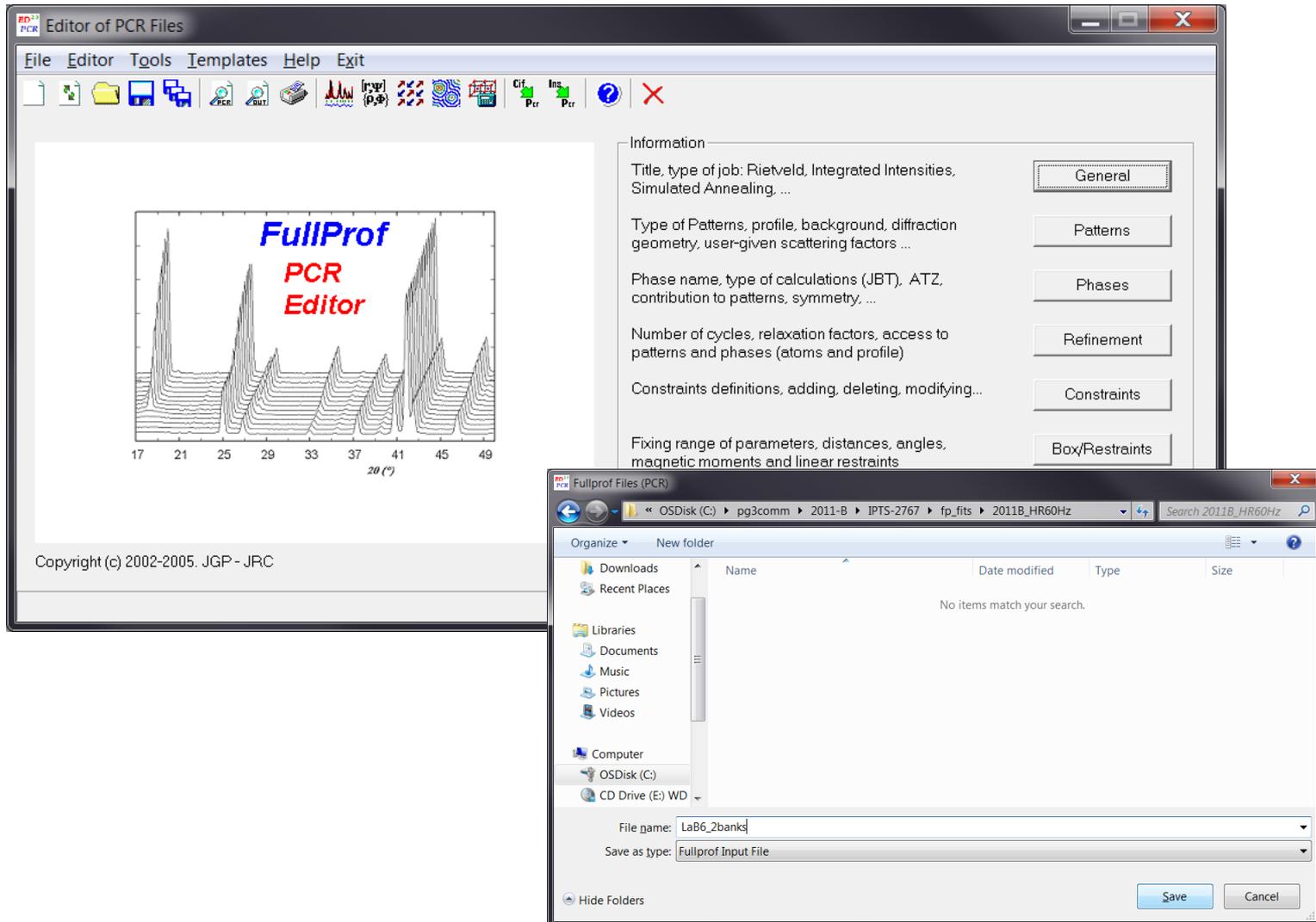
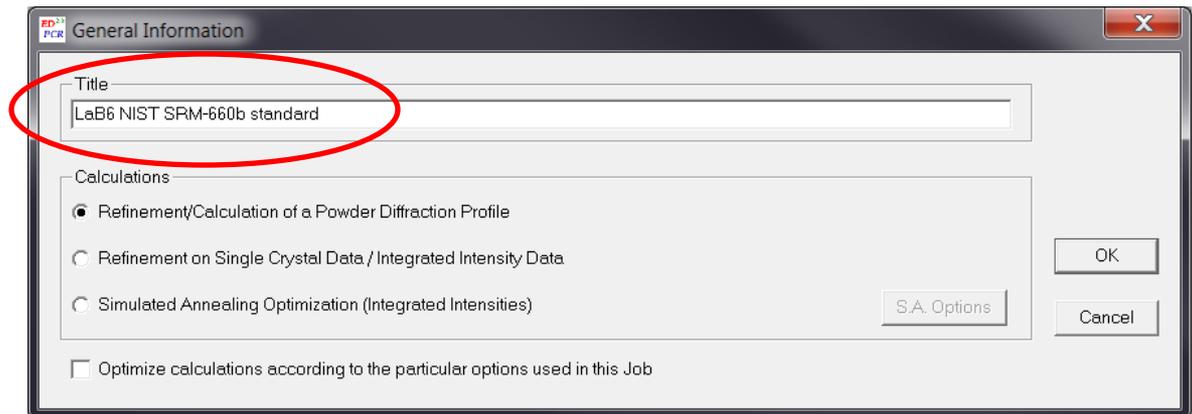
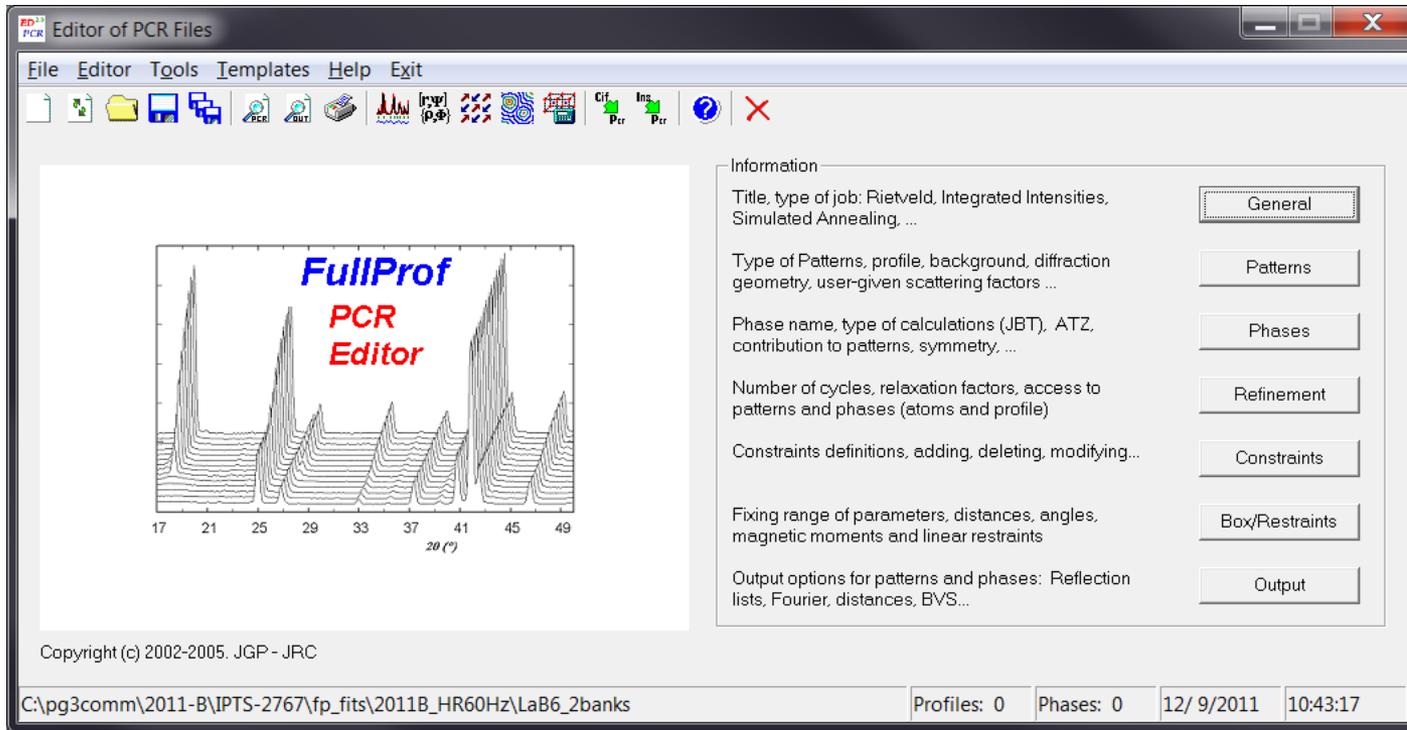


# Fullprof 2-Bank Example

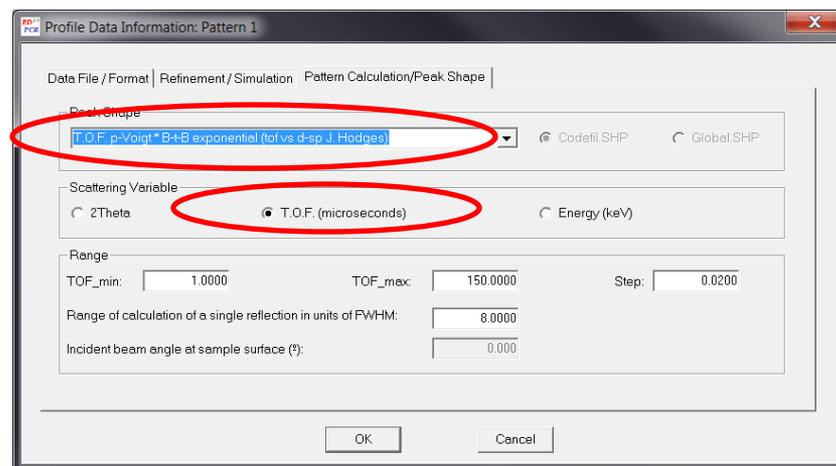
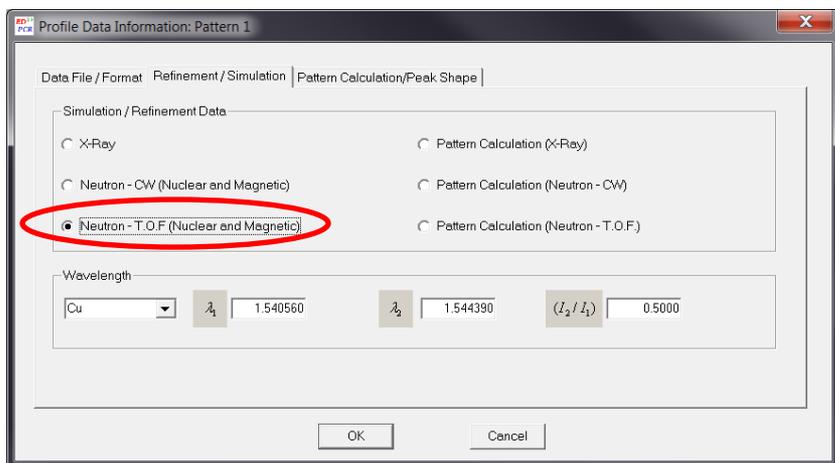
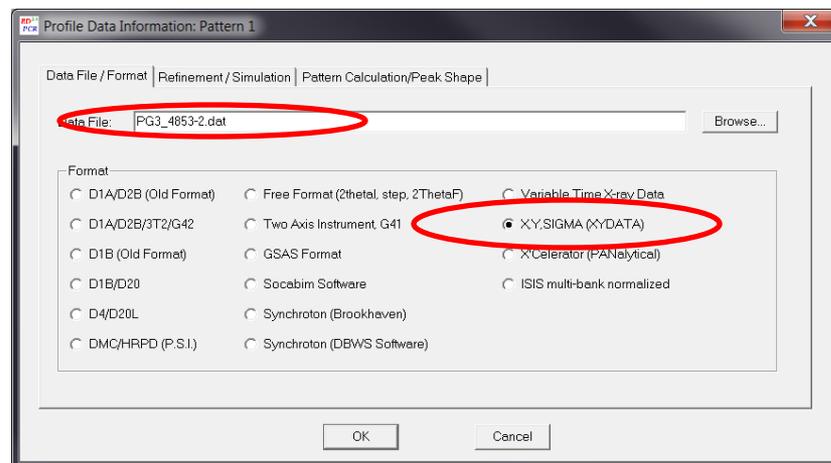
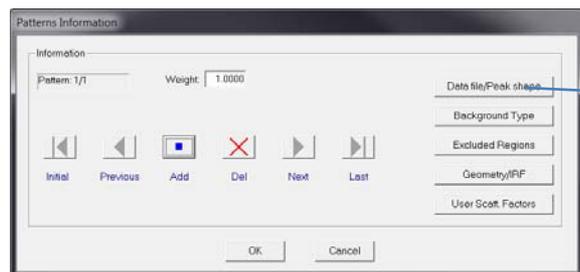
In EdPCR select 'new' and then 'save as' to start a new experiment file



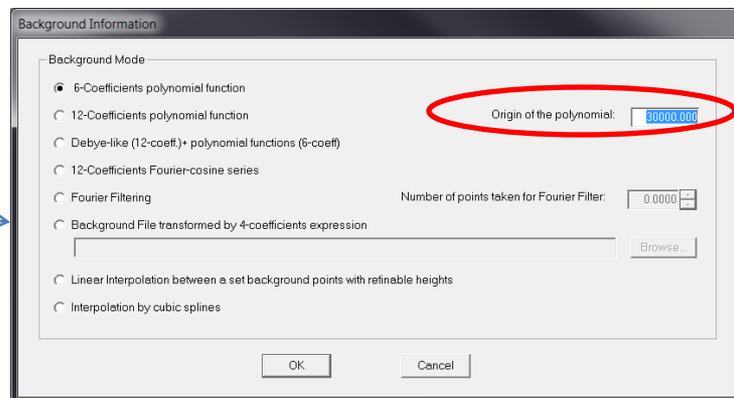
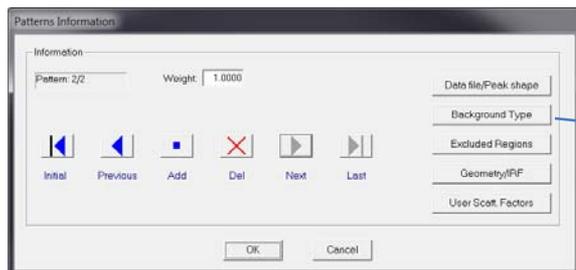
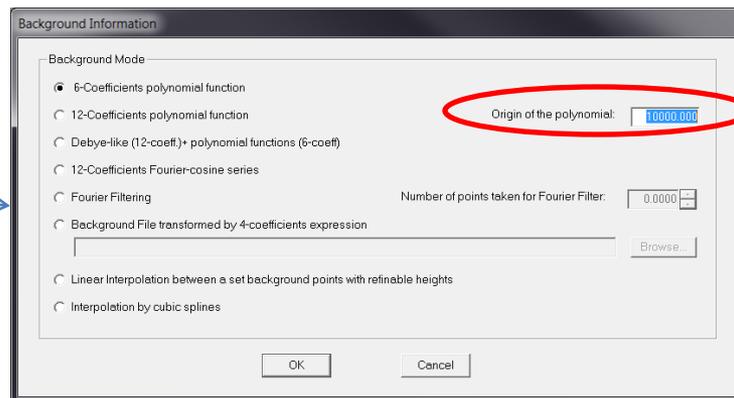
# In [General] add a title



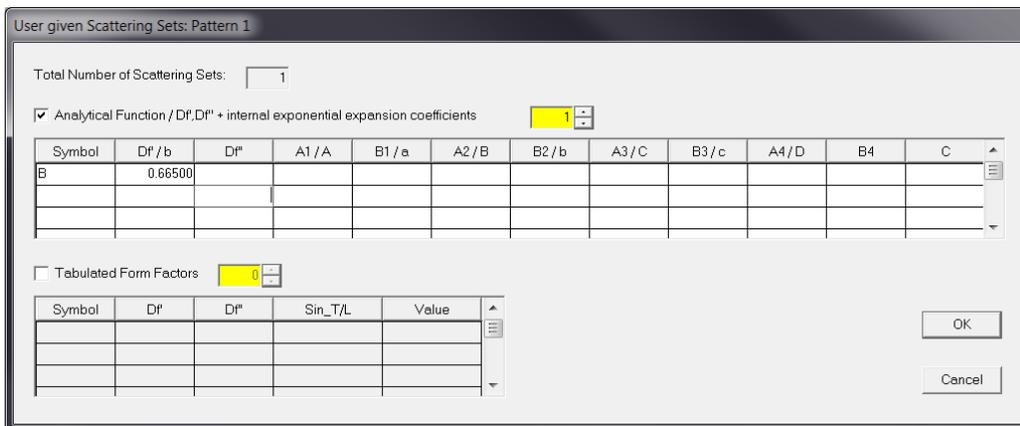
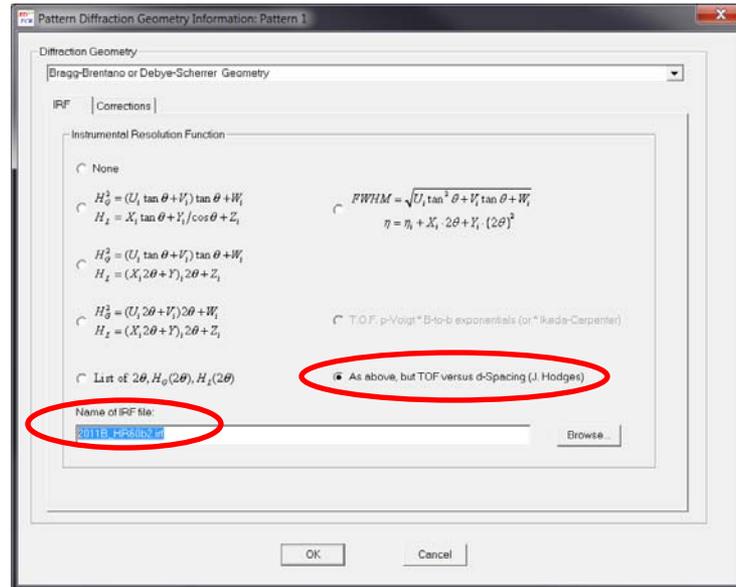
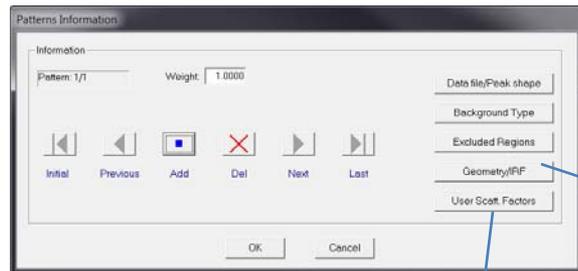
In [Patterns] hit [■] to add a diffraction data set in this way:



# In [Patterns] set background:

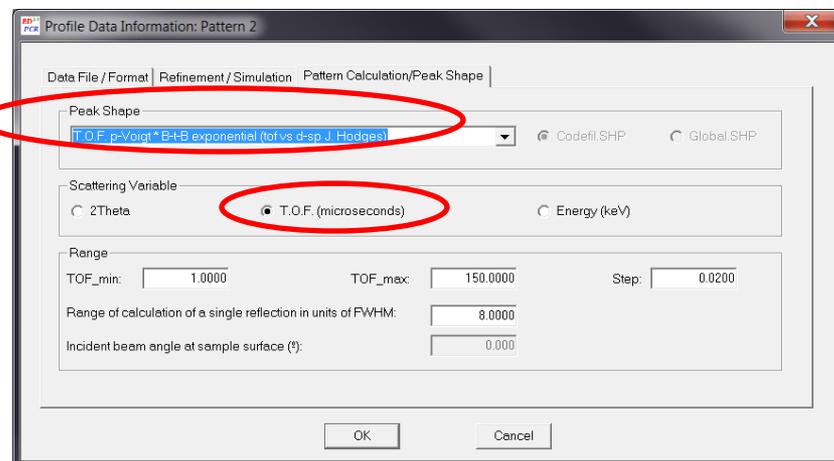
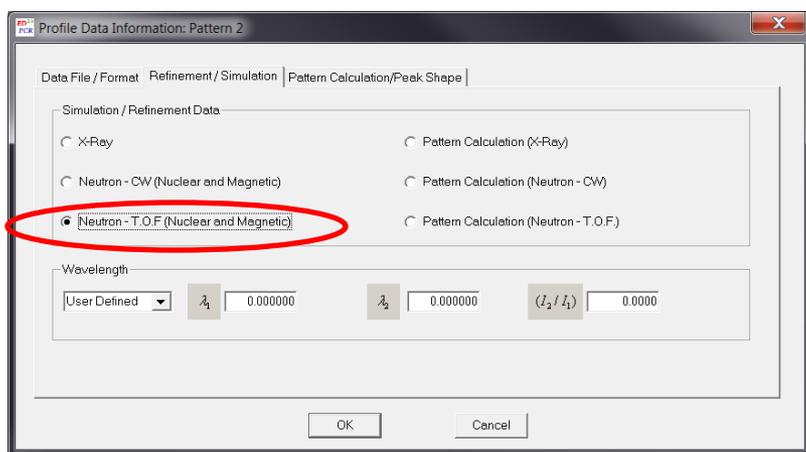
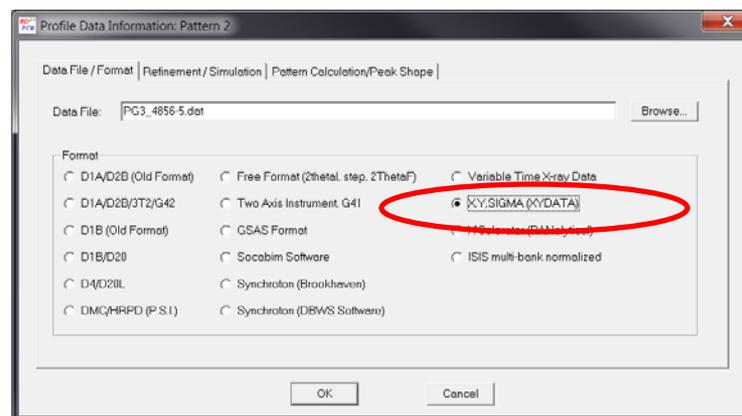
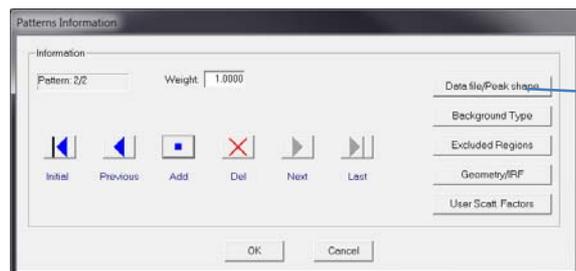


In [Patterns] set the IRF file and scattering factor for 11-B isotope used in this sample:



Don't forget to keep saving your pcr file every few steps

In [Patterns] hit [■] to second diffraction data set in same way as first:



Set IRF file and scattering factor for pattern data set in same way as first.

# In [Phases] hit [■] to add phase information:

Phase Information: Phase 1

General Information on Phases

Name of Phase: [LaB6 NIST 660-b]

Calculation: [Structural Model (Rietveld Method)]

Coefficient to calculate the weight percentage of the Phase: [0.00]  Calculated automatically  Provided by user

Contribution to patterns, preferred orientation direction, reflection list, ...

Space Group symbol/number, symmetry operators, basis functions, etc.

Initial Previous **Add** Del Next Last

OK Cancel

Pattern Contribution Information for Phase 1

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

Current Phase contributes to the pattern

Type of Pattern

X-Ray  Pattern Calculation (X-Ray)

Neutron (Constant Wavelength)  Pattern Calculation (Neutron - Constant Wavelength)

Neutron (T.O.F.)  Pattern Calculation (Neutron - T.O.F.)

Nuclear and Magnetic

Peak Shape

[T.O.F. p.3/098\*64.8 exponential/td/us d. J. Hodgson]

Codef. shp  Global shp

Intensities

Reflection list: [Automatically generated from the Space Group symbol]

Use special control of parameters for peak overlap, rejected reflections for current phase

Brindley coefficient: [0.0000]

Global weight of the integrated intensity data vs profile data: [0.0000]

Factor for excluding reflections [ | < Factor \* Sigma() ]: [0.0000]

Weights are divided by reduced Chi<sup>2</sup> of precedent cycle: [0.0000]

OK Cancel

Symmetry Information

Space Group Properties

Symmetry Operators: [Generated automatically from the symbol]

Space group: [Pm-3m]

Symm. Op. Automatic

Symmetry operators | Magnetic/Displacement Operators | Irreducible representations |

Laue Class: [m3m]  Centrosymmetric Case

Number of Symmetry Operators: [48]

Num	Symmetry	TR	Num	Symmetry	TR
1	x,y,z	<input type="checkbox"/>	2	x,-y,-z	<input type="checkbox"/>
3	-x,y,-z	<input type="checkbox"/>	4	-x,-y,z	<input type="checkbox"/>
5	y,z,x	<input type="checkbox"/>	6	y,-z,x	<input type="checkbox"/>

TR=Time reversal associated to symmetry operator

Time Reversal for Inversion operator

OK Cancel

Pattern Contribution Information for Phase 1

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

Current Phase contributes to the pattern

Type of Pattern

X-Ray  Pattern Calculation (X-Ray)

Neutron (Constant Wavelength)  Pattern Calculation (Neutron - Constant Wavelength)

Neutron (T.O.F.)  Pattern Calculation (Neutron - T.O.F.)

Nuclear and Magnetic

Peak Shape

[T.O.F. p.3/098\*64.8 exponential/td/us d. J. Hodgson]

Codef. shp  Global shp

Intensities

Reflection list: [Automatically generated from the Space Group symbol]

Use special control of parameters for peak overlap, rejected reflections for current phase

Brindley coefficient: [0.0000]

Global weight of the integrated intensity data vs profile data: [0.0000]

Factor for excluding reflections [ | < Factor \* Sigma() ]: [0.0000]

Weights are divided by reduced Chi<sup>2</sup> of precedent cycle: [0.0000]

OK Cancel

In [Refinement] enter phase-1 atoms info:

Refinement Information

Cycles of Refinement: 1

Stop Criterion of Convergence  
Forced Termination when shifts < 0.10 x E.S.D.  
Others: None

Relaxation Factors for Shifts  
Atomic: 0.50 Anisotropic: 0.50 Profile: 0.50 Global: 0.5

Reflections ordering  
 Only at the first cycle  Each cycle  Bragg R-Factor excluding reflections limiting excluded regions

Pattern 1 | **Pattern 2** | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5 | Phase 6 | Phase 7

Refinement weighting model  
 Least Squares  Maximum Likelihood  Unit Weights

Background Instrumental Micro-Absorption

Reduction factor of number of data points: 0

OK Cancel

Atoms Information: Phase 1

List of Atoms  
Number of Atoms: 2

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	La	La	0.0000	0.0000	0.0000	0.50000	1.0000	Isotropic
Atom # 2	B11	B	0.19900	0.50000	0.50000	0.50000	6.0000	Isotropic

Anisotropic Thermal Factors / Form Factors

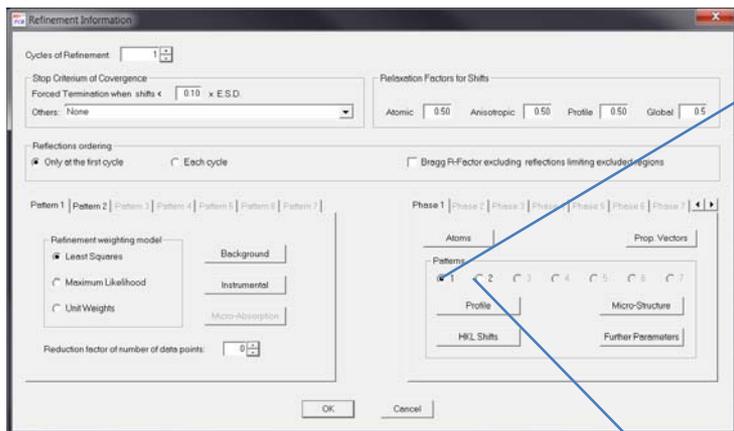
	B11/F1	B22/F2	B33/F3	B12/F4	B13/F5	B23/F6	F7
#							
#							
#							
#							

Special Form Factor

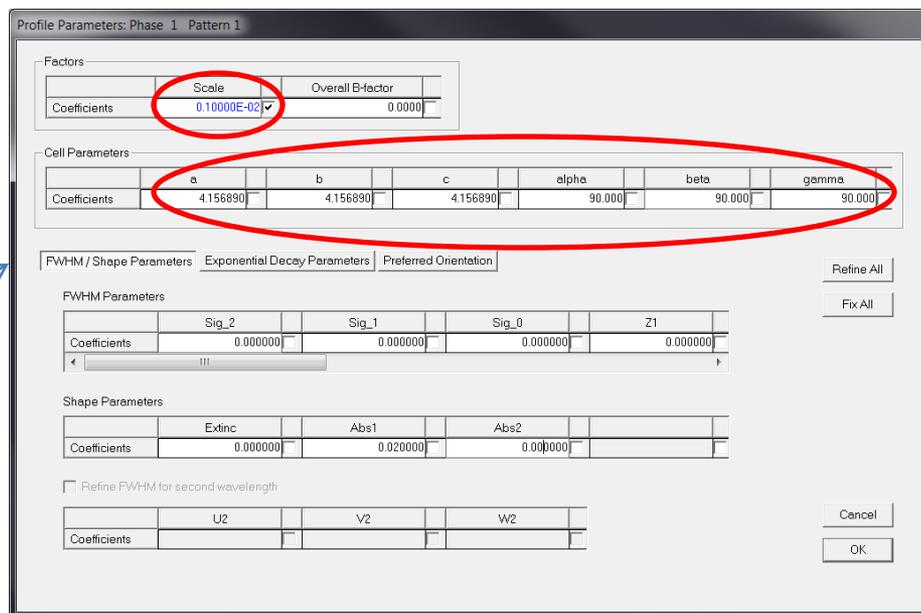
	SASH-Type	Matrix	j=1	j=2	j=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
#	Spherical												
	Spherical												
	Spherical												

Refine Positions  
Refine B\_iso  
Refine B\_aniso  
Fix All  
Cancel  
OK

In [Refinement] enter profile info for both patterns:



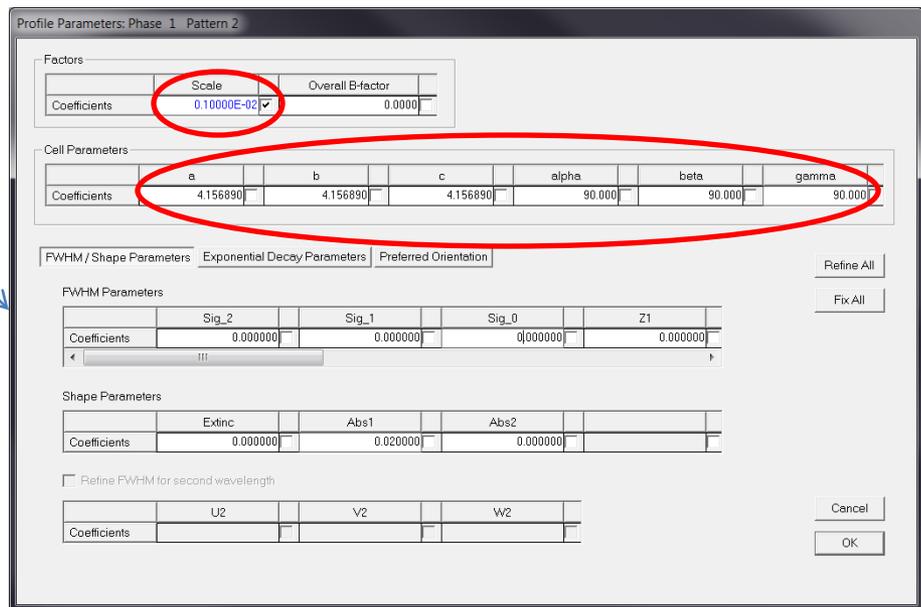
Refinement Information dialog box showing various refinement parameters. The 'Refinement weighting model' section has 'Least Squares' selected. The 'Background' section has 'Background' selected. The 'Refinement weighting model' section has 'Least Squares' selected. The 'Background' section has 'Background' selected. The 'Refinement weighting model' section has 'Least Squares' selected. The 'Background' section has 'Background' selected.



Profile Parameters: Phase 1 Pattern 1 dialog box. The 'Scale' parameter is circled in red. The 'Cell Parameters' section is also circled in red.

Factors	
Scale	0.10000E-02
Overall B-factor	0.0000

Cell Parameters											
a	4.156890	b	4.156890	c	4.156890	alpha	90.000	beta	90.000	gamma	90.000



Profile Parameters: Phase 1 Pattern 2 dialog box. The 'Scale' parameter is circled in red. The 'Cell Parameters' section is also circled in red.

Factors	
Scale	0.10000E-02
Overall B-factor	0.0000

Cell Parameters											
a	4.156890	b	4.156890	c	4.156890	alpha	90.000	beta	90.000	gamma	90.000

Then proceed with refinement as per usual:

Refine parameters such as background, lattice, atomic, profile (sig-2 & gam-1), absorption

