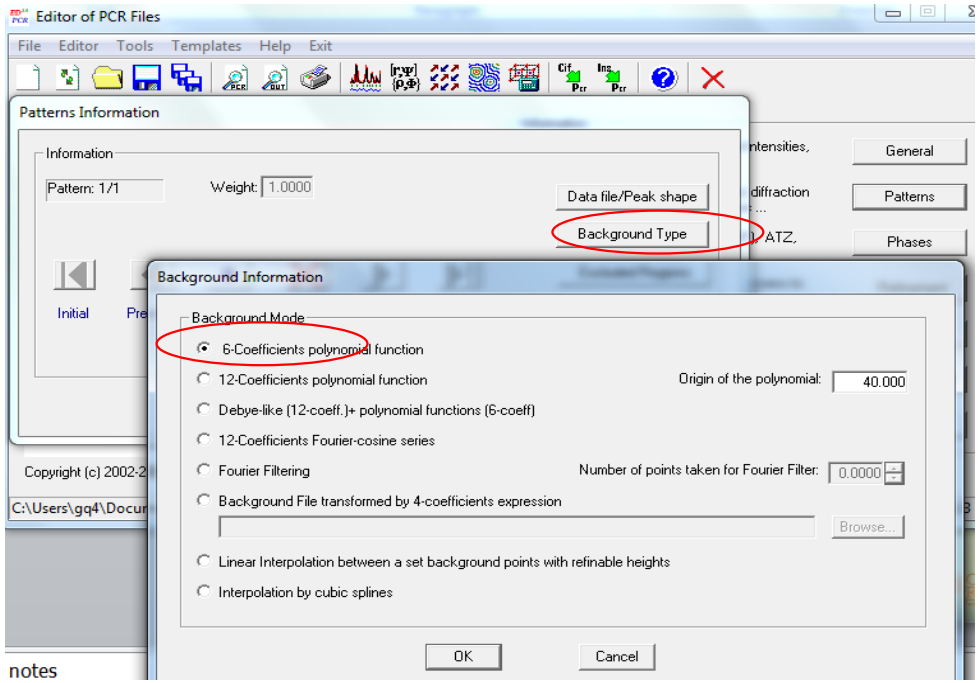
- save the PCR file by clicking the “Save” button



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

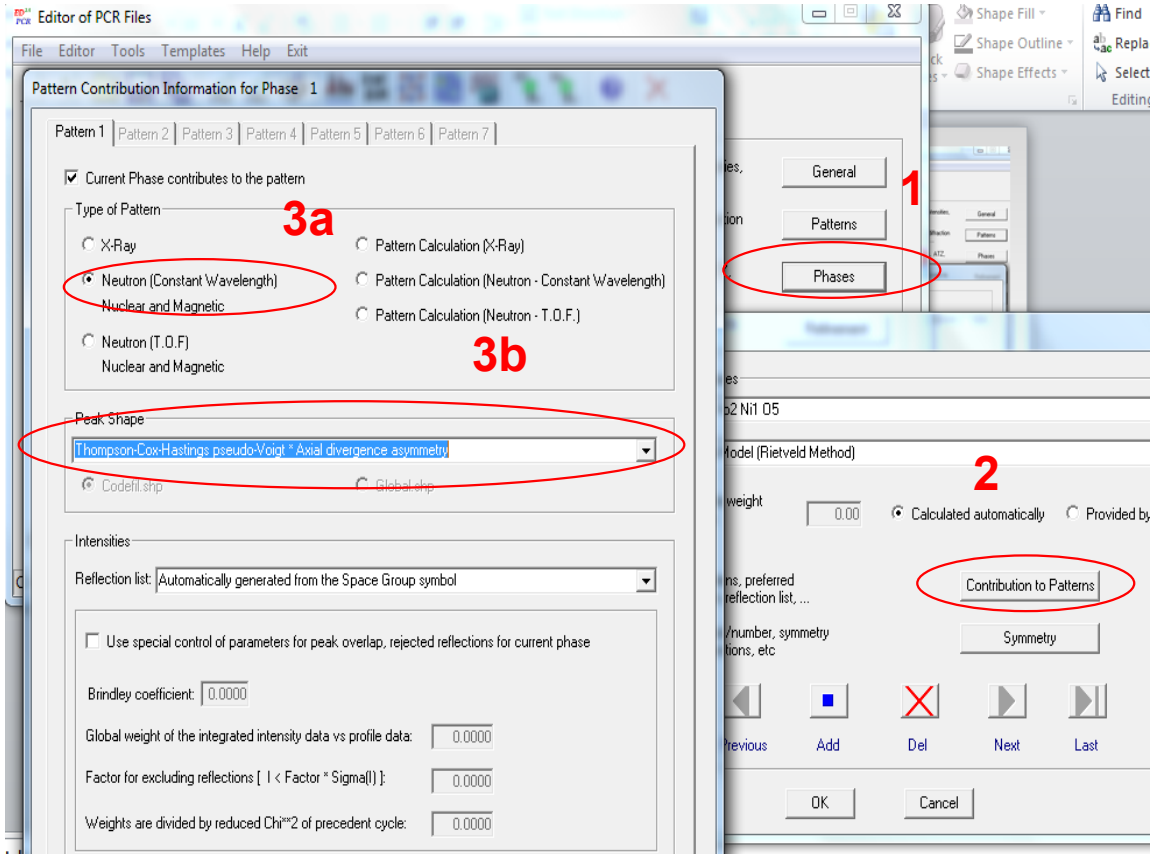
- In the “Patterns” tab , clock on the “Refinement/Simulation”, and make sure that “Neutron-CW” option is selected, and in the “Pattern calculation” the “Thompson-Cox-Hastings pseudo-Voigt” peak shape is chosen

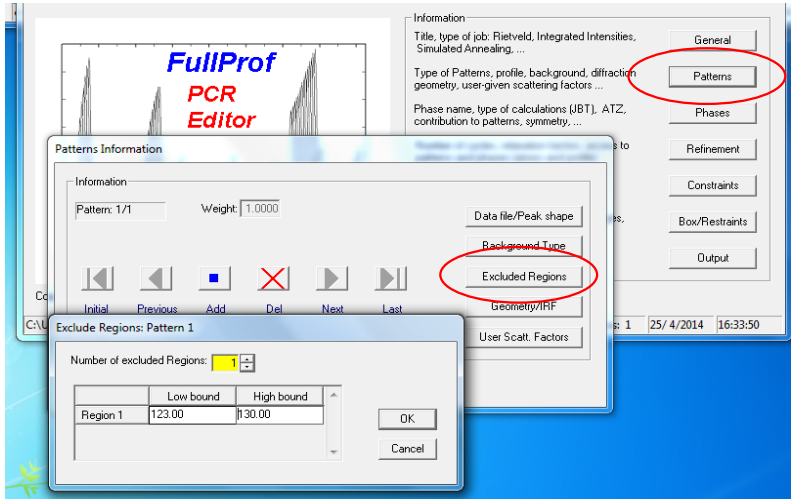




- For the background information, select the “6-coefficients polynomial function”

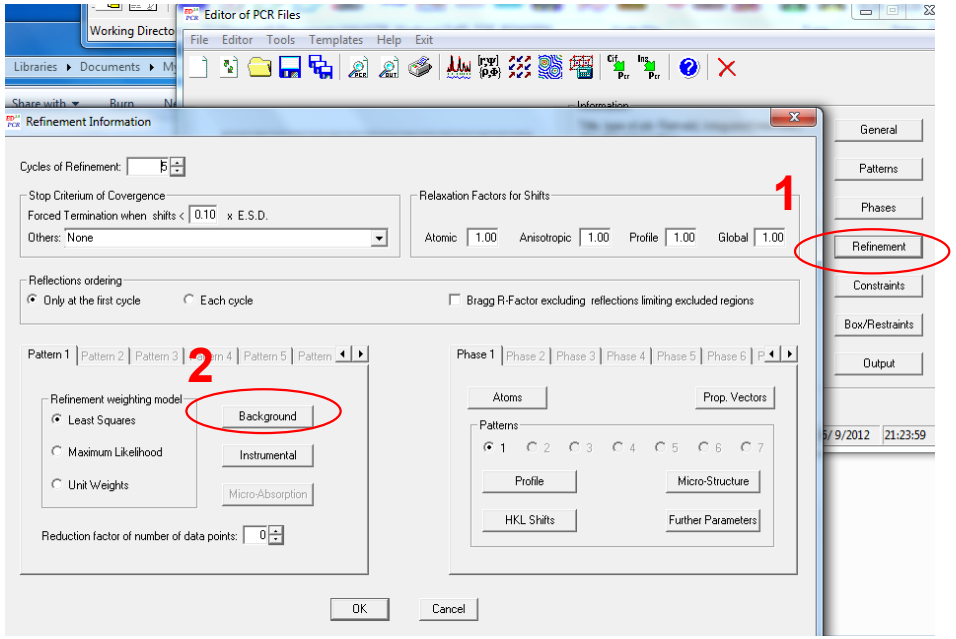
- Add one excluded region with the scattering range 123-130 deg

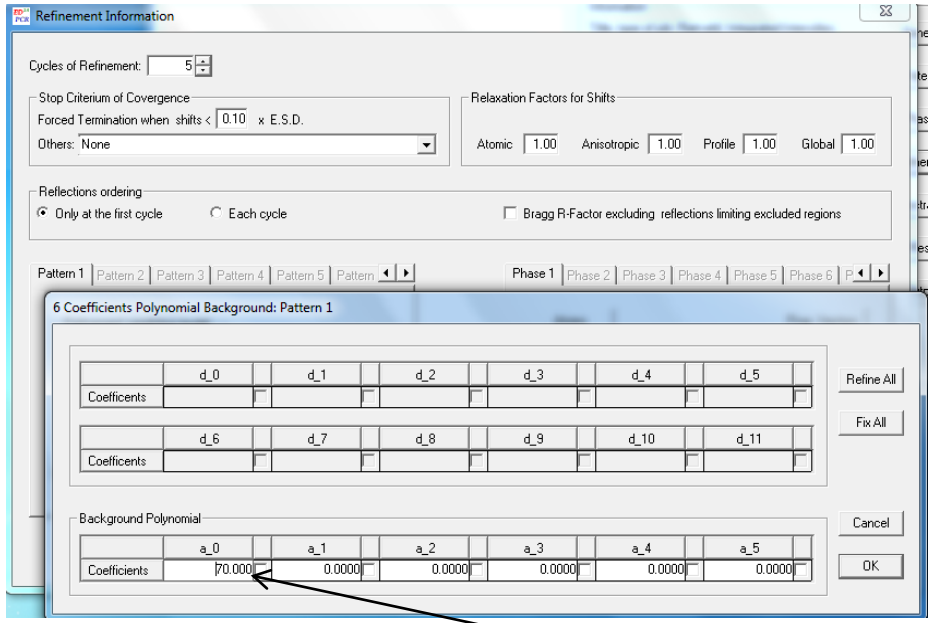


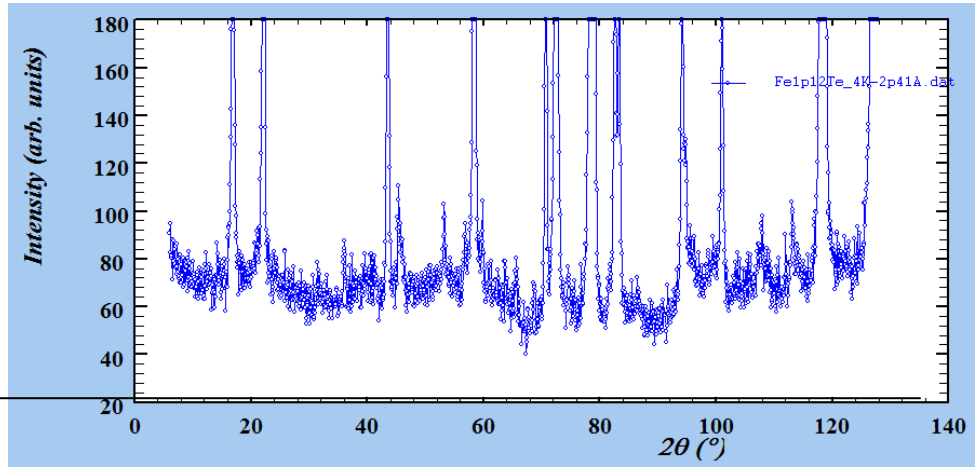


- From the main window of EdPcr, open the “Phases” tab (1) and then click on the “Contribution to patterns” (2) and then select the “current phase contributes to the pattern “ & “neutron (constant wavelength)“(3a) and “Thompson-Cox-Hastings pseudo-Voigt” for the peak shape (3b)

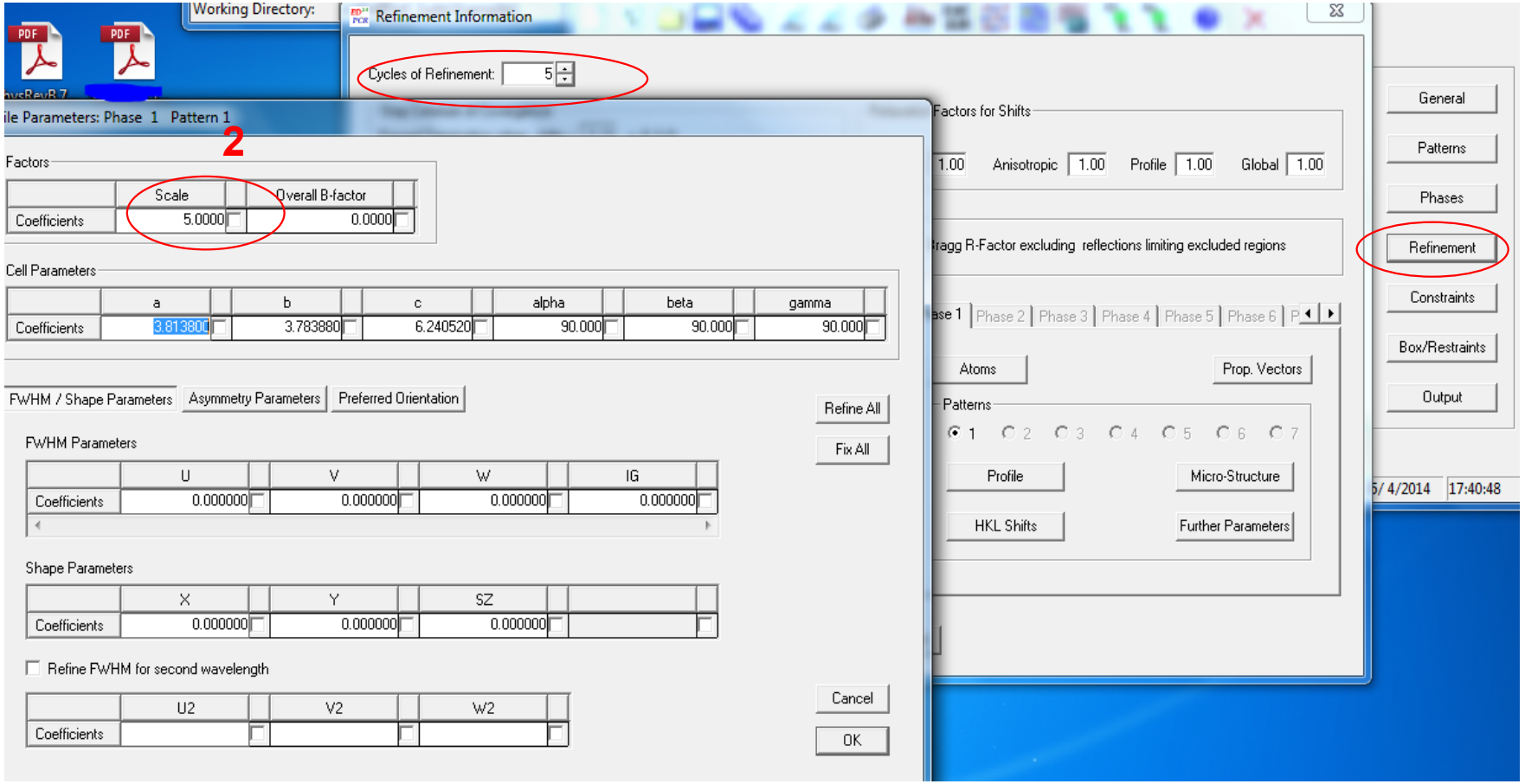
- Open the “Refinement” (1) and then the “Background” and add a value for the “a_o” coefficient that will give a first flat approximation for the background (~70, read it from the data file)



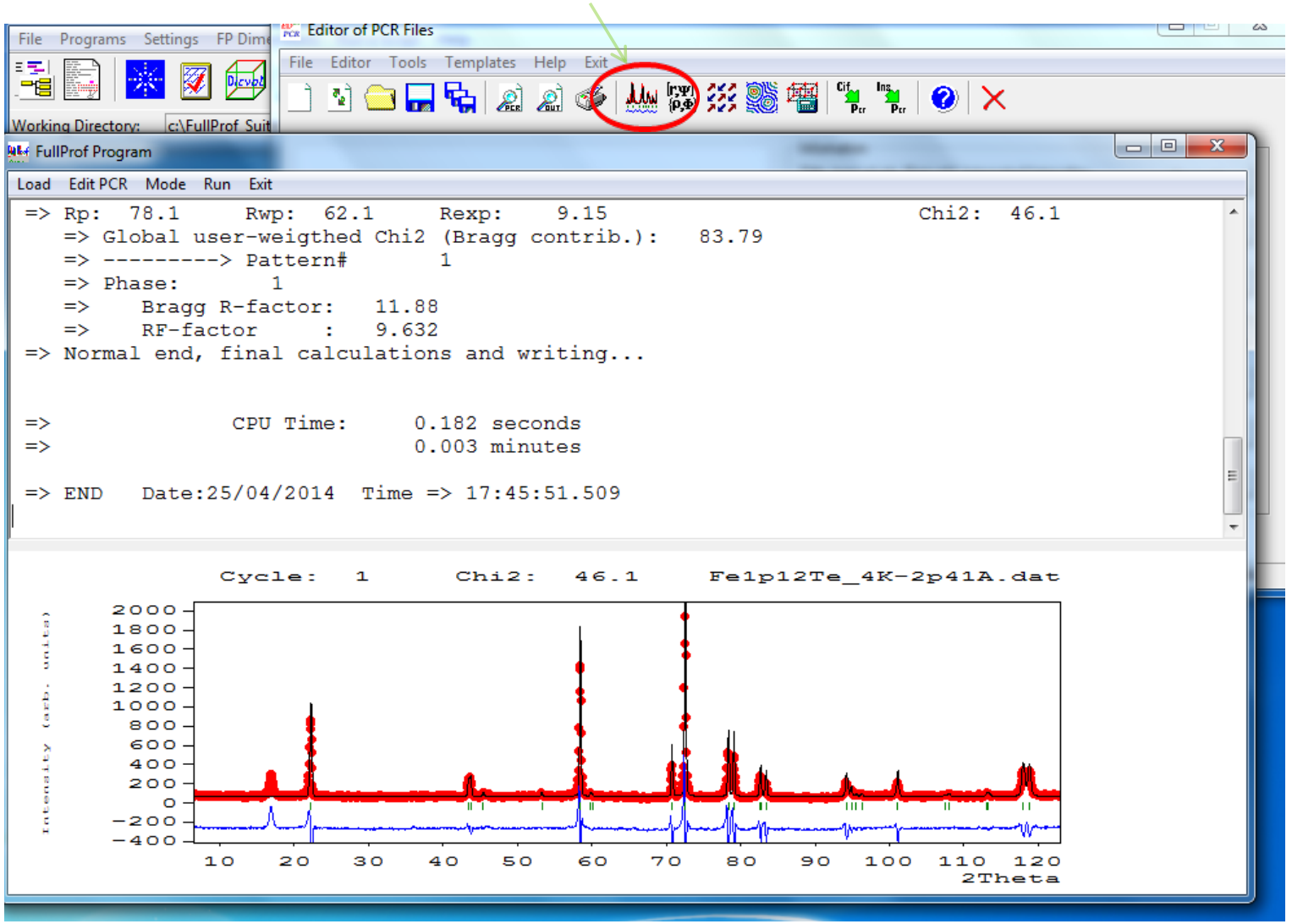




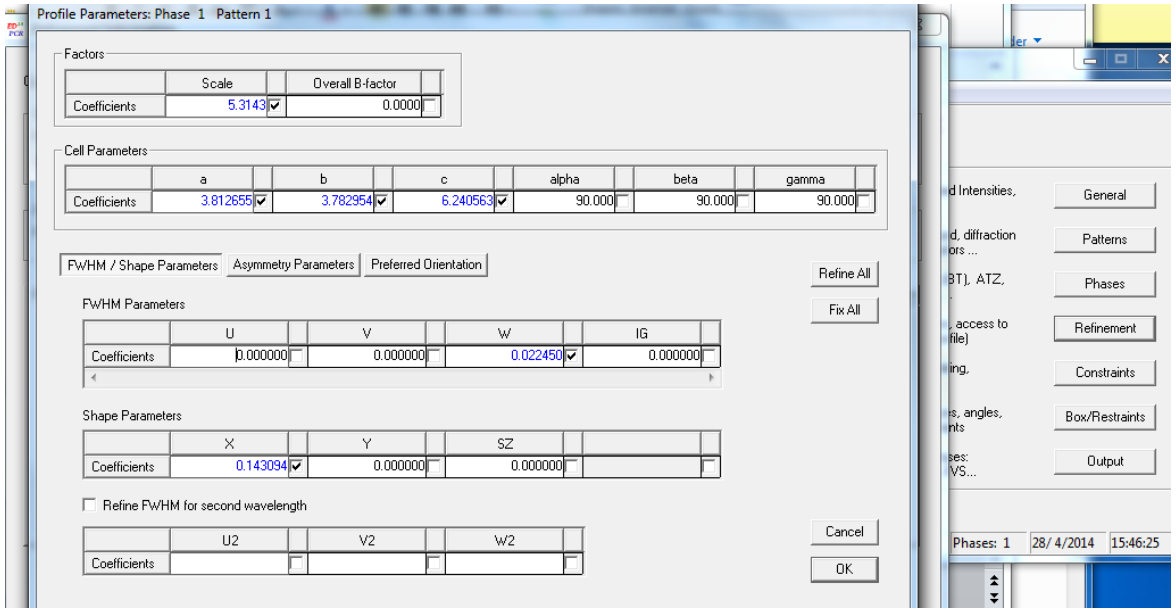
- From the same “Refinement” window (1) , click on the “Profile” tab and set a number for the “scale factor” (~ 5 for this example). The number of “cycles of refinement” can also be increased at this time
- save the PCR file by clicking the “Save” button, every time a change has been made

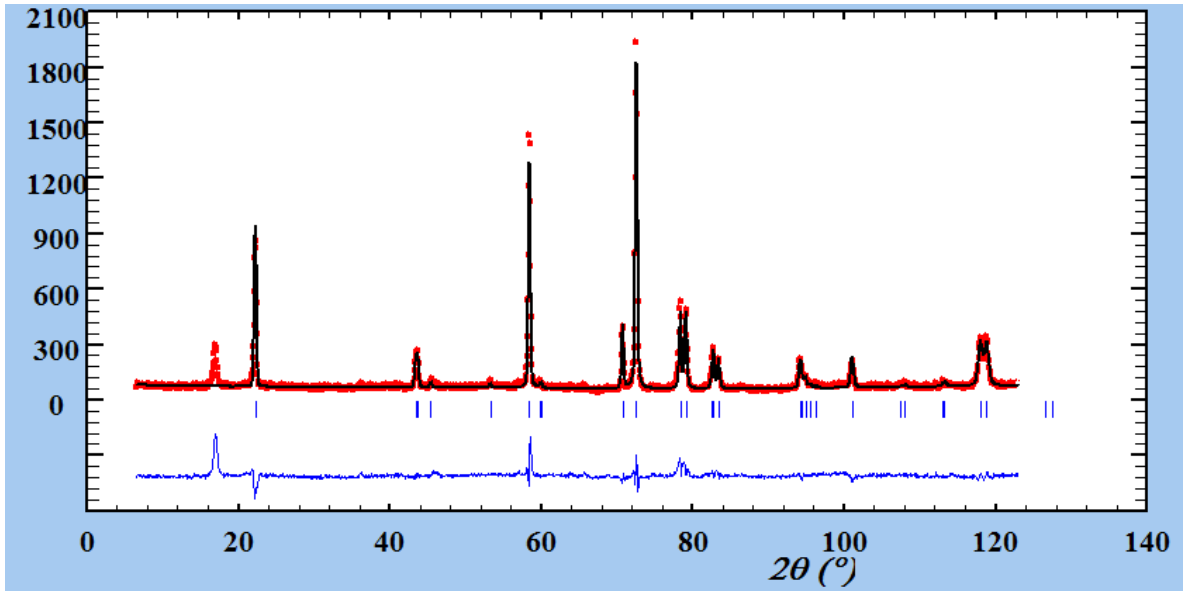


- Run the Fullprof program by click on button indicated below.
  All the parameters are fixed at this time.



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



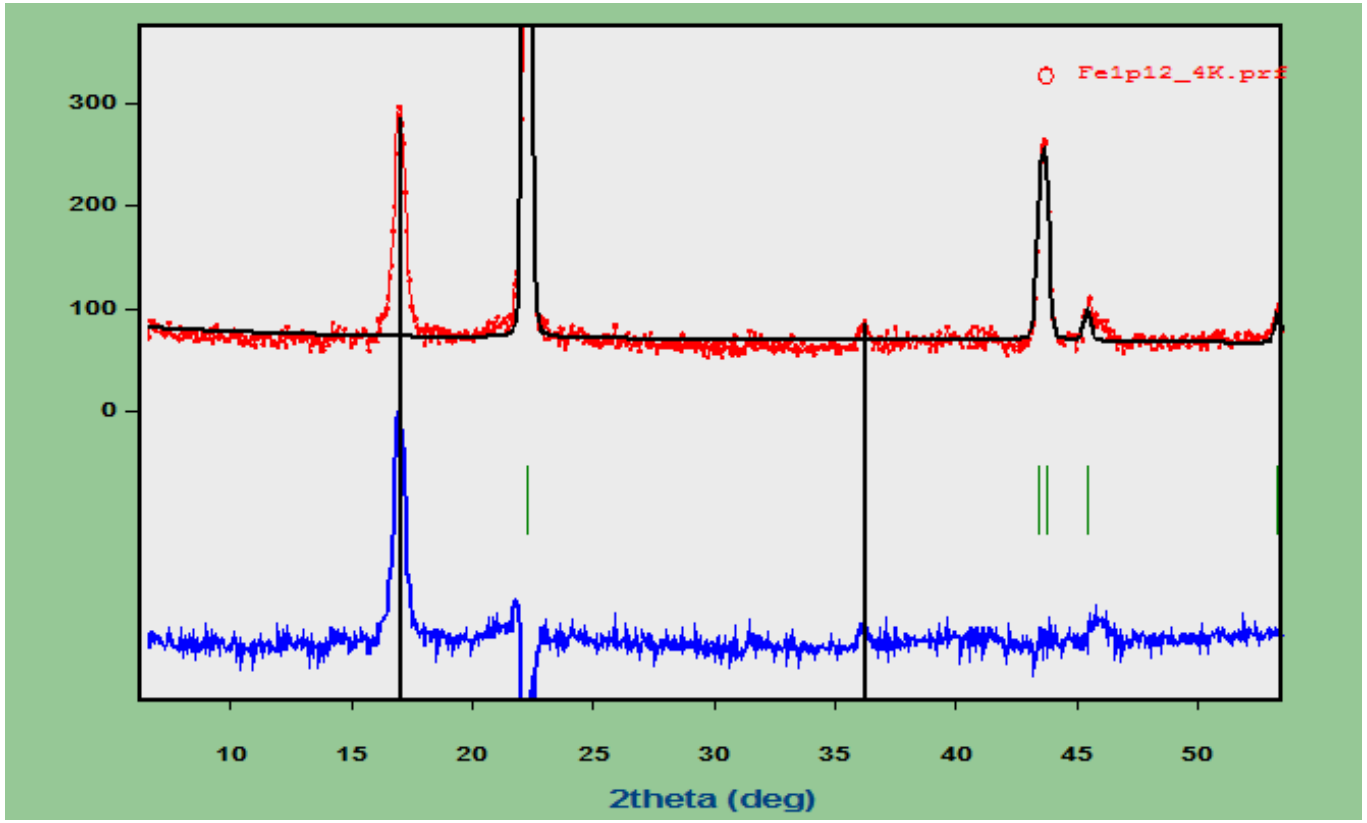


- Open the PRF file using WINPLOTR to observe the quality of the fit.
- Notice the un-indexed peaks that can be associated to the magnetic long range

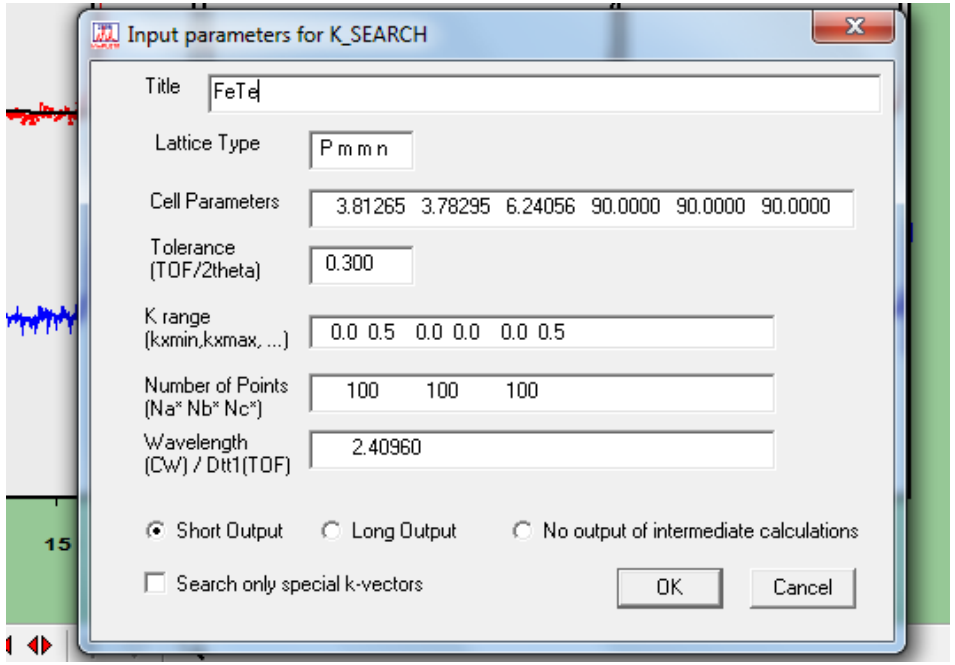
$Fe_{1.16}Te$: Determine the k –wave vector

- 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”)

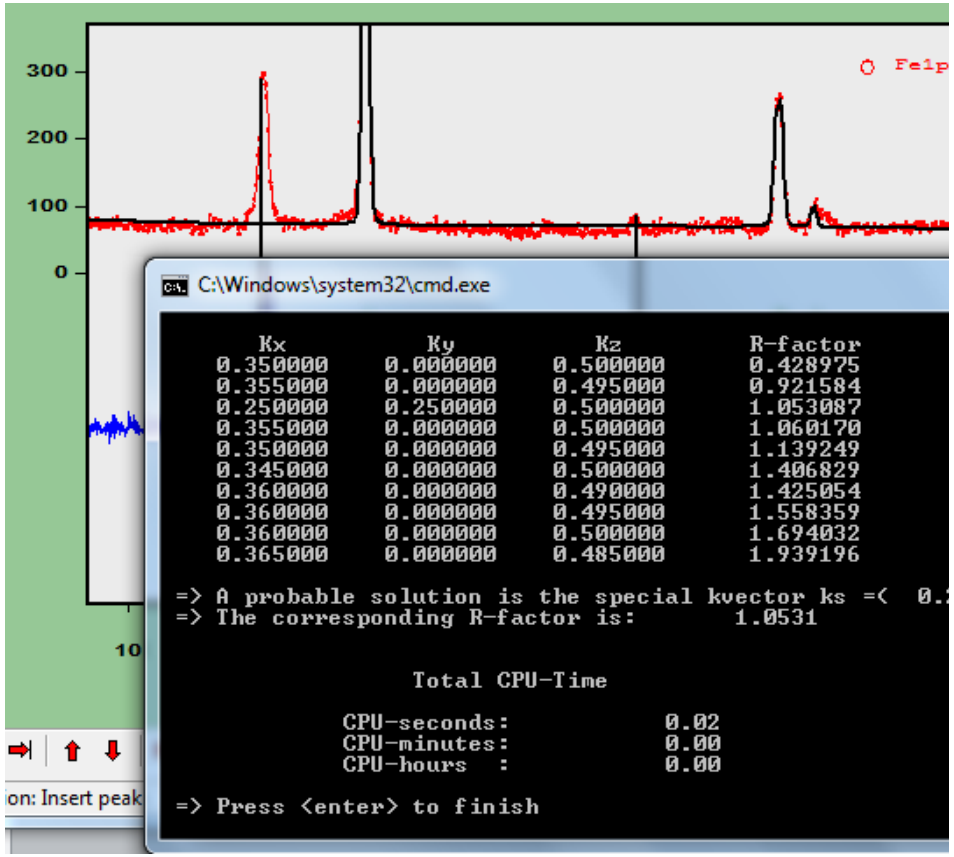


- Run the “k-search “ program to find the propagation vector and see the results listed in the file “k_search.kup”



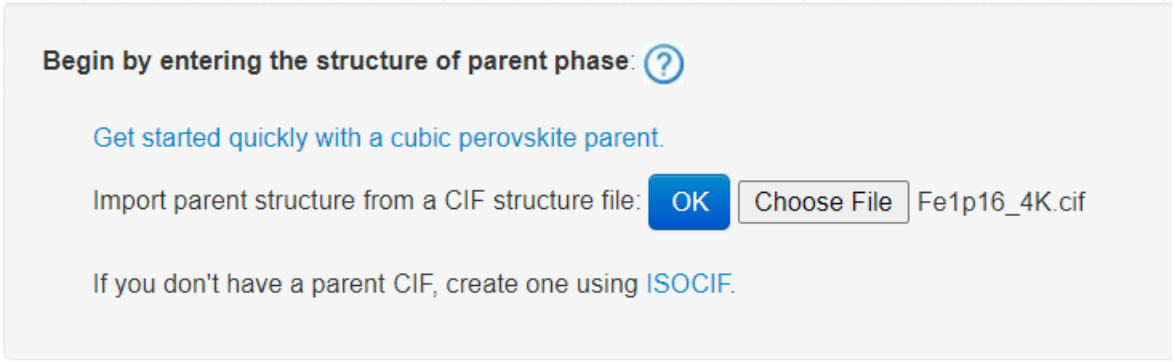
- A number of incommensurate solutions are suggested. Select the **k = (0.35 0 0.5)**

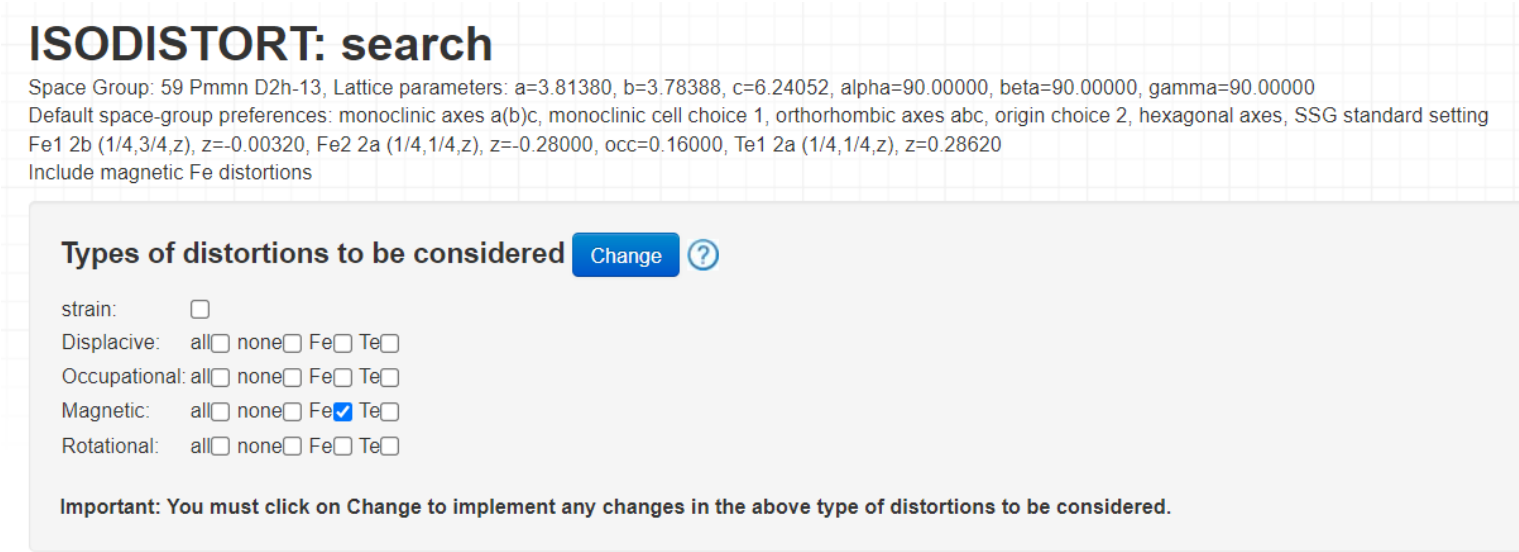
- Make sure to unselect the box “Search only special k-vector” and restrict K range for limiting number of solutions



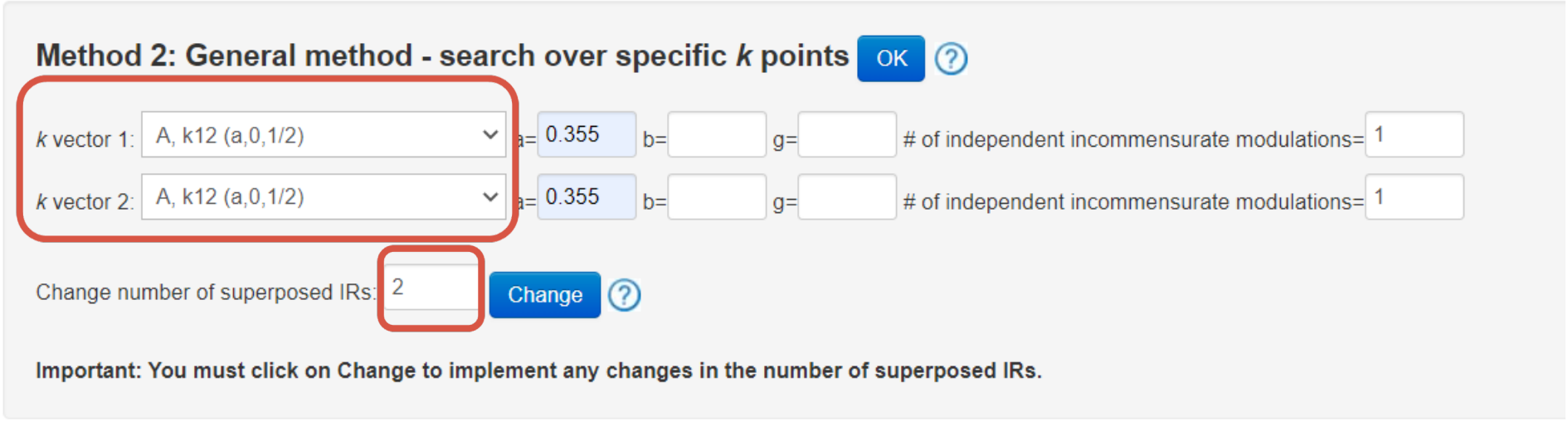
$Fe_{1.16}Te$: Symmetry analysis

- use **ISODISTORT** program (https://stokes.byu.edu/iso/isodistortform.php) to generate the “mcif” file in superspacegroup formalism for the helical structure solution
  - load the provided Fe1p16_4K.cif file in **ISODISTORT**
  - For types of distortions select the magnetic only for Fe atom

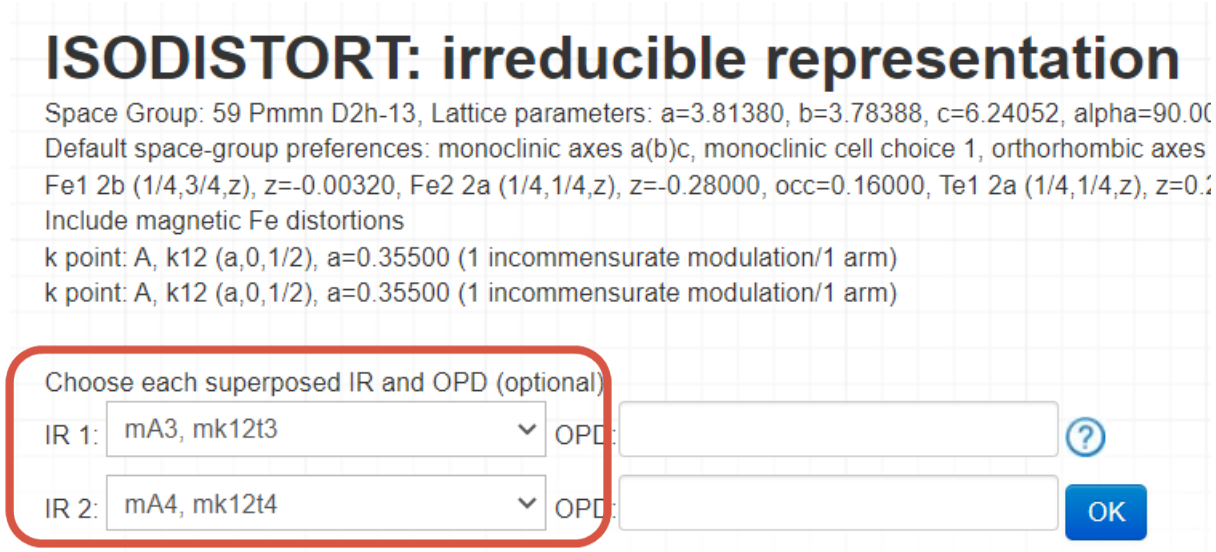




- Use “Method 2” to specify the k point and indicate the number of superimposed IRs

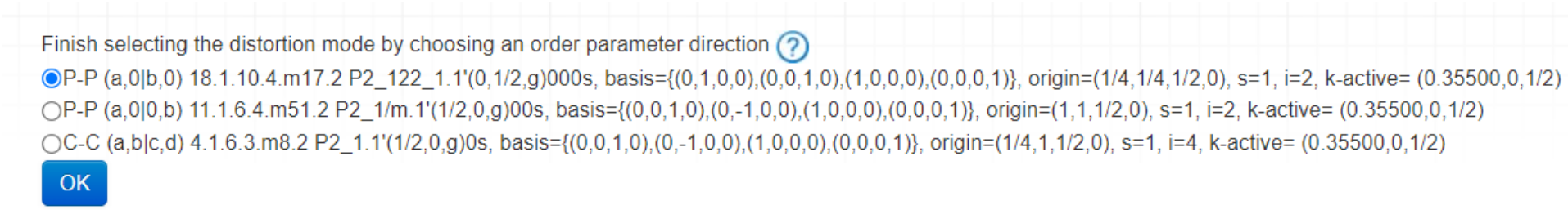


- For the helical structure we will select the IR3 and IR4

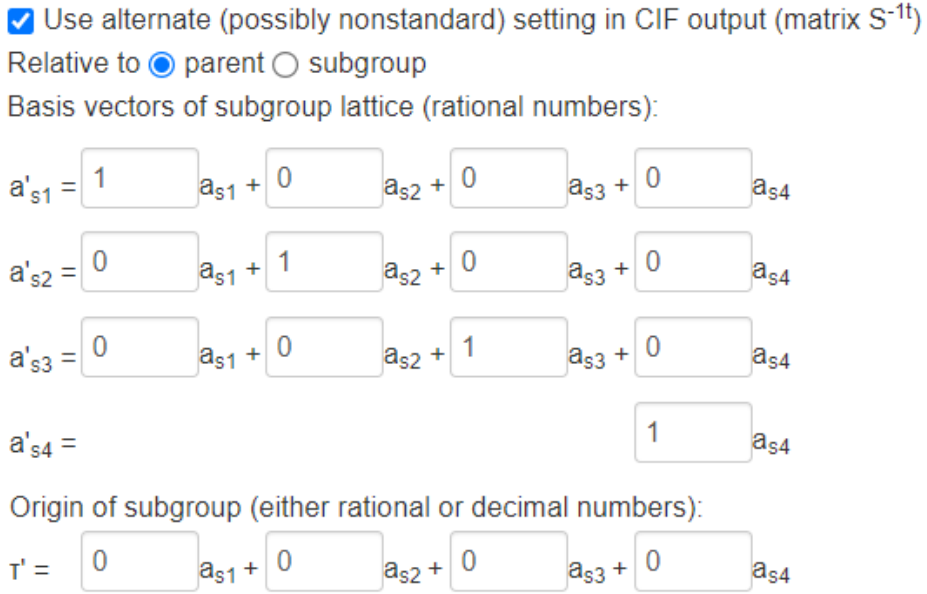


	P mmn	
Irreps	Fe1_1	Fe1_ 2
IR1	(0 1 0)	(0 ξ 0)
IR2	(1 0 0)	(-ξ 0 0)
	(0 0 1)	(0 0 ξ)
IR3	(0 1 0)	(0 -ξ 0)
IR4	(1 0 0)	(ξ 0 0)
	(0 0 1)	(0 0 -ξ)

- Select the first the first option



- Mark the box for using an alternate setting for the lattice, to reverse to the parent setting



- Select the first the first option

Finish selecting the distortion mode by choosing an order parameter direction
- (●) P-P (a,0|b,0) 18.1.10.4.m17.2 P2_122_1.1'(0,1/2,g)000s, basis={(0,1,0,0),(0,0,1,0),(1,0,0,0),(0,0,0,1)}, origin=(1/4,1/4,1/2,0), s=1, i=2, k-active= (0.35500,0,1/2)
- ( ) P-P (a,0|0,b) 11.1.6.4.m51.2 P2_1/m.1'(1/2,0,g)00s, basis={(0,0,1,0),(0,-1,0,0),(1,0,0,0),(0,0,0,1)}, origin=(1,1,1/2,0), s=1, i=2, k-active= (0.35500,0,1/2)
- ( ) C-C (a,b|c,d) 4.1.6.3.m8.2 P2_1.1'(1/2,0,g)0s, basis={(0,0,1,0),(0,-1,0,0),(1,0,0,0),(0,0,0,1)}, origin=(1/4,1,1/2,0), s=1, i=4, k-active= (0.35500,0,1/2)

OK

- Select the "CIF file" box and initialize the moment amplitudes for Fe1

Include magnetic Fe distortions
k point: A, k12 (a,0,1/2), a=0.35500 (1 incommensurate modulation/1 arm)
IR: mA3, mk12t3
k point: A, k12 (a,0,1/2), a=0.35500 (1 incommensurate modulation/1 arm)
IR: mA4, mk12t4
P-P (a,0|b,0) 18.1.10.4.m17.2 P2_122_1.1'(0,1/2,g)000s, basis={(0,1,0,0),(0,0,1,0),(1,0,0,0),(0,0,0,1)}, origin=(1/
Lattice parameters of undistorted supercell: a=3.78388, b=6.24052, c=3.81380, alpha=90.00000, beta=90.00000

( ) Save interactive distortion (?) (●) CIF file (?) ( ) Distortion file (?) ( ) Domains (?) ( ) Modes details ( ) Compl

Enter mode and strain amplitudes: (?)

Pmmn[0.35500,0,1/2]mA3 (a,0) 59.1.10.6.m406.2 Pmnm.1'(0,1/2,g)000s, basis={(1,0,0,0),(0,1,0,0),(0,0,1,0),(0,0

1 [Fe1:b:mag]B1(a)

0 [Fe2:a:mag]B1(a)

Pmmn[0.35500,0,1/2]mA4 (a,0) 59.1.10.7.m406.2 Pmnm.1'(0,1/2,g)s00s, basis={(1,0,0,0),(0,1,0,0),(0,0,1,0),(0,0

1 [Fe1:b:mag]B2(a)

1 [Fe1:b:mag]A2(a)

0 [Fe2:a:mag]B2(a)

0 [Fe2:a:mag]A2(a)

- Mark the box for using an alternate setting for the lattice, to reverse to the parent setting , before saving the CIF file

[x] Use alternate (possibly nonstandard) setting in CIF output (matrix S^{-1t})

Relative to (●) parent ( ) subgroup

Basis vectors of subgroup lattice (rational numbers):

a'_{s1} = 1 a_{s1} + 0 a_{s2} + 0 a_{s3} + 0 a_{s4}

a'_{s2} = 0 a_{s1} + 1 a_{s2} + 0 a_{s3} + 0 a_{s4}

a'_{s3} = 0 a_{s1} + 0 a_{s2} + 1 a_{s3} + 0 a_{s4}

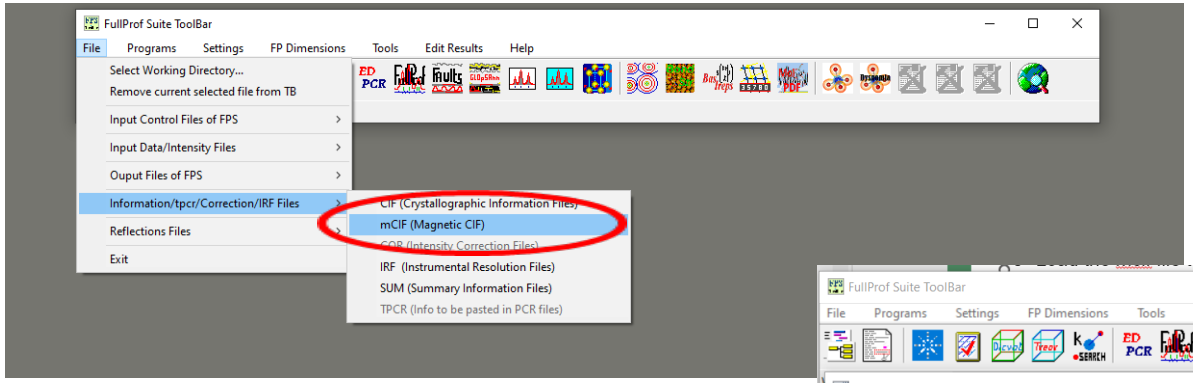
a'_{s4} = 1 a_{s4}

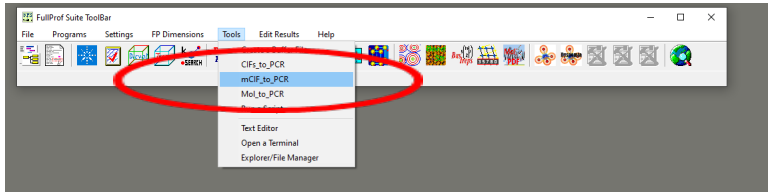
Origin of subgroup (either rational or decimal numbers):

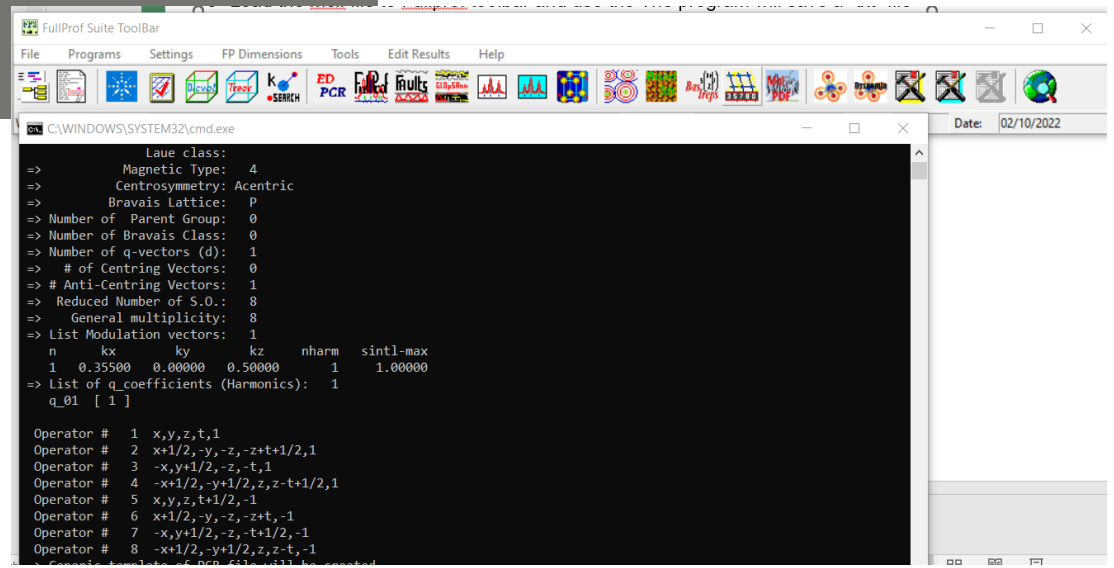
τ' = 0 a_{s1} + 0 a_{s2} + 0 a_{s3} + 0 a_{s4}

- The program will save a “subgroup_cif.txt” file that you need to rename to “anyname.mcif”

- Load the mcif file to FullProf Toolbar and use the “mcif_to_PCR” from “Tools” to convert to file to a PCR . Note : the Fullprog program will be run from the toolbar. The EdPCR is not configured to recognize the pcr format used for this approach.

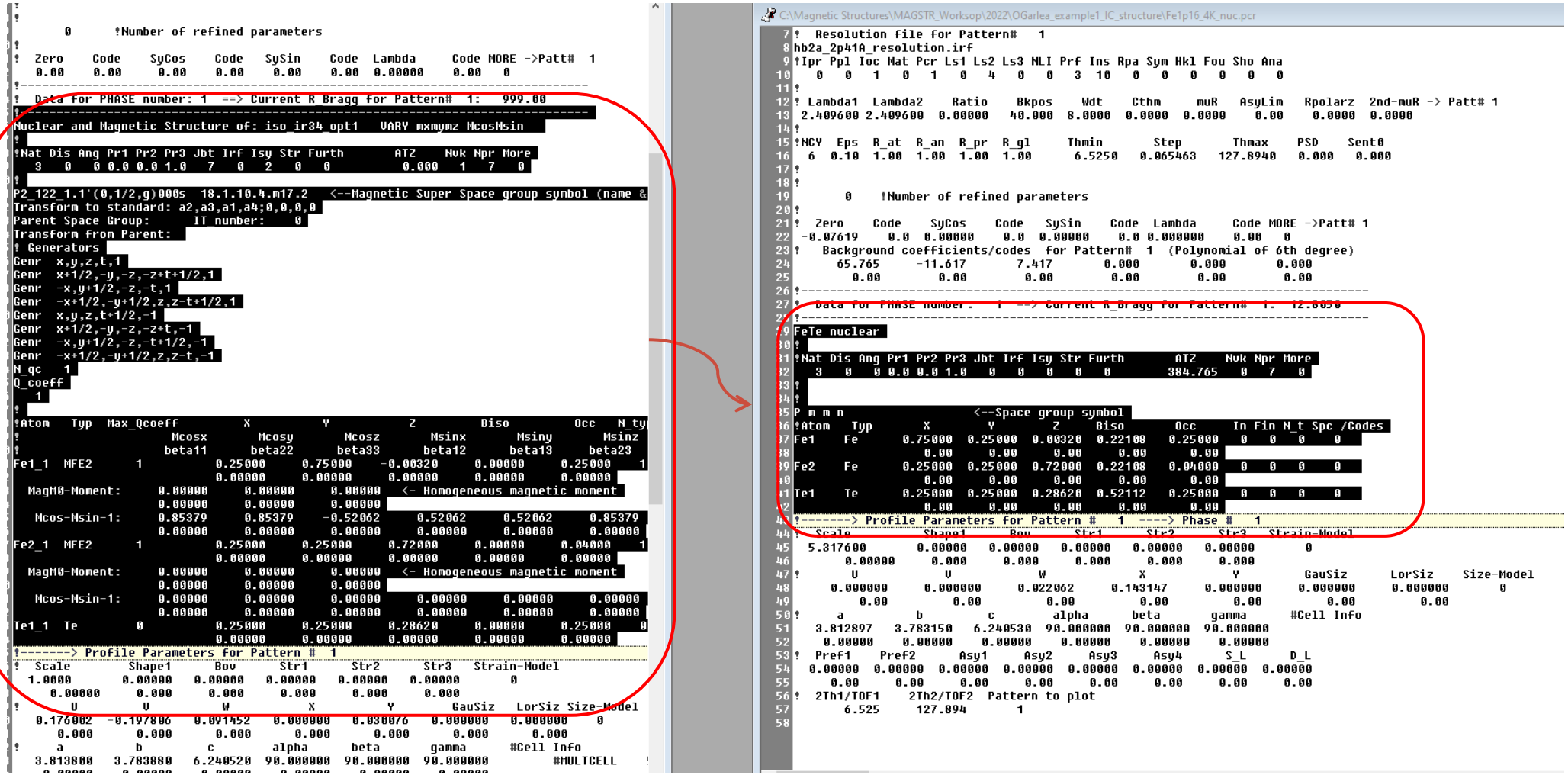






$Fe_{1.16}Te$: Configure the new PCR file and perform the refinement

- Open the new PCR with a text editor and copy the section describing magnetic/nuclear phase into the previously prepared PCR file, used for fitting the nuclear contribution.



```
      0      !Number of refined parameters
!
!  Zero     Code    SyCos    Code   SySin    Code  Lambda     Code MORE ->Patt#  1
   0.00     0.00     0.00    0.00    0.00    0.00  0.00000    0.00   0
!-------------------------------------------------------------------------------
!  Data for PHASE number: 1  ==> Current R_Bragg for Pattern#  1:    999.00
!-------------------------------------------------------------------------------
Nuclear and Magnetic Structure of: iso_ir34_opt1   VARY mxmymz McosMsin
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth        ATZ     Nvk Npr More
  3   0   0 0.0 0.0 1.0   7   0   2   0   0          0.000   1   7   0
!
P2_122_1.1'(0,1/2,g)000s  18.1.10.4.m17.2   <--Magnetic Super Space group symbol (name &
Transform to standard: a2,a3,a1,a4;0,0,0,0
Parent Space Group:       IT_number:    0
Transform from Parent:
! Generators
Genr  x,y,z,t,1
Genr  x+1/2,-y,-z,-z+t+1/2,1
Genr  -x,y+1/2,-z,-t,1
Genr  -x+1/2,-y+1/2,z,z-t+1/2,1
Genr  x,y,z,t+1/2,-1
Genr  x+1/2,-y,-z,-z+t,-1
Genr  -x,y+1/2,-z,-t+1/2,-1
Genr  -x+1/2,-y+1/2,z,z-t,-1
N_qc   1
Q_coeff
   1
!
!Atom   Typ  Max_Qcoeff          X           Y           Z          Biso         Occ    N_ty
!                      Mcosx       Mcosy       Mcosz       Msinx       Msiny       Msinz
!                     beta11      beta22      beta33      beta12      beta13      beta23
Fe1_1  MFE2      1          0.25000     0.75000    -0.00320     0.00000     0.25000     1
                            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:      0.85379     0.85379    -0.52062     0.52062     0.52062     0.85379
                     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Fe2_1  MFE2      1          0.25000     0.25000     0.72000     0.00000     0.04000     1
                            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
                     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Te1_1  Te        0          0.25000     0.25000     0.28620     0.00000     0.25000     0
                            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     0.000     0.000     0.000     0.000     0.000
!       U         V         W         X         Y       GauSiz   LorSiz Size-Model
   0.176002  -0.197806  0.091452  0.000000  0.030076  0.000000  0.000000     0
      0.000     0.000     0.000     0.000     0.000     0.000     0.000
!     a         b         c       alpha      beta       gamma      #Cell Info
   3.813800  3.783880  6.240520 90.000000 90.000000 90.000000          #MULTCELL
```

```
C:\Magnetic Structures\MAGSTR_Worksop\2022\OGarlea_example1_IC_structure\Fe1p16_4K_nuc.pcr
!  Resolution file for Pattern#   1
hb2a_2p41A_resolution.irf
!Ipr  Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
   0    0   1   0   1   0   4   0   0   3  10   0   0   0   0   0   0
!
! Lambda1  Lambda2    Ratio     Bkpos    Wdt     Cthm      muR    AsyLim    Rpolarz  2nd-muR -> Patt# 1
 2.409600 2.409600  0.00000   40.000  8.0000  0.0000  0.0000    0.00     0.0000  0.0000
!
!NCY  Eps  R_at  R_an  R_pr  R_gl     Thmin       Step       Thmax     PSD     Sent0
  6  0.10  1.00  1.00  1.00  1.00      6.5250   0.065463   127.8940   0.000   0.000
!
!
      0    !Number of refined parameters
!
!  Zero     Code    SyCos    Code   SySin    Code  Lambda     Code MORE ->Patt# 1
 -0.07619    0.0  0.00000    0.0  0.00000    0.0 0.000000    0.00   0
!   Background coefficients/codes  for Pattern#  1  (Polynomial of 6th degree)
      65.765     -11.617       7.417       0.000       0.000       0.000
       0.00        0.00        0.00        0.00        0.00        0.00
!-------------------------------------------------------------------------------
!  Data for PHASE number:   1 ==> Current R_Bragg for Pattern#  1:   12.8858
!-------------------------------------------------------------------------------
FeTe nuclear
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth        ATZ     Nvk Npr More
  3   0   0 0.0 0.0 1.0   0   0   0   0   0        384.765   0   7   0
!
!
P m m n                  <--Space group symbol
!Atom   Typ       X           Y           Z          Biso        Occ      In Fin N_t Spc /Codes
Fe1    Fe     0.75000   0.25000   0.00320   0.22108   0.25000   0   0   0   0
                0.00        0.00        0.00        0.00        0.00
Fe2    Fe     0.25000   0.25000   0.72000   0.22108   0.04000   0   0   0   0
                0.00        0.00        0.00        0.00        0.00
Te1    Te     0.25000   0.25000   0.28620   0.52112   0.25000   0   0   0   0
                0.00        0.00        0.00        0.00        0.00
!-------> Profile Parameters for Pattern #   1  ----> Phase #   1
!  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    Size-Model
   0.000000  0.000000  0.022062  0.143147  0.000000  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
   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
!  2Th1/TOF1    2Th2/TOF2  Pattern to plot
      6.525      127.894       1
```

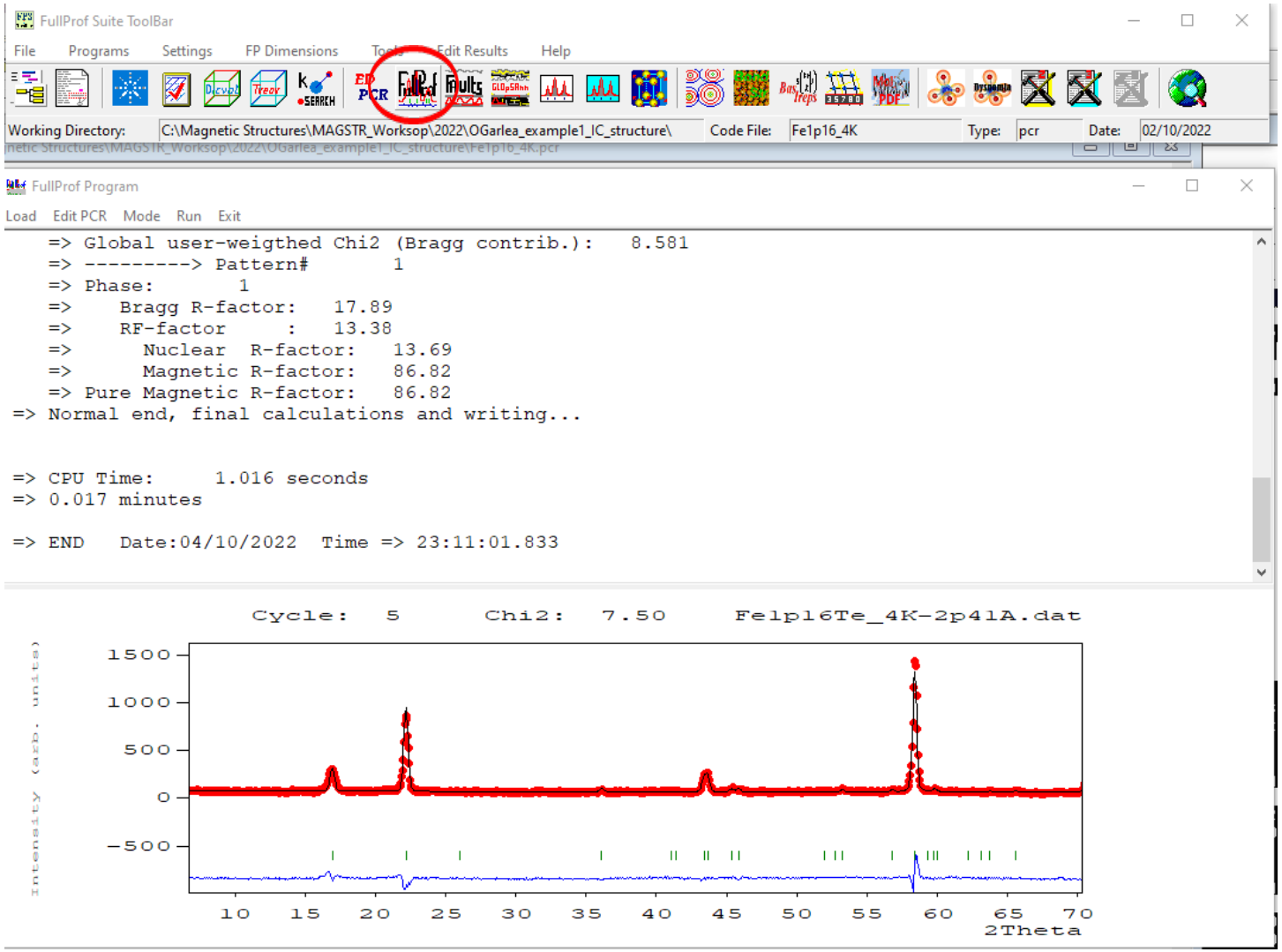
```
!-------------------------------------------------------------------------------
Nuclear and Magnetic Structure of: iso_ir34_mod1    VARY mxmymz McosMsin
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
   3   0   0 0.0 0.0 1.0   7   0   2   0   0       192.383   1   7   0
!
P2_122_1.1'(0,1/2,g)000s  18.1.10.4.m17.2   <--Magnetic Super Space group symbol (name & number)
Transform to standard: a2,a3,a1,a4;0,0,0,0
Parent Space Group:      IT_number:    0
Transform from Parent:
! Generators
Genr  x,y,z,t,1
Genr  x+1/2,-y,-z,-z+t+1/2,1
Genr  -x,y+1/2,-z,-t,1
Genr  -x+1/2,-y+1/2,z,z-t+1/2,1
Genr  x,y,z,t+1/2,-1
Genr  x+1/2,-y,-z,-z+t,-1
Genr  -x,y+1/2,-z,-t+1/2,-1
Genr  -x+1/2,-y+1/2,z,z-t,-1
N_qc   1
Q_coeff
   1
!
!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
Fe1_1  MFE2          1        0.25000    0.75000   -0.00320    0.00000    0.25000    1    0  #
                              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:      1.34601    1.34601   -1.01284    1.01284    1.01284    1.34601   <-Amplitudes of Modulat
                    11.00000   11.00000  -11.00000   11.00000   11.00000   11.00000
Fe2_1  MFE2          1        0.25000    0.25000    0.72000    0.00000    0.04000    1    0  #
                              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 of Modulat
                     0.00000    0.00000    0.00000    0.00000    0.00000    0.00000
Te1_1  Te            0        0.25000    0.25000    0.28620    0.00000    0.25000    0    0  #
                              0.00000    0.00000    0.00000    0.00000    0.00000
!-------> Profile Parameters for Pattern #   1  ----> Phase #   1
!  Scale          Shape1      Bov       Str1      Str2      Str3   Strain-Model
  5.295298       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    0.022601    0.140304    0.000000    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
   3.813800   3.783880   6.240520  90.000000  90.000000  90.000000   #MULTCELL    5    1    4
     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:
   0.3550000   0.0000000   0.5000000      1    1.0000  <-- Propagation Vector, nharm, sintl_lim  1
    0.000000    0.000000    0.000000
!  2Th1/TOF1    2Th2/TOF2  Pattern to plot
       4.525      123.000        1
```

- The command line VARY mxmymz McosMsin is automatically varying all allowed magnetic moment projections for all sites. Remove that command as we will set the refinements flags manualy
- Make sure that the atoms identifiers (for magnetic form factor) are correct. Here the label must be MFE2. If you are dealing with a rare-earths, then the format is: JRE3 (e.g. JDY3)
- For the first refinement of magnetic moments, fix all the other parameters, that have been varied for nuclear refinement.
- Copy to your new PCR the line at the end of the file that defines the propagation vectors. Make sure that you have the same lattice definition as given for the parent phase.

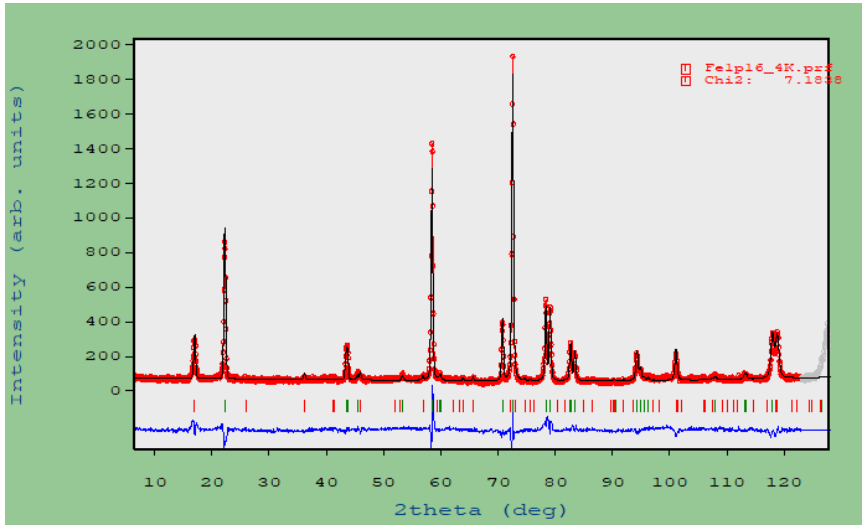
```
   3    0    0 0.0 0.0 1.0    7    0    2    0    0        192.383    1    7    0
!
P2_122_1.1'(0,1/2,g)000s  18.1.10.4.m17.2   <--Magnetic Super Space group symbol (name & number)
Transform to standard: a2,a3,a1,a4;0,0,0,0
Parent Space Group:      IT_number:    0
Transform from Parent:
! Generators
Genr  x,y,z,t,1
Genr  x+1/2,-y,-z,-z+t+1/2,1
Genr  -x,y+1/2,-z,-t,1
Genr  -x+1/2,-y+1/2,z,z-t+1/2,1
Genr  x,y,z,t+1/2,-1
Genr  x+1/2,-y,-z,-z+t,-1
Genr  -x,y+1/2,-z,-t+1/2,-1
Genr  -x+1/2,-y+1/2,z,z-t,-1
N_qc   1
Q_coeff
   1
!
!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
Fe1_1  MFE2      1          0.25000     0.75000    -0.00320     0.00000     0.25000    1    0  #
                            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     1.34601     0.00000     0.00000     0.00000     1.34601   <-Amplitudes of Modulated m
                     0.00000    11.00000     0.00000     0.00000     0.00000    11.00000
Fe2_1  MFE2      1          0.25000     0.25000     0.72000     0.00000     0.04000    1    0  #
                            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 of Modulated m
                     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
Te1_1  Te        0          0.25000     0.25000     0.28620     0.00000     0.25000    0    0  #
                            0.00000     0.00000     0.00000     0.00000     0.00000
!-------> Profile Parameters for Pattern #   1  ----> Phase #   1
!  Scale          Shape1      Bov       Str1       Str2       Str3   Strain-Model
  5.295298       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    0.022601    0.140304    0.000000    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
   3.813800    3.783880    6.240520   90.000000   90.000000   90.000000   #MULTCELL    5    1    4
    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:
   0.3550000   0.0000000   0.5000000      1    1.0000  <-- Propagation Vector, nharm, sintl_lim  1
    0.000000    0.000000    0.000000
!  2Th1/TOF1    2Th2/TOF2  Pattern to plot
```

- To create a helix we only need two orthogonal components (Mcosy and Msinz) that are perpendicular to the IC kx direction.
- Since the data only shows one magnetic peak, we will constrain the two amplitudes to be equal for a circular helix

- Load the new PCR into the Toolbar and run FullProf refinement



- the fit can be improved by refining the k-vector, lattice parameters, profile parameter, background.



$Fe_{1.16}Te$: Display the magnetic structure using *Vesta*

- to visualize the magnetic structure one can use ***VESTA*** program, which reads the *.mcif file, generated automatically by Fullprof.

- The mcif created by FullProf is set to display the moment modulation across preselected multiple unit cells

```
! Scale          Shape1       Bov        Str1       Str2       Str3    Strain-Model
  5.295298      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    0.022601    0.153345    0.000000    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
  3.813800   3.783880   6.240520  90.000000  90.000000  90.000000  #MULTCELL    5    1    4
   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:
  0.3543174   0.0000000   0.5000000      1    1.0000  <-- Propagation Vector, nharm, sintl_lim  1
  0.000000    0.000000    0.000000
!  2Th1/TOF1    2Th2/TOF2  Pattern to plot
      6.525      123.000       1
```