

Magnetic structure determination of $\text{Ho}_2\text{BaNiO}_5$ using FullProf Suite and SARAh

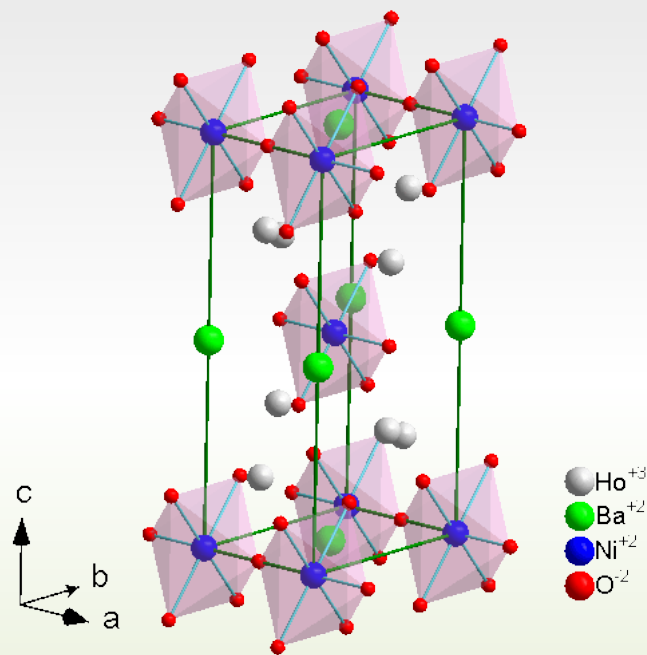


Orthorhombic (Space group: $Immm$)

$a=3.764 \text{ \AA}$, $b=5.761 \text{ \AA}$, $c=11.336 \text{ \AA}$

NiO_6 octahedra form chains along the a -axis.

3D Antiferromagnetic ordering at $T_N \sim 53 \text{ K}$



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Neutron diffraction study of the magnetic ordering in the series R_2BaNiO_5 (R = Rare Earth)

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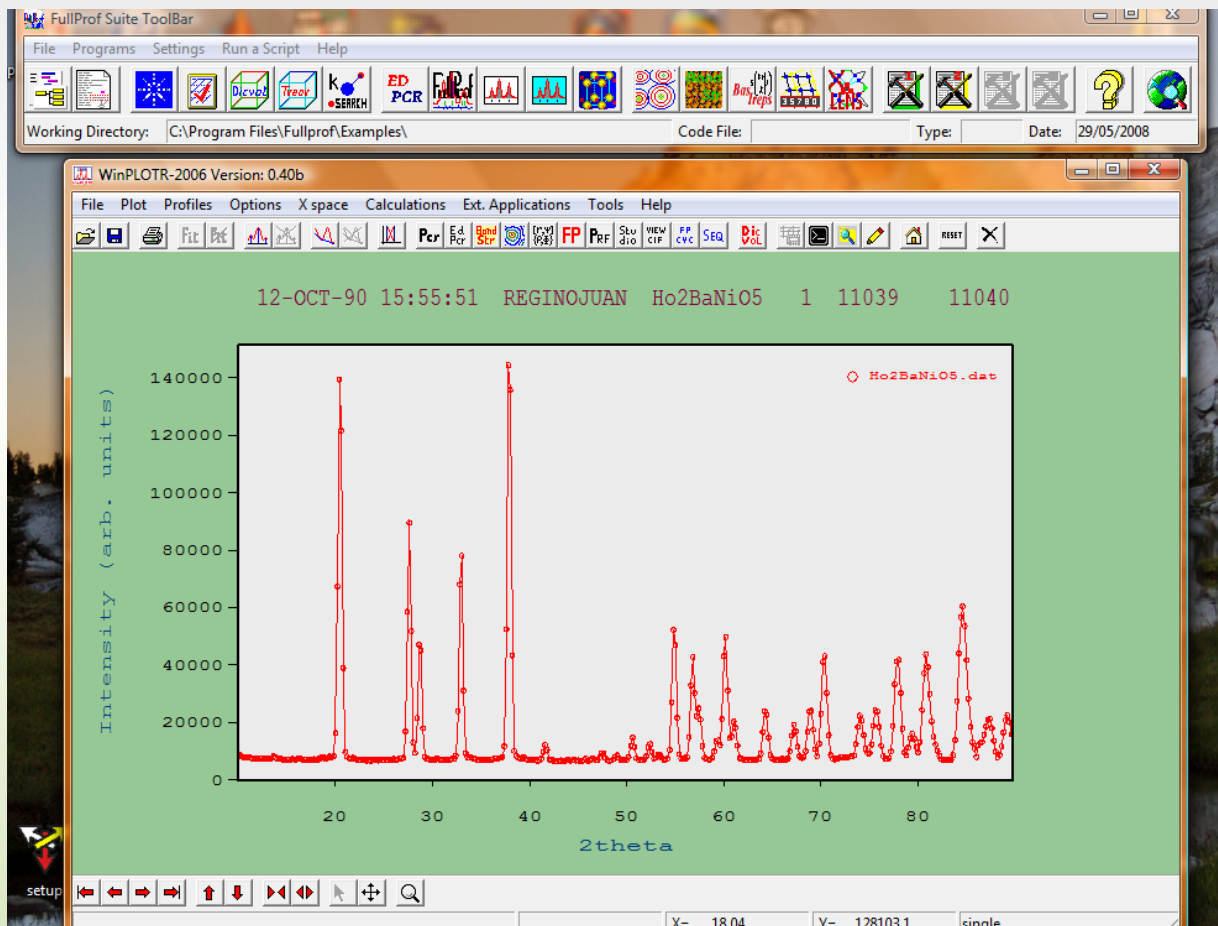
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Atom	Wyck.	Site	x/a	y/b	z/c
Ho	4j	mm2	1/2	0	0.2025(4)
Ni	2a	mmm	0	0	0

STARTING INFORMATION

- Neutron powder diffraction data collected at D1B –ILL at 1.5 K using $\lambda = 2.524 \text{ \AA}$ (File : Ho2BaNiO5.dat)
- Instrument resolution file: (d1b_ill.irf)
- Crystal structure known (File: Ho2BaNiO5.cif)

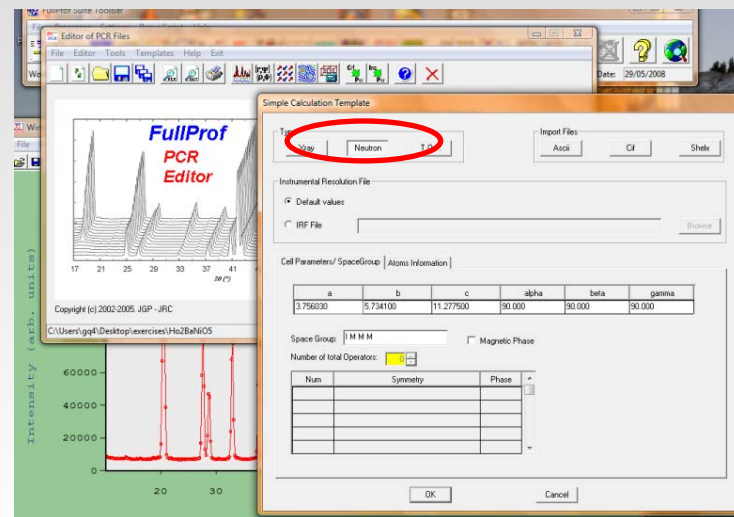
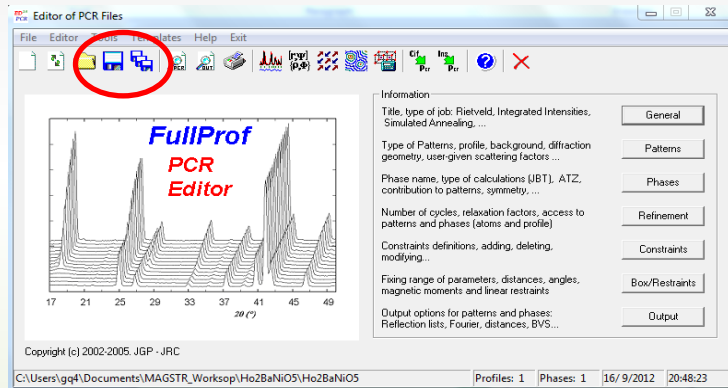


STEPS FOR MAGNETIC STRUCTURE DETERMINATION

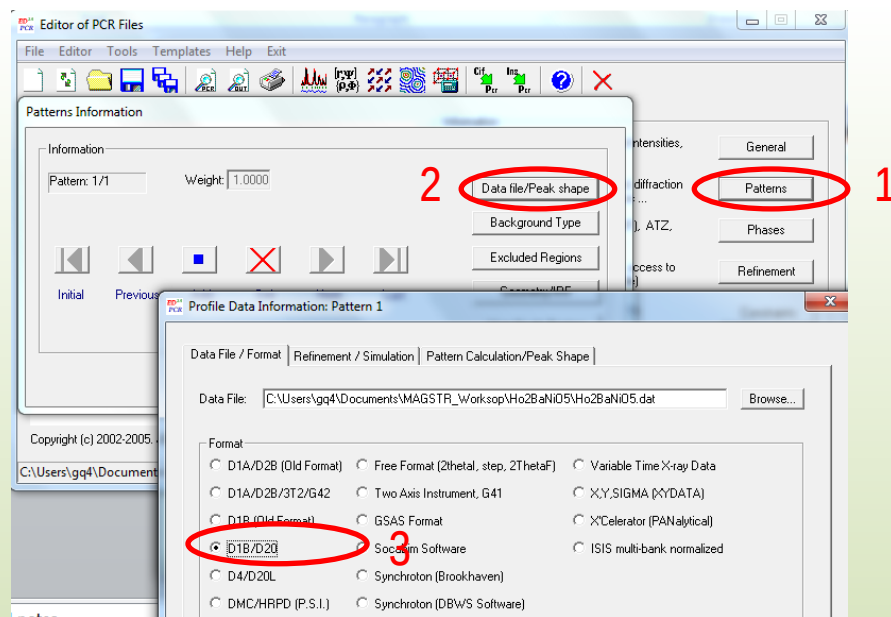
- ✓ refining the crystal structure for the paramagnetic state ($T > T_N$ or T_C)
→ **obtain all the relevant structural and profile parameters**
- ✓ preparing a PCR file and performing a refinement of the low temperature data ($T < T_N$) with fixed structural parameters (without a magnetic model)
→ **identify 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 *Baslreps* 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)

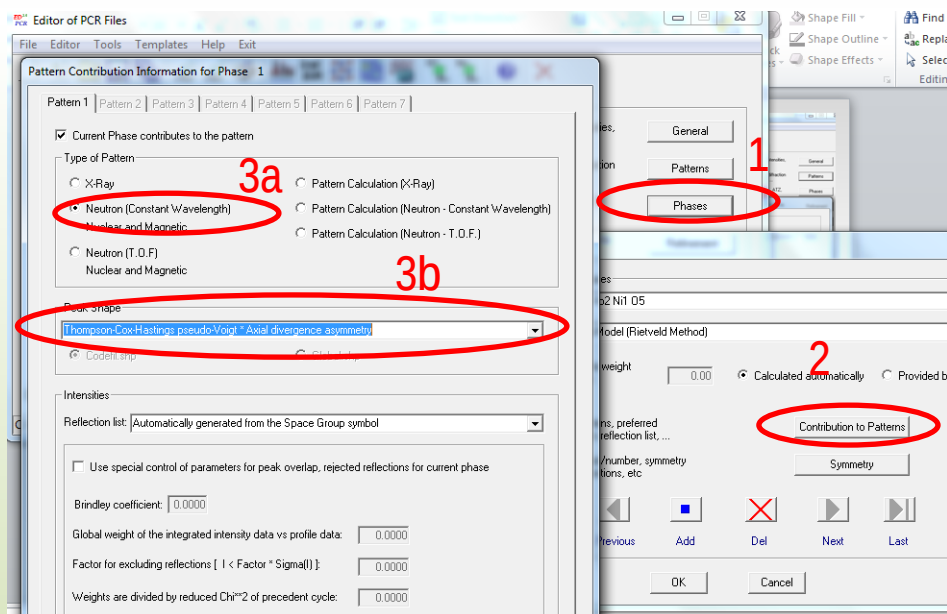
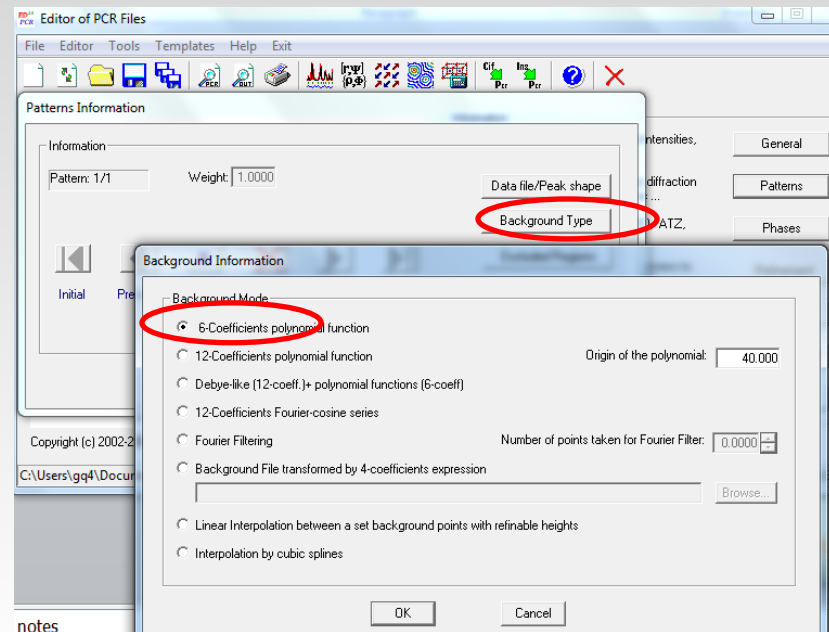
- o import the crystallographic information by clicking on “CIF to PCR”
- o in the new window, select the “Neutron” tab for the type of calculations
- o use the “Browse” button to upload the instrument resolution file “IRF” (d1b_ill.irf)



- o save the PCR file by clicking the “Save” button
- o open the “Patterns” tab (1) and then the “Data file/ peak shape” (2) and select the “D1B/D20” for the data file format (3)

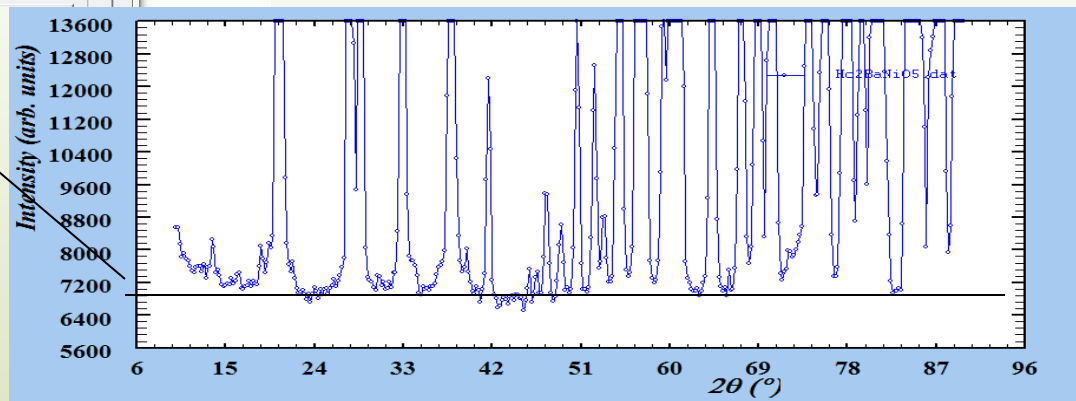
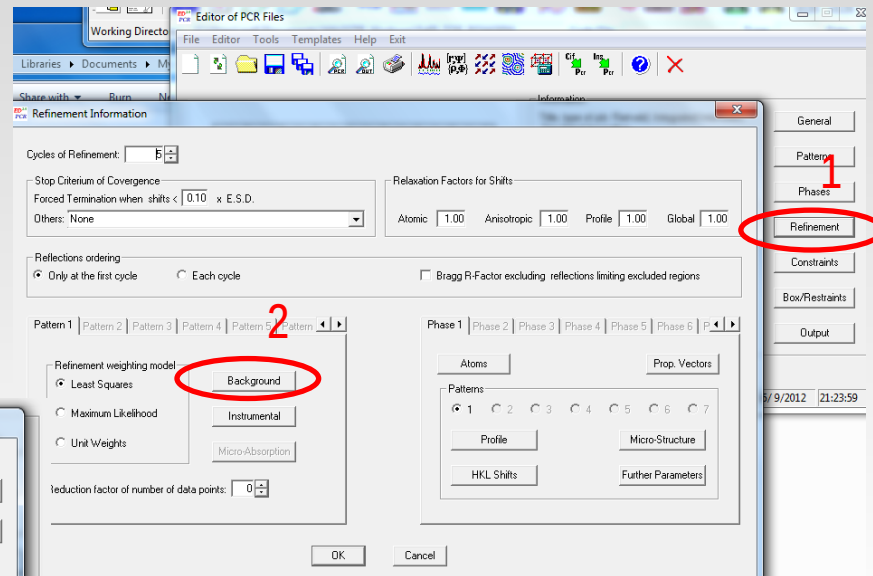
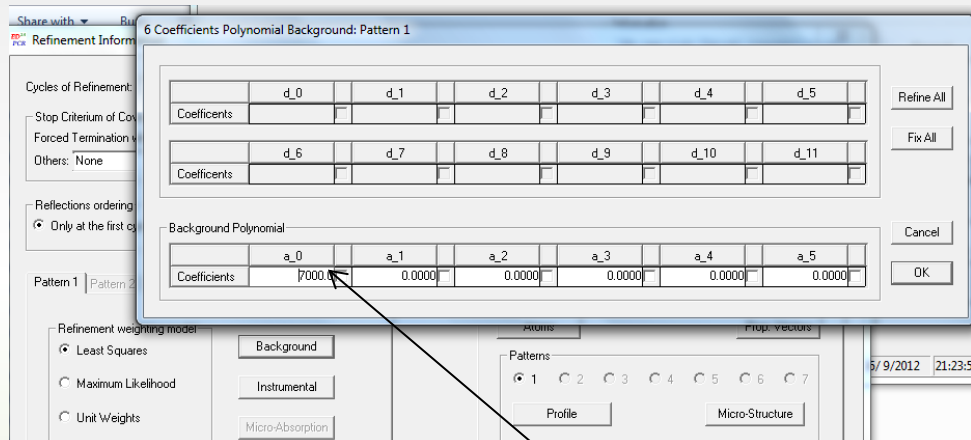


- o “Refinement/Simulation” tab, make sure that “Neutron-CW” option is selected, wavelength is “User defined”
 $\lambda_1 = \lambda_2 = 2.524 \text{ \AA}$
- o “pattern calculation” the “Thompson-Cox-Hastings pseudo-Voigt” peak shape is chosen
- o For the background information, select the “6-coefficients polynomial function”



- o 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”

- o Open the “Refinement” (1) and then the “Background” and add value for the “a₀” coefficient (~7000, read from the data file) that will give a first flat approximation for the background



- o 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
- o save the PCR file by clicking the “Save” button, every time a change has been made

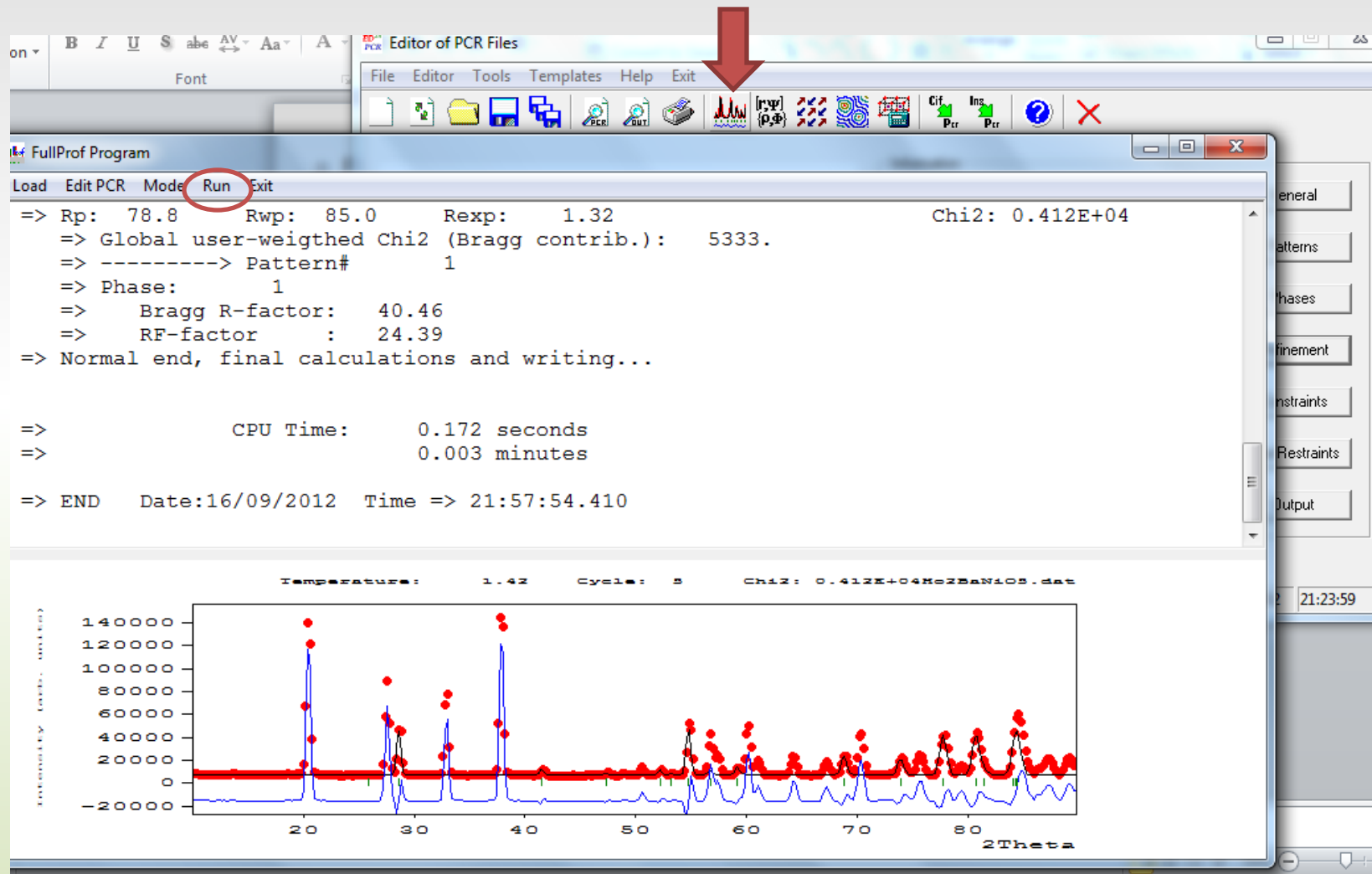
The screenshot displays the MAGSTR software interface. The 'Refinement Information' window is open, showing 'Cycles of Refinement' set to 5, which is circled in red. Below it, the 'Profile Parameters: Phase 1 Pattern 1' dialog box is open. In this dialog, the 'Scale' factor is set to 50.000, also circled in red, with a red number '2' above it. The 'Cell Parameters' table shows values for a, b, c, alpha, beta, and gamma. The 'FWHM / Shape Parameters' section includes tables for FWHM Parameters and Shape Parameters. On the right side, the 'Refinement' tab is selected in the sidebar, circled in red, with a red number '1' above it. The 'Profile' sub-tab is also visible.

	a	b	c	alpha	beta	gamma
Coefficients	3.756031	5.734100	11.277499	90.000	90.000	90.000

	U	V	W	IG
Coefficients	0.000000	0.000000	0.000000	0.000000

	X	Y	SZ
Coefficients	0.000000	0.000000	0.000000

- o Run the Fullprof program by click on button indicated below. 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)

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	52.856	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	3.751848	5.733387	11.270996	90.000	90.000	90.000

FWHM / Shape Parameters Asymmetry Parameters Preferred Orientation

FWHM Parameters

	U	V	W	IG
Coefficients	0.000000	0.000000	0.000000	0.000000

Refine All Fix All

- ✓ **Atomic parameters** (fractional atomic positions, thermal factors, occupation) can be accessed through **Refinement** → **Phase #** tab → **Atoms**

Phase 1 Phase 2 Phase 3 Phase 4 Phase 5 Phase 6

Atoms Prop. Vectors

Atoms Information: Phase 1

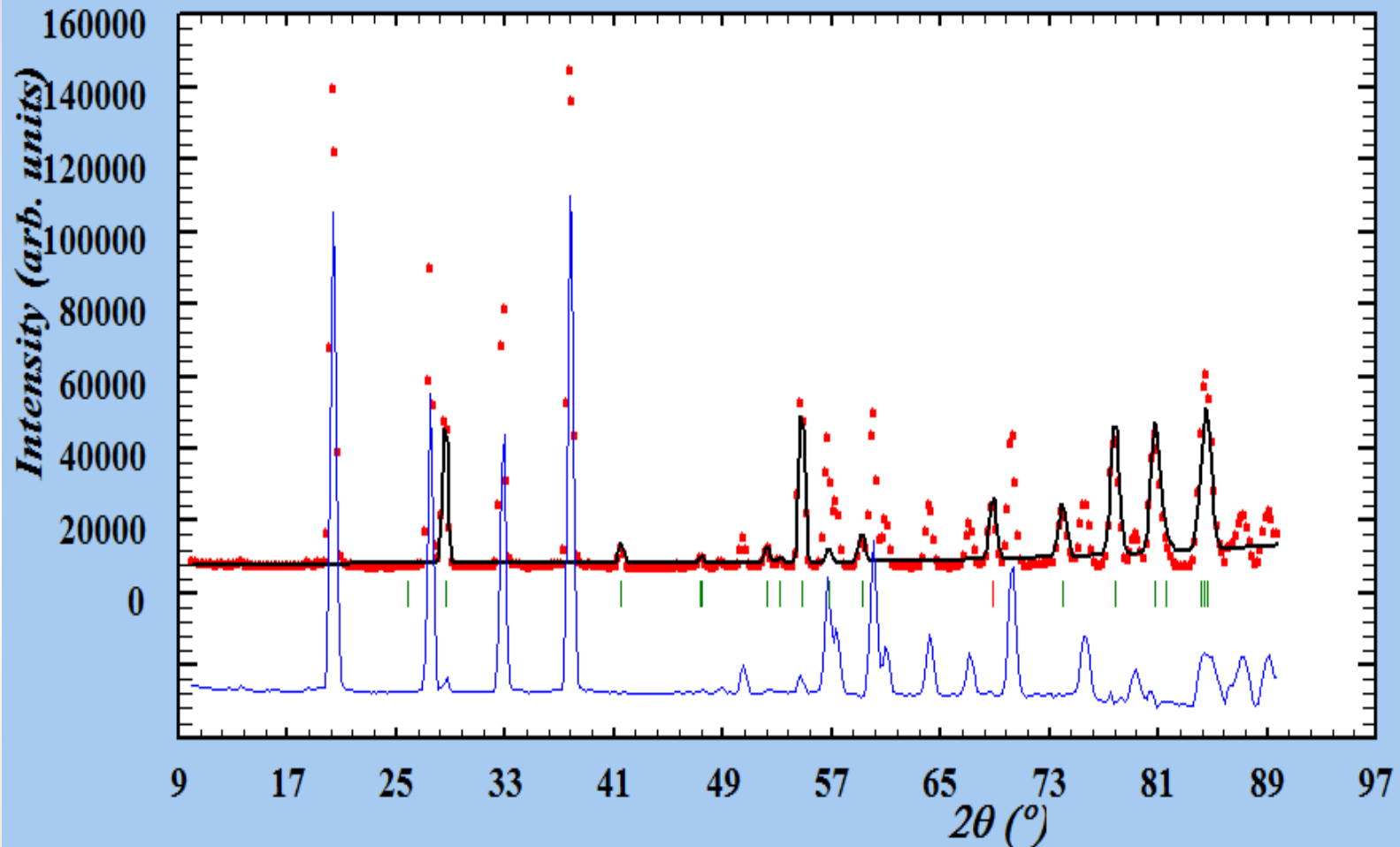
List of Atoms

Number of Atoms: 5

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Ho1	Ho	0.50000	0.00000	0.20178	0.30000	0.25000	Isotropic
Atom # 2	Ba1	Ba	0.50000	0.50000	0.00000	0.30000	0.12500	Isotropic
Atom # 3	Ni1	Ni	0.00000	0.00000	0.00000	0.30000	0.12500	Isotropic
Atom # 4	O1	O	0.00000	0.24224	0.14892	0.30000	0.50000	Isotropic

Anisotropic Thermal Factors / Form Factors

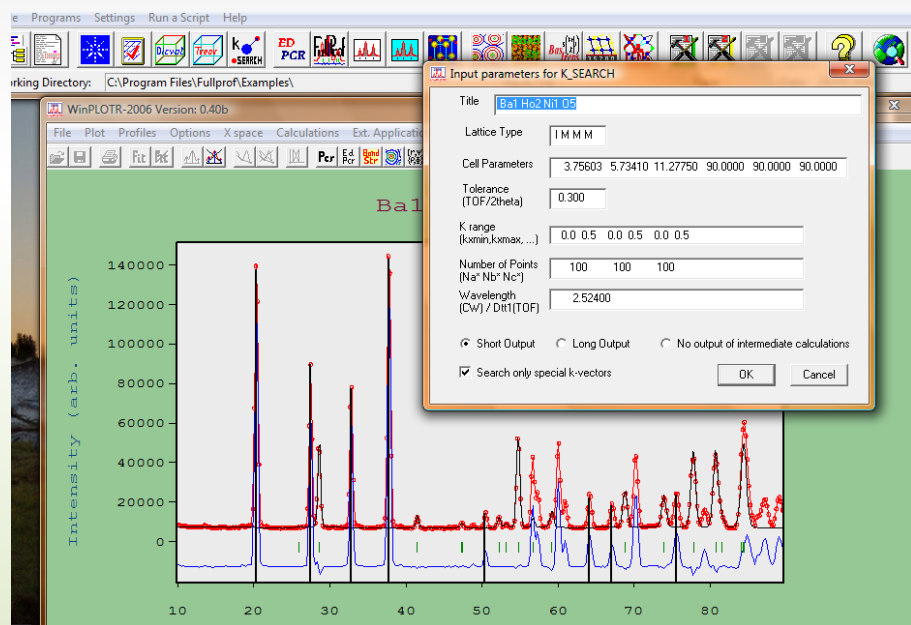
Ba1 Ho2 Ni1 O5



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

➤ INDEX THE MAGNETIC REFLECTIONS USING THE k-search program

- o 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”



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

=> List of satellites (hkl)+(Kx,Ky,Kz) for the best solution:

				Kx=0.5000	Ky=0.0000	Kz=0.5000			
H	K	L	n	D* (cal)	D* (obs)	2Th (cal)	2Th (obs)	2Th (obs-cal)	
1	0	1	1	0.1403	0.1398	20.3982	20.3261	-0.0721	
1	0	-1	1	0.1882	0.1880	27.4762	27.4512	-0.0250	
1	1	0	1	0.2238	0.2237	32.8159	32.7950	-0.0209	
1	1	2	1	0.2566	0.2564	37.7840	37.7571	-0.0269	
1	0	-3	1	0.3377	0.3371	50.4500	50.3532	-0.0968	
1	0	5	1	0.4206	0.4205	64.1262	64.0944	-0.0318	
-1	1	0	1	0.4380	0.4375	67.1170	67.0208	-0.0962	
1	2	-3	1	0.4855	0.4854	75.5671	75.5454	-0.0217	

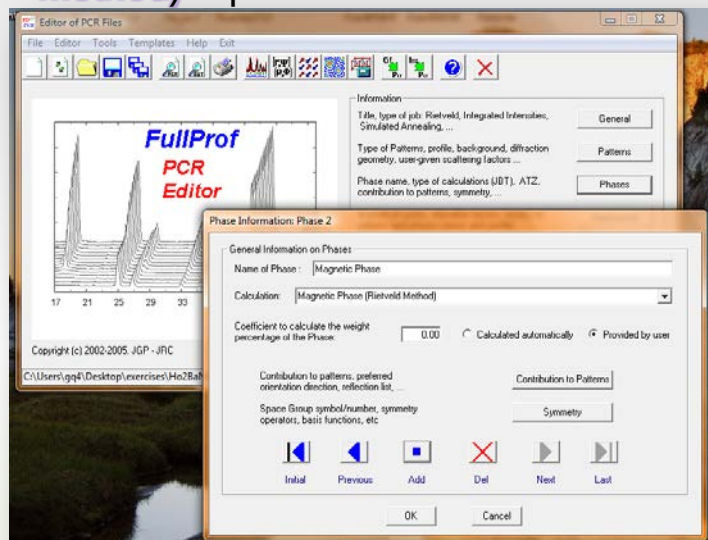
=> Best R-factor: 0.9461 % for propagation vector:

k = (0.5000 0.0000 0.5000)

for the $\text{Ho}_2\text{BaNiO}_5 \rightarrow k_m = (0.5, 0, 0.5)$

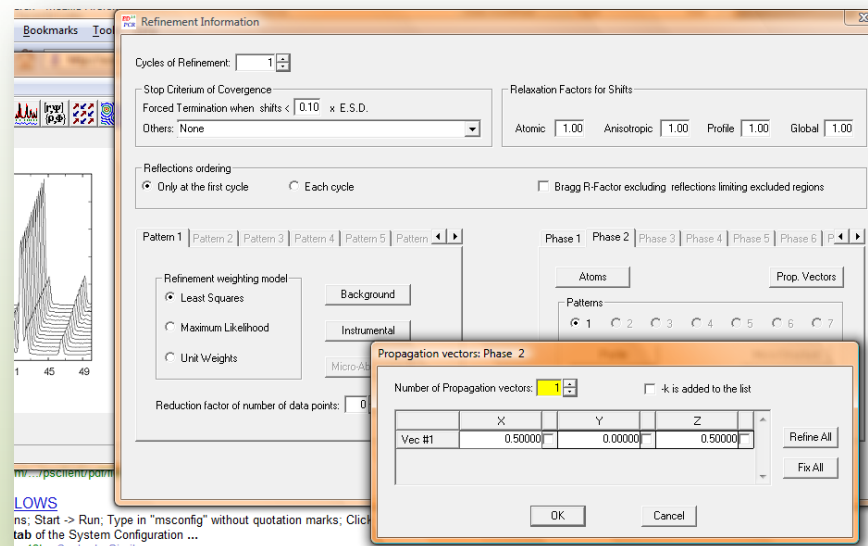
➤ ADDING THE MAGNETIC PHASE AS A SECOND PHASE TO THE PCR

- ✓ 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.



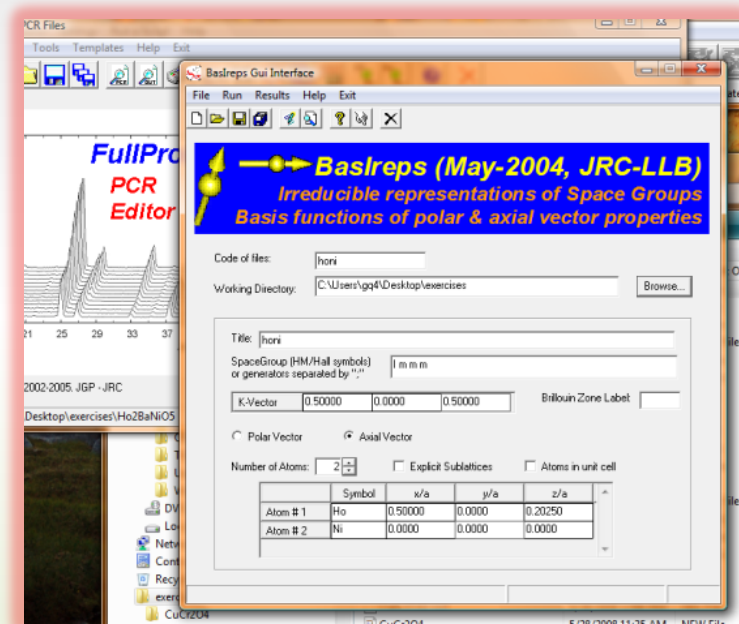
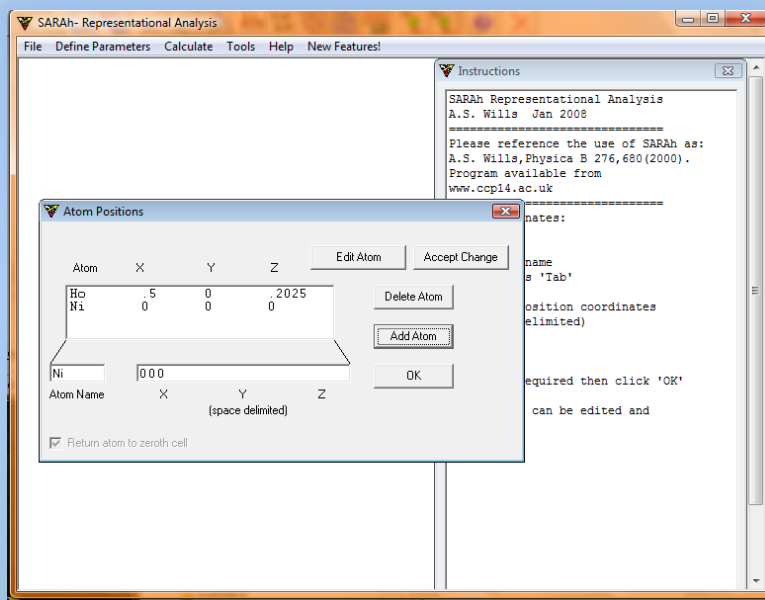
- ✓ you can also open the PCR file using your default text editor at this time and verify that the second phase has been successfully added. Don't worry about the symmetry at this time.

- ✓ 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 the **SARAh** program or **Baslreps** to generate the Irreducible representations and basis vectors associated with $k_m = (0.5, 0, 0.5)$. Both programs require 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.

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

Ho

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_1	ψ_1	1	0	4	0	0	0	0
		2	0	4	0	0	0	0
Γ_2	ψ_2	1	4	0	0	0	0	0
		2	-4	0	0	0	0	0
	ψ_3	1	0	0	4	0	0	0
		2	0	0	-4	0	0	0
Γ_3	ψ_4	1	4	0	0	0	0	0
		2	4	0	0	0	0	0
	ψ_5	1	0	0	4	0	0	0
		2	0	0	4	0	0	0
Γ_4	ψ_6	1	0	4	0	0	0	0
		2	0	-4	0	0	0	0

Table 1: Basis vectors for the space group $I m m m$ with $k_{-55} = (.5, 0, .5)$. The decomposition of the magnetic representation for the Ho site $(.5, 0, .2025)$ is $\Gamma_{Mag} = 1\Gamma_1^1 + 2\Gamma_2^1 + 2\Gamma_3^1 + 1\Gamma_4^1$. The atoms of the nonprimitive basis are defined according to 1: $(.5, 0, .2025)$, 2: $(.5, 0, .7975)$.

Γ_1 constraints moments to lie along the *b*-axis

Γ_3 constraints moments to lie in the *ac*-plane

Ni

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_1	ψ_1	1	0	4	0	0	0	0
Γ_3	ψ_2	1	4	0	0	0	0	0
	ψ_3	1	0	0	4	0	0	0

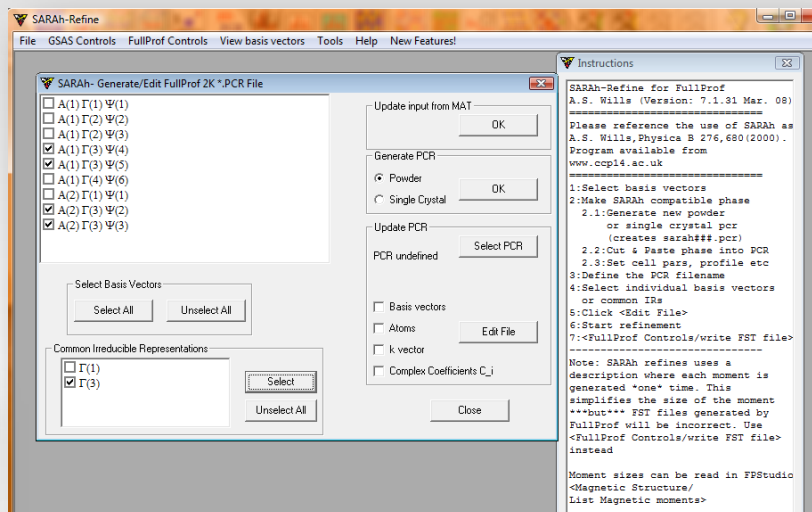
Table 2: Basis vectors for the space group $I m m m$ with $k_{-55} = (.5, 0, .5)$. The decomposition of the magnetic representation for the Ni site $(0, 0, 0)$ is $\Gamma_{Mag} = 1\Gamma_1^1 + 0\Gamma_2^1 + 2\Gamma_3^1 + 0\Gamma_4^1$. The atom of the primitive basis is defined according to 1: $(0, 0, 0)$.

- ✓ If the two sites (Ni and Ho) order according to the same representation only the representations 1 and 3 are allowed.

- ✓ “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 “sarah71.pcr”

- ✓ You’ll need to select the basis vectors corresponding to one of the two common Irreducible Representations (gamma3 or Γ_3 in our case).

```
sarah71.pcr - Notepad
File Edit Format View Help
! Real(0)-Imaginary(1) indicator for C1
0 0
!
SYMM X, Y, Z
BASR 2 0 0 0 0 0 2
BASR 0 0 0 0 0 0 0
BASR 4 0 0 0 0 0 4
BASR 0 0 0 0 0 0 0
SYMM -X+1, Y, -Z+1
BASR 2 0 0 0 0 0 2
BASR 0 0 0 0 0 0 0
BASR 0 0 0 0 0 0 0
BASR 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
HO1 MHO3 1 0 .500000 .000000 .20250 .30000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 .000000 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
NI2 MN13 2 0 .000000 .000000 .30000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 .000000 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1
! Scale Shape1 Bv Str1 Str2 Str3 Strain-Model
10.0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0
0.00000 0.00 0.00 0.00 0.00 0.00 0.00
! U V W X Y GauSiz Lrsiz Size-Model
1.08239 -0.23233 0.25618 0.00000 0.00000 0.00000 0.00000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma
273
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
.5000000 .0000000 .5000000
0.000000 0.000000 0.000000 Propagation Vector 1
```



- ✓ Note that the selected model Γ_3 constraints the magnetic moments of Ho and Ni to lie in the ac-plane
- ✓ Open the PCR file generated by Sarah (“sarah71.pcr”), copy the entire content of the file and PASTE it over the section of the second phase of your Ho₂BaNiO₅ 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.

External EdPCR Text Editor - C:\Users\j7zu\Desktop\MAGSTR2014\cdelacruz_example1\ho2banio5.pcr

File Edit Search

! Real(0)-Imaginary(0) indicator for Ci

0 0

! SVHM X, V

BASR 2 0 0 0 0 2

BASI 0 0 0 0 0 0

BASR 4 0 0 0 0 4

BASI 0 0 0 0 0 0

SVHM -X+1, V, -Z+1

BASR 2 0 0 0 0 2

BASI 0 0 0 0 0 0

BASR 0 0 0 0 0 0

BASI 0 0 0 0 0 0

! Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3

H01 C4 C5 C6 C7 C8 C9 MagPh

JH03 1 1 0.50000 0.00000 0.20284 0.30000 1.00000 0.046 4.576 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 11.00 21.00 0.00

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

H12 MN13 2 1 0.00000 0.00000 0.00000 0.30000 1.00000 0.187 -0.316 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 31.00 41.00 0.00

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

! Profile Parameters for Pattern # 1

Scale Shape1 Bov Str1 Str2 Str3 Strain-Model

55.467 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0

91.00000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

U U U X Y GauSiz LorSiz Size-Model

0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

a b c alpha beta gamma #Cell Info

3.754295 5.730079 11.269611 90.000000 90.000000 90.000000 0.000000

81.00000 101.00000 111.00000 0.00000 0.00000 0.00000 0.00000

Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S L D I

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

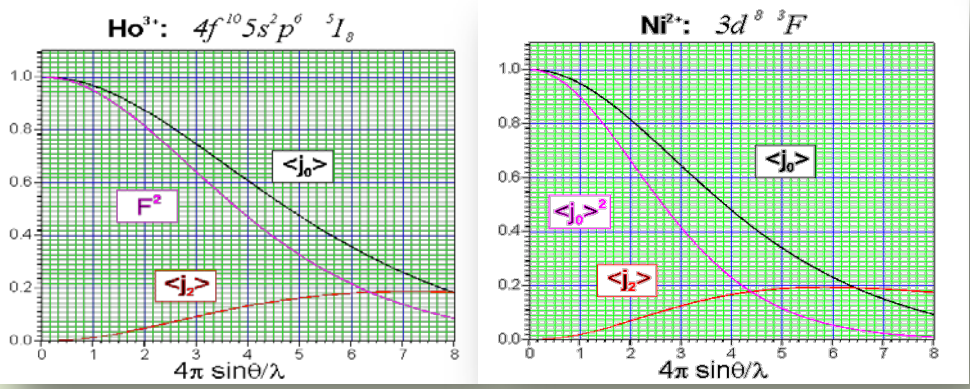
! Propagation vectors:

0.5000000 0.0000000 0.5000000 Propagation Vector 1

0.0000000 0.0000000 0.0000000

2Th1/TOF1 2Th2/TOF2 Pattern # 1

10.010 20.010 1



$$S_{kjs} = \sum_{n\lambda} C_{n\lambda}^v S_{n\lambda}^{k v} (js)$$

Fourier coefficient for calculation of m_{ijs} at each site

$$S_k = C_1 S^1 + C_2 S^2$$

✓ make sure that the correct parameters for the magnetic scattering form factors are used **JH03** for the magnetic rare earth Ho³⁺ and **MN13** for the transition metal ion Ni³⁺

$$I(\delta) = \langle I^0(\delta) \rangle + \left(1 - \frac{\delta}{5}\right) \langle I^5(\delta) \rangle$$

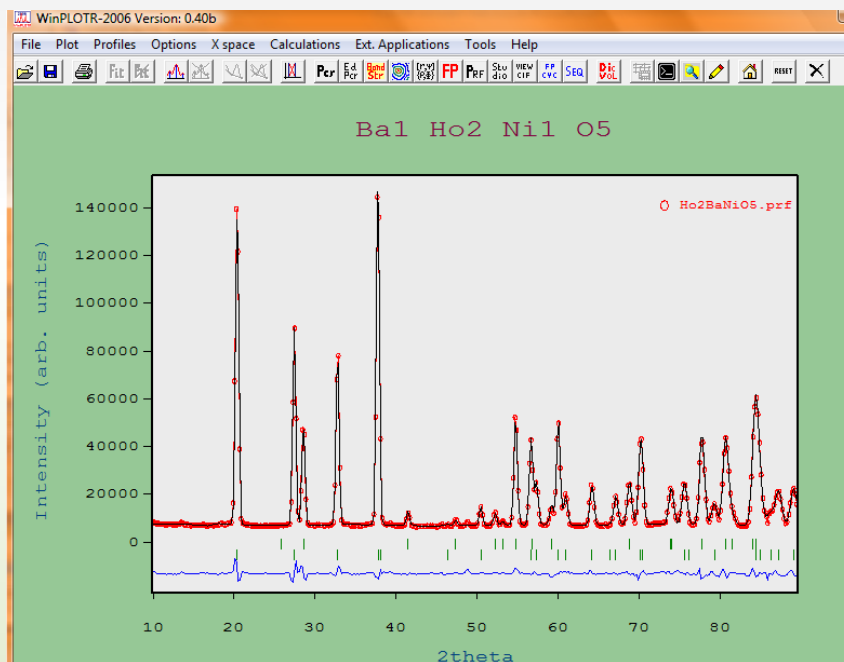
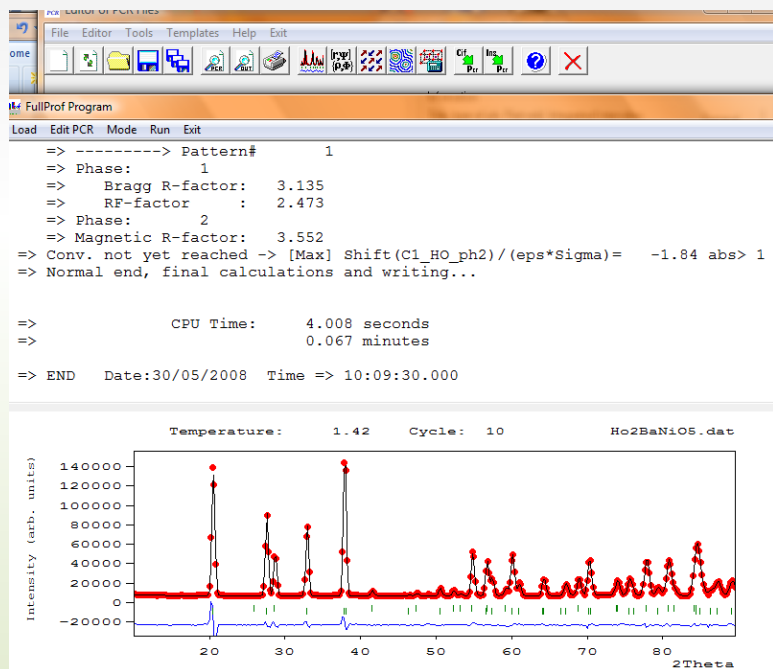
International Tables of Crystallography, Volume C, ed. by AJC Wilson, Kluwer Ac. Pub., 1998, p. 513

➤ MAGNETIC STRUCTURE REFINEMENT

- ✓ select the basis vector coefficients C1 and C2 for the two independent magnetic ions (Ho and Ni) to be refined
- ✓ run the refinement using the FullProf program
- ✓ start to refine additional parameters (profile, lattice ...) to obtain a good quality fit.

Basis Functions Coefficients

	C1		C2		C3		C4	
Atom # 1	2.00000	☒	2.00000	☒	0.00000	☐	0.00000	☐
Atom # 2	0.12300	☒	0.18300	☒	0.00000	☐	0.00000	☐



MAGNETIC MOMENT DETERMINATION

- ✓ Check the output file (*.out) from FullProf. Verify that the magnetic structure model and the magnitude of the Ho and Ni moments are meaningful

External EdPCR Text Editor - [C:\Users\7zu\Desktop\MAGSTR2014\Cdelacruz_example1\Ho2BaNiO5.out]

File Edit Search

=> Phase 2 Name: Magnetic Phase

=> New parameters, shifts, and standard deviations

Atom	x	dx	sx	y	dy	sy	z	dz	sz	B	dB	SB	occ.
HO1	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20250	0.00000	0.00000	0.30000	0.00000	0.00000	1.00000
NI2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.30000	0.00000	0.00000	1.00000

=> Coefficients of basis vectors, shifts, and standard deviations:

Atom	C1	dc1	sc1	C2	dc2	sc2	C3	dc3	sc3
	C4	dc4	sc4	C5	dc5	sc5	C6	dc6	sc6
	C7	dc7	sc7	C8	dc8	sc8	C9	dc9	sc9
	MPhas	dMPhas	sMPhas						
HO1	0.089718	0.000000	0.065527	9.029646	0.000000	0.054908	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NI2	0.765226	0.000000	0.125650	-1.242781	0.000000	0.050806	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Line:1708 Col:30

The moment $\mathbf{m}_{ljs}$ is calculated from the refined values of the Fourier components S_{kjs}

$$\mathbf{m}_{ljs} = \sum_{\{k\}} S_{kjs} \exp\{-2\pi i k \mathbf{R}_l\}$$

$$S_{kjs} = \sum_{n\lambda} C_{n\lambda}^v S_{n\lambda}^{kv}(js)$$

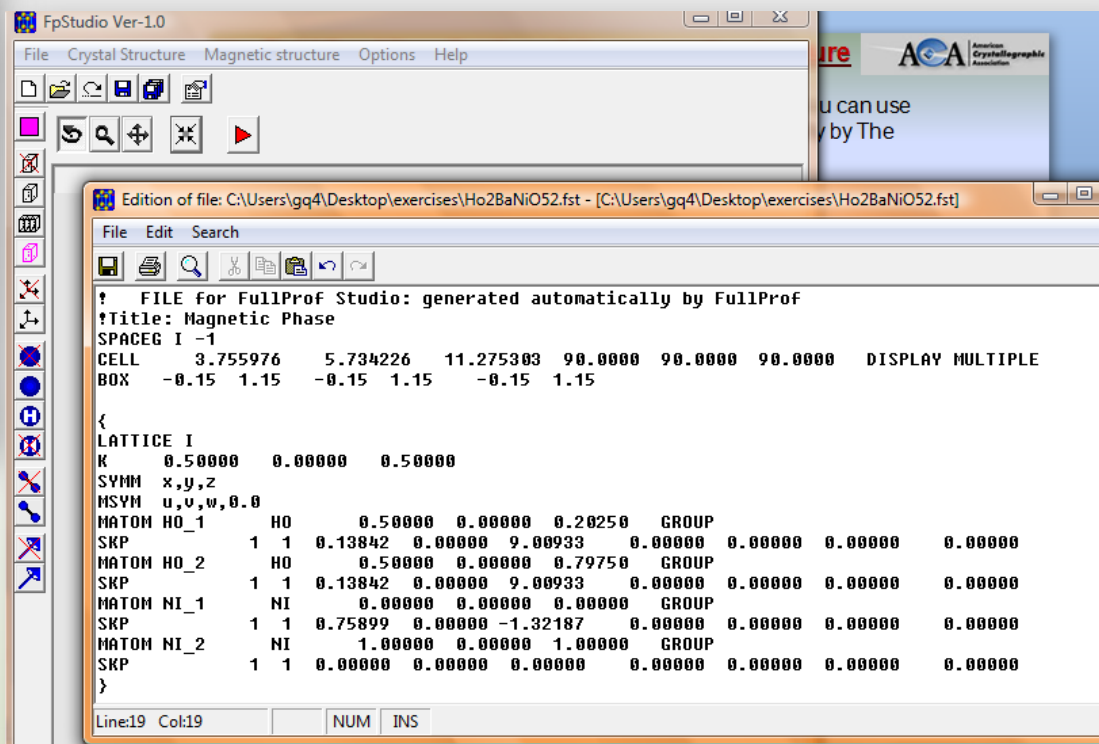
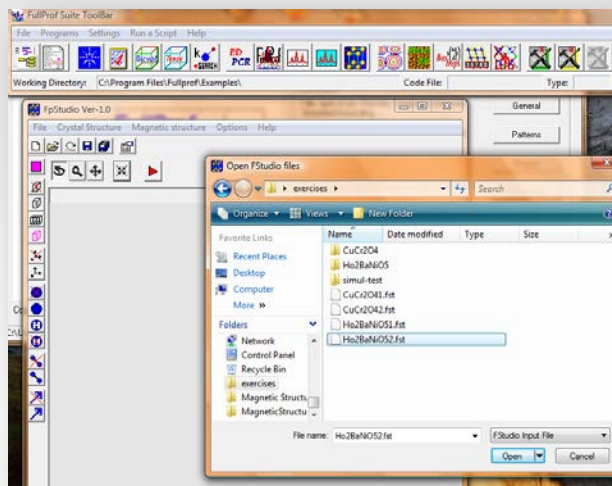
Ho: $M_x = 0.09(6) \mu_B$; $M_z = 9.03(5) \mu_B$

Ni: $M_x = 0.77(12) \mu_B$; $M_z = -1.24(5) \mu_B$

the moment of Ho is nearly parallel to the c-axis and the Ni-moment is canted by ~ 29 deg with respect to the c-axis

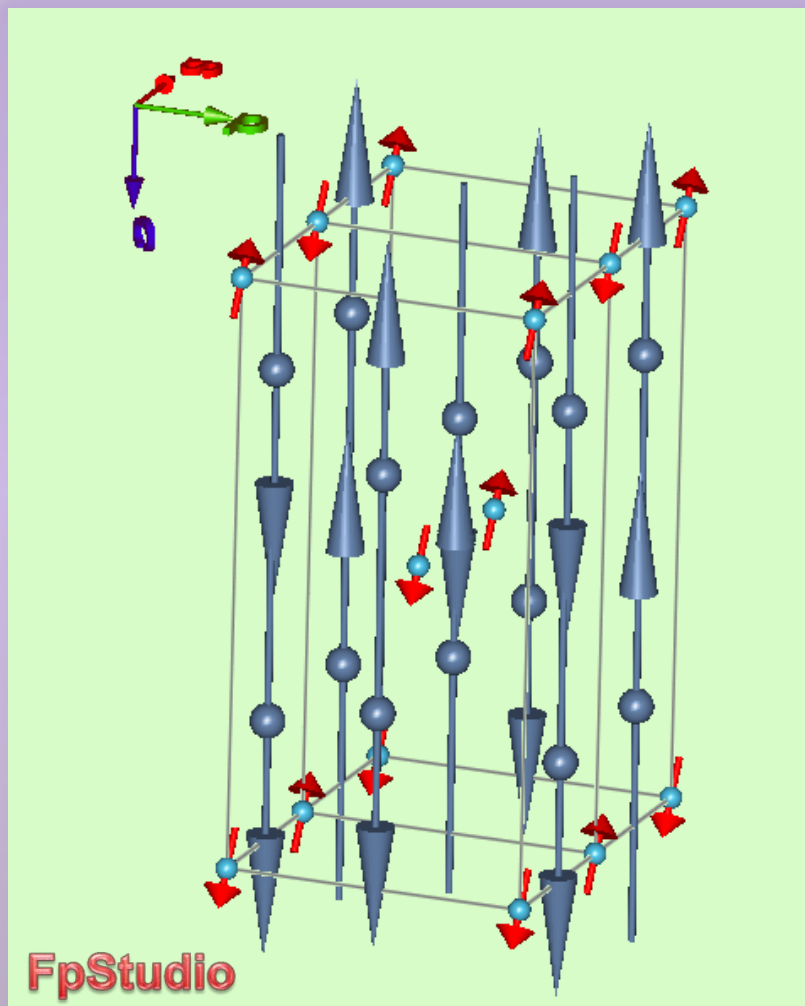
➤ VISUALIZATION OF THE MAGNETIC STRUCTURE

- ✓ 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..

CONGRATULATIONS ! Here is your magnetic structure



- ✓ To see list of magnetic moments at each site:
Magnetic structure → List magnetic moments

Atom : H01_1 H0									
x	y	z	Translation	k	MSYM	m(a)	m(b)	m(c)	Mtot
0.500	0.000	0.203	(0, 0, 0)	1	1	0.090	0.000	9.030	
						0.090	0.000	9.030	9.030
Ho									
			(0, 1, 0)	1	1	0.090	0.000	9.030	
						0.090	0.000	9.030	9.030
0.000	0.500	0.703	(0, 0, 0)	1	1	0.090	0.000	9.030	
						0.090	0.000	9.030	9.030
			(1, 0, 0)	1	1	-0.090	0.000	-9.030	
Atom : NI2_1 NI									
x	y	z	Translation	k	MSYM	m(a)	m(b)	m(c)	Mtot
0.000	0.000	0.000	(0, 0, 0)	1	1	0.765	0.000	-1.243	
						0.765	0.000	-1.243	1.459
Ni									
			(0, 0, 1)	1	1	-0.765	0.000	1.243	
						-0.765	0.000	1.243	1.459
			(0, 1, 0)	1	1	0.765	0.000	-1.243	
						0.765	0.000	-1.243	1.459
			(0, 1, 1)	1	1	-0.765	0.000	1.243	
						-0.765	0.000	1.243	1.459
			(1, 0, 0)	1	1	-0.765	0.000	1.243	
						-0.765	0.000	1.243	1.459
			(1, 0, 1)	1	1	0.765	0.000	-1.243	
						0.765	0.000	-1.243	1.459