

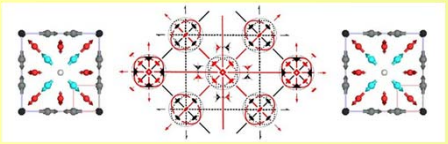
CMS 2014 workshop



Jana2006 – hands on (magnetic option)

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Institute of Physics
Academy of Sciences of the Czech Republic

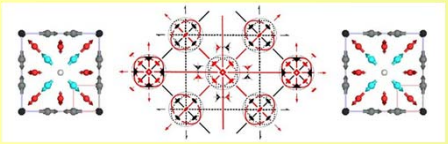




Jana2006 features

General options

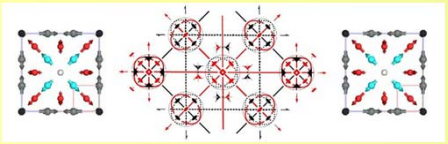
- Crystallographic program focused to solution, refinement and interpretation of difficult, especially modulated structures
- Applicable to powder and single crystal data. It allows also a joint refinement
- Structure solution preferably made by the program Superflip (Palatinus &Chapuis, *J.Appl.Cryst.* (2007). **40**, 786-790)
- Allows refinement of twinned and multiphase crystals
- Powerful tool also for disordered structures - constrains, restrains, rigid body description, local symmetry etc.
- ADP parameters up 6^{th} order tensors
- Charge density studies



Jana2006 features

Handling symmetry in Jana2006

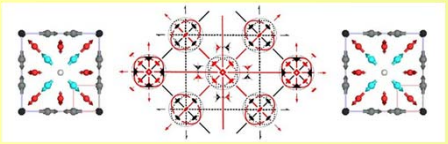
- The program accepts any reasonable setting of space groups and superspace groups including non-standard centering vectors
- Systematical extinctions are derived from symmetry operations
- All symmetry restrictions of structural parameters are derived mathematically from symmetry operations and from the actual position of the atom. This works ADP's up to 6^{th} order, multipole and modulation parameters.
- Program supports an interactive transformation to lower symmetry
- A local symmetry can be applied to individual atoms and also to rigid body groups



Jana2006 features

What Jana could offer for magnetic structures?

- Solution and refinement of magnetic structures for positionally and/or occupationally modulated structures and composite structures – multiferroic refinements
- Application of higher harmonics and special modulation functions for magnetic modulations
- Using (3+2) and (3+3) nuclear and magnetic modulations
- Handling of twinned (multidomains) magnetic structures
- Combined study of charge densities and magnetic ordering



Magnetic symmetry

Laue symmetry

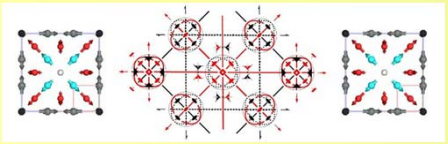
Magnetic diffraction pattern produced by circularly polarized neutron beam follows the Laue symmetry:

- Merging of equivalent reflections
- Smaller number of reflections generated for powder refinement

Can we recognize Laue symmetry from diffraction pattern?

Single crystal data: any lowering point group symmetry during the phase transition is usually almost fully “compensated” by creation of equally populated magnetic domains.

Powder data: Even worse – reflections which could help are completely overlapped.



Magnetic symmetry

Systematic extinctions

Reflections from invariant subspace associated with symmetry operations $\mathbf{h} = \boldsymbol{R}.\boldsymbol{h}$:

$$F_{nucl}(\boldsymbol{h}) = \exp(-2\pi i \boldsymbol{h}.\boldsymbol{s}) F_{nucl}(\boldsymbol{h})$$

Present only if $\boldsymbol{h}.\boldsymbol{s}$ is an integer. For magnetic reflections:

$$\boldsymbol{F}_{mag}(\boldsymbol{h}) = \exp(-2\pi i \boldsymbol{h}.\boldsymbol{s}) \theta^{-1} \det(\boldsymbol{R}^{-1}) \boldsymbol{R}^{-1} \boldsymbol{F}_{mag}(\boldsymbol{h})$$

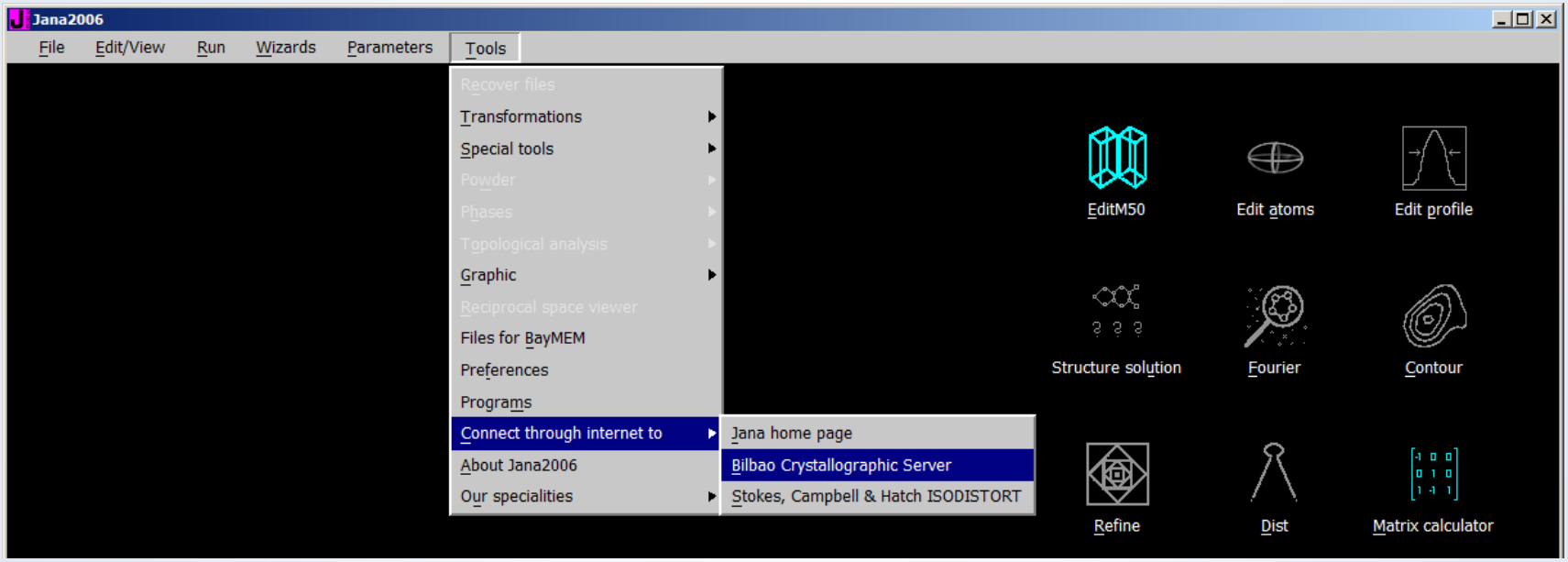
- magnetic reflections can have different extinction conditions
- three equations must but fulfilled simultaneously
- centering conditions – three equations are reduced one equivalent with nuclear centering conditions

Number of magnetic atoms small and often located at special positions → specific extinctions

Magnetic symmetry

Systematic extinctions

Great help: Bilbao Crystallographic Server – can be called form Jana2006:



Magnetic symmetry

Systematic extinctions



Sections

- Retrieval Tools
- Magnetic Space Groups
- Group-Subgroup
- Representations
- Solid State
- Structure Utilities
- Subperiodic
- Incommensurate Structures Database
- Raman and Hyper-Raman scattering
- Contact us
- About us
- Links
- Publications
- How to cite the server
- Tutorials

Material from the ITOnline Workshop (September 2011)

Material from the school on the server (June 2009)

MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations

Magnetic Space Groups

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector

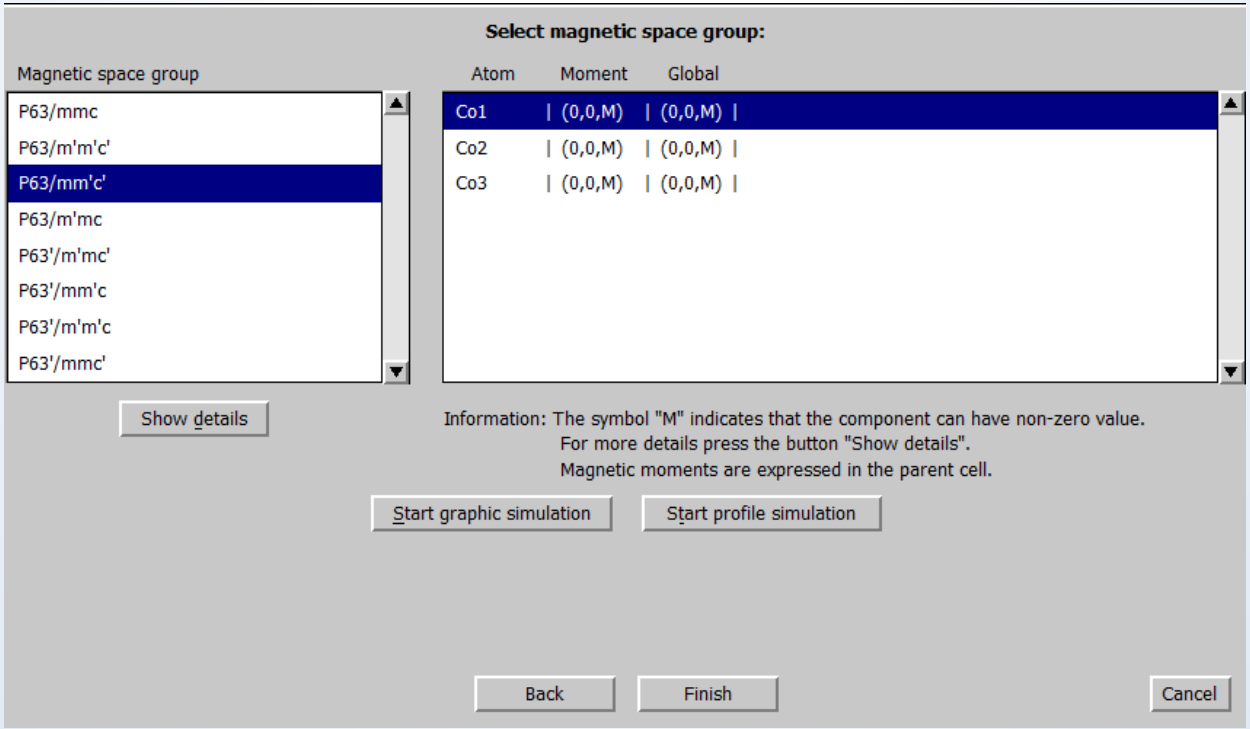
Group - Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups

Magnetic symmetry

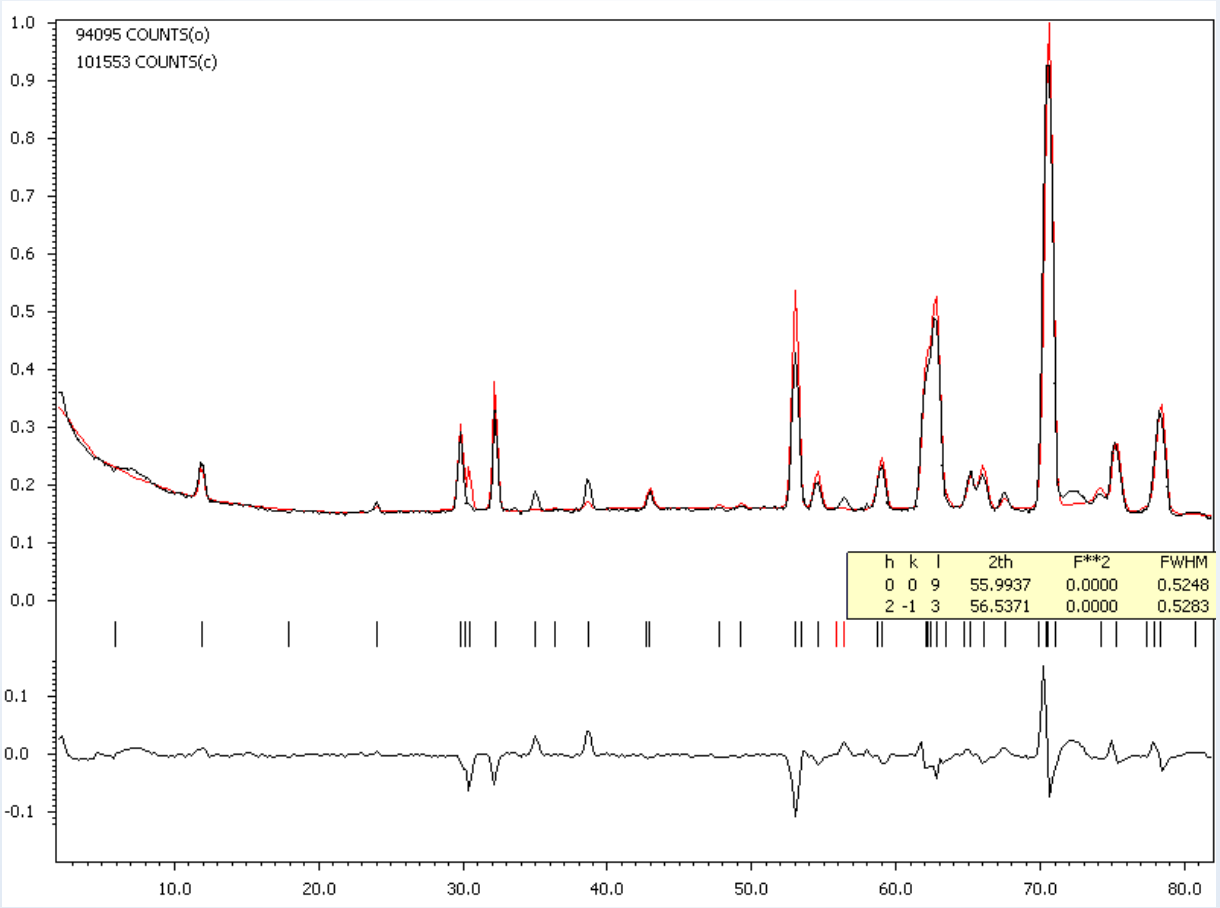
Systematic extinctions

Extinctions can also be tested in Jana2006 by a simulation:
Example 12.1 from Jana2006 Cookbook: Ba5Co5ClO13, Mentré, O., Kauffmann, M., Ehora, G., Daviero-Minaud, S., Abraham F. and Roussel, P. (2008). *Solid State Sciences* **10**, 471-475.



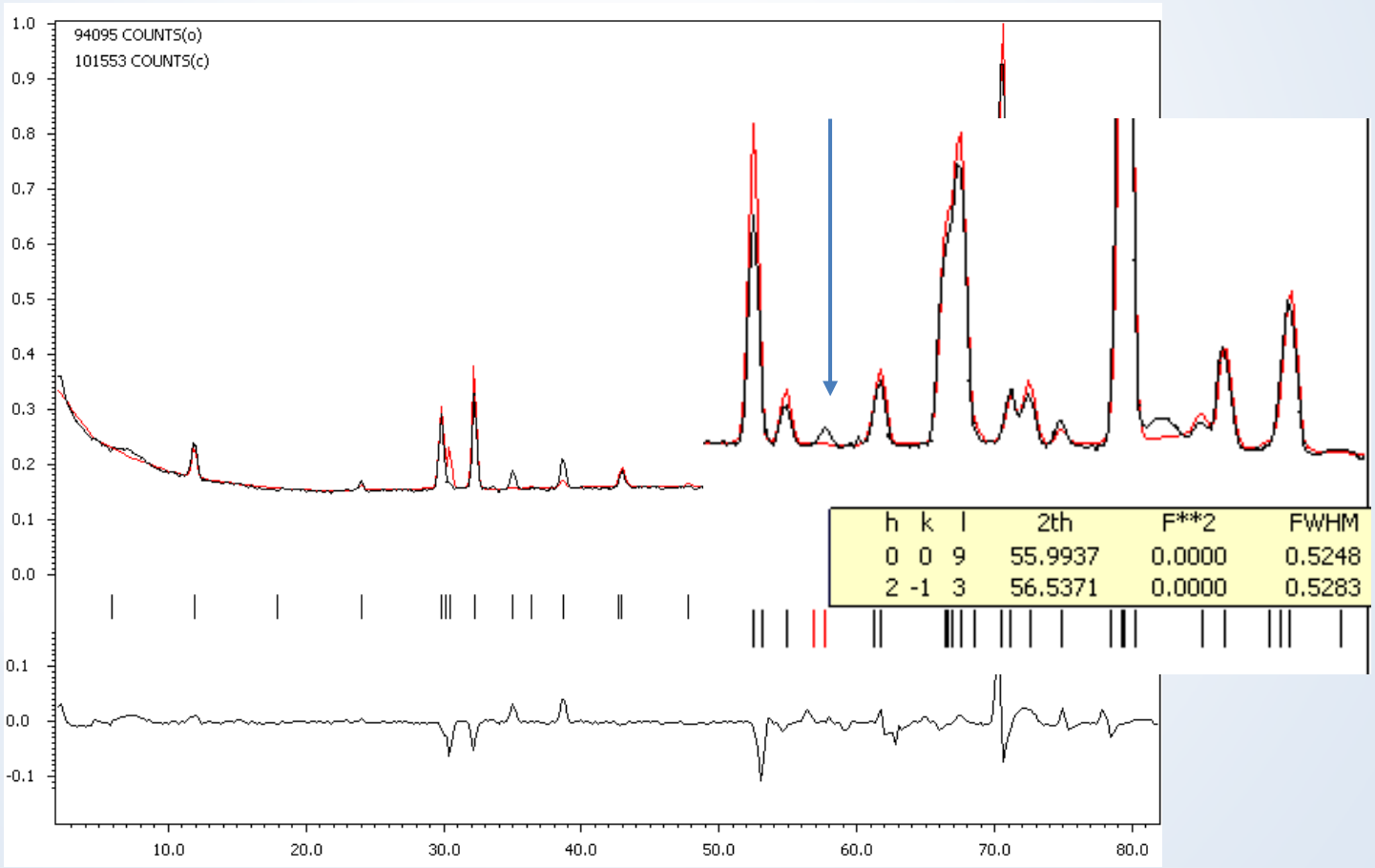
Magnetic symmetry

Systematic extinctions



Magnetic symmetry

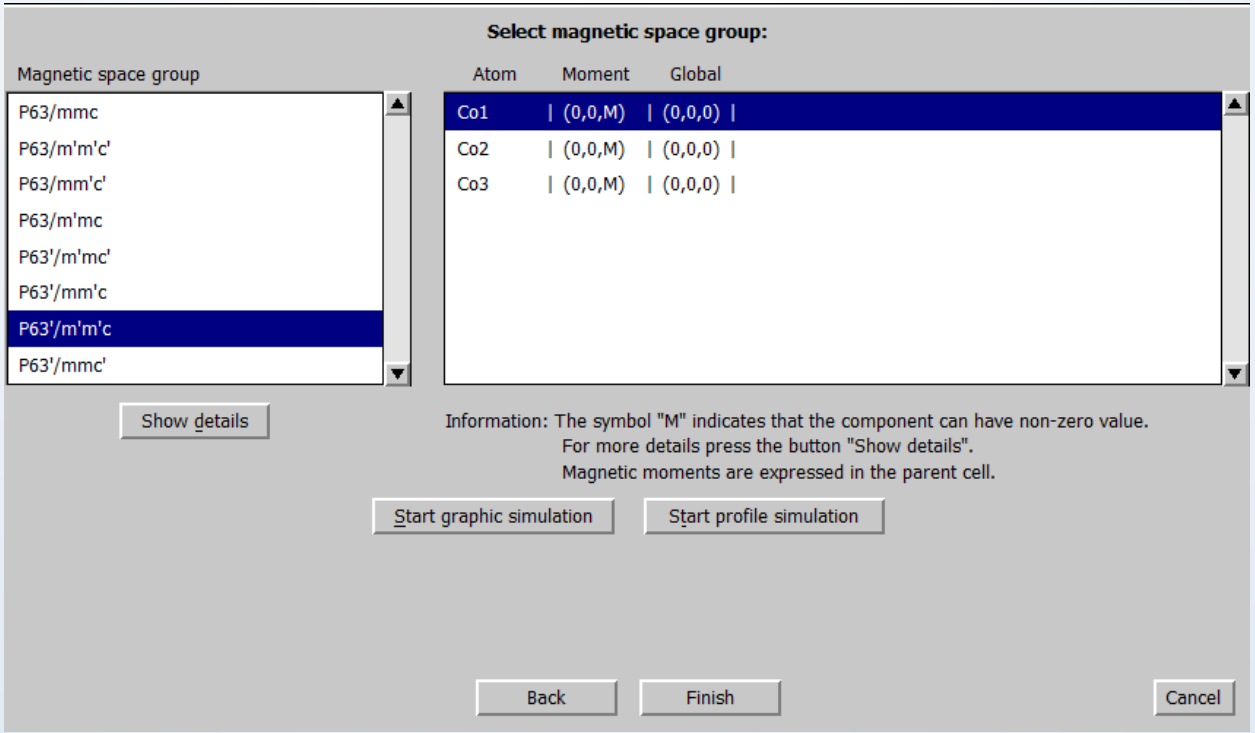
Systematic extinctions



Magnetic symmetry

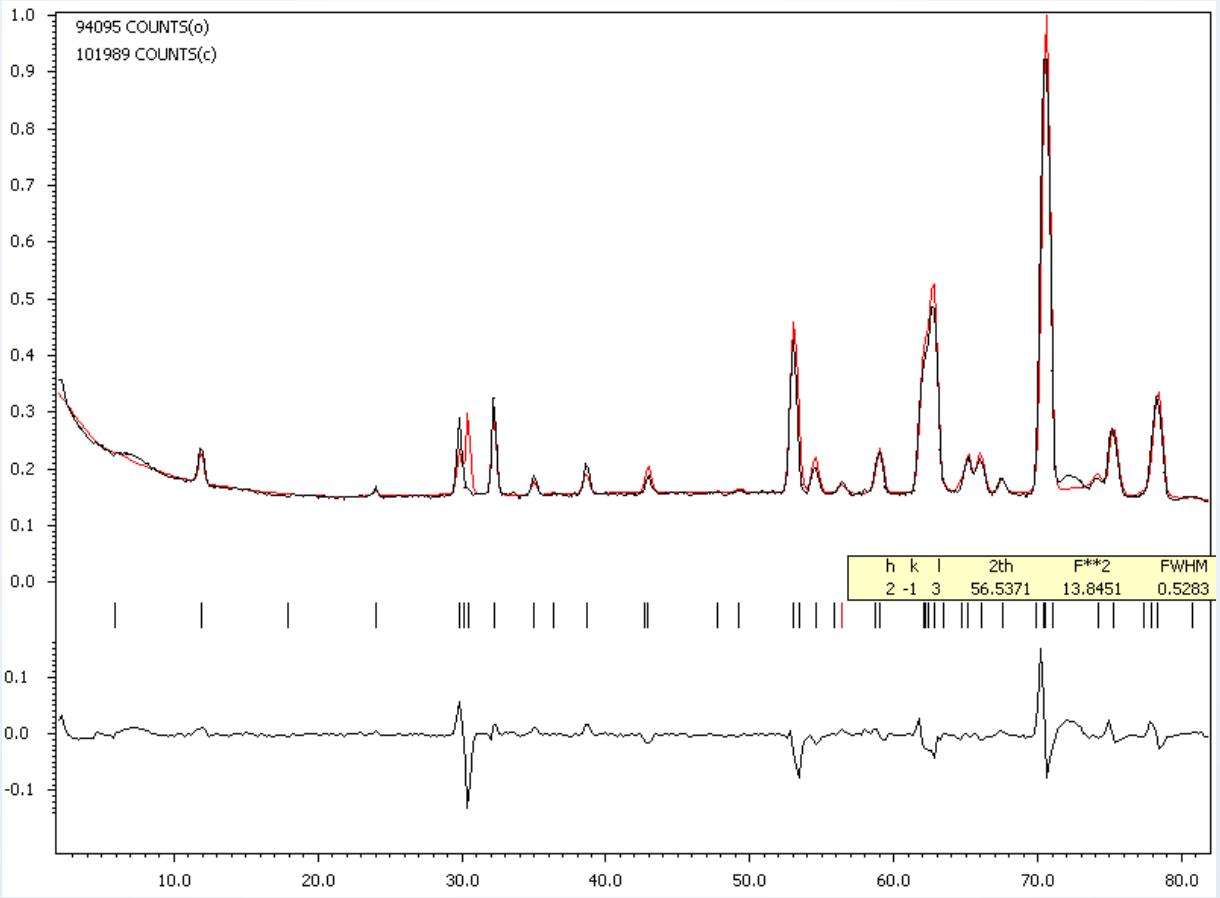
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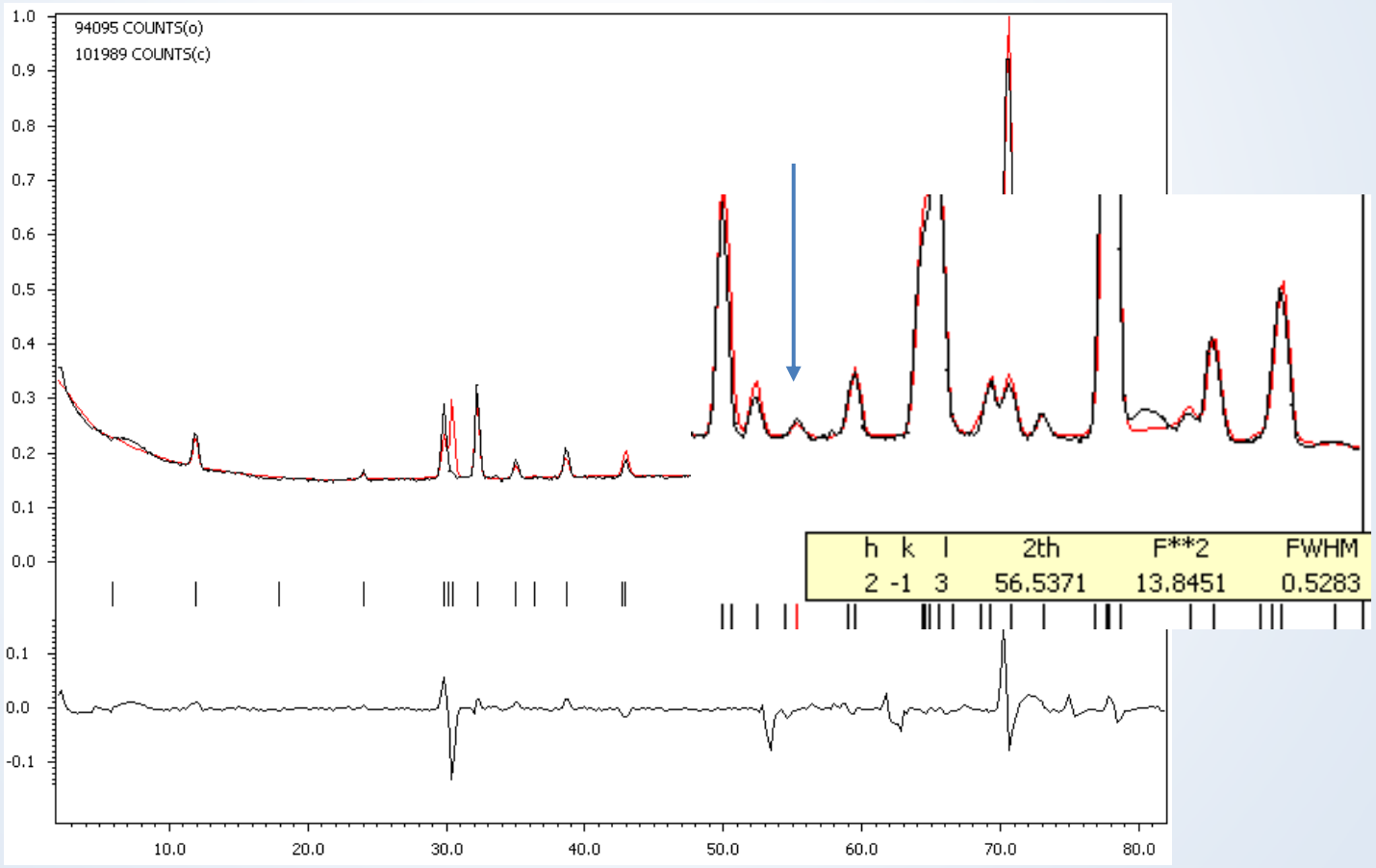
Magnetic symmetry

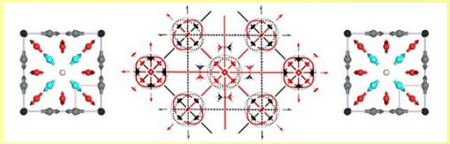
Systematic extinctions



Magnetic symmetry

Systematic extinctions





Jana2006 info

Program Scheme

Reading of one or more data sets

M95 + M50

Determining symmetry, merging symmetry equivalent reflections, absorption correction
Refinement of powder profile parameters

M90, M41

Solution (by calling external programs)

M40

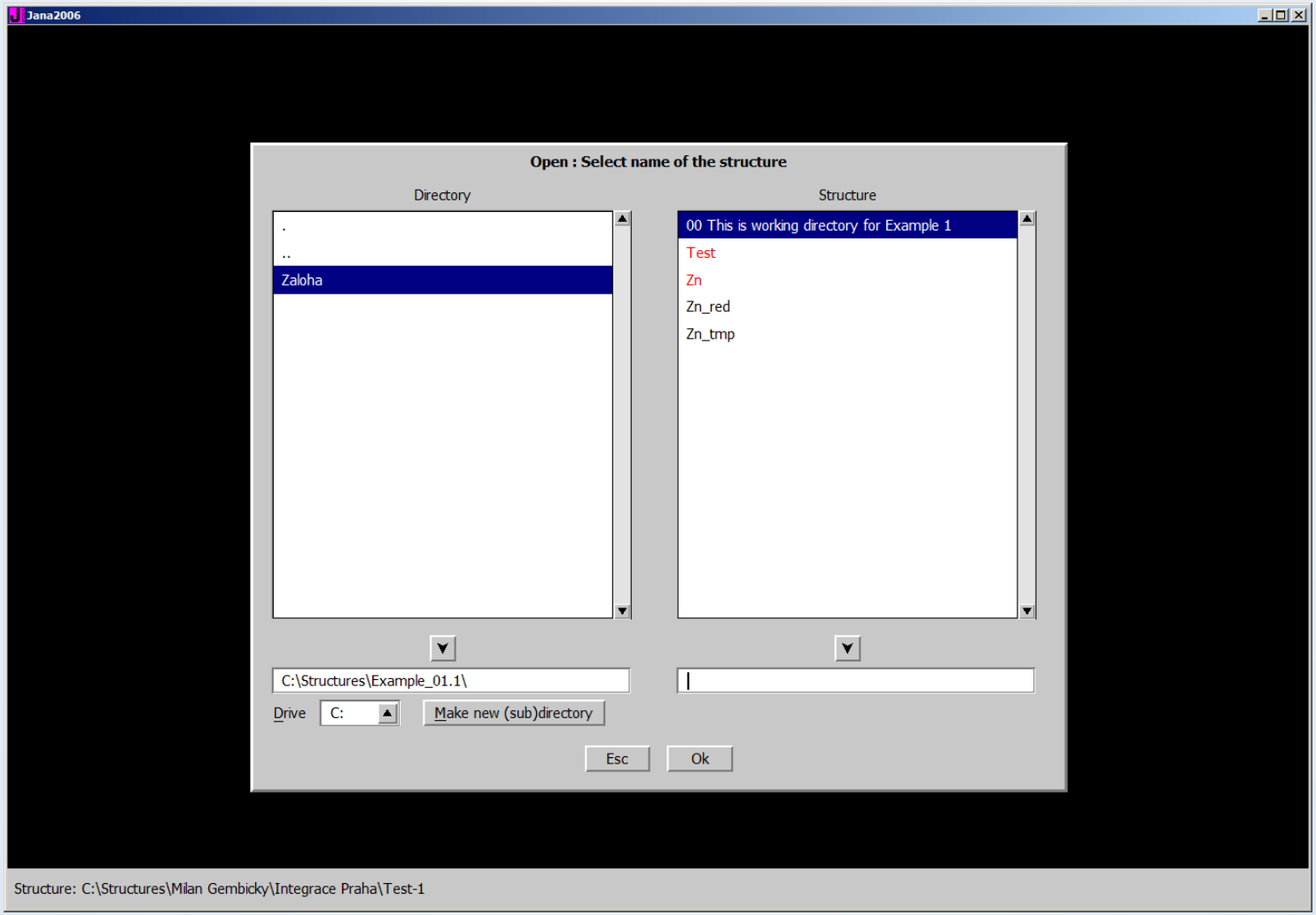
Refinement
Transformation
Introduction of twinning
Change of symmetry

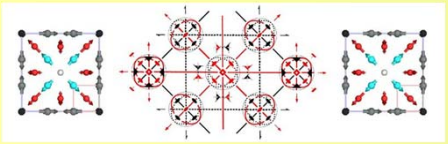
Plotting, geometry parameters, Fourier maps ….

M95	data repository
M90	refinement reflection file
M50	basic crystal information, form factors, program options
M40	structure model

Jana2006 info

File/directory manager



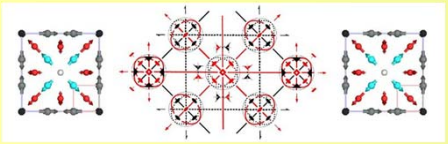


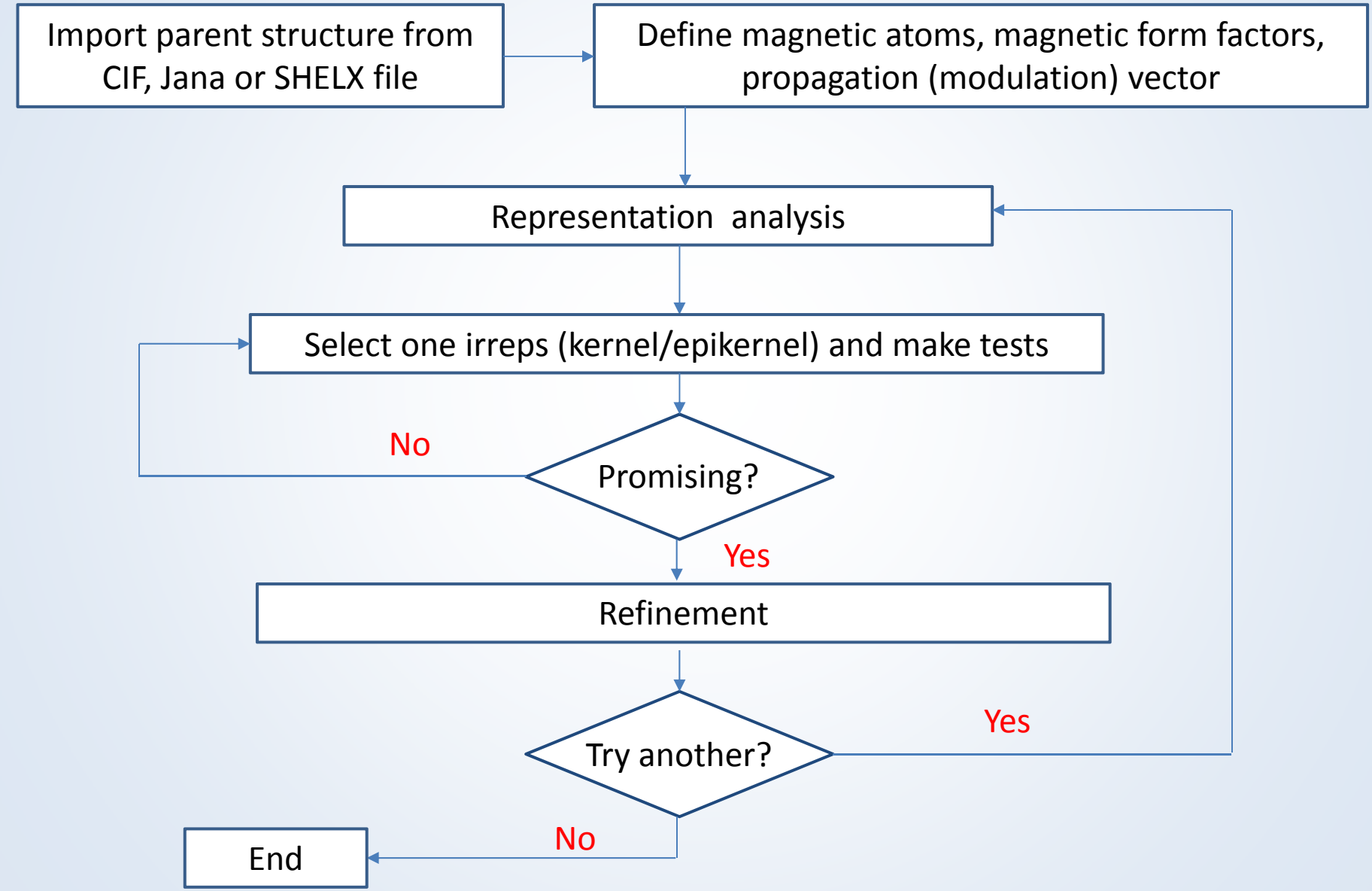
Jana2006 tools

A specific wizard has been developed to make first steps:

- Import a parent structure from CIF, Jana, SHELX
- Define magnetic atoms and magnetic propagation (modulation) vector
- Representation analysis
- Testing
- Refinement

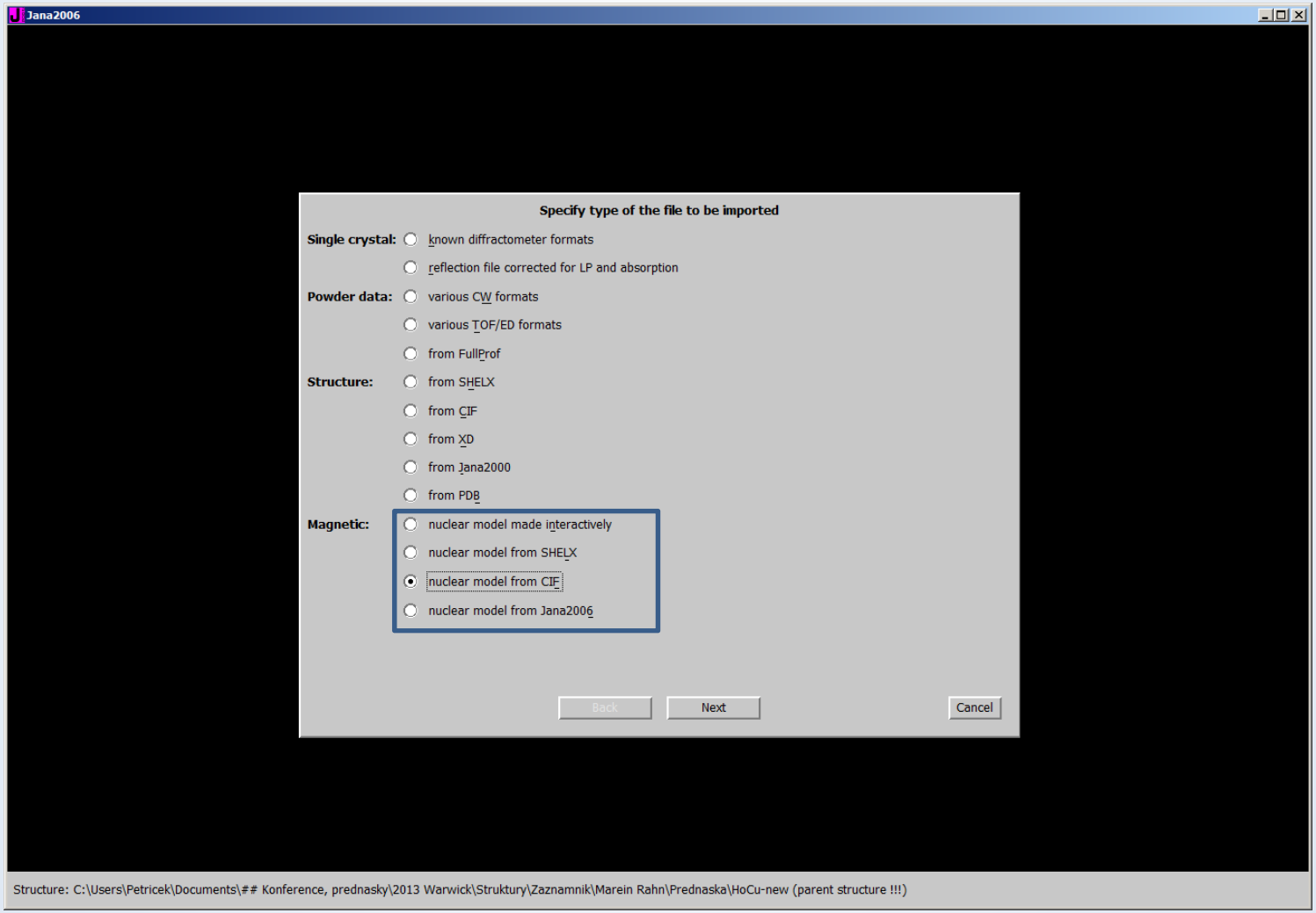
Jana2006 tools





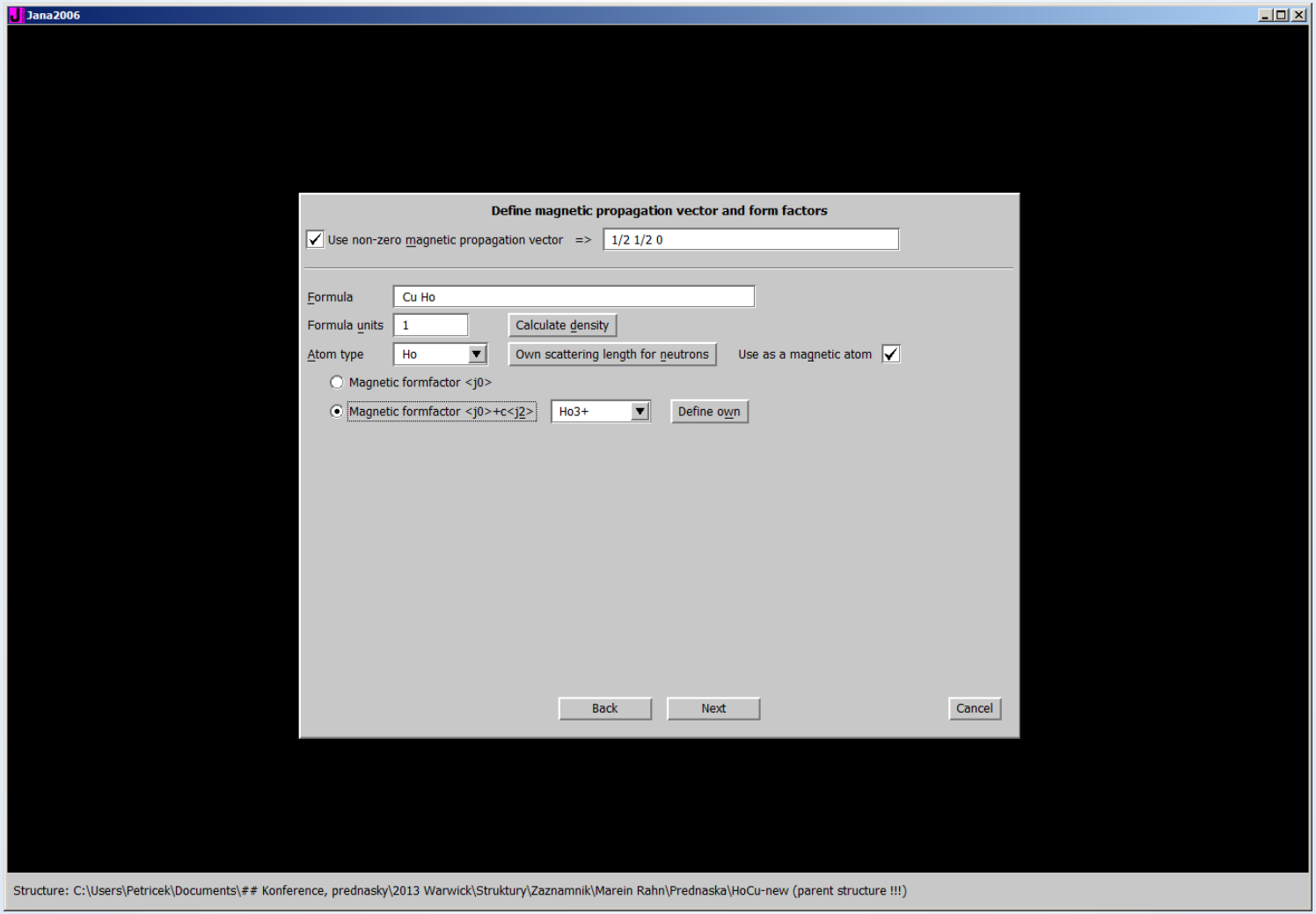
Jana2006 tools

Import the parent structure



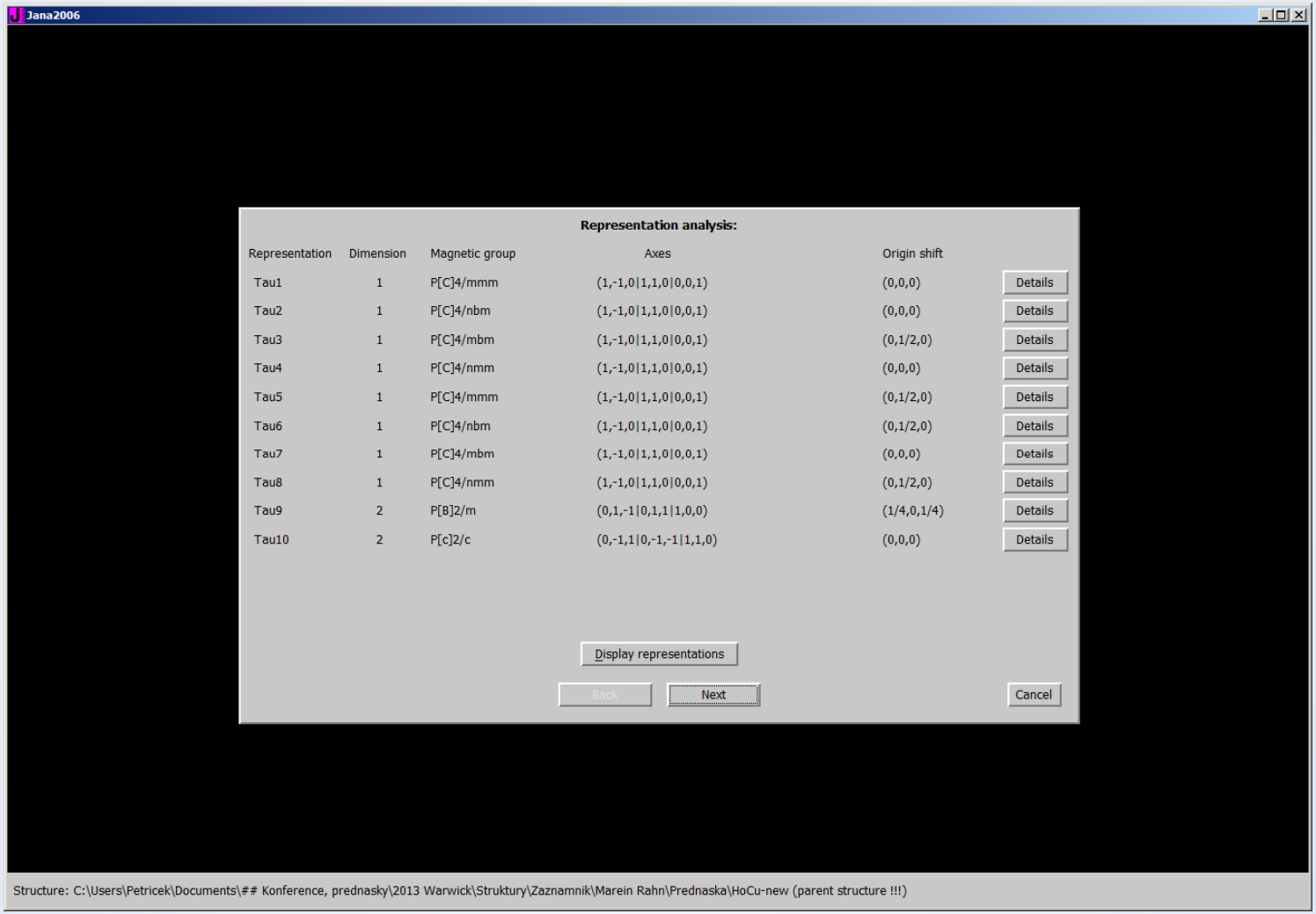
Jana2006 tools

Define propagation (modulation) vector and magnetic atoms



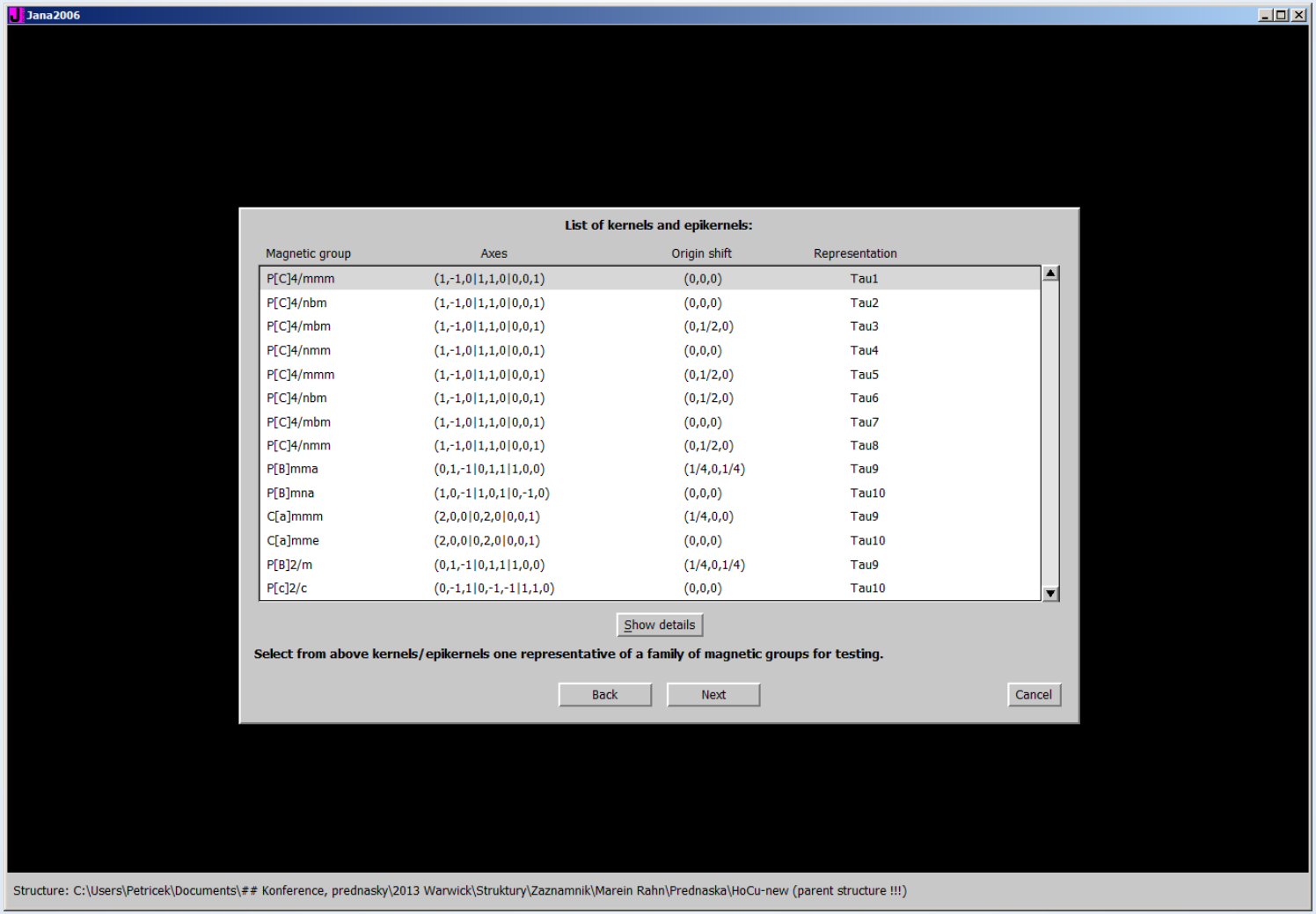
Jana2006 tools

Representation analysis



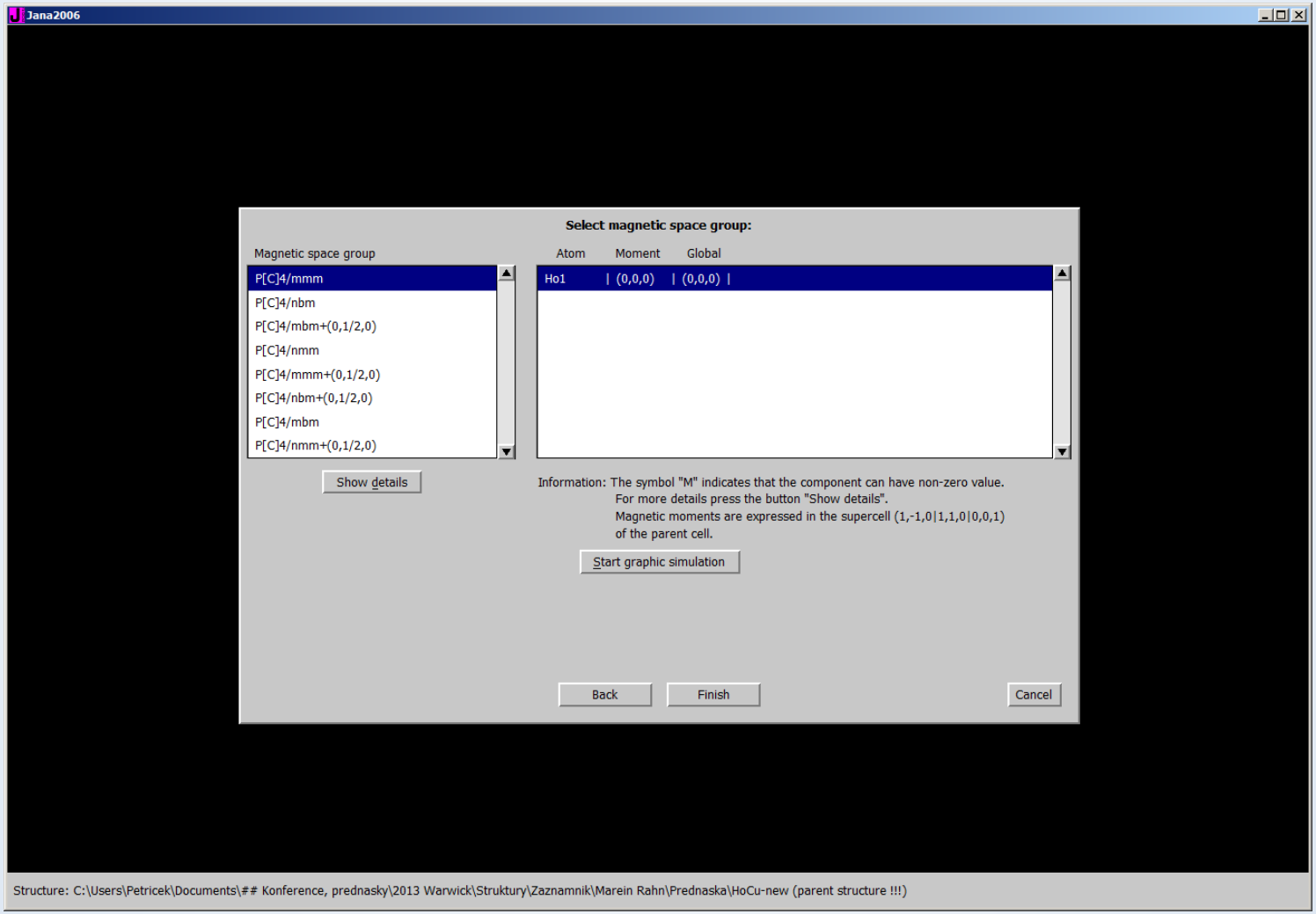
Jana2006 tools

List of kernels and epikernels (isotropic subgroups):



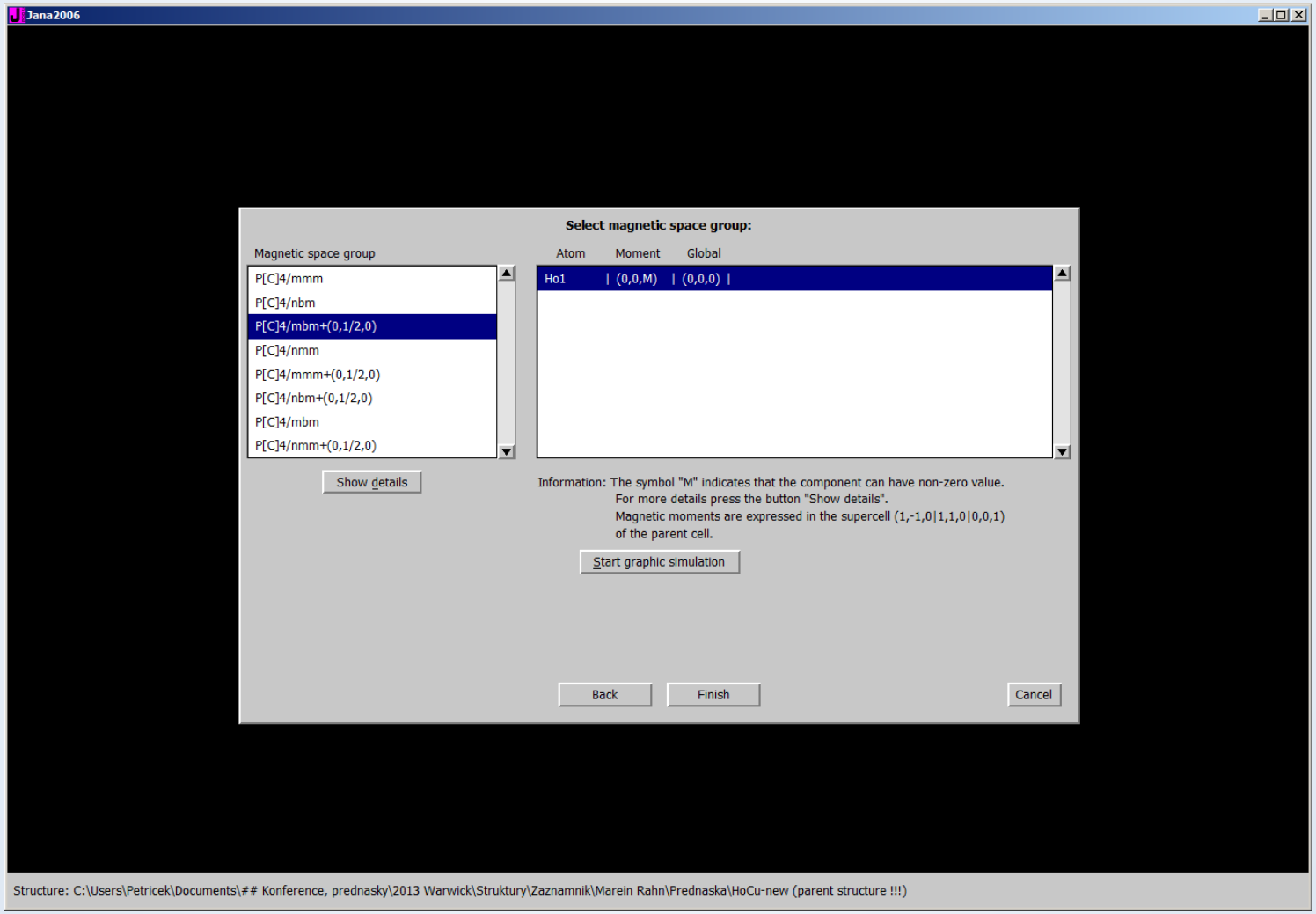
Jana2006 tools

Test of the selected kernel/epikernel “family”



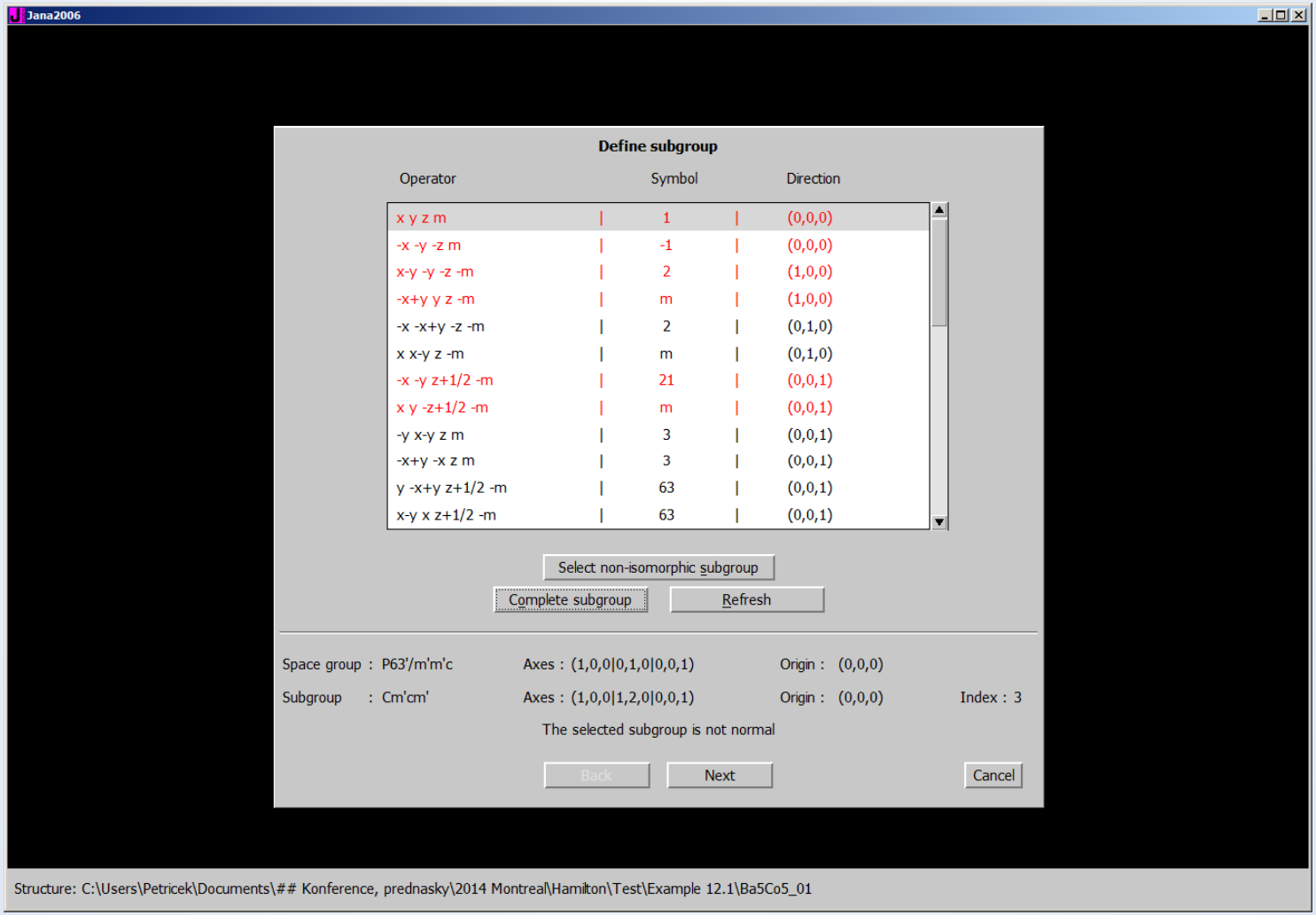
Jana2006 tools

Test of the selected kernel/epikernel “family”

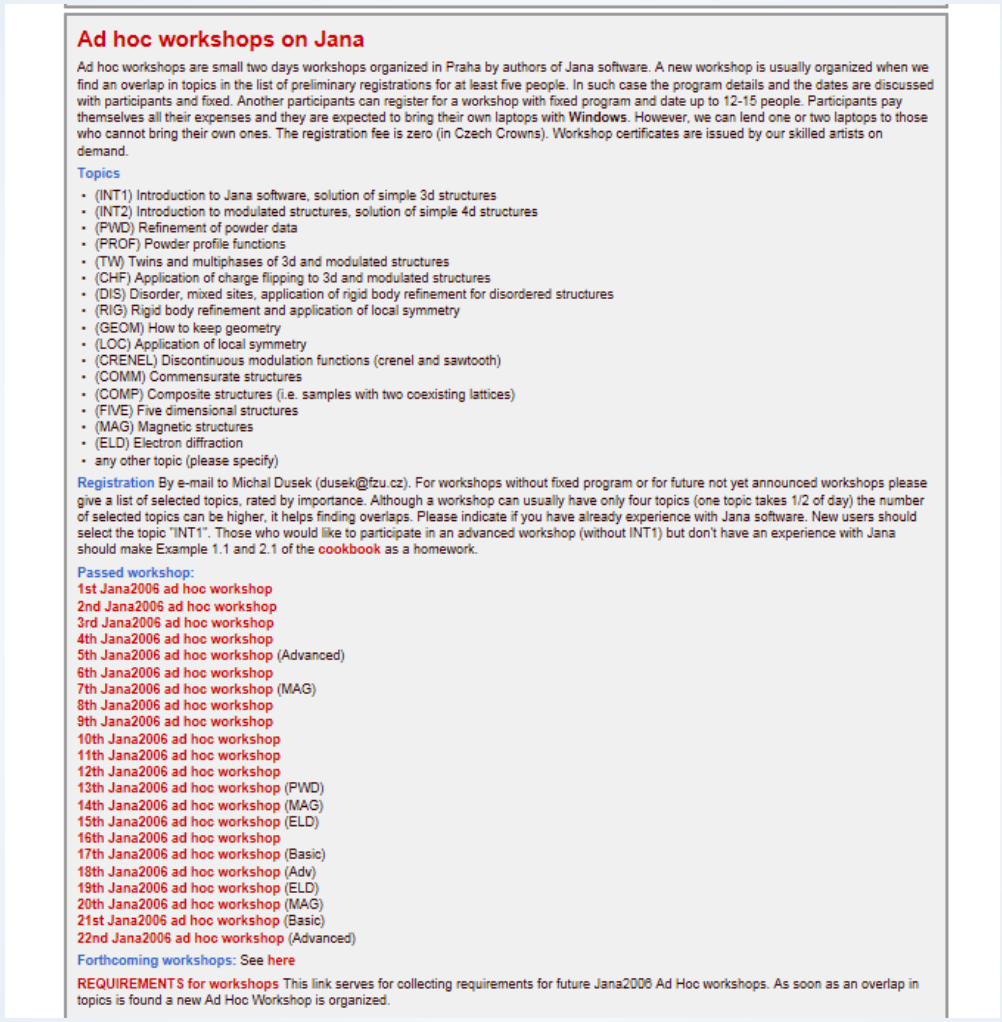


Jana2006 tools

Group/subgroup transformation



Ad hoc workshops on Jana



Ad hoc workshops on Jana

Ad hoc workshops are small two days workshops organized in Praha by authors of Jana software. A new workshop is usually organized when we find an overlap in topics in the list of preliminary registrations for at least five people. In such case the program details and the dates are discussed with participants and fixed. Another participants can register for a workshop with fixed program and date up to 12-15 people. Participants pay themselves all their expenses and they are expected to bring their own laptops with **Windows**. However, we can lend one or two laptops to those who cannot bring their own ones. The registration fee is zero (in Czech Crowns). Workshop certificates are issued by our skilled artists on demand.

Topics

- (INT1) Introduction to Jana software, solution of simple 3d structures
- (INT2) Introduction to modulated structures, solution of simple 4d structures
- (PWD) Refinement of powder data
- (PROF) Powder profile functions
- (TW) Twins and multiphases of 3d and modulated structures
- (CHF) Application of charge flipping to 3d and modulated structures
- (DIS) Disorder, mixed sites, application of rigid body refinement for disordered structures
- (RIG) Rigid body refinement and application of local symmetry
- (GEOM) How to keep geometry
- (LOC) Application of local symmetry
- (CRENEL) Discontinuous modulation functions (crenel and sawtooth)
- (COMM) Commensurate structures
- (COMP) Composite structures (i.e. samples with two coexisting lattices)
- (FIVE) Five dimensional structures
- (MAG) Magnetic structures
- (ELD) Electron diffraction
- any other topic (please specify)

Registration By e-mail to Michal Dusek (dusek@fzu.cz). For workshops without fixed program or for future not yet announced workshops please give a list of selected topics, rated by importance. Although a workshop can usually have only four topics (one topic takes 1/2 of day) the number of selected topics can be higher, it helps finding overlaps. Please indicate if you have already experience with Jana software. New users should select the topic "INT1". Those who would like to participate in an advanced workshop (without INT1) but don't have an experience with Jana should make Example 1.1 and 2.1 of the **cookbook** as a homework.

Passed workshop:
1st Jana2006 ad hoc workshop
2nd Jana2006 ad hoc workshop
3rd Jana2006 ad hoc workshop
4th Jana2006 ad hoc workshop
5th Jana2006 ad hoc workshop (Advanced)
6th Jana2006 ad hoc workshop
7th Jana2006 ad hoc workshop (MAG)
8th Jana2006 ad hoc workshop
9th Jana2006 ad hoc workshop
10th Jana2006 ad hoc workshop
11th Jana2006 ad hoc workshop
12th Jana2006 ad hoc workshop
13th Jana2006 ad hoc workshop (PWD)
14th Jana2006 ad hoc workshop (MAG)
15th Jana2006 ad hoc workshop (ELD)
16th Jana2006 ad hoc workshop
17th Jana2006 ad hoc workshop (Basic)
18th Jana2006 ad hoc workshop (Adv)
19th Jana2006 ad hoc workshop (ELD)
20th Jana2006 ad hoc workshop (MAG)
21st Jana2006 ad hoc workshop (Basic)
22nd Jana2006 ad hoc workshop (Advanced)

Forthcoming workshops: See **here**

REQUIREMENTS for workshops This link serves for collecting requirements for future Jana2006 Ad Hoc workshops. As soon as an overlap in topics is found a new Ad Hoc Workshop is organized.

For more details: http://jana.fzu.cz/
Praha – Prague (Czech Republic)

Installation

Installation notes

For the workshop following programs are necessary:

- **Jana2006 for most tasks**
- **Superflip (part of Jana2006 distribution) for solution of phase problem**
- **Vesta for visualization of electron density with isosurfaces and for magnetic structures**

Installation of Jana2006

Execute janainst.msi from the directory Setup\Jana2006 and follow instructions.
The installation creates shortcut to Jana2006 in the desktop and in Start → Programs

Start Jana2006, go to "Tools → About Jana2006" and verify the version string.
The version date should 30/07/2014 or newer

- Don't use your "old" preinstalled versions of Jana2006
- Don't use flash disk for calculation. Copy the example files to hard disk.
- Don't install Jana2006 to desktop or flash disk

Installation of Vesta

Unpack the archive "Vesta.zip" or "Vesta-win64.zip" from the directory Setup\Vesta to a directory of your choice

Installation

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Version you have used for Bilbao Crystallographic Server Tutorial should be OK.

Installation

Configuration of Jana2006

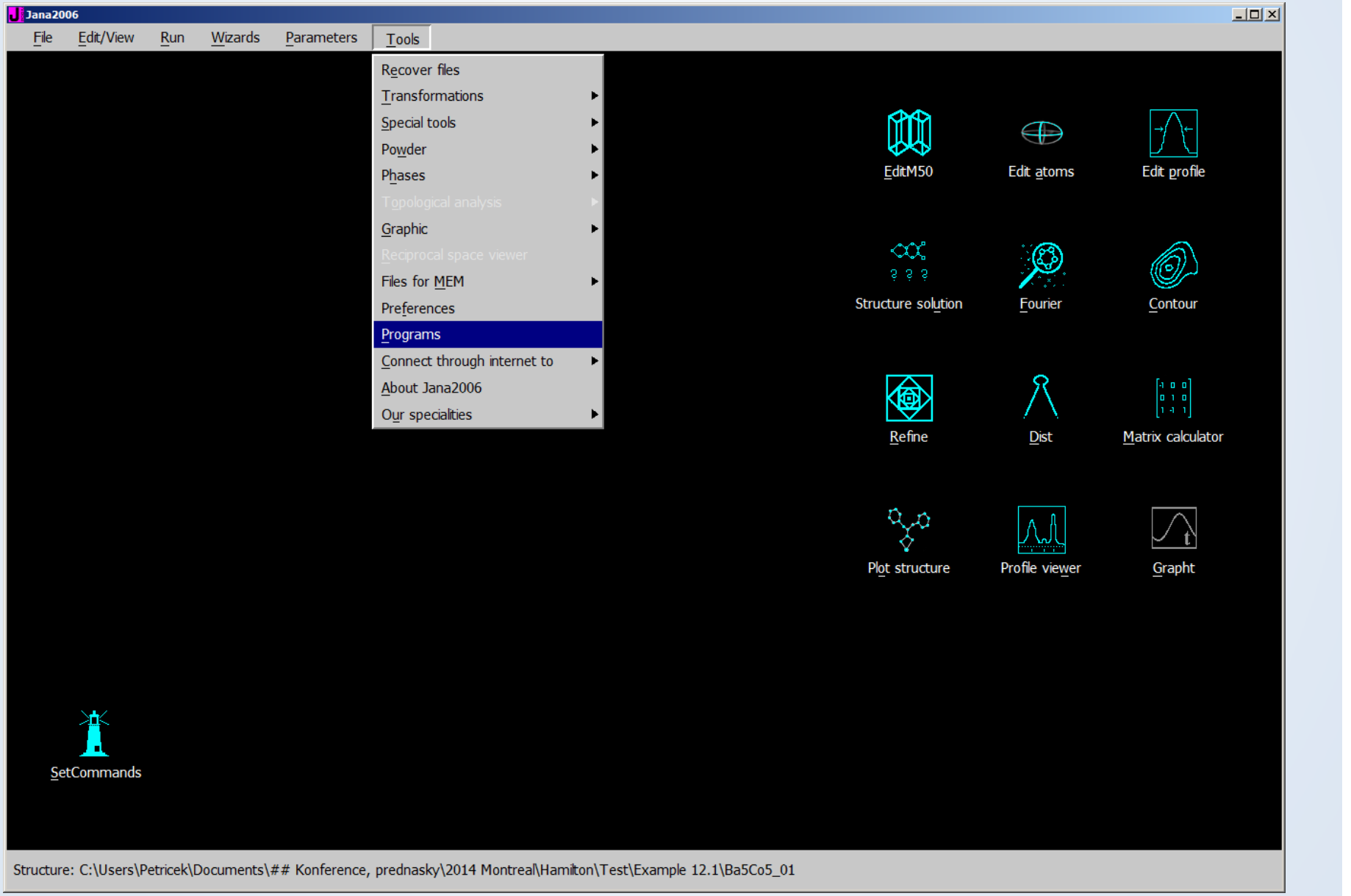
Start Jana2006

Go to "Tools → Programs", select with mouse the textbox "Graphic viewer" and define (using "Browse" button) the pathname of Vesta.exe

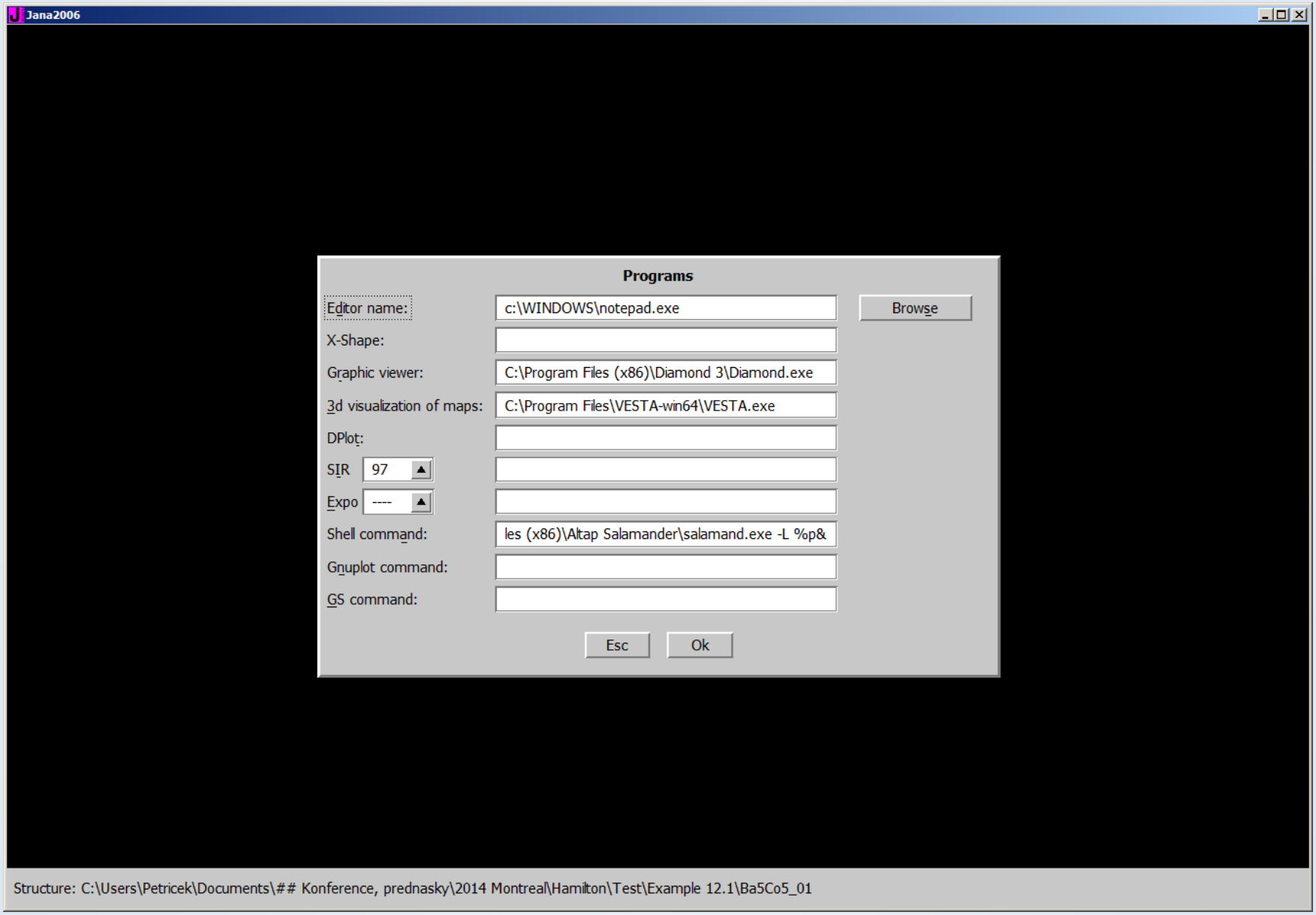
For using a different text editor than Notepad define its pathname in the textbox "Editor name".

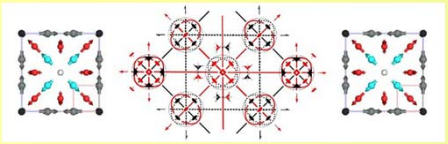
For using Vesta define its pathname in the textbox "3d visualization of maps"

Installation



Installation





Examples

Example 12.1 – simple magnetic structure **k=0**

Example 12.2 – commensurate magnetic structure **k=**(0,0,1/2)

Example 12.3 – commensurate magnetic structure **k=**(1,0,0)

Example 12.4 – incommensurate magnetic structure

Example 12.6 – Jana2006-ISODISTORT communication