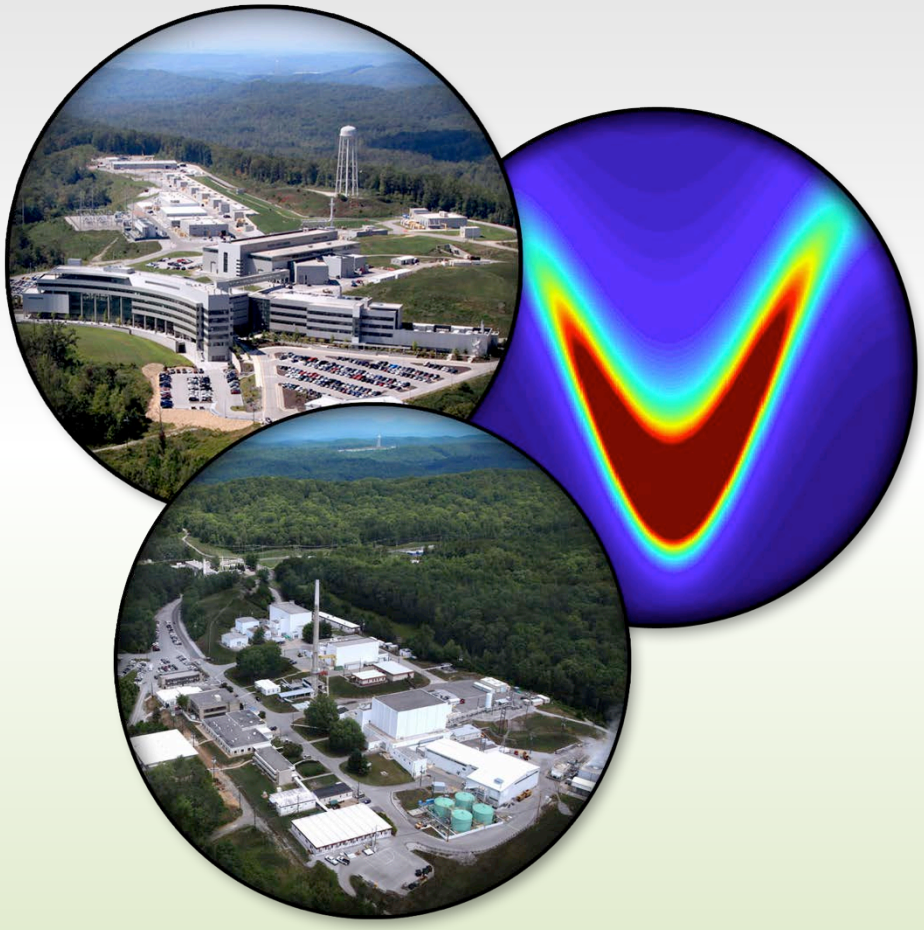
Magnetic structure determination of Cr_2WO_6 using FullProf Suite and SARAh



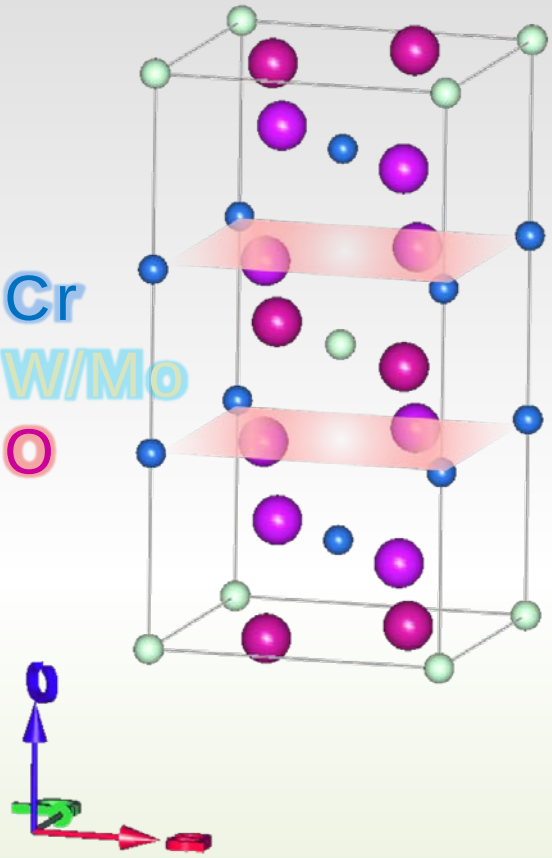
Clarina dela Cruz

Lead Instrument Scientist

HB2a High Resolution Powder Diffractometer

https://neutrons.ornl.gov/powder

Introduction to Cr_2WO_6, Cr_2MoO_6 and similar compounds



Cr_2MoO_5 and Cr_2WO_5

Tetragonal (Space group #136: $P4_2/mnm$)
$a=b=4.58328$ Å $c=8.85289$ Å)

3D Antiferromagnetic ordering at T_N (Mo)~ 93 K and
T_N (Mo)~ 93 K

PRL 113, 076406 (2014) PHYSICAL REVIEW LETTERS week ending 15 AUGUST 2014

Tuning the Magnetic Exchange via a Control of Orbital Hybridization in $Cr_2(Te_{1-x}W_x)O_6$

M. Zhu,[1] D. Do,[1] C. R. Dela Cruz,[2] Z. Dun,[3] H. D. Zhou,[3,4] S. D. Mahanti,[1] and X. Ke[1,*]

[1]Departme
[2]Quantum C
[3]Depart
[4]National

PHYSICAL REVIEW B 92, 094419 (2015)

Ferromagnetic superexchange in insulating Cr_2MoO_6 by controlling orbital hybridization

M. Zhu,[1] D. Do,[1] C. R. Dela Cruz,[2] Z. Dun,[3] J.-G. Cheng,[4,5] H. Goto,[5] Y. Uwatoko,[5] T. Zou,[1] H. D. Zhou,[3]
Subhendra D. Mahanti,[1] and X. Ke[1]

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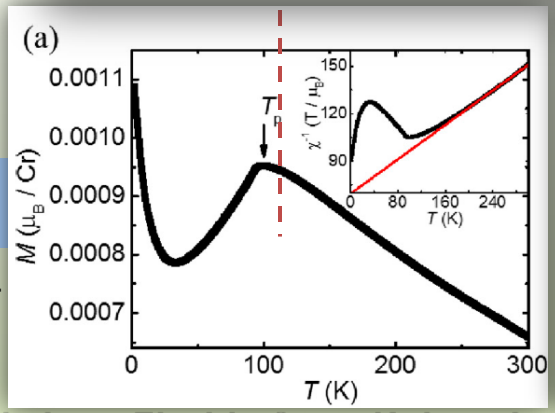
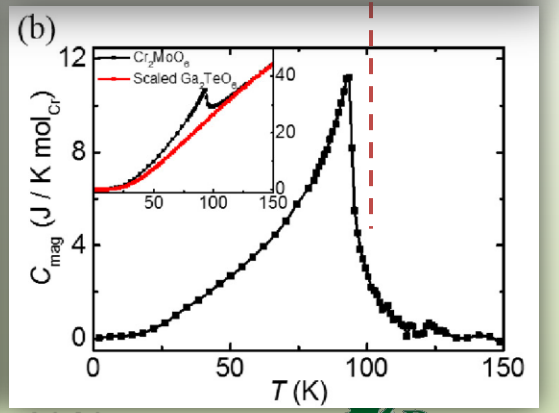
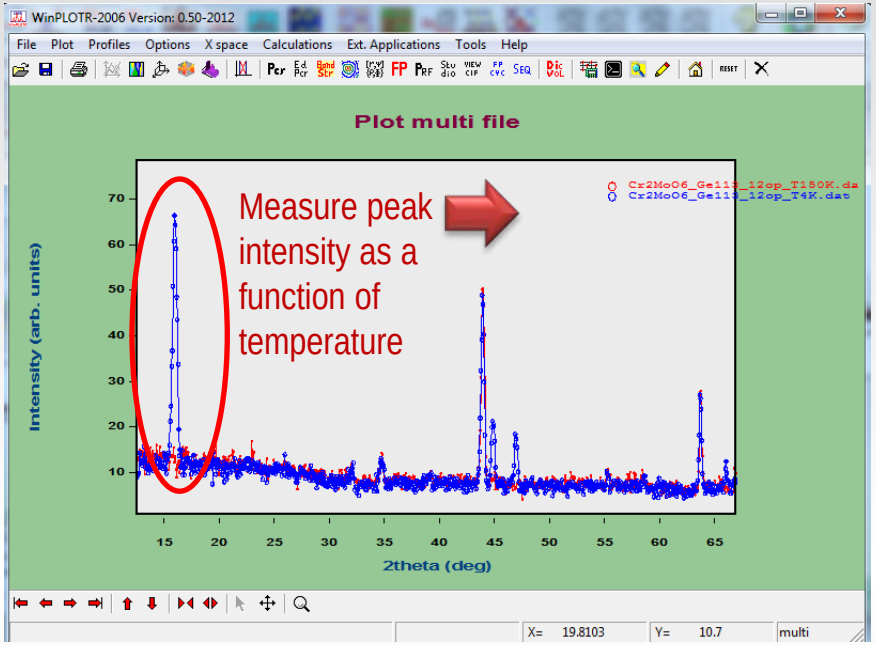
[5]Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277–8581, Japan

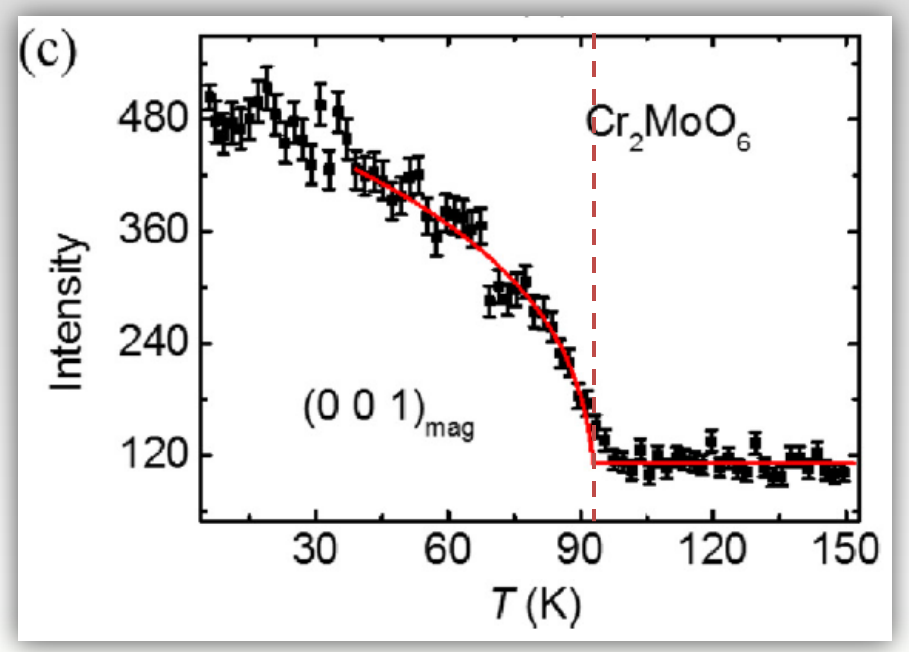


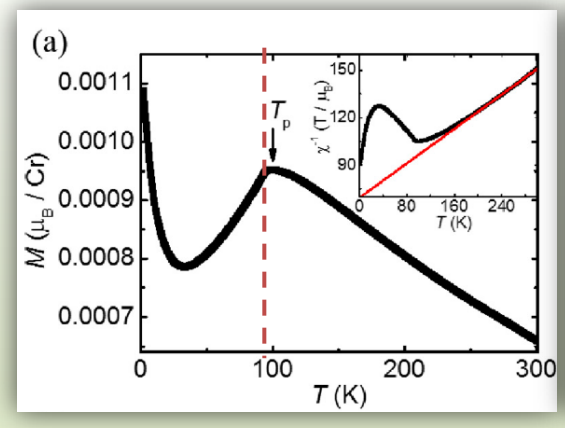


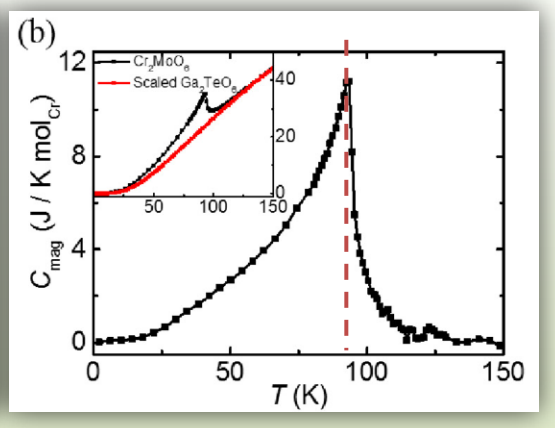
Atom	Wyckoff site	Site symmetry	x/a	y/b	z/c
Cr^{3+}	4e	2mm	0	0	0.334

ORDER PARAMETER MEASUREMENTS



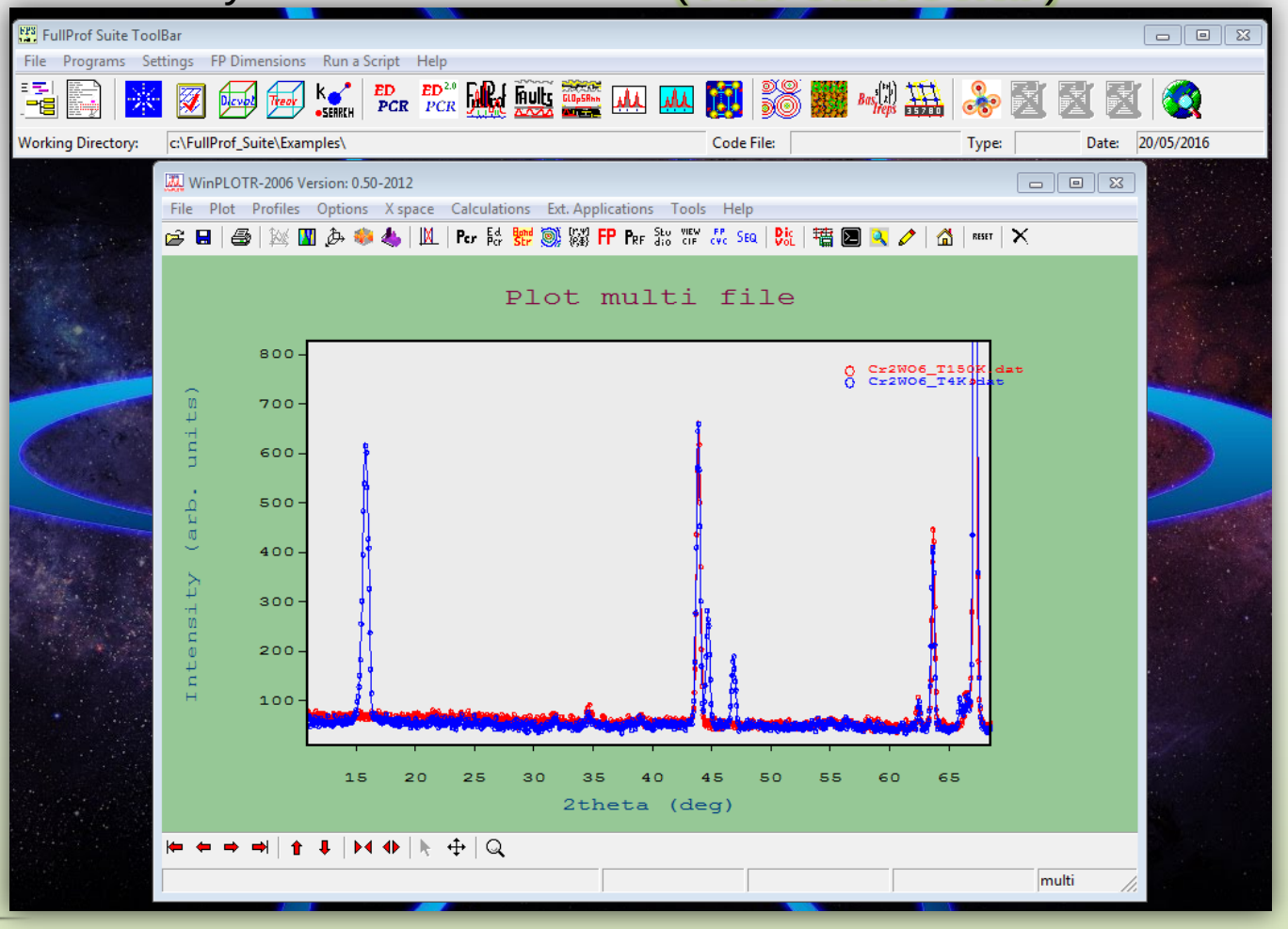






STARTING INFORMATION

- Neutron powder diffraction data collected at HB2a at HFIR, λ = 2.4097 Å and a collimation of 12'-open-6' at 4 K (File : Cr2WO6_T4K.dat AND Cr2WO6_T150K.dat)
- Instrument resolution file: (hb2a_Ge113_irf_FP.irf)
- Crystal structure known (File: Cr2WO6.cif)



STEPS FOR MAGNETIC STRUCTURE DETERMINATION

✓ refining the crystal structure for the paramagnetic state ($T > T_N$ or T_C)
→ **obtain all the relevant structural and profile parameters**

✓ preparing a PCR file and performing a refinement of the low temperature data ($T < T_N$) with fixed structural parameters (without a magnetic model)
→ **identify the magnetic contribution to the diffraction pattern**

✓ indexing the magnetic reflections
→ **use *k-search* to determine the propagation vector(s) k_m**

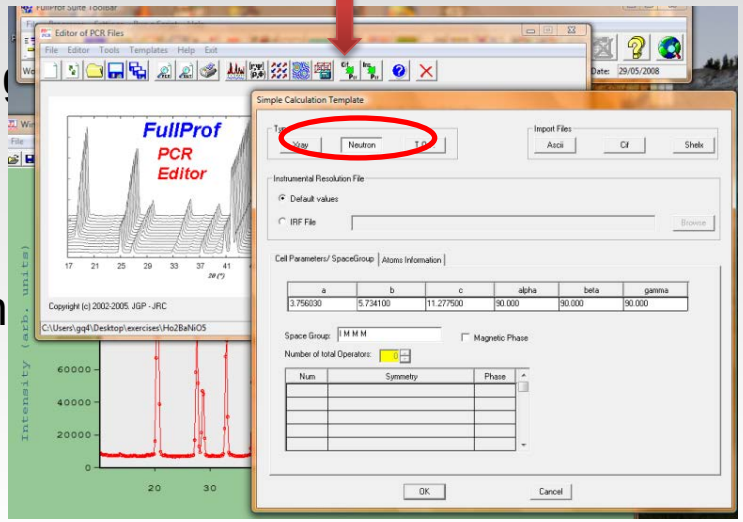
✓ Performing symmetry analysis (propagation vector, space group, atomic position)
→ **use *BasIreps* or *SARAh* to get IRs and Basis vectors**

✓ Adding the magnetic phase to the PCR file (using the symmetry information) and **solve the magnetic structure using trial and error methods**

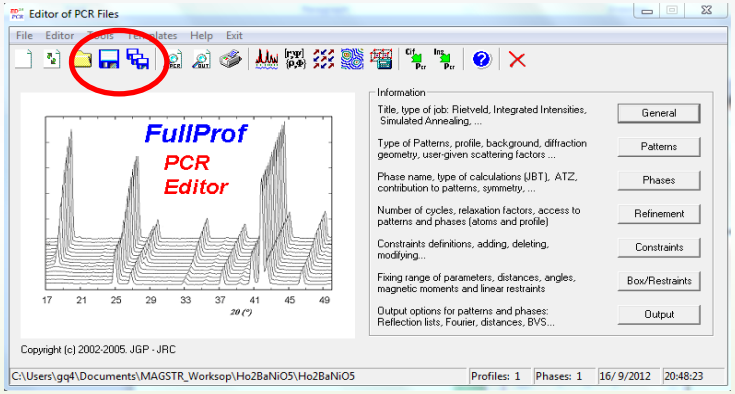
✓ **Magnetic structure model visualization using FpStudio program**

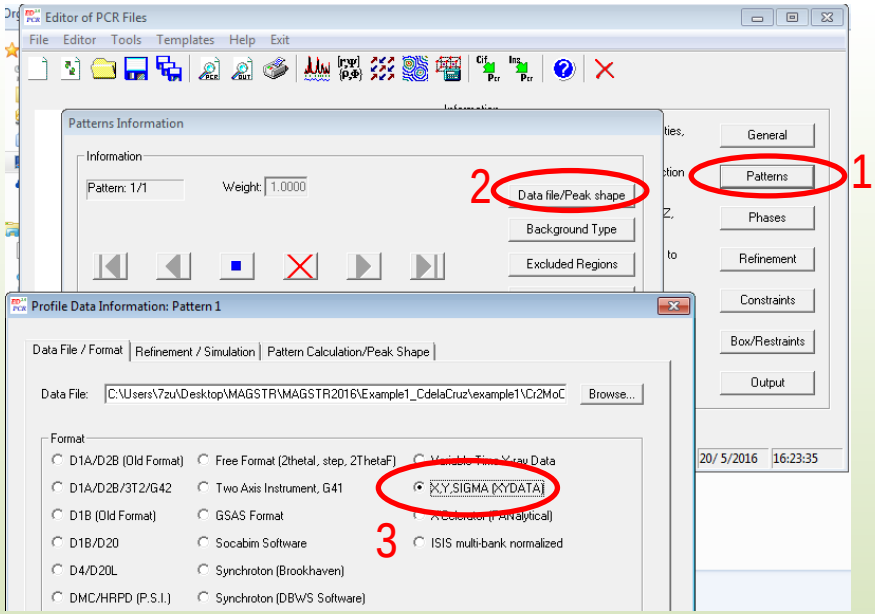
- use **EdPCR** to create the input file for FullProf (*.PCR)

Cif ➔ Pcr



- import the crystallographic information by clicking on “CIF to PCR”
- in the new window, select the “Neutron” tab for the type of calculations
- use the “Browse” button to upload the instrumental resolution file “IRF” (hb2a_Ge113_irf_FP.irf)



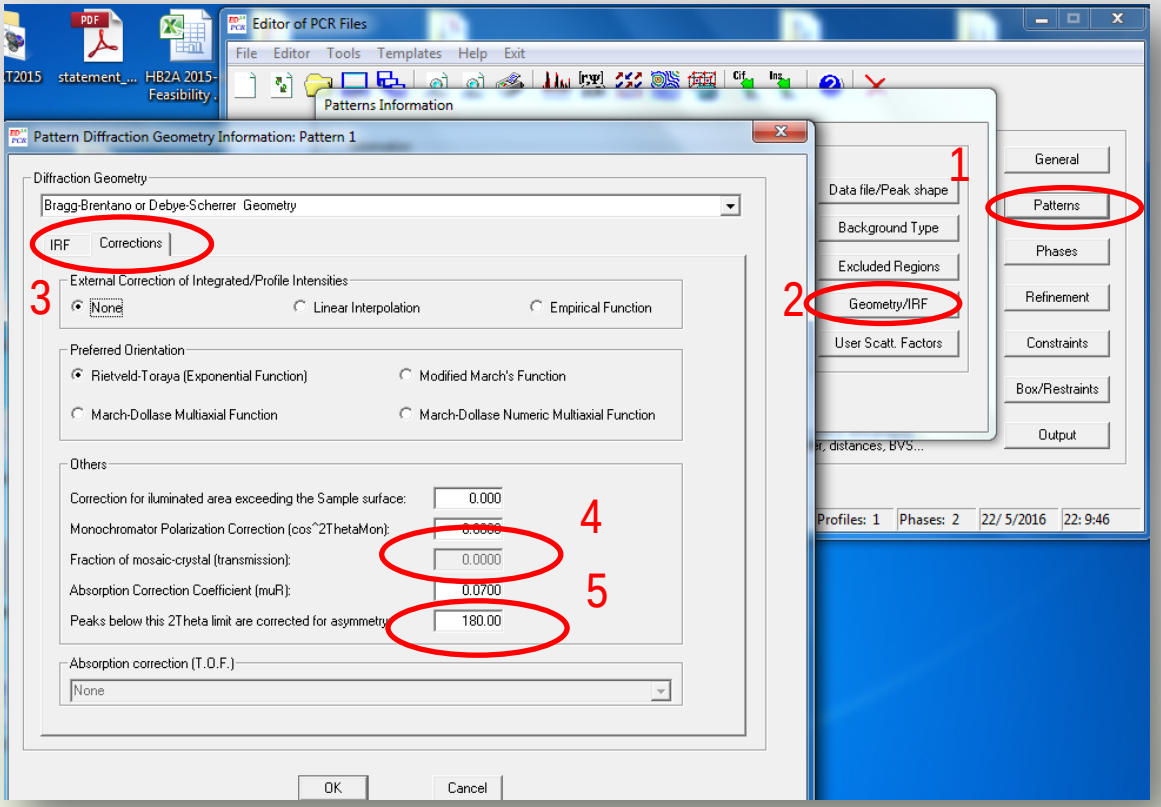


- save the PCR file by clicking the “Save” button
- open the “Patterns” tab (1) and then the “Data file/ peak shape” (2) and select the “X,Y,SIGMA(XYDATA)” for the data file format (3)

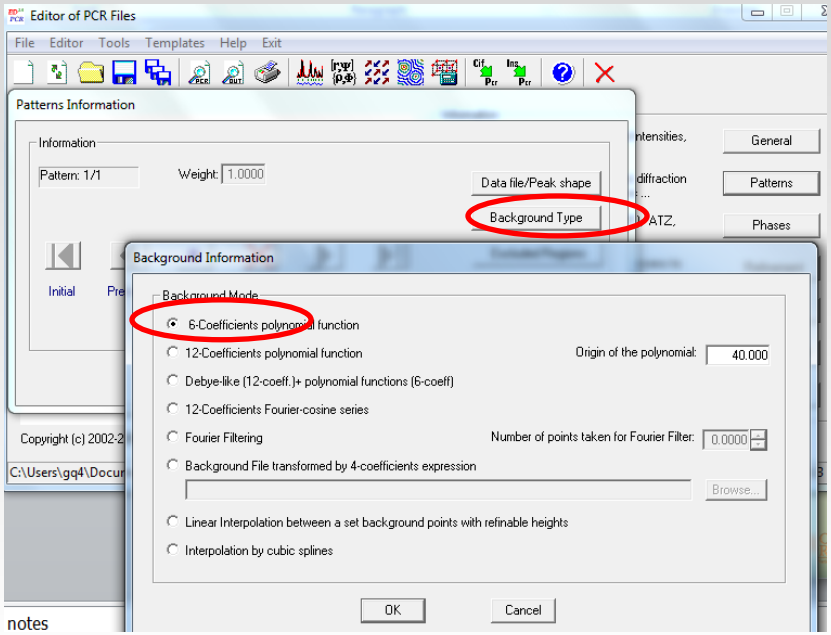
- open the “Patterns” tab (1) and then the “Geometry/IRF” (2) and select the “Corrections” tab (3)
- Input the calculated absorption correction coefficient (4)

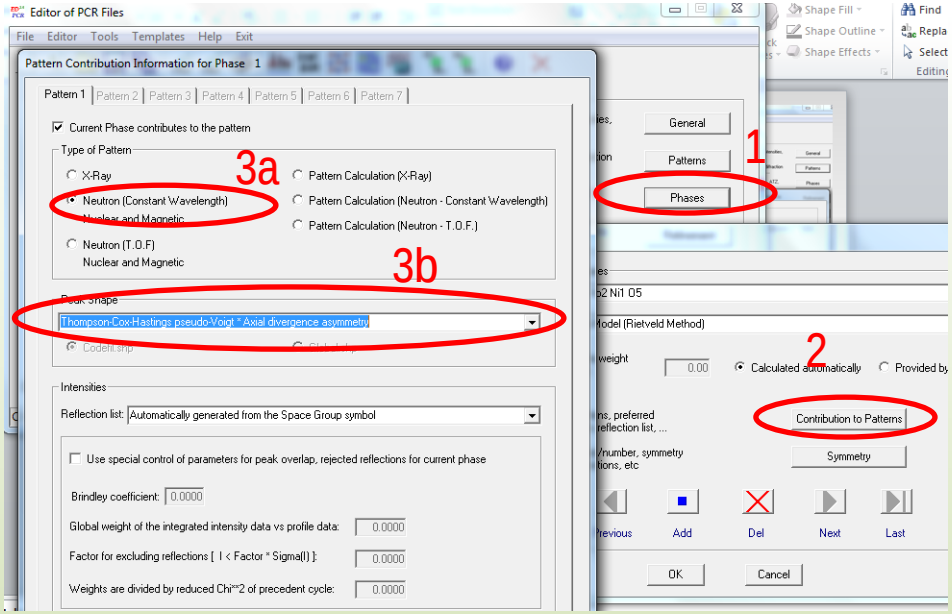
➔ Refer to NCNR website on how to determine absorption correction http://www.ncnr.nist.gov/instruments/bt1/neutron.html

- For HB2a data, enter 180 degrees for Peaks below this 2theta are corrected for asymmetry (5)



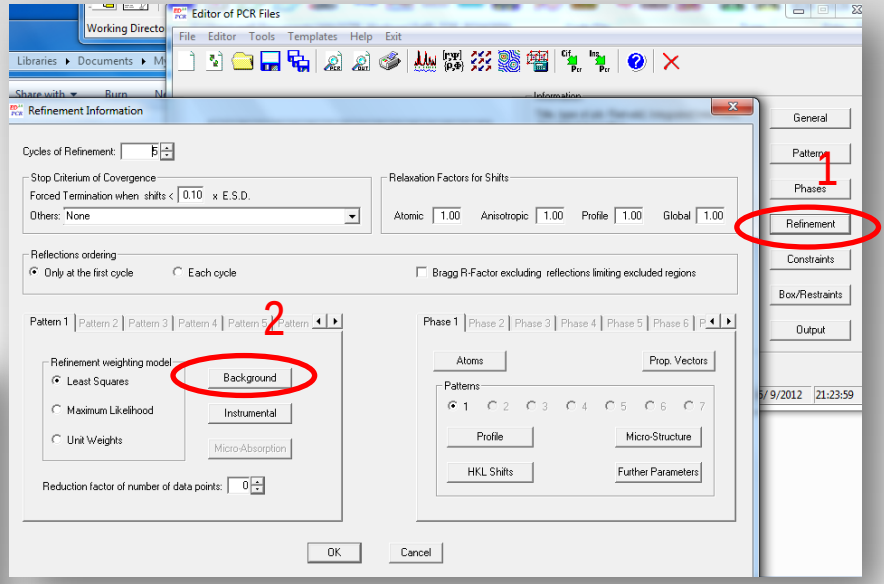
- “Refinement/Simulation” tab, make sure that “Neutron-CW” option is selected, wavelength is “**User defined**” $\lambda_1=\lambda_2=2.4097$Å
- “pattern calculation” the “Thompson-Cox-Hastings pseudo-Voigt * Axial divergence asymmetry” peak shape is chosen
- For the background information, select the “6-coefficients polynomial function”

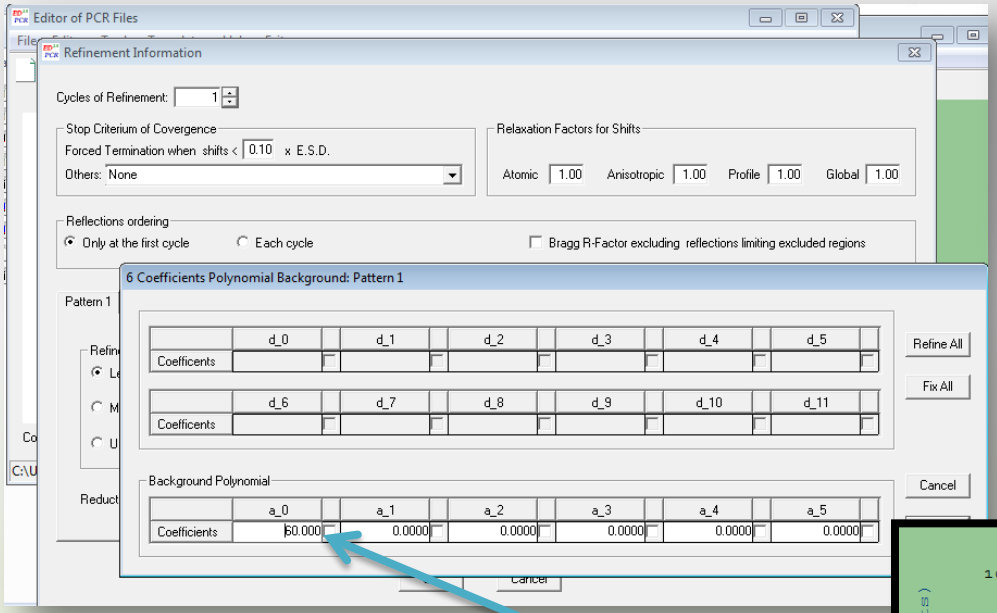


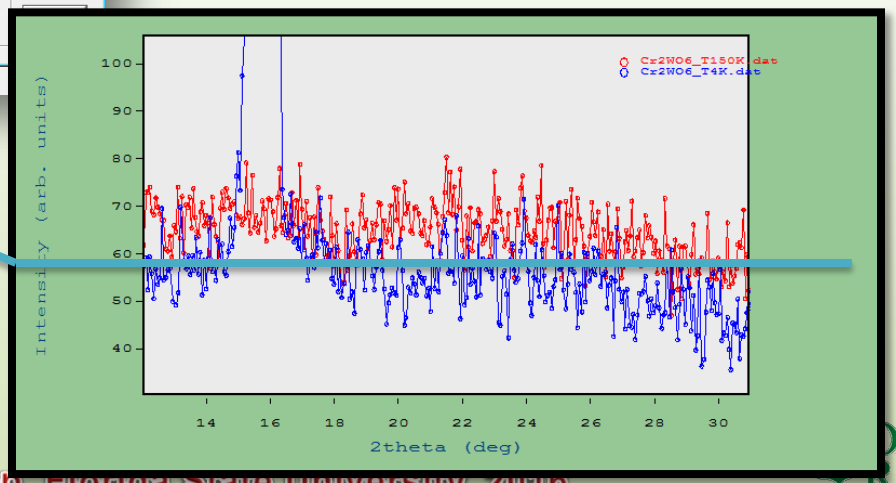


- From the main window of EdPcr, open the “Phases” tab (1) and then click on the “Contribution to patterns” (2) and then select the “current phase contributes to the pattern” & “neutron (constant wavelength)” (3a) and “Thompson-Cox-Hastings pseudo-Voigt” for the peak shape (3b), Reflection list : “Automatically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

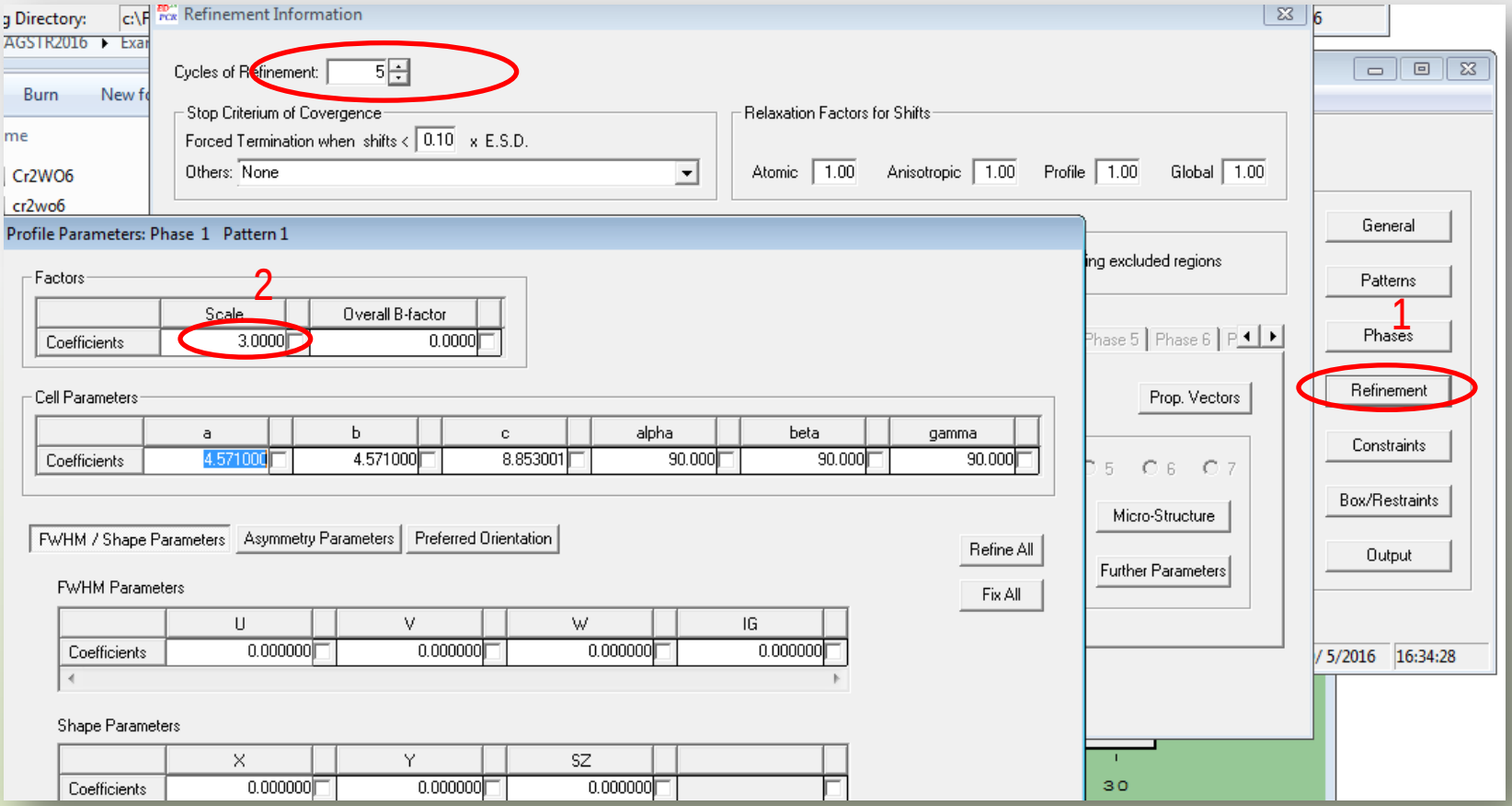
- Open the “Refinement” (1) and then the “Background” and add value for the “a_o” coefficient (~60, read from the data file) that will give a first flat approximation for the background



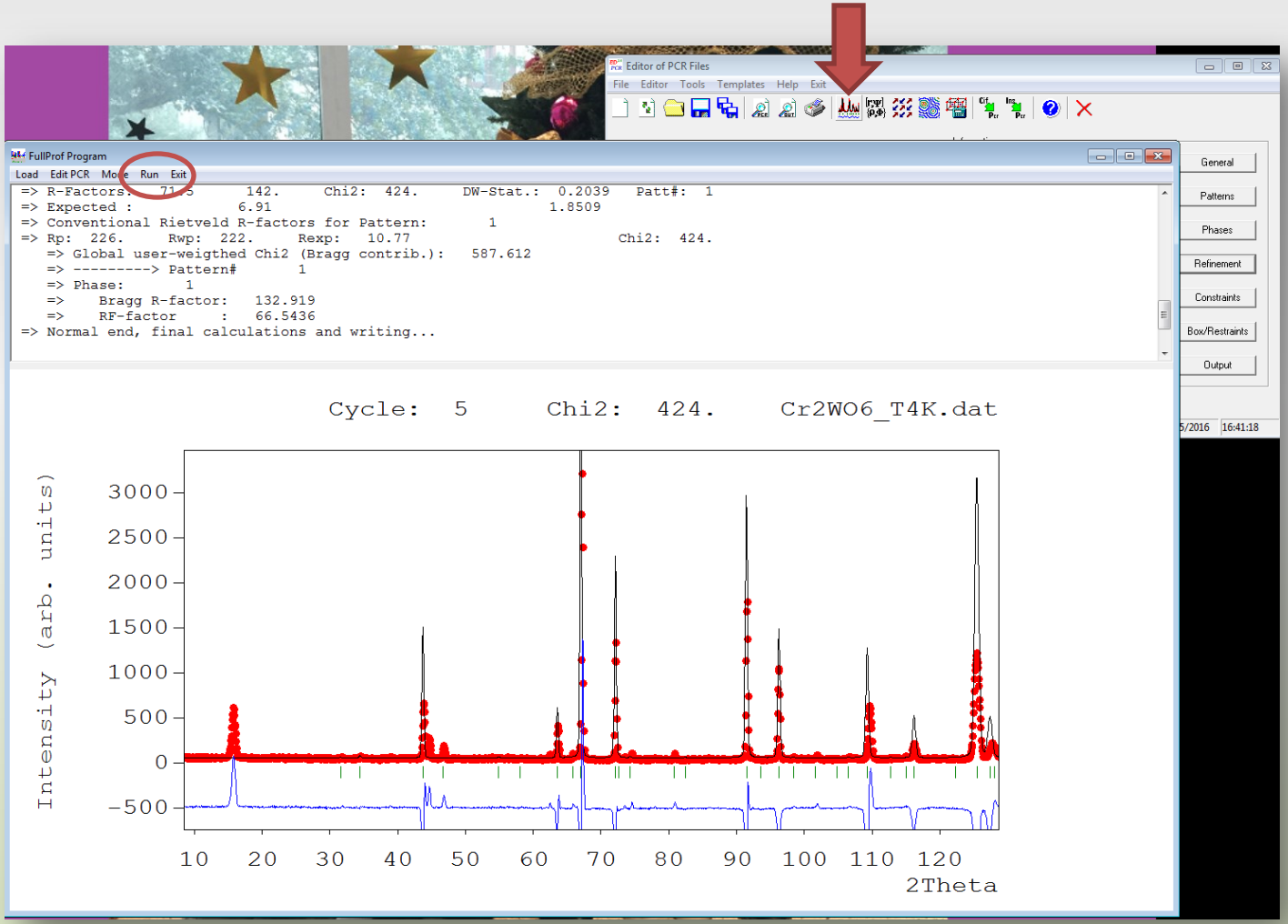




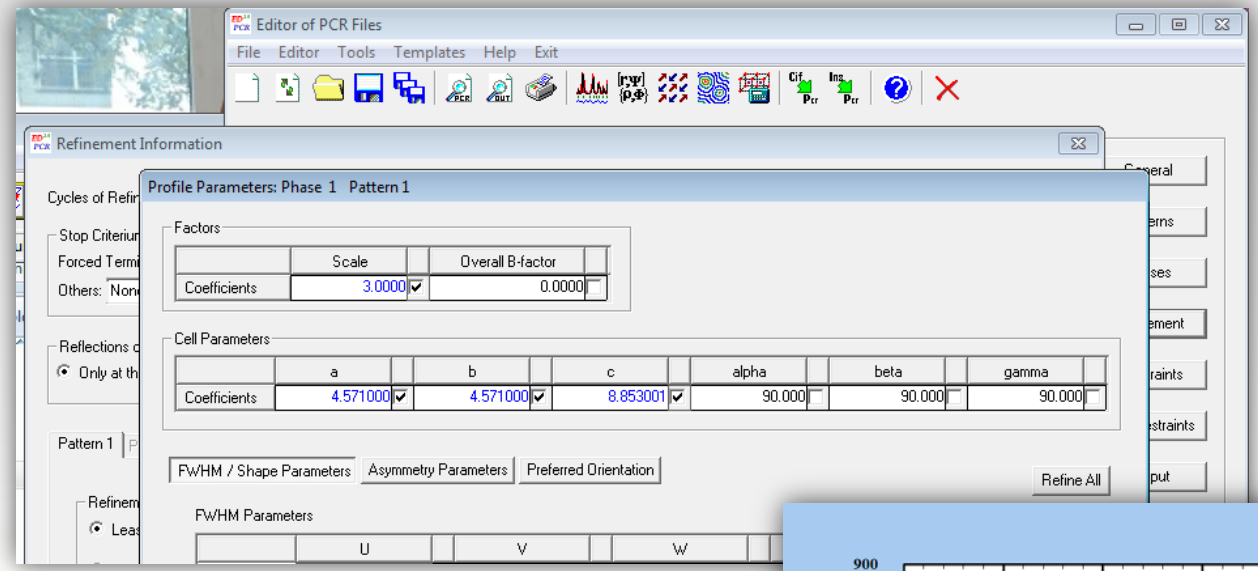
- From the same “Refinement” window (1) , click on the “Profile” tab and and set a number for the “Scale factor” (~ 50 for this example). The number of “cycles of refinement” can also be increased at this time
- save the PCR file by clicking the “Save” button, every time a change has been made



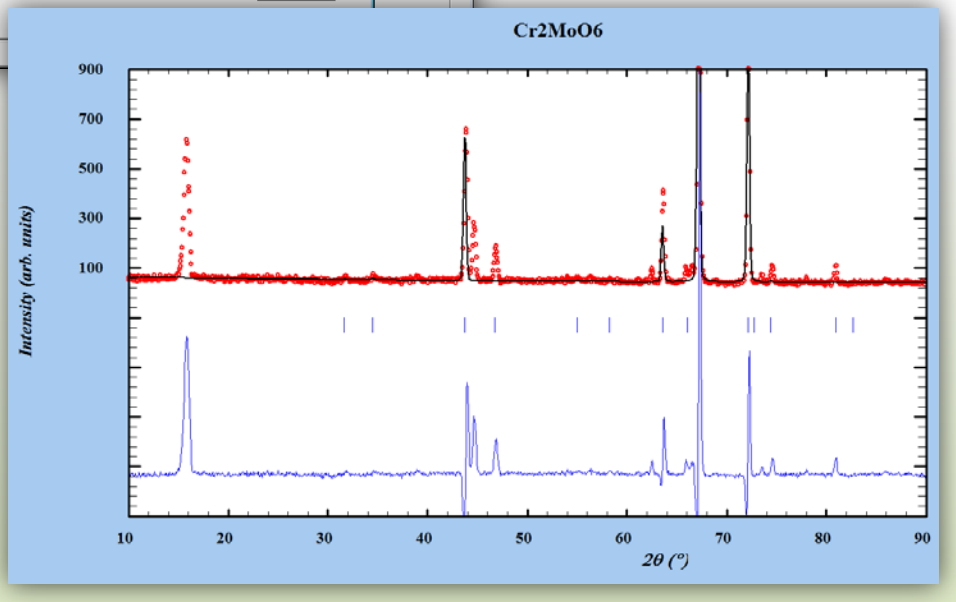
- Run the Fullprof program by click on button indicated below.
- Choose the Cr2WO6_T4K.dat
- All the parameters are fixed at this time.



- ✓ You can run the refinement again by allowing the scale factor, lattice parameters, some of the background coefficients and the 2theta zero to vary
- ✓ Refined parameters appear in blue or red (with additional constraints)

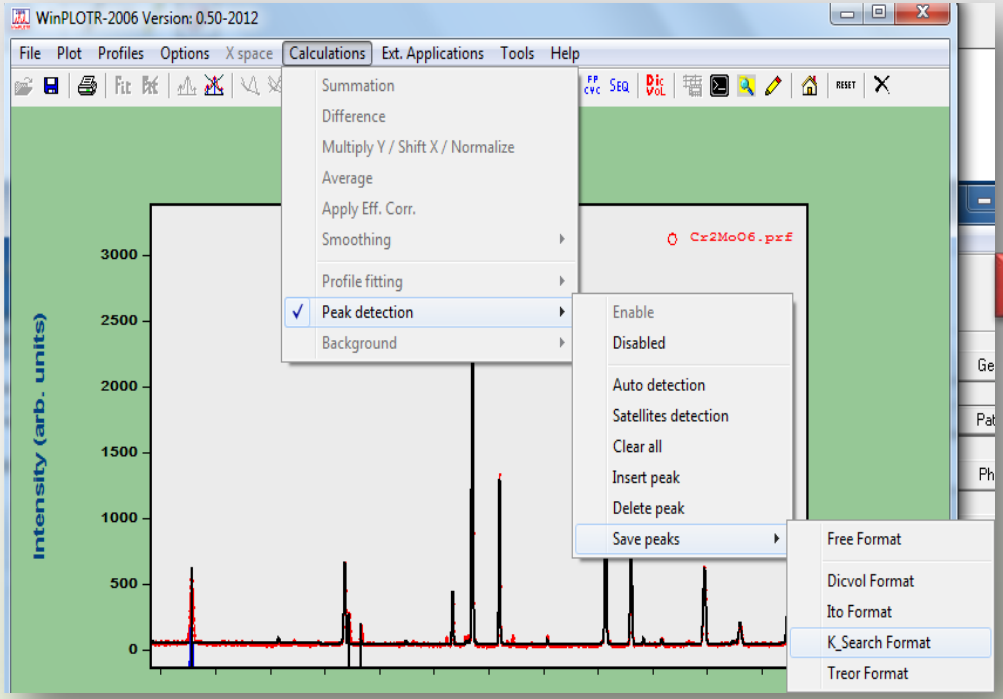


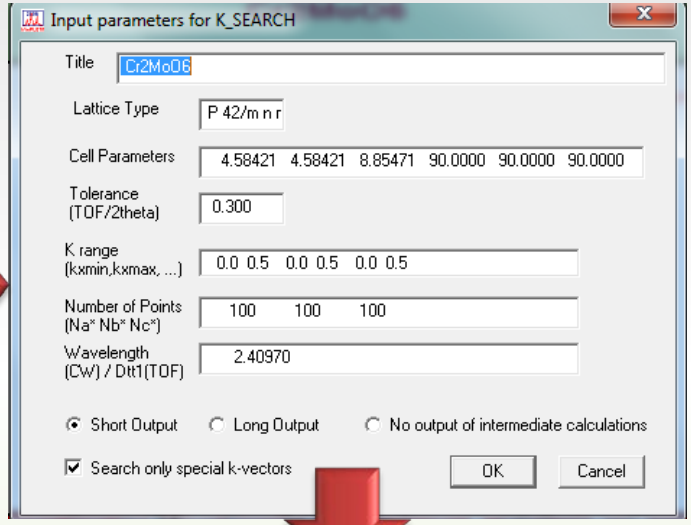
o Open the PRF file (Rietveld plot) by using the Winplotr program. The result will look something similar to the figure on the right. The reflections that are left unindexed are all magnetic in origin



INDEX THE MAGNETIC REFLECTIONS USING THE k-search program

- open the PRF file using WinPlotr-2006 program and select the un-indexed reflections to create the input file for “k-search” program. For doing this, in the menu of winplotr click on “Calculations”- “peak detection”-”enable” . After enabling, go again to “Calculations”- “peak detection” and “ insert peak”. After selecting the magnetic peaks, go to “save peaks” to save them as “K-search format”





for the Cr_2WO_6 → k_m= (0, 0, 0)

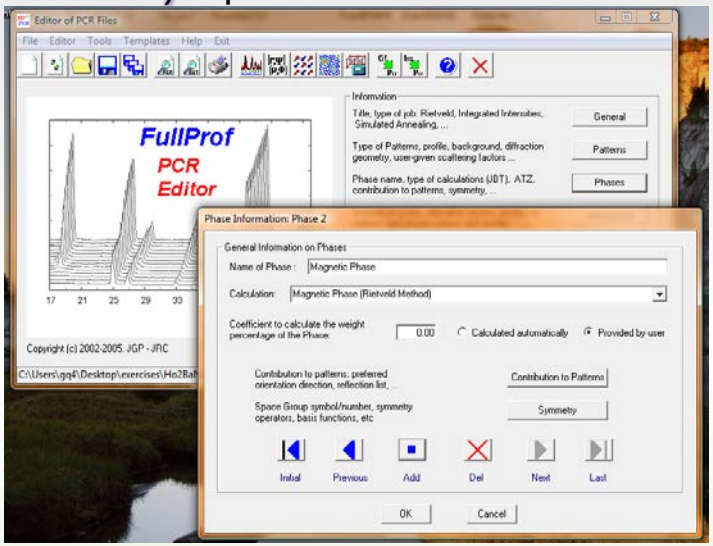
```
=> Special k-vector solutions found!

=> List of the best 10 solutions for  3 satellites

      Kx          Ky          Kz        R-factor
 0.500000    0.000000    0.250000    0.118863
 0.000000    0.500000    0.250000    0.118863
 0.000000    0.000000    0.000000    0.181839
 0.500000    0.125000    0.000000    0.724201
 0.125000    0.500000    0.000000    0.724201

=> A probable solution is the special kvector ks =(  0.0000   0.5000   0.2500)
=> The corresponding R-factor is:       0.1189
```

Need to check these possible solutions!

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

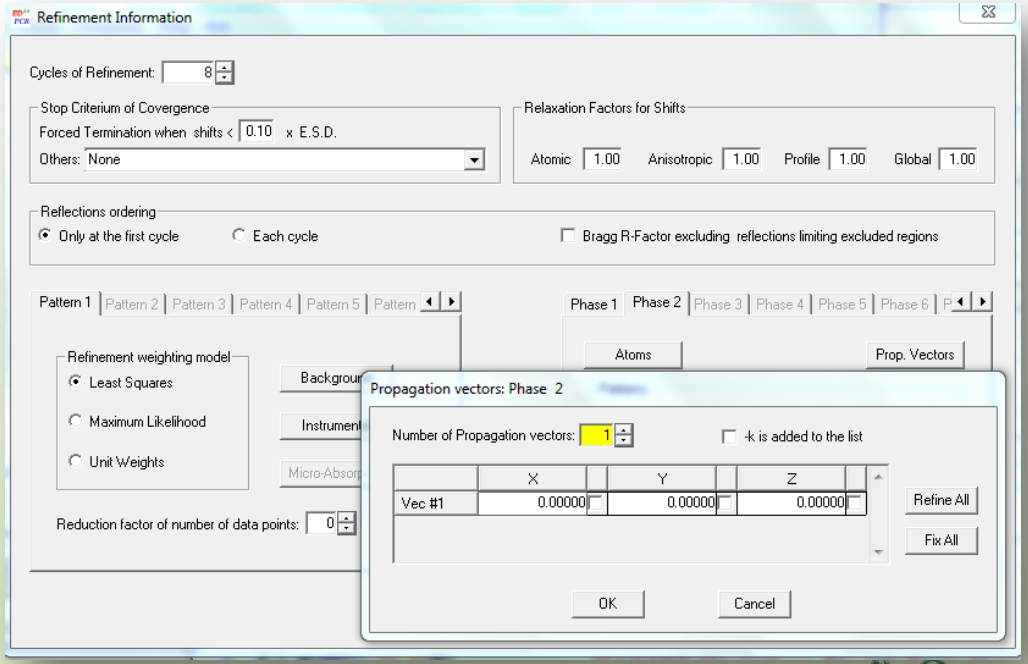
➢ ADDING THE MAGNETIC PHASE AS A SECOND PHASE TO THE PCR

- use PCR Editor to introduce the magnetic phase as a second phase. Go to the "Phases" tab and click on the "Add" button. You can name (ex. *magphase*) the new phase as you wish, and in the "calculation" tab select the "Magnetic phase (Rietveld Method)" option.



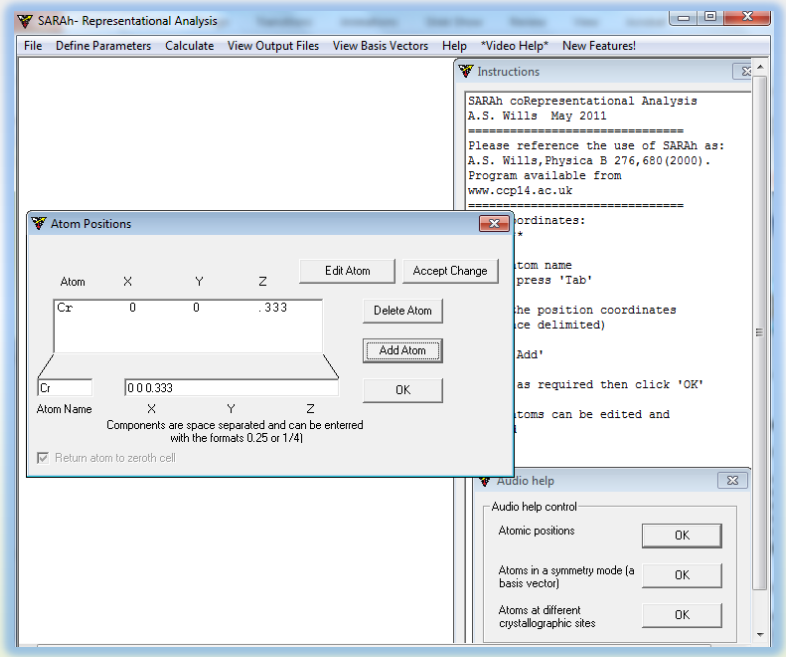
- you can also open the PCR file using your default text editor at thins time and verify that the second phase has been successfully added . Don't worry about the symmetry at this time.

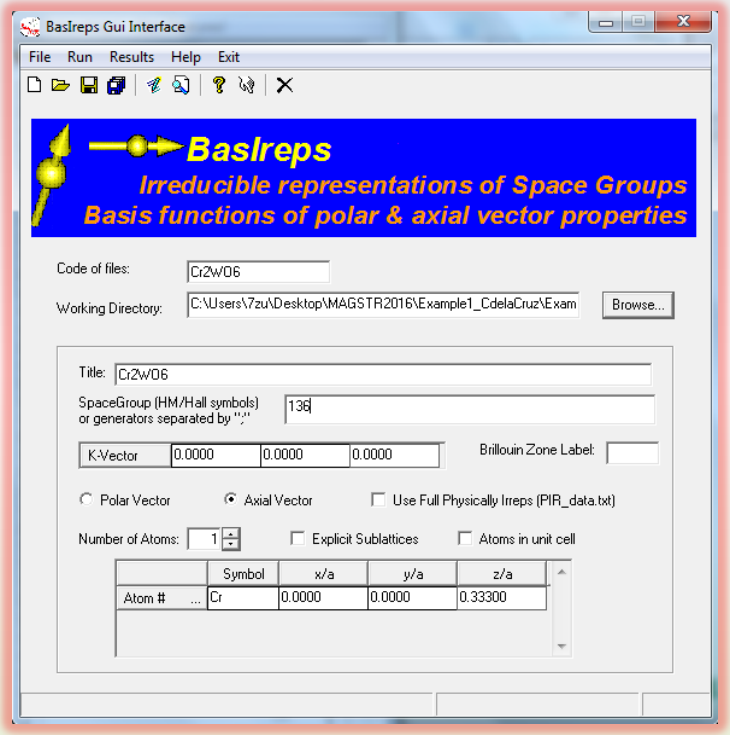
- the propagation vector for the magnetic phase needs to be added into the PCR file. For doing that, you need to click on "Refinement" button and then select the "Phase 2" and "Prop. Vectors"



PERFORM SYMMETRY ANALYSIS

- use SARAh program or **BasIrreps** to generate the Irreducible representations and basis vectors associated with k_m= (0, 0, 0). Both programs required as an input the k_m vector, space group and atom positions of the magnetic ion.





- for this example we will use the program SARAh. See the software's website for the tutorial on how to run the program. The program generates a summary file containing the basis vectors components for the two magnetic ions. The file is located in SARAh program's folder.

IR	BV	Atom	BV components					
			$m_{\|\|a}$	$m_{\|\|b}$	$m_{\|\|c}$	$im_{\|\|a}$	$im_{\|\|b}$	$im_{\|\|c}$
Γ_2	ψ_1	1	0	0	4	0	0	0
		2	0	0	-4	0	0	0
		3	0	0	-4	0	0	0
		4	0	0	4	0	0	0
Γ_3	ψ_2	1	0	0	4	0	0	0
		2	0	0	4	0	0	0
		3	0	0	4	0	0	0
		4	0	0	4	0	0	0
Γ_5	ψ_3	1	0	0	4	0	0	0
		2	0	0	-4	0	0	0
		3	0	0	4	0	0	0
		4	0	0	-4	0	0	0
Γ_8	ψ_4	1	0	0	4	0	0	0
		2	0	0	4	0	0	0
		3	0	0	-4	0	0	0
		4	0	0	-4	0	0	0
Γ_9	ψ_5	1	2	0	0	0	0	0
		2	2	0	0	0	0	0
		3	2	0	0	0	0	0
		4	2	0	0	0	0	0
	ψ_6	1	0	2	0	0	0	0
		2	0	-2	0	0	0	0
		3	0	2	0	0	0	0
		4	0	-2	0	0	0	0
	ψ_7	1	0	-2	0	0	0	0
		2	0	-2	0	0	0	0
		3	0	-2	0	0	0	0
		4	0	-2	0	0	0	0
	ψ_8	1	-2	0	0	0	0	0
		2	2	0	0	0	0	0
		3	-2	0	0	0	0	0
		4	2	0	0	0	0	0
Γ_{10}	ψ_9	1	2	0	0	0	0	0
		2	2	0	0	0	0	0
		3	-2	0	0	0	0	0
		4	-2	0	0	0	0	0
	ψ_{10}	1	0	2	0	0	0	0
		2	0	-2	0	0	0	0
		3	0	-2	0	0	0	0
		4	0	2	0	0	0	0
	ψ_{11}	1	0	2	0	0	0	0
		2	0	2	0	0	0	0
		3	0	-2	0	0	0	0
		4	0	-2	0	0	0	0
	ψ_{12}	1	2	0	0	0	0	0
		2	-2	0	0	0	0	0
		3	-2	0	0	0	0	0
		4	2	0	0	0	0	0

FM //a

FM //b

- The result of the symmetry analysis is also summarized in a TEX file, in Sarah directory, as shown in this capture

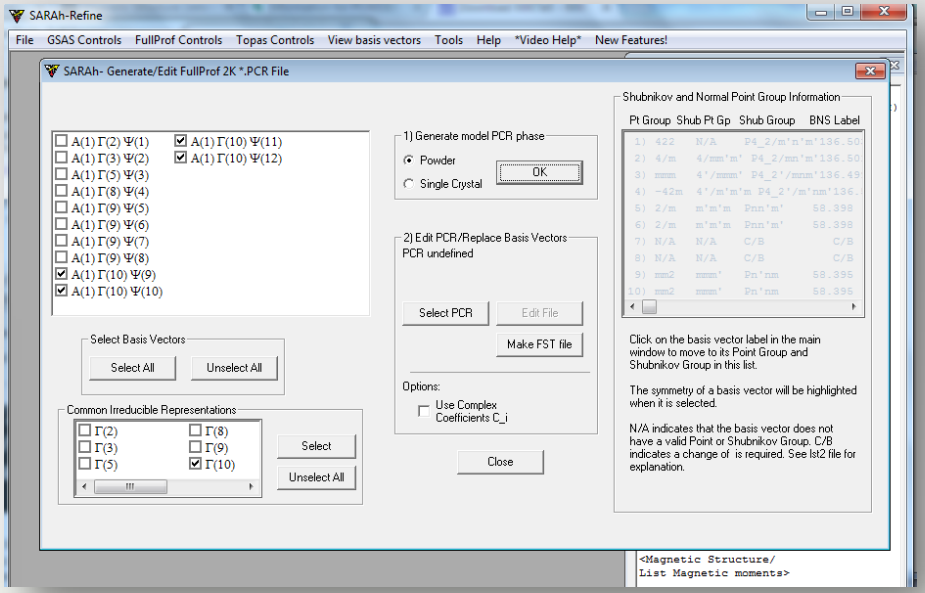
Γ_2, Γ_3, Γ_5 and Γ_8 constraints the moments to lie along the *c-axis*

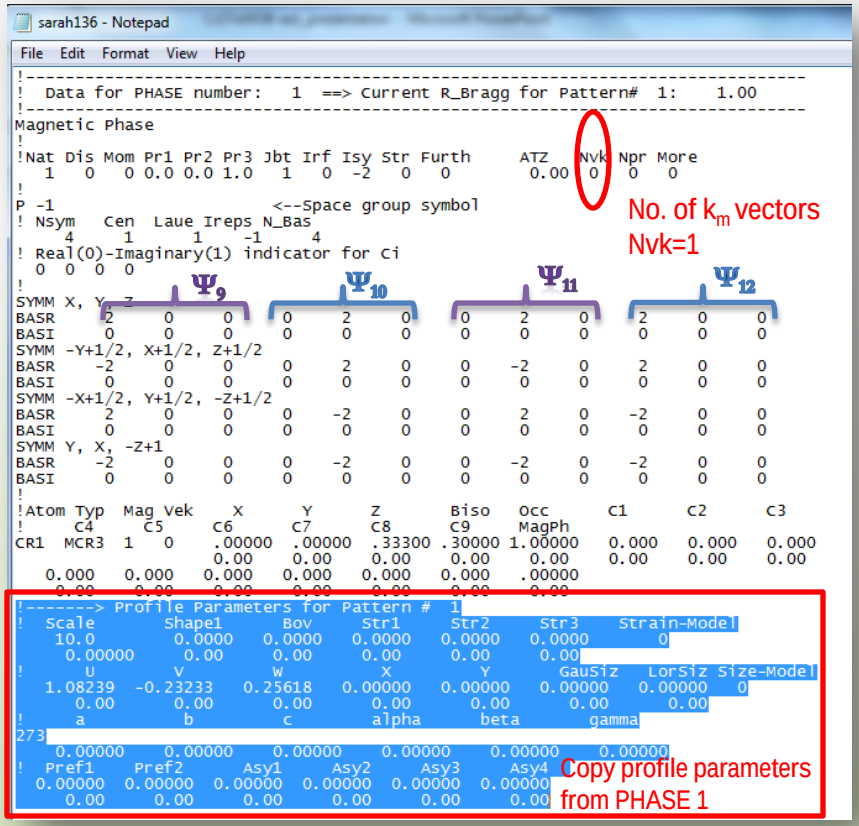
Γ_9 and Γ_{10} constraints moments to lie in the *ab-plane*

- The index (0 0 1) of the strongest magnetic peak at Q= 0.7096A^{-1} suggests that the moments are in the ab-plane
- Bulk magnetic measurements did not show any Ferromagnetic (FM) behavior

- ✓ "SARAh Refine" program can be used to generate the magnetic phase for the PCR (FullProf) format (see Sarah manual for more details). In our case , it will generate the file "sarah136.pcr"

- ✓ You'll need to select the basis vectors corresponding to one of the Irreducible Representations (gamma10 or Γ10 in our case).





No. of k_m vectors Nvk=1

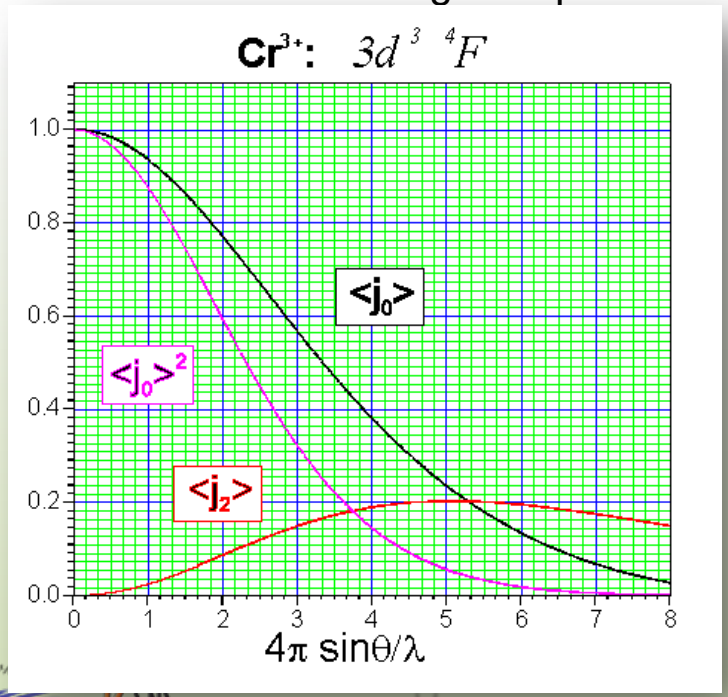
Copy profile parameters from PHASE 1

- ✓ Note that the selected model Γ10 constraints the magnetic moments of Cr to lie in the *ab*-plane

- ✓ Open the PCR file generated by Sarah ("sarah136.pcr"), copy the entire content of the file and PA STE it over the section of the second phase of your Cr2WO6 PCR file.

- ✓ once the magnetic phase is defined into your PCR file, examine the profile parameter section; you'll need to set the profile parameters for the magnetic phase (phase 2) the same as you have in the structural phase (phase 1). Copy/paste that section from the phase1 to the phase 2. Make sure that you are not removing the line defining the propagation vector, at the end of the phase 2 section.
- ✓ note that the scale factor and the lattice parameters of the structural and magnetic phase need to be constrained to have the same values in both the nuclear and magnetic phases.

```
Magnetic Phase
!
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
   1   0   0 0.0 0.0 1.0   1  -1  -2   0   0         0.000   1   7   0
!
P -1                    <--Space group symbol for hkl generation
! Nsym   Cen  Laue Ireps N_Bas
     4     1     1    -1     4
! Real(0)-Imaginary(1) indicator for Ci
  0  0  0  0
!
SYMM X, Y, Z
BASR     2     0     0     0     2     0     0     2     0     2     0     0
BASI     0     0     0     0     0     0     0     0     0     0     0     0
SYMM -Y+1/2, X+1/2, Z+1/2
BASR    -2     0     0     0     2     0     0    -2     0     2     0     0
BASI     0     0     0     0     0     0     0     0     0     0     0     0
SYMM -X+1/2, Y+1/2, -Z+1/2
BASR     2     0     0     0    -2     0     0     2     0    -2     0     0
BASI     0     0     0     0     0     0     0     0     0     0     0     0
SYMM Y, X, -Z+1
BASR    -2     0     0     0    -2     0     0    -2     0    -2     0     0
BASI     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
CR1    MCR3  1  1  0.00000 0.00000 0.33300 0.30000  1.00000   3.000    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
!  Scale          Shape1       Bov        Str1       Str2       Str3    Strain-Model
  1.8681        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
   0.431390   -0.698147    0.340387    0.042805    0.000000   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
   4.584211    4.584211    8.854706   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  -0.13759    0.00000    0.00000    0.00000   0.03400   0.03500
     0.00      0.00       0.00       0.00       0.00       0.00      0.00       0.00
! Propagation vectors:
   0.0000000   0.0000000   0.0000000          Propagation Vector  1
    0.000000    0.000000    0.000000
!  2Th1/TOF1    2Th2/TOF2  Pattern to plot
      8.500      128.694        1
```



- ✓ make sure that the correct parameters for the magnetic scattering form factors are used for the magnetic transition metal ion Cr^{3+} MCR3

International Tables of Crystallography, Volume C, ed. by AJC Wilson, Kluwer Ac. Pub., 1998, p. 513

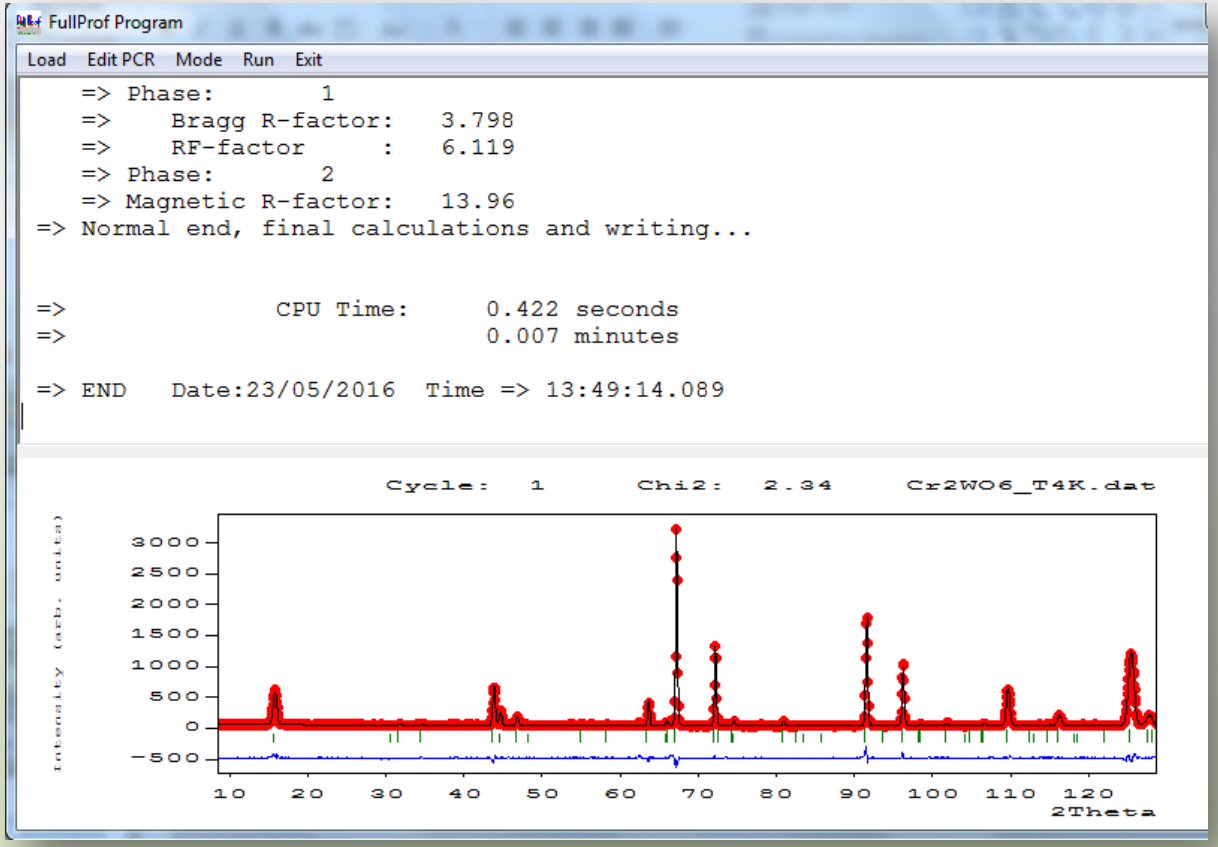
MAGNETIC STRUCTURE REFINEMENT

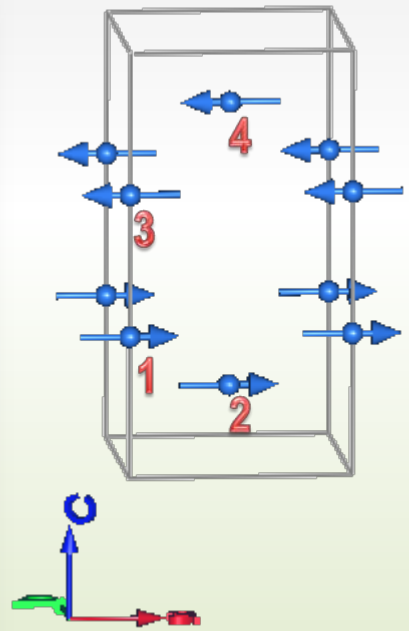
- ✓ select the basis vector coefficients C1 to be refined, this corresponds to the first basis vector Ψ_9 as a trial solution

Basis Functions Coefficients

	C1	C2	C3	C4
Atom # 1	3.00000 ☑	0.00000 ☐	0.00000 ☐	0.00000 ☐

- ✓ run the refinement using the FullProf program
- ✓ start to refine additional parameters (profile, lattice …) to obtain a good quality fit.





MAGNETIC MOMENT DETERMINATION

- Check the summary file (*.sum) from FullProf. Verify that the magnetic structure model and the magnitude Cr moments are meaningful. The output file has similar information (*.out)

```
==> ATOM PARAMETERS:

 Name      x      sx       y      sy       z      sz      B   sB   occ. socc.  Mult
CR1     0.00000(   0)  0.00000(   0)  0.33300(   0)  0.300(  0)  1.000(  0)    0


==>  COEFFICIENTS OF BASIS VECTORS:

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

  CR1    C1=   1.0176( 105) C2=   0.0000(   0) C3=   0.0000(   0)
         C4=   0.0000(   0) C5=   0.0000(   0) C6=   0.0000(   0)
         C7=   0.0000(   0) C8=   0.0000(   0) C9=   0.0000(   0)
         Phase/2pi=   0.0000(   0)
```

In general, the moment is calculated from the refined values of the Fourier components (i.e. C_i's)

Ex. Cr(1)➔ m[Cr(1)]= 1.018* $\begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$ exp $\left[-2\pi i \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 0 \\ 0.333 \end{bmatrix} \right]$

$$\vec{m}_j = \sum_{\nu,\vec{k}} C_\nu^{\vec{k}} \, \psi_{i,\nu}^{\vec{k}} \, e^{-2\pi i \vec{k}\cdot\vec{t}_{ij}}$$

$C_1 * \Psi_9(Cr1)\ exp\ (-2\pi\ k \cdot t(Cr1))$

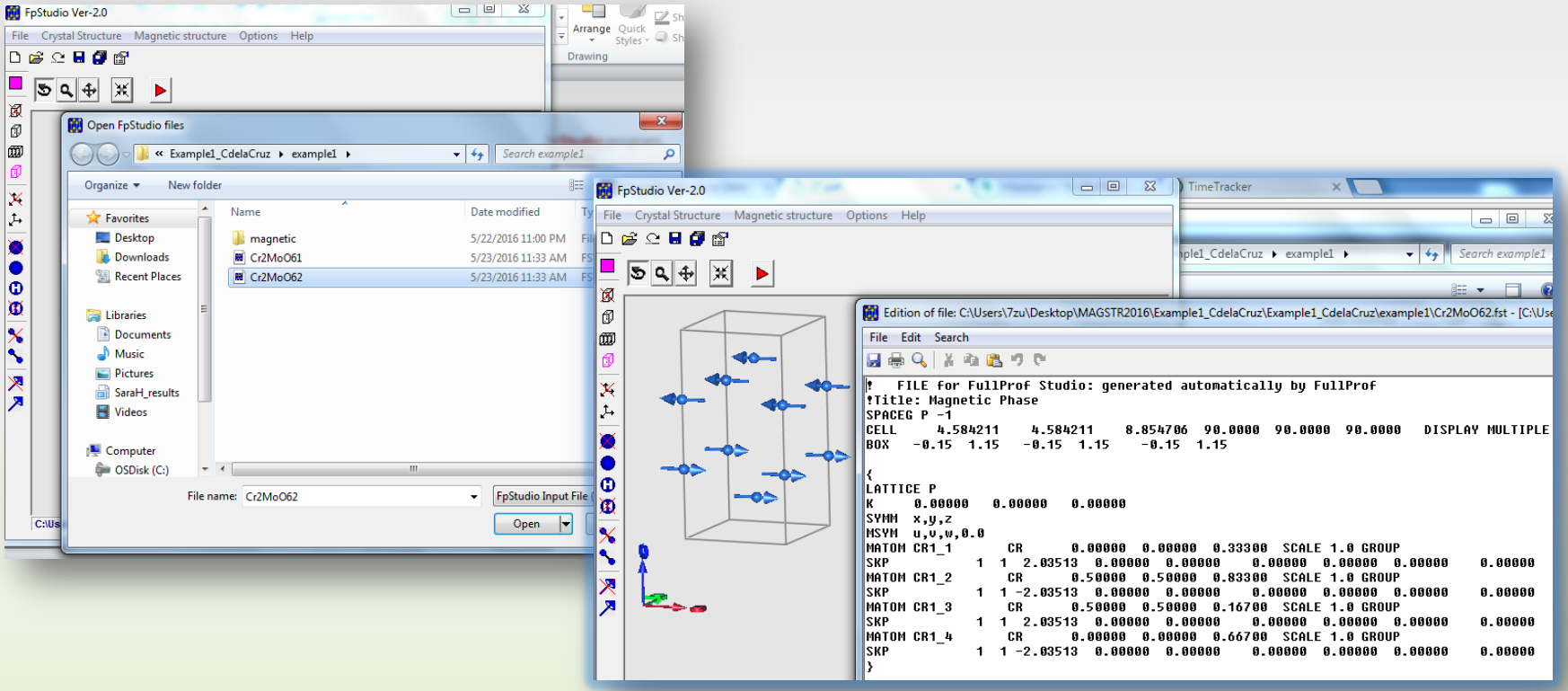
Cr: Mx = 2.036(20) μ_B

➔ Due to the symmetry of the crystal structure being tetragonal, one cannot uniquely determine the direction of the spin within the plane.

➔ From this refinement you may describe your structure as the Cr moments lying on the a-b plane with a magnitude of 2.036(20)/ μ_B per Cr site

VISUALIZATION OF THE MAGNETIC STRUCTURE

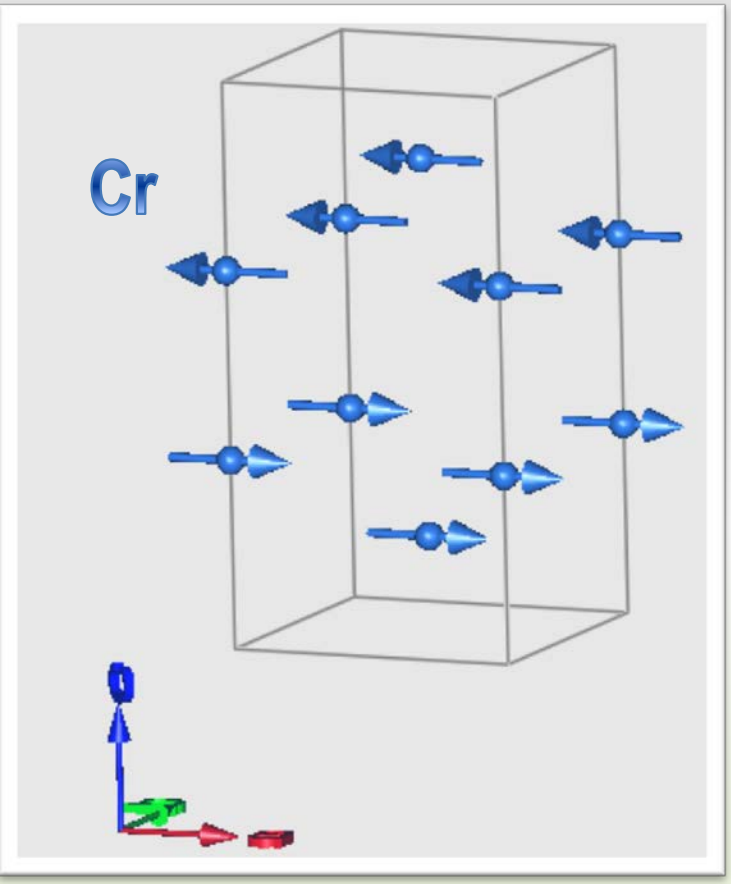
- to visualize the determined magnetic structure you can use **FpStudio** program. It reads *.fst files, generated automatically by The Fullprof or SARAh



- FpStudio uses Fourier coefficients notation (u,v,w). You can edit the input file if necessary to see how the structure changes as you change the coefficients or the k vector

CONGRATULATIONS ! Here is your magnetic structure

- ✓ To see list of magnetic moments at each site using the FPstudio: Magnetic structure ➔ List magnetic moments



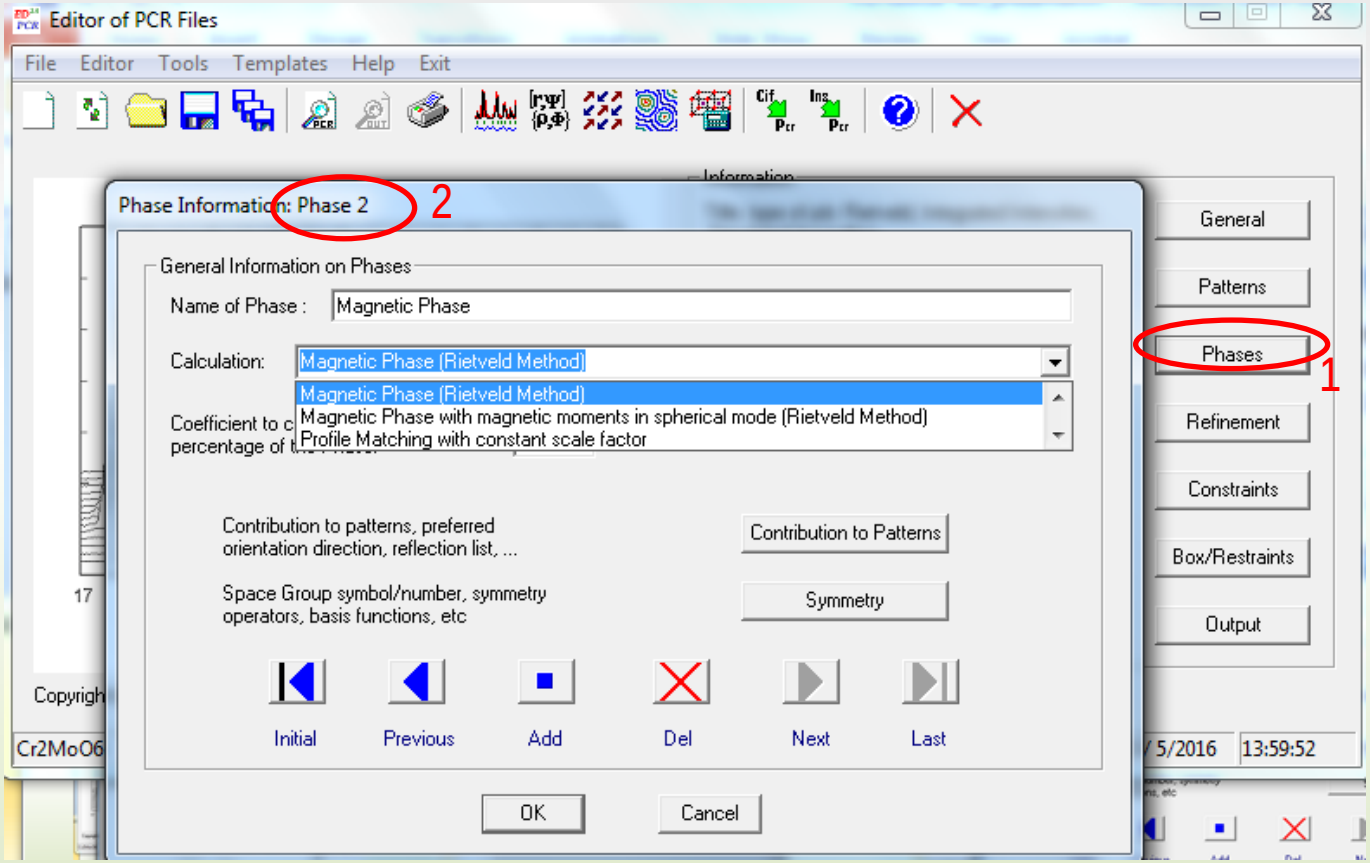
Fp-Studio Magnetic list - [C:\Users\7zu\Desktop\MAGSTR2016\Example1_CdelaCruz\Example1_CdelaCruz\example1\temp.dat]

File Edit Search

```
 Magnetic lattice type : P

 Magnetic k-vectors :
   0.000   0.000   0.000

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

Atom : CR1_1     CR
------------------------------------------------------------------------------
        x       y       z        Translation     k MSYM     m(a)     m(b)     m(c)     Mtot
    0.000   0.000   0.333
                             (   0,   0,   0)
                                                1    1    2.035    0.000    0.000
                                                          ---------------------------------
                                                          2.035    0.000    0.000    2.035
                             (   0,   1,   0)
                                                1    1    2.035    0.000    0.000
                                                          ---------------------------------
                                                          2.035    0.000    0.000    2.035
                             (   1,   0,   0)
                                                1    1    2.035    0.000    0.000
                                                          ---------------------------------
                                                          2.035    0.000    0.000    2.035
                             (   1,   1,   0)
                                                1    1    2.035    0.000    0.000
                                                          ---------------------------------
                                                          2.035    0.000    0.000    2.035
Atom : CR1_2     CR
------------------------------------------------------------------------------
        x       y       z        Translation     k MSYM     m(a)     m(b)     m(c)     Mtot
    0.500   0.500   0.833
                             (   0,   0,   0)
                                                1    1   -2.035    0.000    0.000
                                                          ---------------------------------
                                                         -2.035    0.000    0.000    2.035
Atom : CR1_3     CR
------------------------------------------------------------------------------
        x       y       z        Translation     k MSYM     m(a)     m(b)     m(c)     Mtot
    0.500   0.500   0.167
                             (   0,   0,   0)
                                                1    1    2.035    0.000    0.000
                                                          ---------------------------------
                                                          2.035    0.000    0.000    2.035
Atom : CR1_4     CR
------------------------------------------------------------------------------
        x       y       z        Translation     k MSYM     m(a)     m(b)     m(c)     Mtot
    0.000   0.000   0.667
                             (   0,   0,   0)
                                                1    1   -2.035    0.000    0.000
                                                          ---------------------------------
```

DESCRIBING THE MAGNETIC STRUCTURE USING MAGNETIC MATRICES

- In this method, we describe the magnetic moments on each site freely using only the k-vector, in either cartesian or spherical coordinates
- This is set as you choose how the magnetic phase (Phase 2) is described.



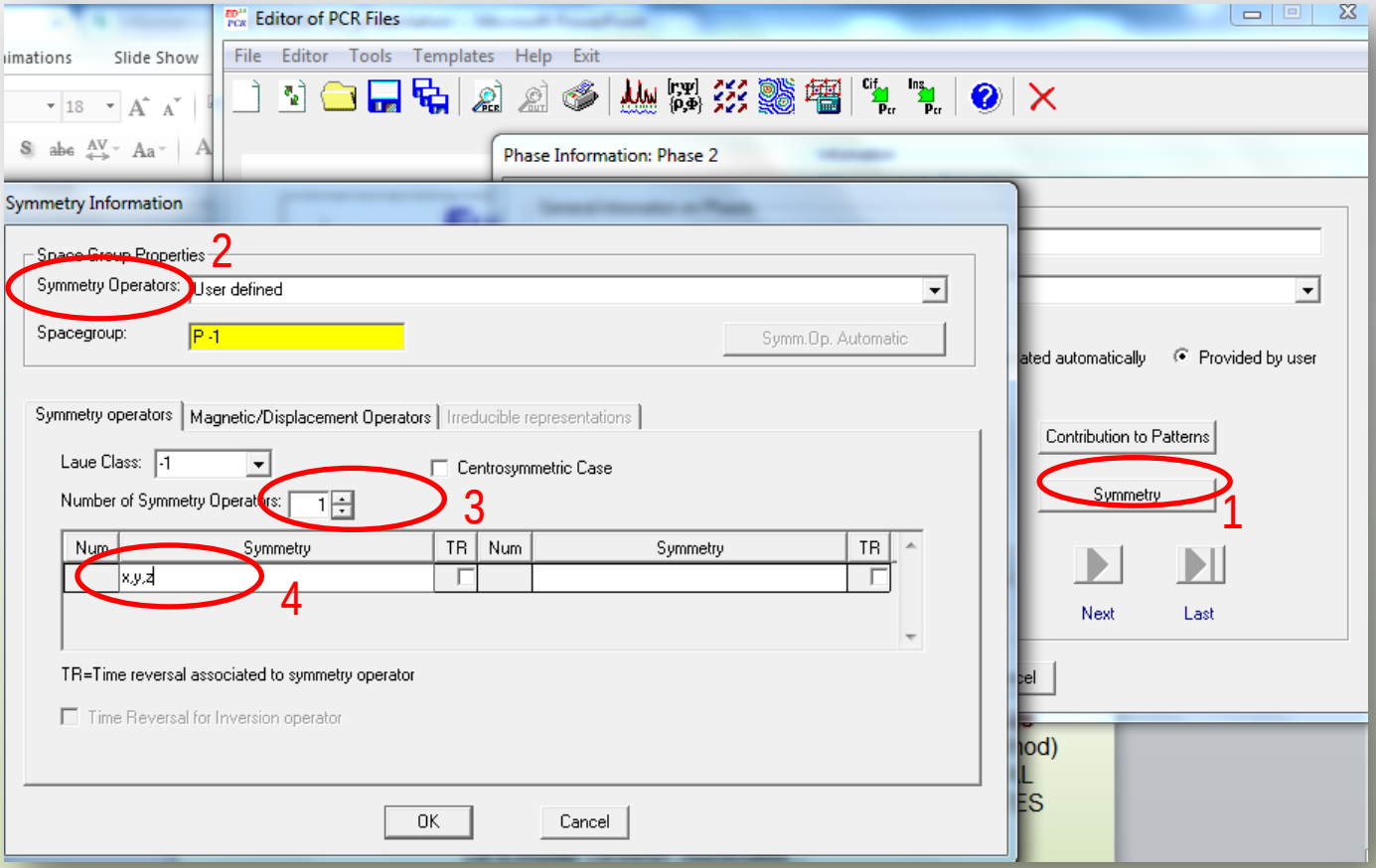
Choose the Calculation: Magnetic Phase (Rietveld Method) ➔CARTESIAN COORDINATES

Magnetic Phase with magnetic moments in spherical mode (Rietveld Method) ➔SPHERICAL COORDINATES

Let's choose Cartesian coordinates…

DESCRIBING THE MAGNETIC STRUCTURE USING MAGNETIC MATRICES

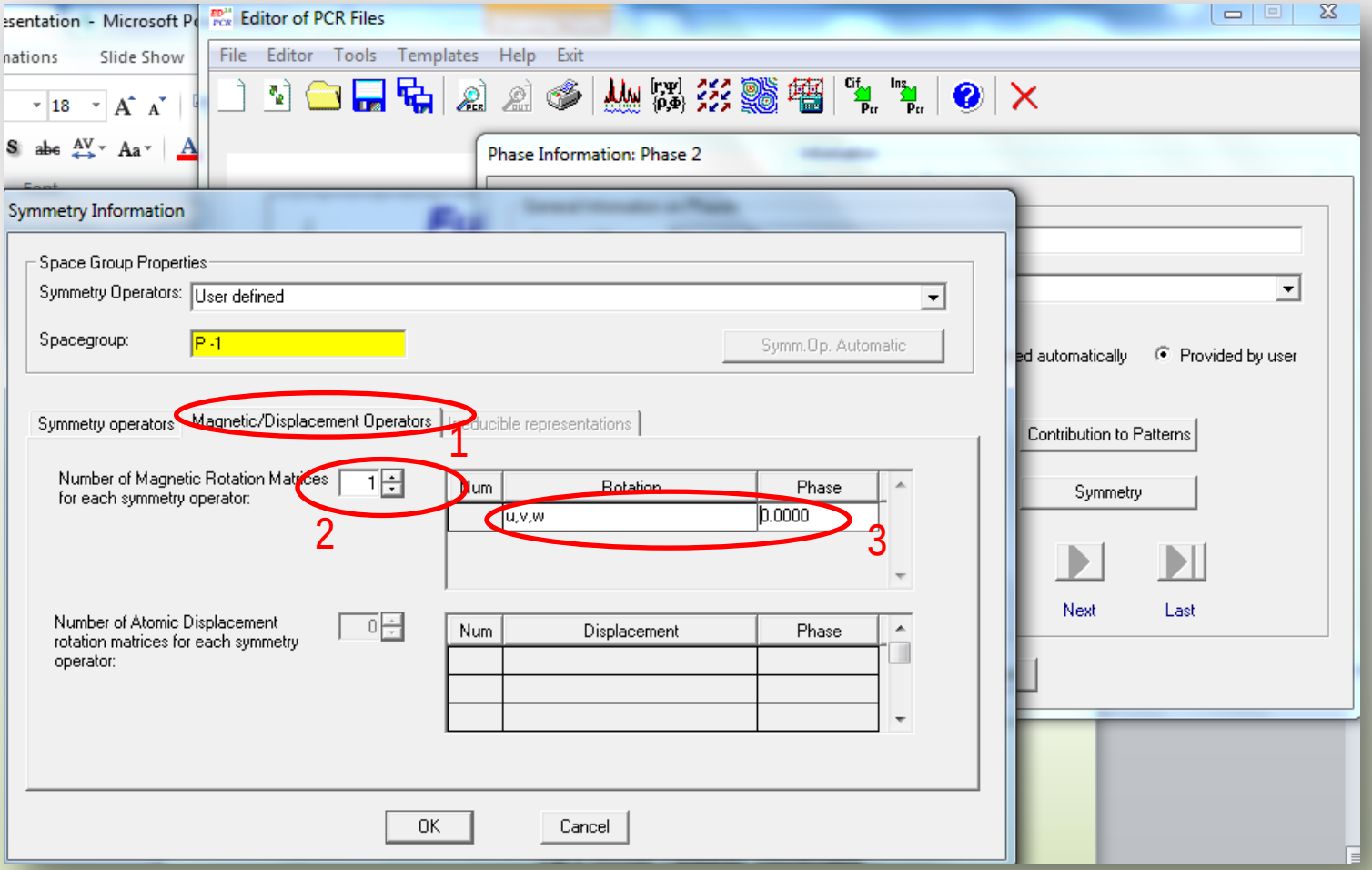
- Go into the Symmetry section (1), and set the Symmetry Operators to be “User defined” (2)
- Set the number of symmetry operators to 1 (3) and type **x,y,z** in the symmetry box (4)



Let’s choose Cartesian coordinates…

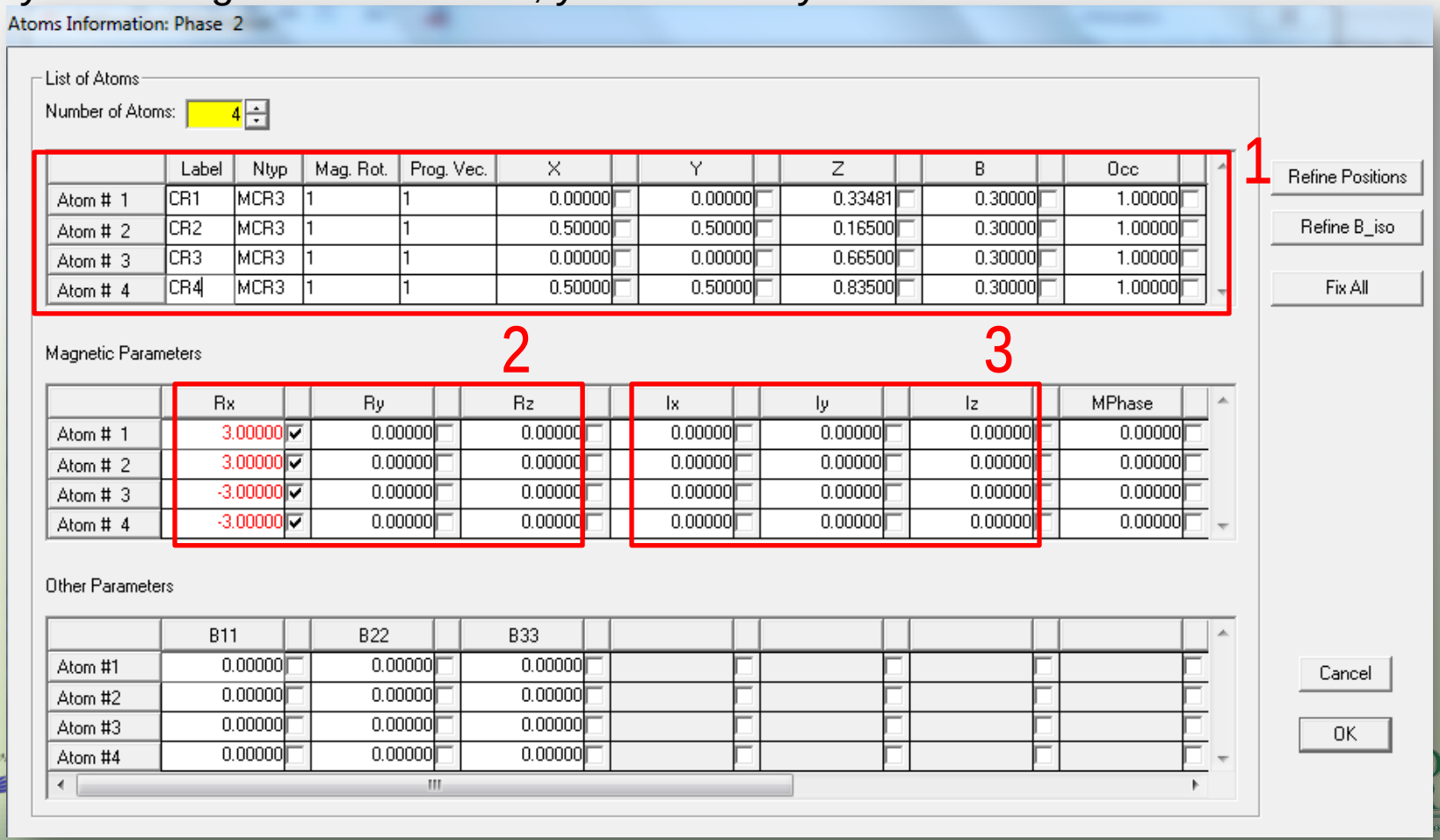
DESCRIBING THE MAGNETIC STRUCTURE USING MAGNETIC MATRICES

- Go into the Magnetic/Displacement Operators tab (1)
- Enter 1 for the no. of Magnetic Rotation matrices (2) Type **u,v,w** for the Rotation and 0.0 for the Phase (3)



DESCRIBING THE MAGNETIC STRUCTURE USING MAGNETIC MATRICES

- Enter Refinement ➔ Phase 2 ➔ Atoms to provide input for the magnetic structures
- Enter the magnetic ion information for all the inequivalent magnetic ion positions (1)
- The Magnetic parameters are described with real components along x,y and z (Rx, Ry,Rz) (2) and imaginary components (Ix, Iy, Iz) (3) in unit of μ_B
- The model desrcibed below is exactly the Ψ_9 of $\Gamma 10$ from the representational analysis. Though in this method, you can freely refine each of the moments.



DESCRIBING THE MAGNETIC STRUCTURE USING MAGNETIC MATRICES

- Below is the how the pcr looks like when using magnetic displacement vectors (MSYM) to describe the magnetic structure
- Note how the constraint on this refinement was implemented to have the magnetic moment magnitude equal on all Cr sites. All four variables have the same refinement flag 11.00 with the appropriate sign (+ or -)

```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   2  ==> Current R_Bragg for Pattern#  1:    11.87
!-------------------------------------------------------------------------------
Magnetic Phase
!
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
   4   0   0 0.0 0.0 1.0   1  -1  -1   0   0         0.000   1   7   0
!
P -1                        <--Space group symbol for hkl generation
!Nsym Cen Laue MagMat
   1   1   1   1
!
SYMM x,y,z
MSYM u,v,w, 0.000
!
!Atom   Typ  Mag Vek    X       Y       Z       Biso    Occ      Rx      Ry      Rz
!     Ix      Iy      Iz     beta11  beta22  beta33    MagPh
CR1    MCR3  1  1  0.00000 0.00000 0.33481 0.30000  1.00000   2.090   0.000   0.000
                     0.00    0.00    0.00    0.00     0.00    11.00    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
CR2    MCR3  1  1  0.50000 0.50000 0.16500 0.30000  1.00000   2.090   0.000   0.000
                     0.00    0.00    0.00    0.00     0.00    11.00    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
CR3    MCR3  1  1  0.00000 0.00000 0.66500 0.30000  1.00000  -2.090   0.000   0.000
                     0.00    0.00    0.00    0.00     0.00   -11.00    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
CR4    MCR3  1  1  0.50000 0.50000 0.83500 0.30000  1.00000  -2.090   0.000   0.000
                     0.00    0.00    0.00    0.00     0.00   -11.00    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
```