Hands-on half-polarized single-crystal data from DEMAND

Polarized Neutron Diffraction and Spectroscopy: Applications to Quantum Materials Workshop, 2026

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Software: Cryspy

CrysPy

Crystallographic Python library

Leon Brillouin Laboratory UMR12 CEA-CNRS

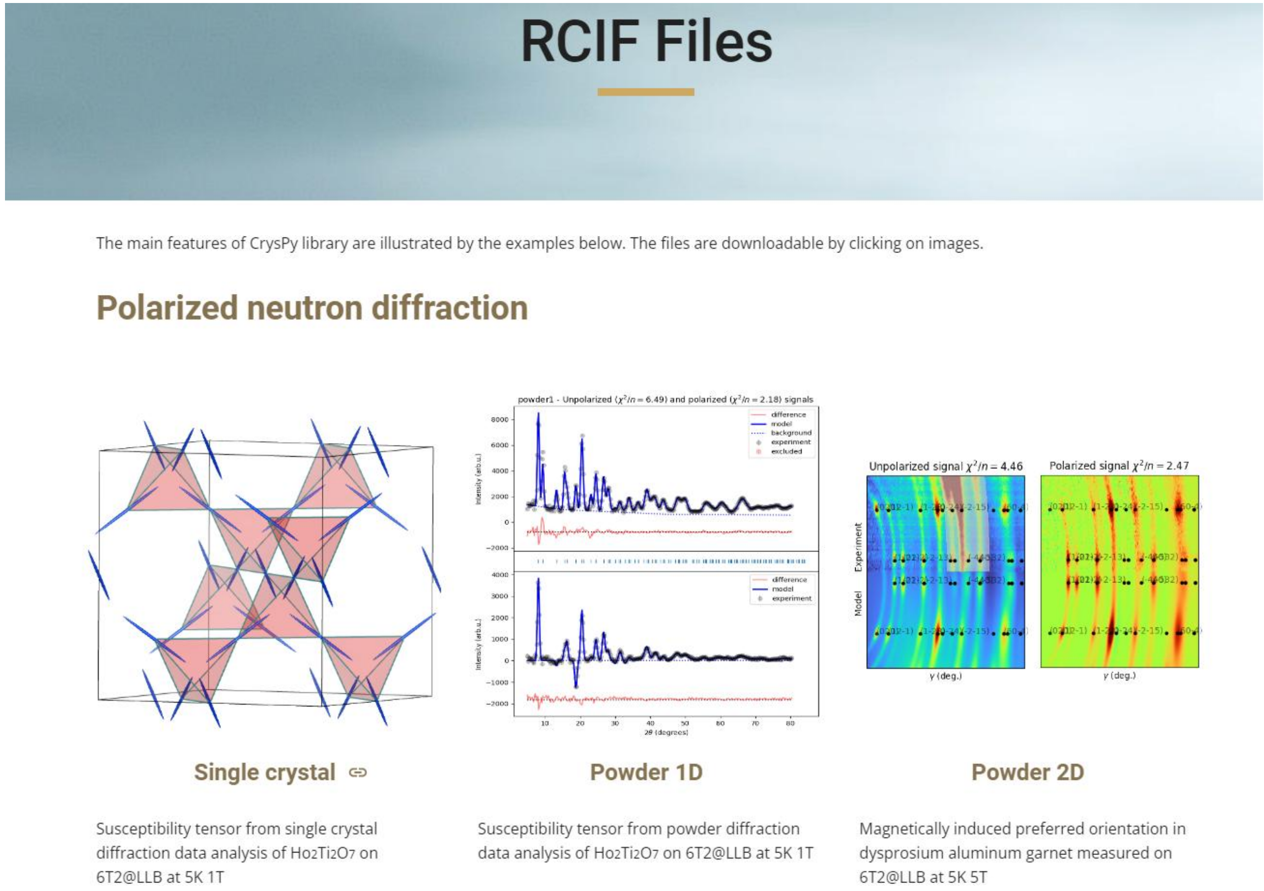
EURIZON 2020 (871072)

CrysPy is an open source program package that was originally developed for polarized neutron diffraction data analysis. The package allows the data treatment both for powders and single-crystal samples. Nuclear and (commensurate) magnetic structures refinement can be also perfomed based on the unpolarized neutron diffraction and X-ray diffraction data.

Before installing CrysPy on your computer, try it in a Web Browser by clicking on the link.

https://www.cryspy.fr/main

Examples in Cryspy



RCIF Files

The main features of CrysPy library are illustrated by the examples below. The files are downloadable by clicking on images.

Polarized neutron diffraction

Single crystal

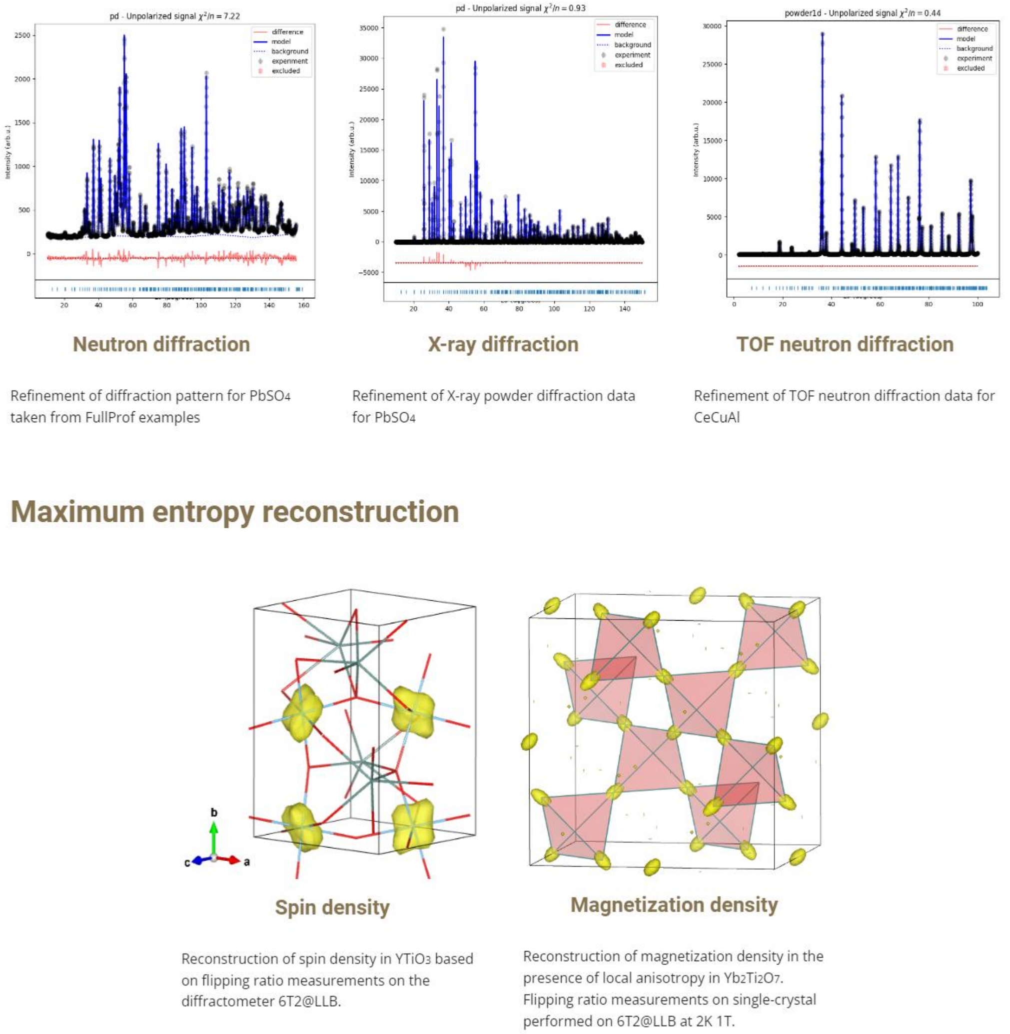
Susceptibility tensor from single crystal diffraction data analysis of $Ho_2Ti_2O_7$ on 6T2@LLB at 5K 1T

Powder 1D

Susceptibility tensor from powder diffraction data analysis of $Ho_2Ti_2O_7$ on 6T2@LLB at 5K 1T

Powder 2D

Magnetically induced preferred orientation in dysprosium aluminum garnet measured on 6T2@LLB at 5K 5T



Neutron diffraction

Refinement of diffraction pattern for $PbSO_4$ taken from FullProf examples

X-ray diffraction

Refinement of X-ray powder diffraction data for $PbSO_4$

TOF neutron diffraction

Refinement of TOF neutron diffraction data for CeCuAl

Maximum entropy reconstruction

Spin density

Reconstruction of spin density in $YTiO_3$ based on flipping ratio measurements on the diffractometer 6T2@LLB.

Magnetization density

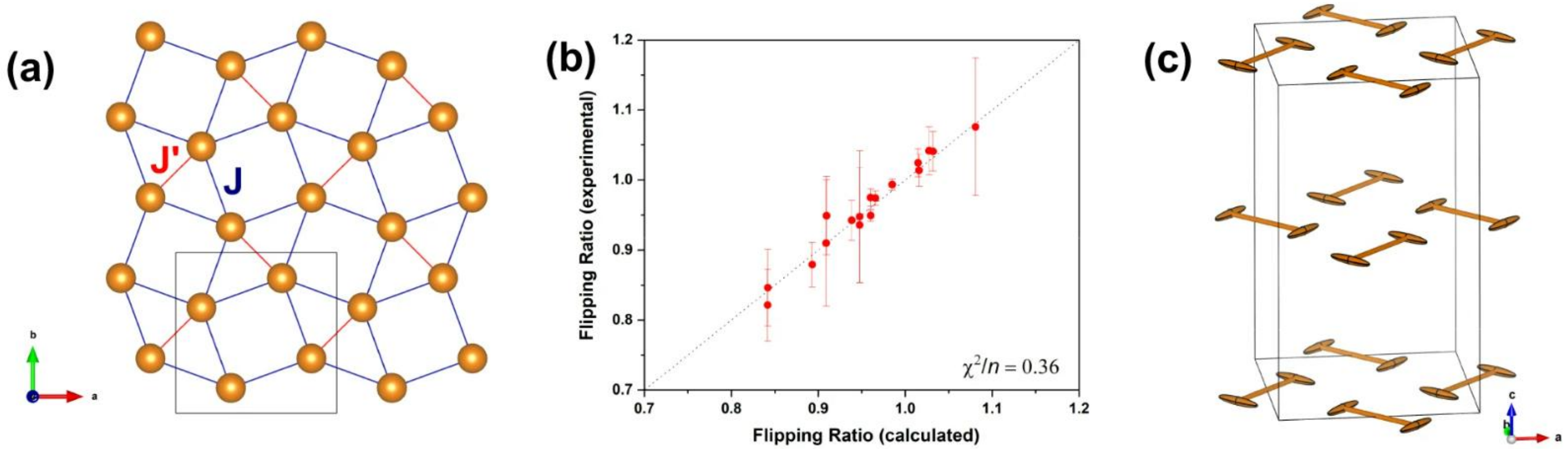
Reconstruction of magnetization density in the presence of local anisotropy in $Yb_2Ti_2O_7$. Flipping ratio measurements on single-crystal performed on 6T2@LLB at 2K 1T.

Example used in this tutorial

Field-induced partial disorder in a Shastry-Sutherland lattice

Madalynn Marshall, Brianna R. Billingsley, Xiaojian Bai, Qianli Ma, Tai Kong & Huibo Cao

Nature Communications **14**, Article number: 3641 (2023) | Cite this article



Step 0: Install Cryspy

- Step 0.0: Install Python 3 environment (if not already
  - Download Python 3 install package at python.org/downloads/

Download the latest version for Windows

Download Python 3.12.4

Looking for Python with a different OS? Python for Windows, Linux/UNIX, macOS, Other

Want to help test development versions of Python 3.13? Prereleases, Docker images

  - Install Python 3 with **Add python.exe to PATH option**

Install Python 3.12.4 (64-bit)

Select Install Now to install Python with default settings, or choos
Customize to enable or disable features.

→ Install Now
C:\Users\yho\AppData\Local\Programs\Python\Python312

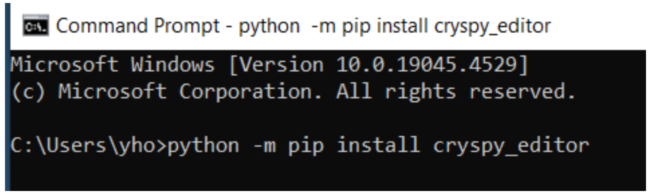
Includes IDLE, pip and documentation
Creates shortcuts and file associations

→ Customize installation
Choose location and features

☐ Use admin privileges when installing py.exe
☑ Add python.exe to PATH

- Step 0.1: Install Cryspy
  - Open command prompt (cmd)
  - Install Cryspy with command:

python –m pip install cryspy_editor

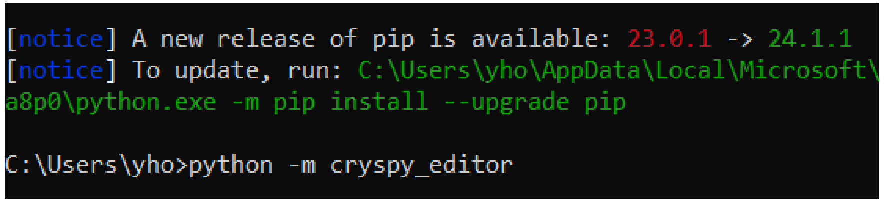


Command Prompt - python -m pip install cryspy_editor

```
Microsoft Windows [Version 10.0.19045.4529]
(c) Microsoft Corporation. All rights reserved.

C:\Users\yho>python -m pip install cryspy_editor
```

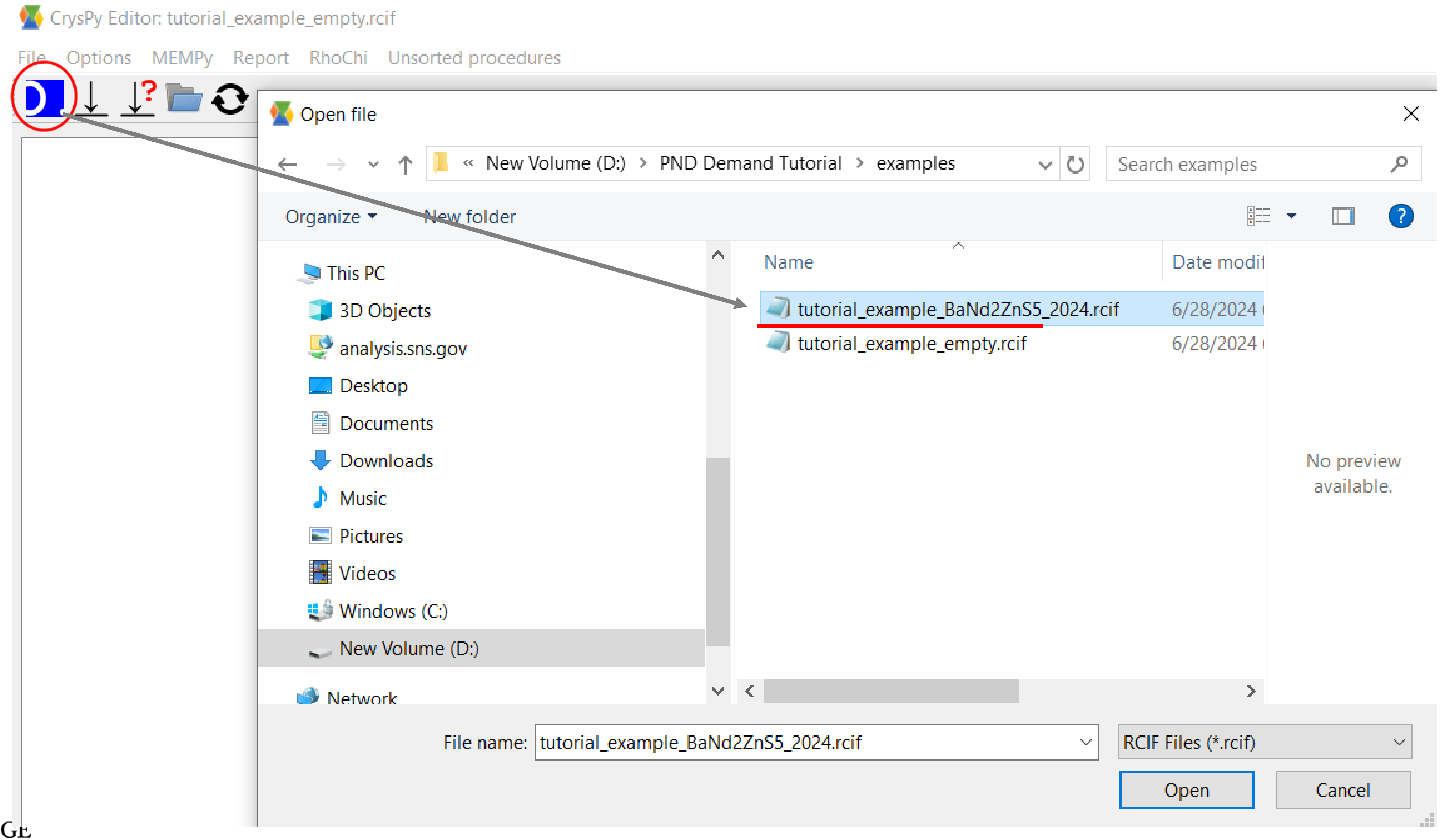
  - Open Cryspy with command:

python –m cryspy_editor



```
[notice] A new release of pip is available: 23.0.1 -> 24.1.1
[notice] To update, run: C:\Users\yho\AppData\Local\Microsoft\
a8p0\python.exe -m pip install --upgrade pip

C:\Users\yho>python -m cryspy_editor
```

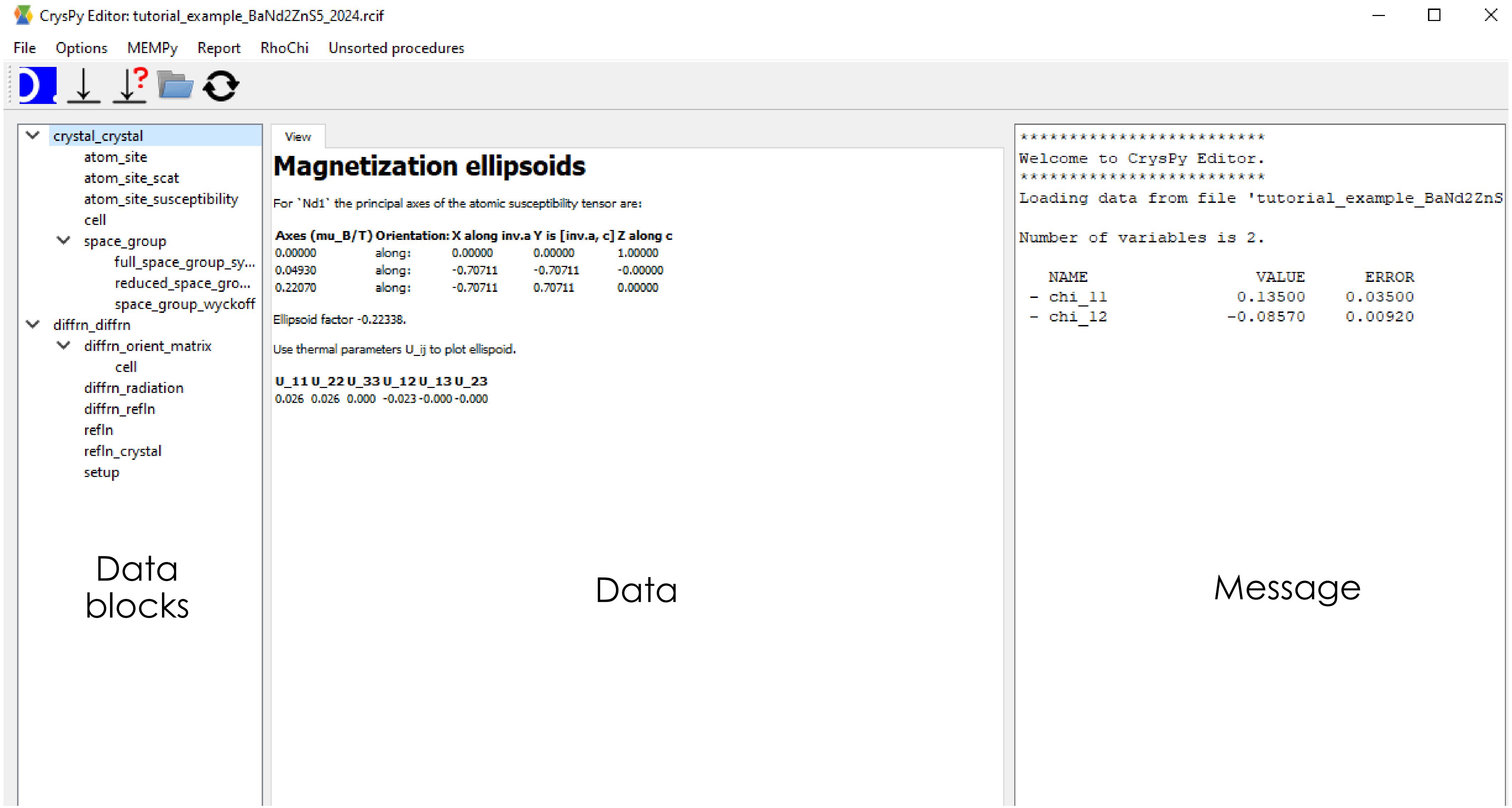
Step 0.5: Reading the tutorial example .rcif file



Name	Date modi
tutorial_example_BaNd2ZnS5_2024.rcif	6/28/2024
tutorial_example_empty.rcif	6/28/2024

File name: tutorial_example_BaNd2ZnS5_2024.rcif

Step 0.5: Reading the tutorial example .rcif file



Magnetization ellipsoids

For `Nd1` the principal axes of the atomic susceptibility tensor are:

Axes (mu_B/T)	Orientation:	X along inv.a	Y is [inv.a, c]	Z along c
0.00000	along:	0.00000	0.00000	1.00000
0.04930	along:	-0.70711	-0.70711	-0.00000
0.22070	along:	-0.70711	0.70711	0.00000

Ellipsoid factor -0.22338.

Use thermal parameters U_ij to plot ellipsoid.

U_11	U_22	U_33	U_12	U_13	U_23
0.026	0.026	0.000	-0.023	-0.000	-0.000

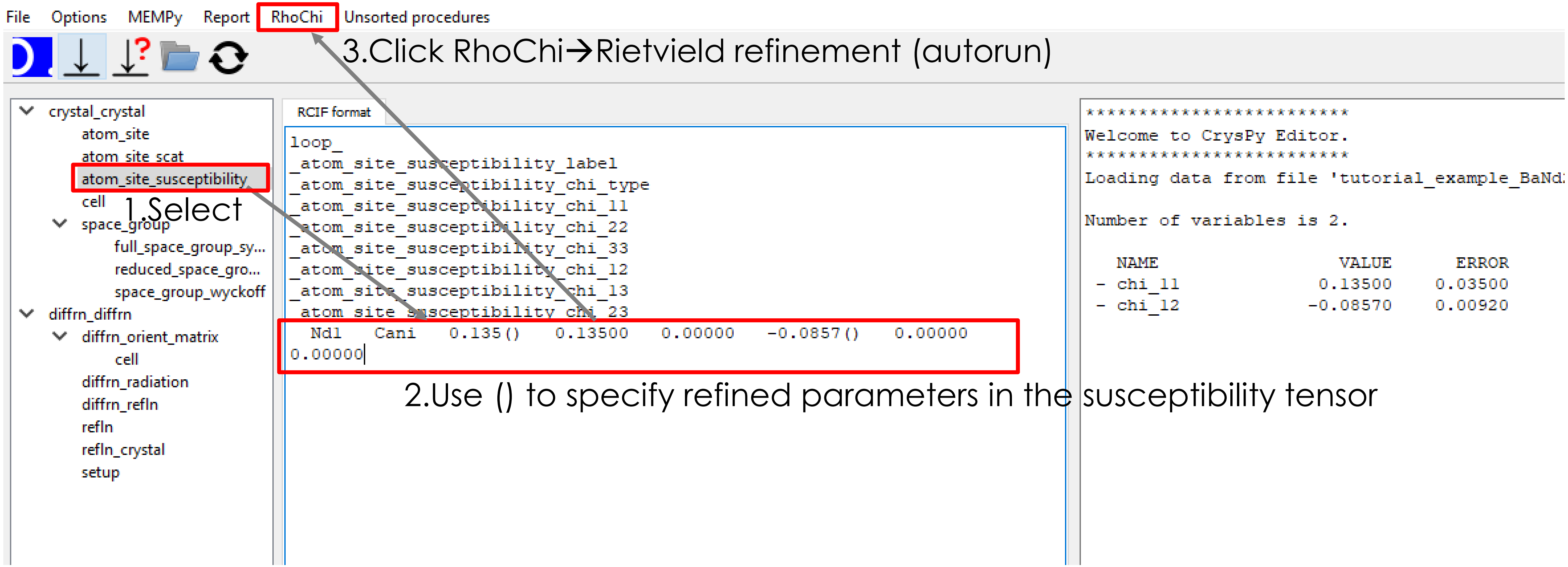
```
*************************
Welcome to CrysPy Editor.
*************************
Loading data from file 'tutorial_example_BaNd2ZnS

Number of variables is 2.

   NAME                   VALUE      ERROR
 - chi_11               0.13500    0.03500
 - chi_12              -0.08570    0.00920
```

Data blocks

Data

Message

Step 0.6: Refining the tutorial example .rcif file



1.Select

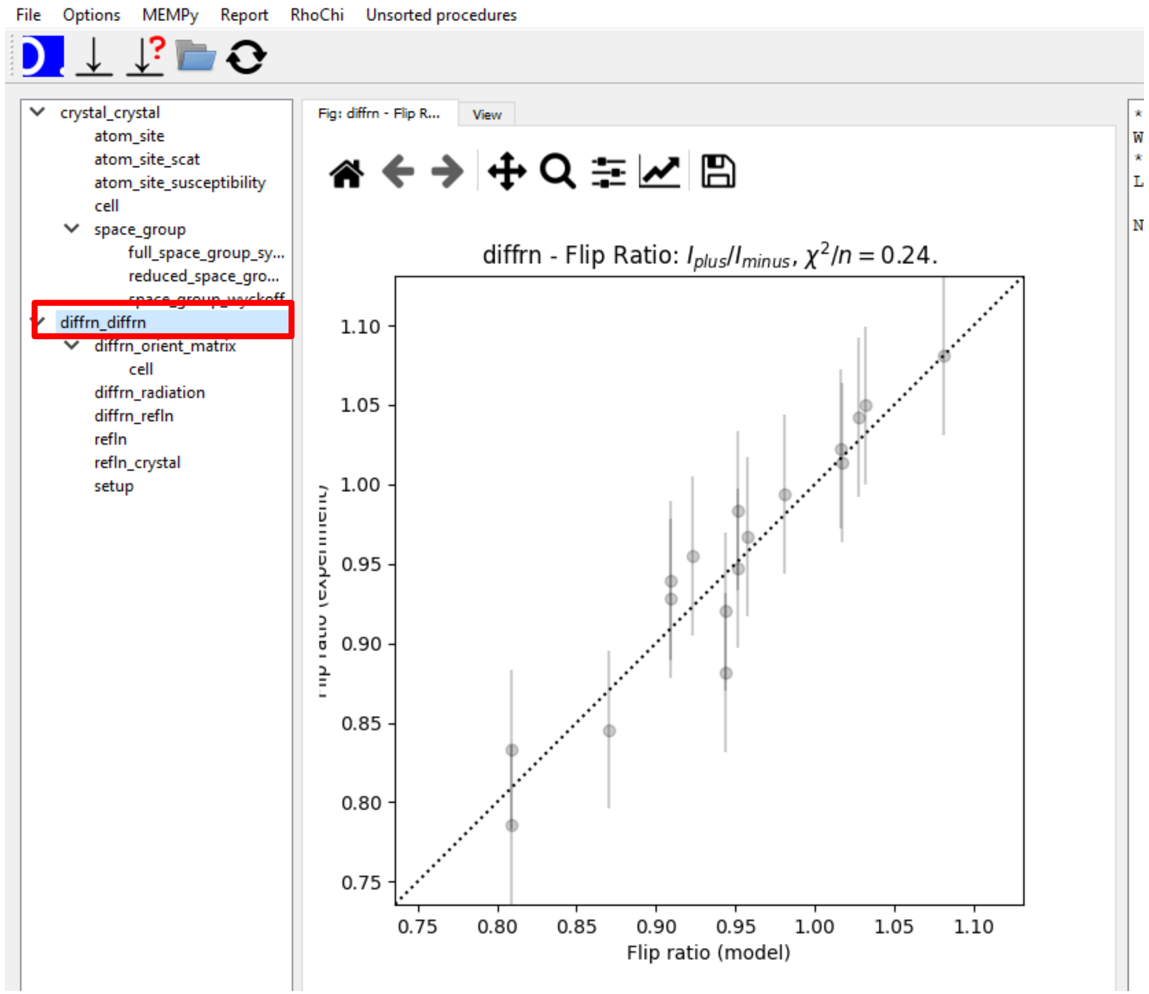
2.Use () to specify refined parameters in the susceptibility tensor

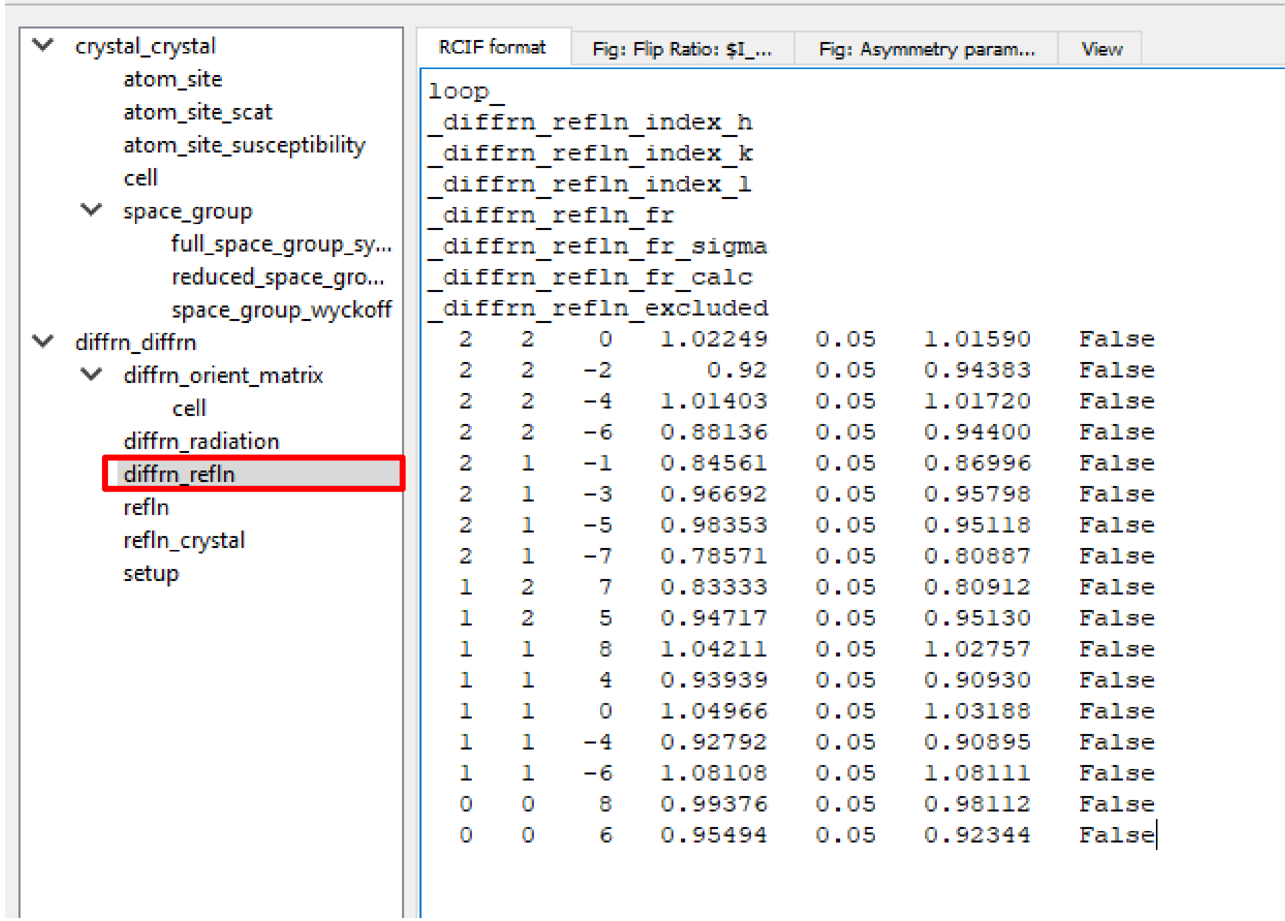
3.Click RhoChi→Rietvield refinement (autorun)

```
loop_
_atom_site_susceptibility_label
_atom_site_susceptibility_chi_type
_atom_site_susceptibility_chi_11
_atom_site_susceptibility_chi_22
_atom_site_susceptibility_chi_33
_atom_site_susceptibility_chi_12
_atom_site_susceptibility_chi_13
_atom_site_susceptibility_chi_23
 Nd1   Cani   0.135()   0.13500   0.00000   -0.0857()   0.00000
0.00000
```

```
************************
Welcome to CrysPy Editor.
************************
Loading data from file 'tutorial_example_BaNd

Number of variables is 2.

   NAME                    VALUE       ERROR
 - chi_11                0.13500     0.03500
 - chi_12               -0.08570     0.00920
```

Step 0.7: Examining the fitting quality

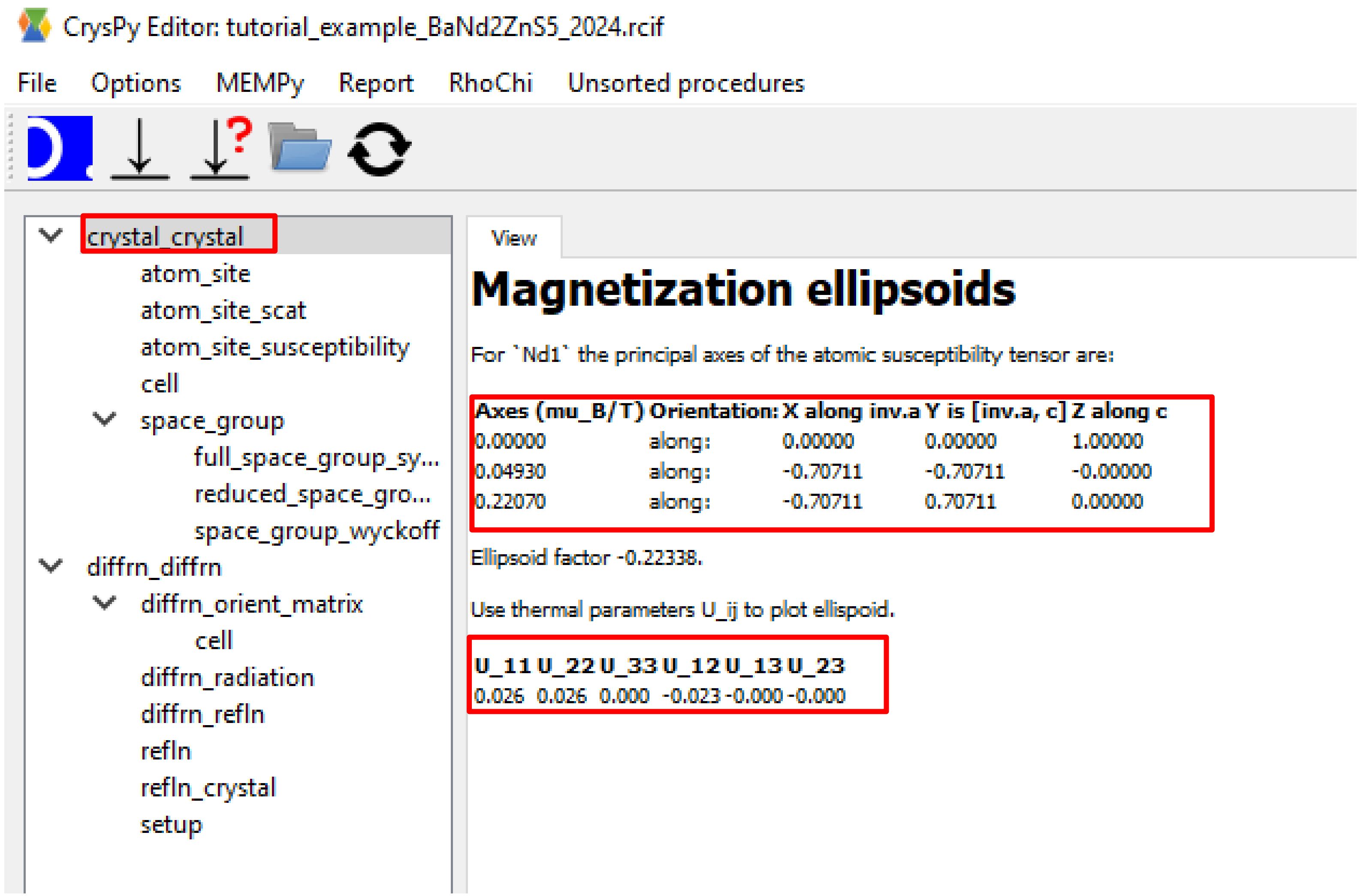




```
loop_
_diffrn_refln_index_h
_diffrn_refln_index_k
_diffrn_refln_index_l
_diffrn_refln_fr
_diffrn_refln_fr_sigma
_diffrn_refln_fr_calc
_diffrn_refln_excluded
  2   2    0   1.02249   0.05   1.01590   False
  2   2   -2      0.92   0.05   0.94383   False
  2   2   -4   1.01403   0.05   1.01720   False
  2   2   -6   0.88136   0.05   0.94400   False
  2   1   -1   0.84561   0.05   0.86996   False
  2   1   -3   0.96692   0.05   0.95798   False
  2   1   -5   0.98353   0.05   0.95118   False
  2   1   -7   0.78571   0.05   0.80887   False
  1   2    7   0.83333   0.05   0.80912   False
  1   2    5   0.94717   0.05   0.95130   False
  1   1    8   1.04211   0.05   1.02757   False
  1   1    4   0.93939   0.05   0.90930   False
  1   1    0   1.04966   0.05   1.03188   False
  1   1   -4   0.92792   0.05   0.90895   False
  1   1   -6   1.08108   0.05   1.08111   False
  0   0    8   0.99376   0.05   0.98112   False
  0   0    6   0.95494   0.05   0.92344   False
```

4. Examine the fitting quality in the flipping ratio plot and the peak list

Step 0.8: Reading the refinement results



Magnetization ellipsoids

For `Nd1` the principal axes of the atomic susceptibility tensor are:

Axes (mu_B/T)	Orientation:	X along inv.a	Y is [inv.a, c]	Z along c
0.00000	along:	0.00000	0.00000	1.00000
0.04930	along:	-0.70711	-0.70711	-0.00000
0.22070	along:	-0.70711	0.70711	0.00000

Ellipsoid factor -0.22338.

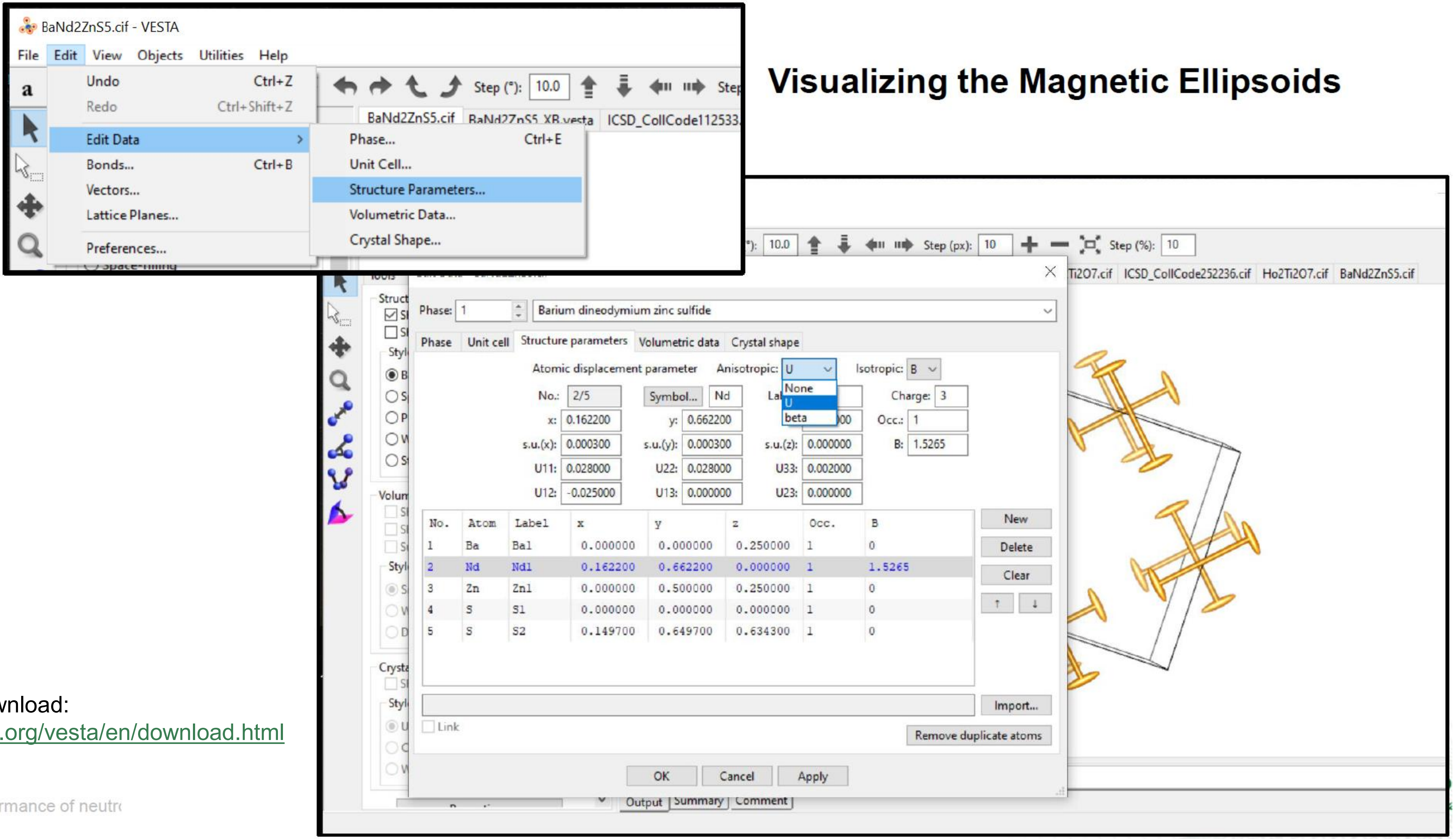
Use thermal parameters U_ij to plot ellispoid.

U_11	U_22	U_33	U_12	U_13	U_23
0.026	0.026	0.000	-0.023	-0.000	-0.000

5. Find the local susceptibility tensor and ellipsoid U_ij

Step 0.9: Visualize the results in VESTA

Visualizing the Magnetic Ellipsoids



Phase: 1 Barium dineodymium zinc sulfide

Anisotropic: U Isotropic: B

No.: 2/5 Symbol: Nd Charge: 3

x: 0.162200 y: 0.662200 Occ.: 1

s.u.(x): 0.000300 s.u.(y): 0.000300 s.u.(z): 0.000000 B: 1.5265

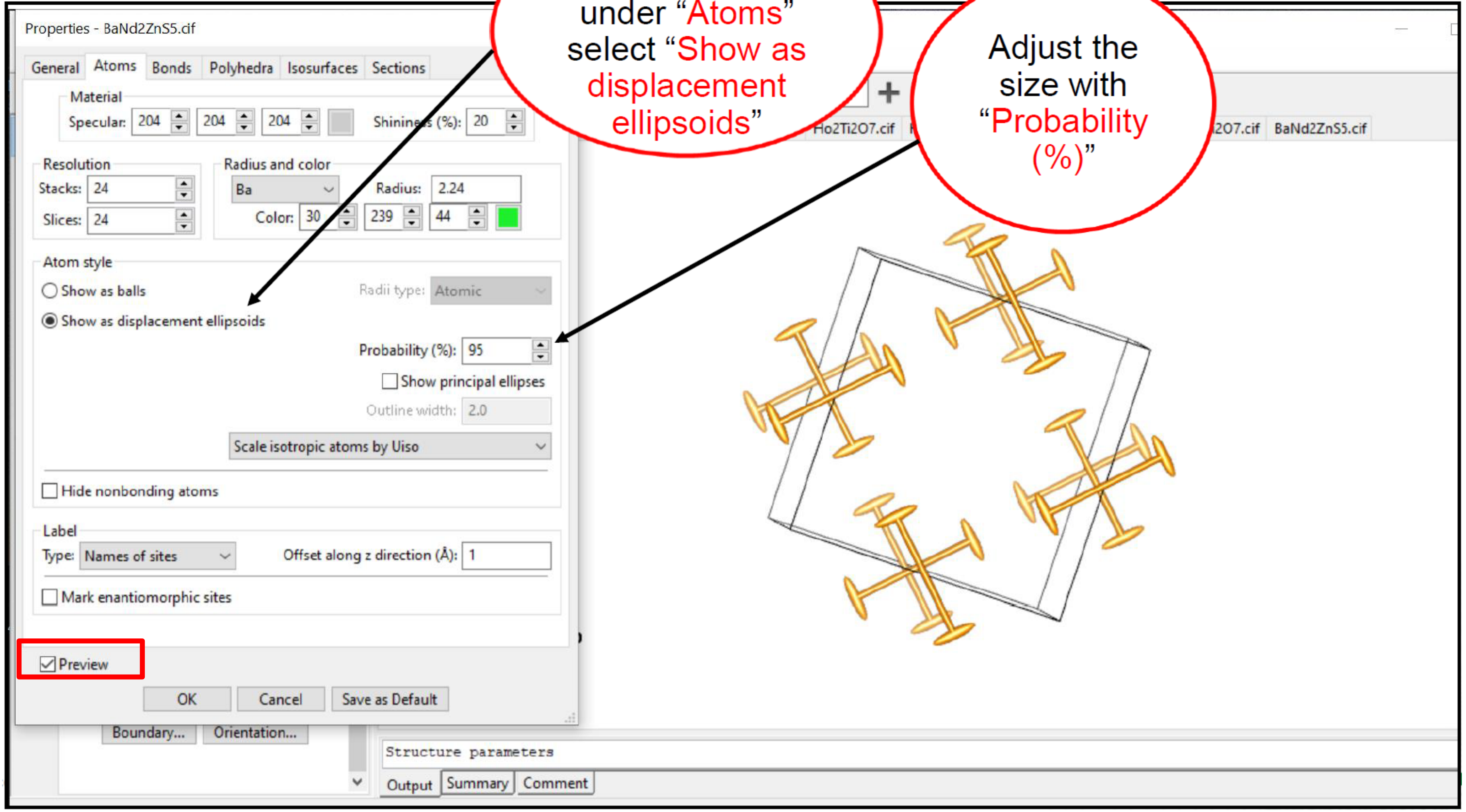
U11: 0.028000 U22: 0.028000 U33: 0.002000

U12: -0.025000 U13: 0.000000 U23: 0.000000

No.	Atom	Label	x	y	z	Occ.	B
1	Ba	Ba1	0.000000	0.000000	0.250000	1	0
2	Nd	Nd1	0.162200	0.662200	0.000000	1	1.5265
3	Zn	Zn1	0.000000	0.500000	0.250000	1	0
4	S	S1	0.000000	0.000000	0.000000	1	0
5	S	S2	0.149700	0.649700	0.634300	1	0

VESTA download:
jp-minerals.org/vesta/en/download.html

Step 0.9: Visualize the results in VESTA



Properties - BaNd2ZnS5.cif

Material
Specular: 204 204 204 Shininess (%): 20

Resolution
Stacks: 24
Slices: 24

Radius and color
Ba
Radius: 2.24
Color: 30 239 44 🟩

Atom style
○ Show as balls
● Show as displacement ellipsoids
Radii type: Atomic
Probability (%): 95
☐ Show principal ellipses
Outline width: 2.0
Scale isotropic atoms by Uiso

☐ Hide nonbonding atoms

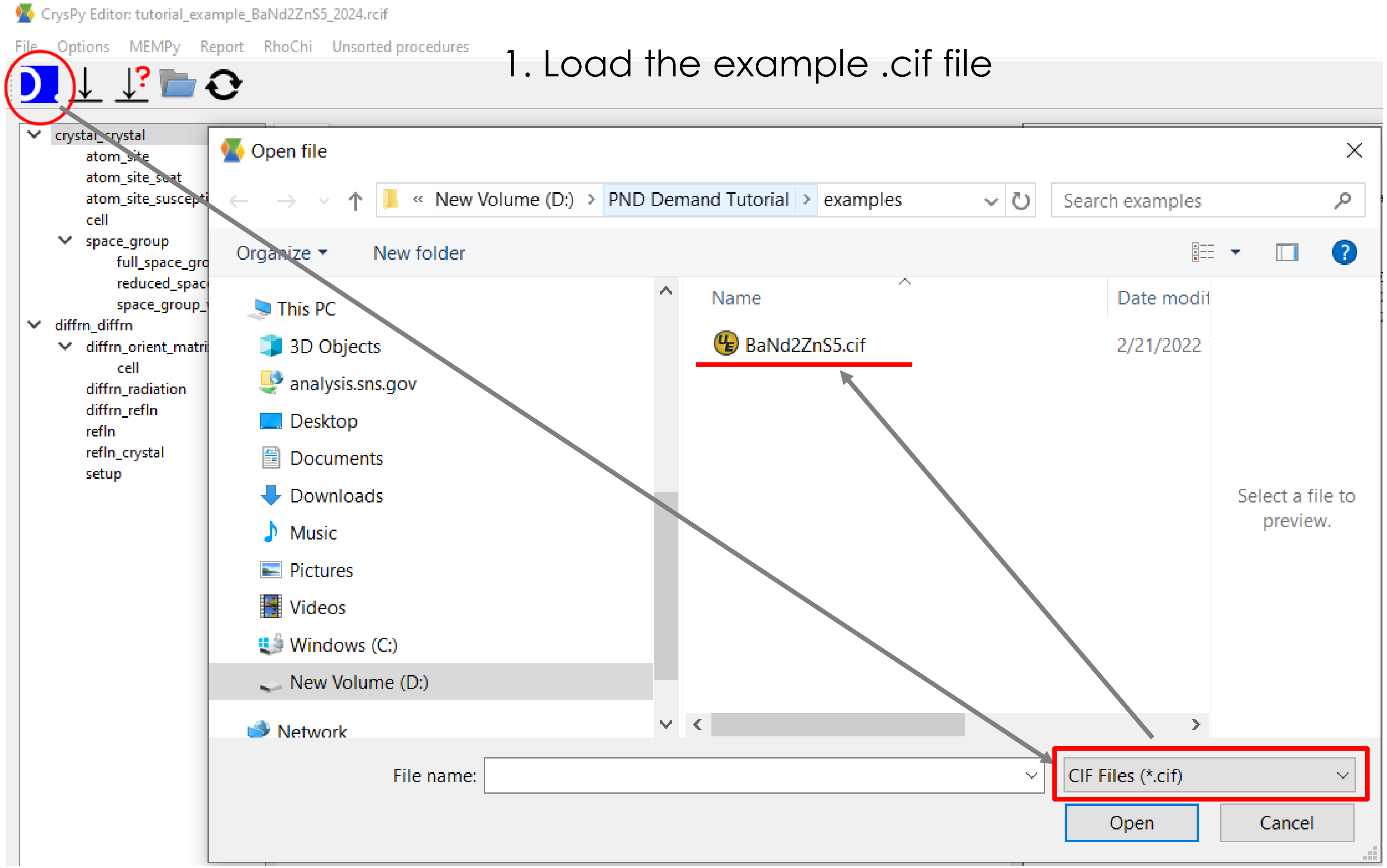
Label
Type: Names of sites
Offset along z direction (Å): 1
☐ Mark enantiomorphic sites

☑ Preview

Select “Properties” then under “Atoms” select “Show as displacement ellipsoids”

Adjust the size with “Probability (%)”

Step 1: Create an .rcif file from Scratch



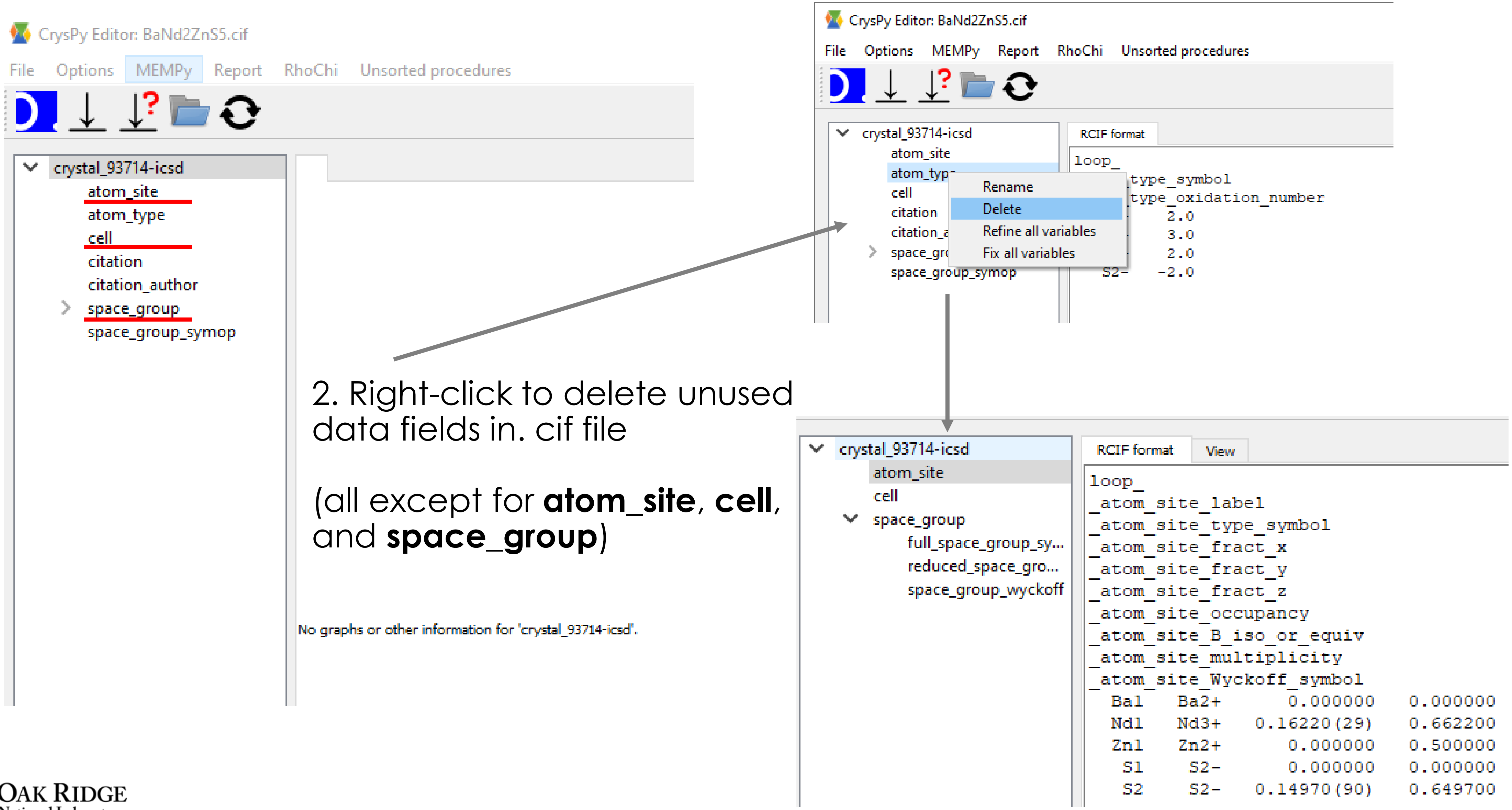
1. Load the example .cif file

BaNd2ZnS5.cif 2/21/2022

File name:

CIF Files (*.cif)

Step 1.1: Modify the .cif file



No graphs or other information for 'crystal_93714-icsd'.

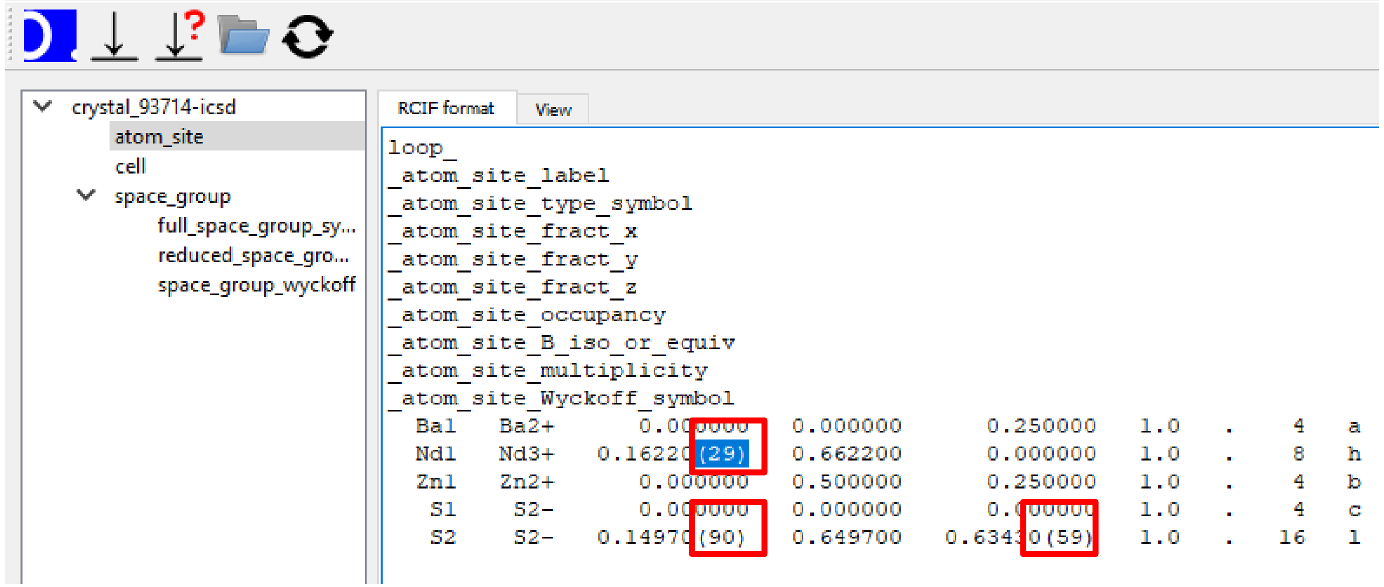
```
loop_
_type_symbol
_type_oxidation_number
   2.0
   3.0
   2.0
S2-   -2.0
```

2. Right-click to delete unused data fields in. cif file

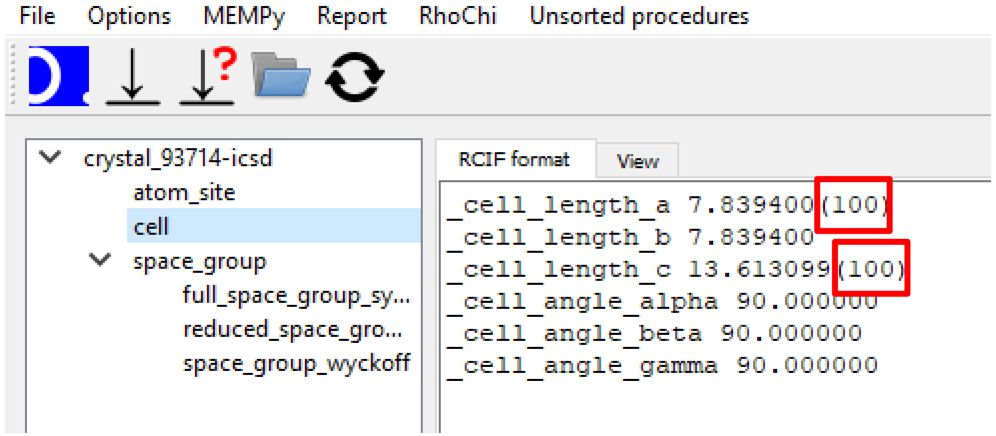
(all except for **atom_site**, **cell**, and **space_group**)

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
_atom_site_multiplicity
_atom_site_Wyckoff_symbol
  Ba1    Ba2+      0.000000    0.000000
  Nd1    Nd3+   0.16220(29)    0.662200
  Zn1    Zn2+      0.000000    0.500000
   S1     S2-      0.000000    0.000000
   S2     S2-   0.14970(90)    0.649700
```

Step 1.1: Modify the .cif file



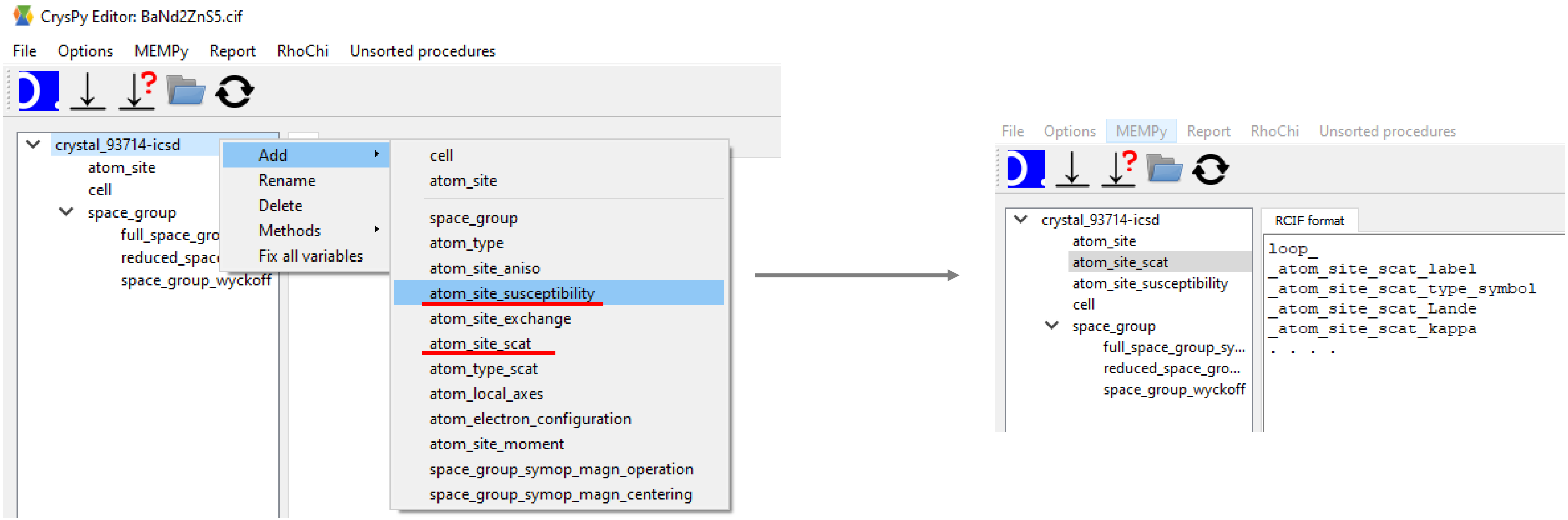
```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
_atom_site_multiplicity
_atom_site_Wyckoff_symbol
  Ba1    Ba2+      0.000000   0.000000      0.250000   1.0    .    4   a
  Nd1    Nd3+    0.16220(29)  0.662200      0.000000   1.0    .    8   h
  Zn1    Zn2+      0.000000   0.500000      0.250000   1.0    .    4   b
   S1     S2-      0.000000   0.000000      0.000000   1.0    .    4   c
   S2     S2-    0.14970(90)  0.649700    0.63430(59)  1.0    .   16   l
```



```
_cell_length_a 7.839400(100)
_cell_length_b 7.839400
_cell_length_c 13.613099(100)
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 90.000000
```

3. Remove all (..) in atom positions and lattice parameters, so Cryspy will not treat them as refined parameters

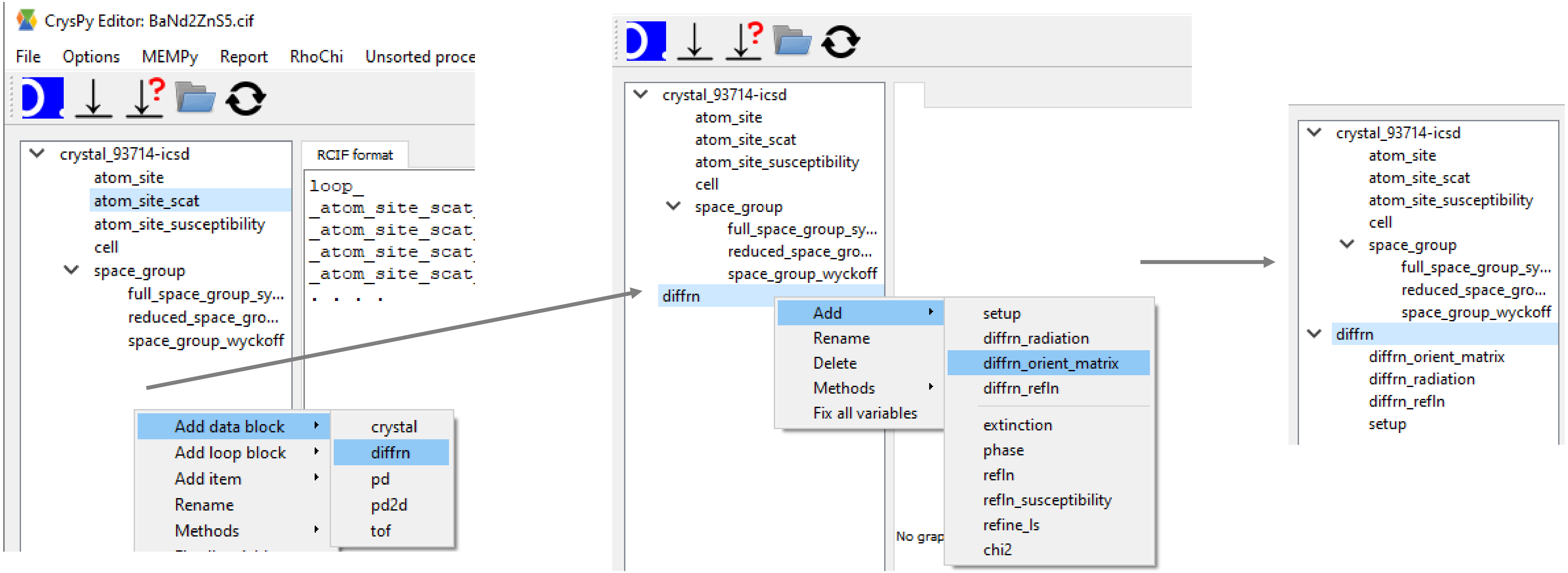
Step 1.1: Modify the .cif file



```
loop_
_atom_site_scat_label
_atom_site_scat_type_symbol
_atom_site_scat_Lande
_atom_site_scat_kappa
. . . .
```

4. Right-click on the **Crystal_...** data block to add new data fields: **atom_site_susceptibility** and **atom_site_scat** for local susceptibility

Step 1.1: Modify the .cif file



```
loop_
 _atom_site_scat
 _atom_site_scat
 _atom_site_scat
 _atom_site_scat
 . . . .
```

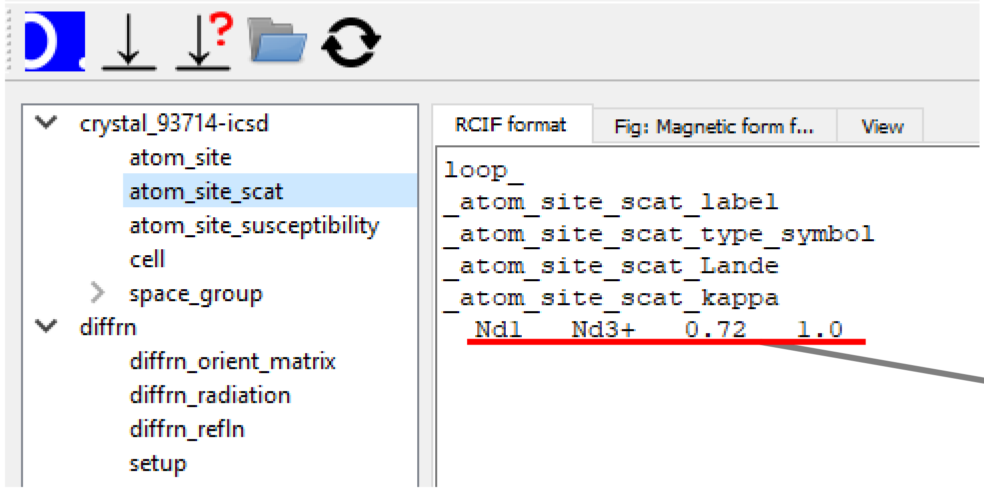
5. Right-click on empty space to add the data block **diffrn** for diffraction data

6. Right-click on **diffrn** to add the upper 4 data fields: **setup, diffrn_radiation, diffrn_orient matrix, and diffrn_refln**

Congrats! You now have a complete (but mostly empty) .rcif file!

Step 1.2: Fill in the new .rcif fields

1. Fill in the magnetic atom and its Lande g-factor



```
loop_
_atom_site_scat_label
_atom_site_scat_type_symbol
_atom_site_scat_Lande
_atom_site_scat_kappa
 Nd1   Nd3+   0.72   1.0
```

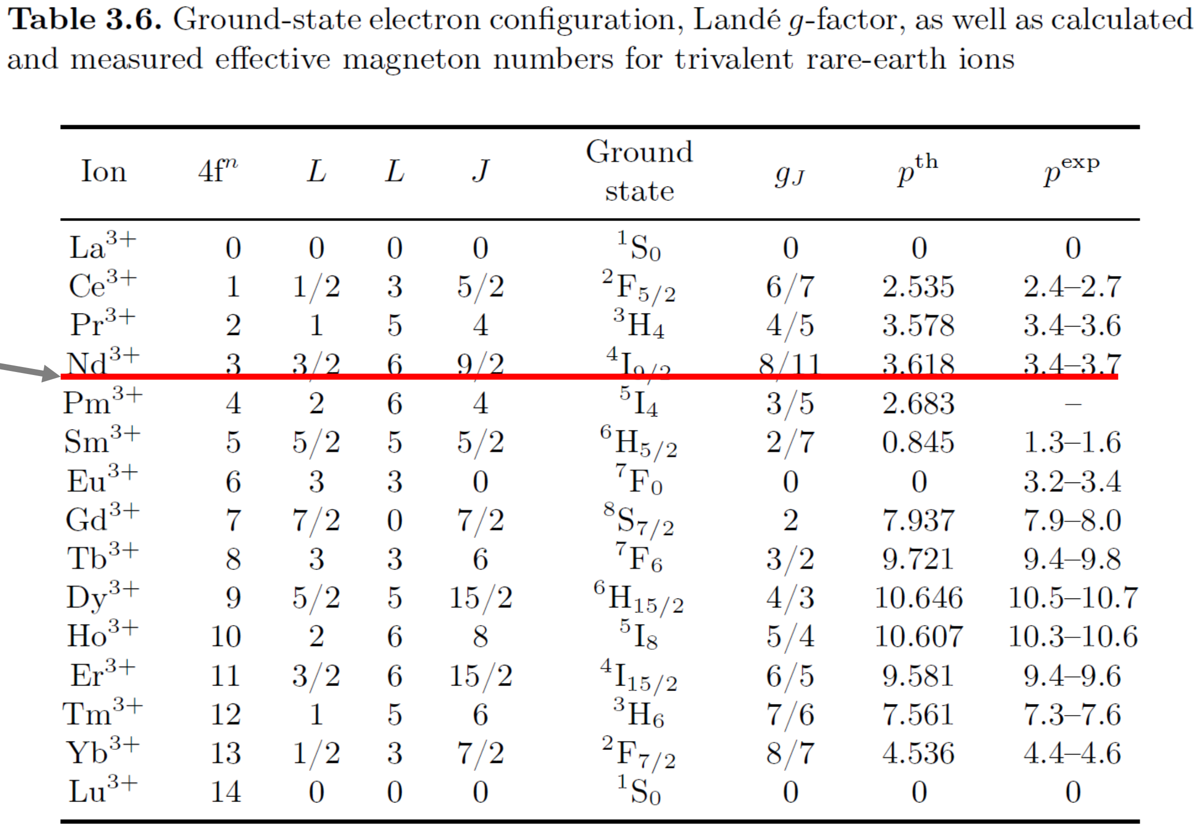
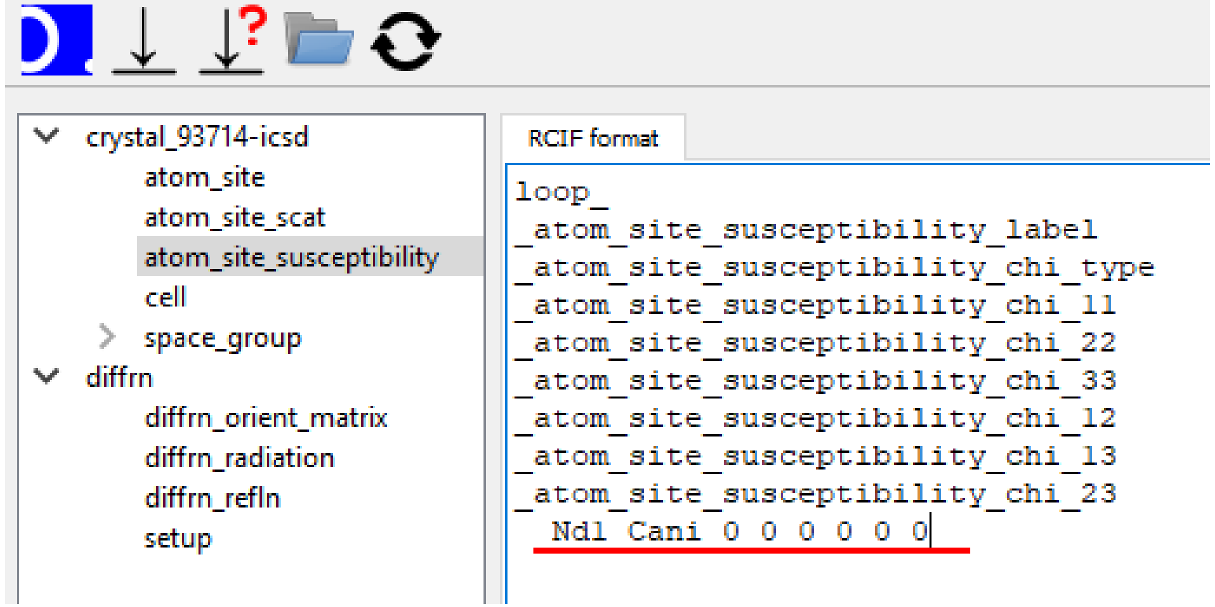


Table 3.6. Ground-state electron configuration, Landé g-factor, as well as calculated and measured effective magneton numbers for trivalent rare-earth ions

Ion	$4f^n$	L	L	J	Ground state	g_J	p^{th}	p^{exp}
La^{3+}	0	0	0	0	$^1S_0$	0	0	0
Ce^{3+}	1	1/2	3	5/2	$^2F_{5/2}$	6/7	2.535	2.4–2.7
Pr^{3+}	2	1	5	4	$^3H_4$	4/5	3.578	3.4–3.6
Nd^{3+}	3	3/2	6	9/2	$^4I_{9/2}$	8/11	3.618	3.4–3.7
Pm^{3+}	4	2	6	4	$^5I_4$	3/5	2.683	–
Sm^{3+}	5	5/2	5	5/2	$^6H_{5/2}$	2/7	0.845	1.3–1.6
Eu^{3+}	6	3	3	0	$^7F_0$	0	0	3.2–3.4
Gd^{3+}	7	7/2	0	7/2	$^8S_{7/2}$	2	7.937	7.9–8.0
Tb^{3+}	8	3	3	6	$^7F_6$	3/2	9.721	9.4–9.8
Dy^{3+}	9	5/2	5	15/2	$^6H_{15/2}$	4/3	10.646	10.5–10.7
Ho^{3+}	10	2	6	8	$^5I_8$	5/4	10.607	10.3–10.6
Er^{3+}	11	3/2	6	15/2	$^4I_{15/2}$	6/5	9.581	9.4–9.6
Tm^{3+}	12	1	5	6	$^3H_6$	7/6	7.561	7.3–7.6
Yb^{3+}	13	1/2	3	7/2	$^2F_{7/2}$	8/7	4.536	4.4–4.6
Lu^{3+}	14	0	0	0	$^1S_0$	0	0	0

Step 1.2: Fill in the new .rcif fields

2. Use **Cani** for atom_site_susceptibility_chi_type, type in all 0 for site susceptibilities

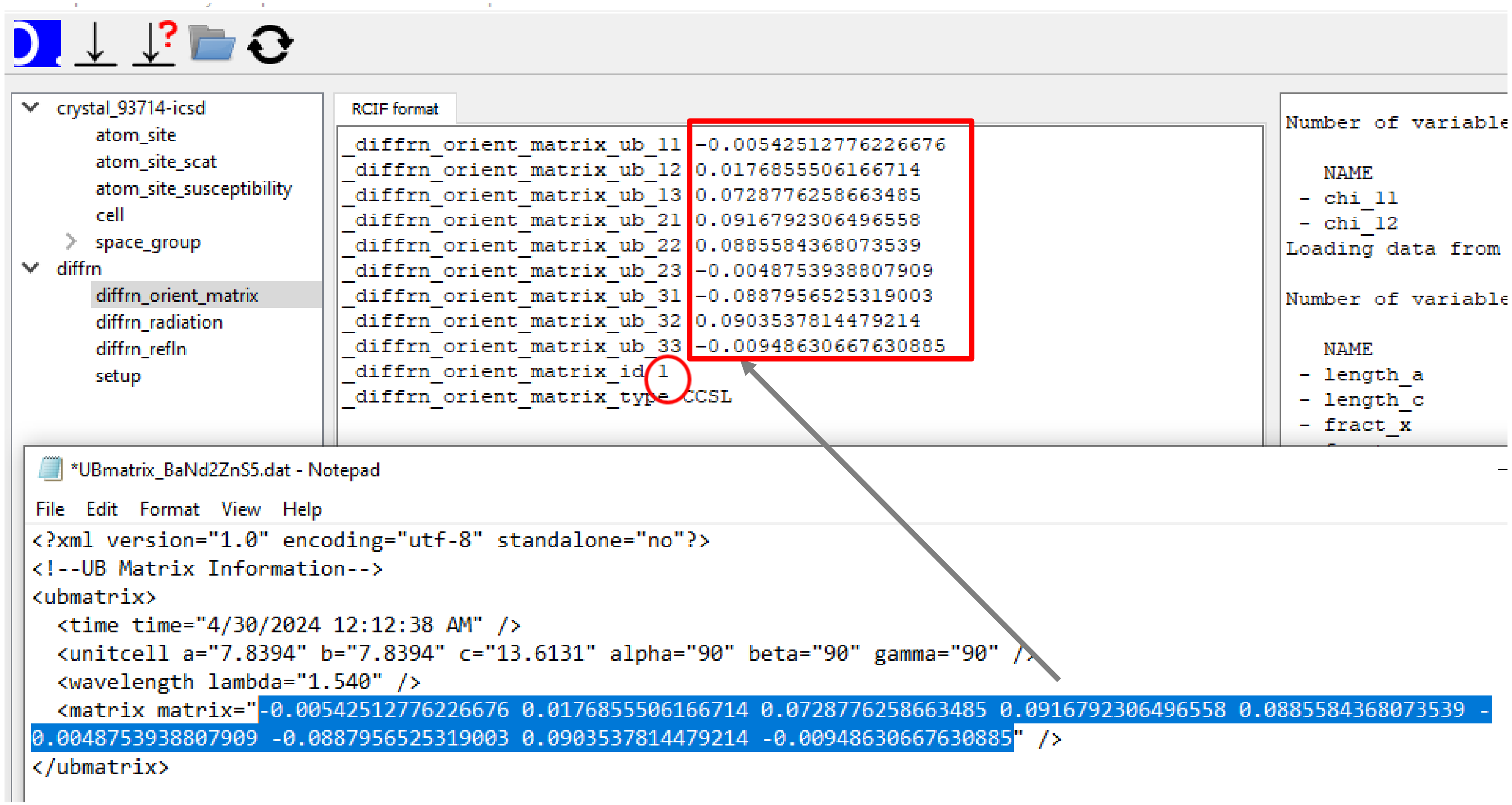


```
loop_
_atom_site_susceptibility_label
_atom_site_susceptibility_chi_type
_atom_site_susceptibility_chi_11
_atom_site_susceptibility_chi_22
_atom_site_susceptibility_chi_33
_atom_site_susceptibility_chi_12
_atom_site_susceptibility_chi_13
_atom_site_susceptibility_chi_23
 Nd1 Cani 0 0 0 0 0 0
```

Step 1.2: Fill in the new .rcif fields

2. Fill in the UB-matrix from experiment. For HB-3A **SPICE** Format UB, fill in the elements by the order of UB_11, UB_12, .. to UB_33.

(Do not use HB-3A **MANTID(ISAW)** Format UB as it uses a different set of coordination)



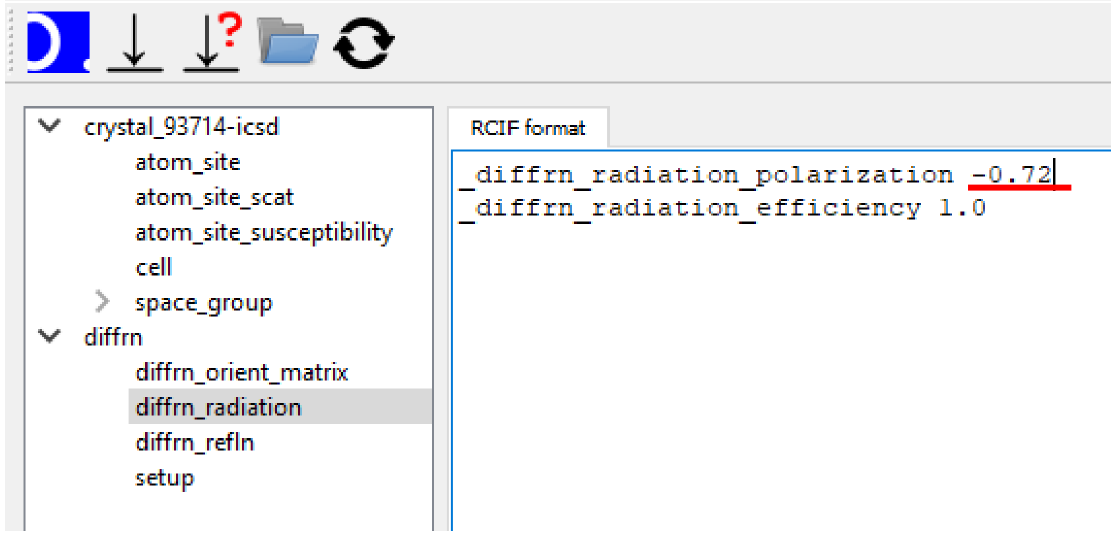
```
_diffrn_orient_matrix_ub_11 -0.00542512776226676
_diffrn_orient_matrix_ub_12 0.0176855506166714
_diffrn_orient_matrix_ub_13 0.0728776258663485
_diffrn_orient_matrix_ub_21 0.0916792306496558
_diffrn_orient_matrix_ub_22 0.0885584368073539
_diffrn_orient_matrix_ub_23 -0.0048753938807909
_diffrn_orient_matrix_ub_31 -0.0887956525319003
_diffrn_orient_matrix_ub_32 0.0903537814479214
_diffrn_orient_matrix_ub_33 -0.00948630667630885
_diffrn_orient_matrix_id 1
_diffrn_orient_matrix_type CCSL
```

```
Number of variable

  NAME
 - chi_11
 - chi_12
Loading data from

Number of variable

  NAME
 - length_a
 - length_c
 - fract_x
```

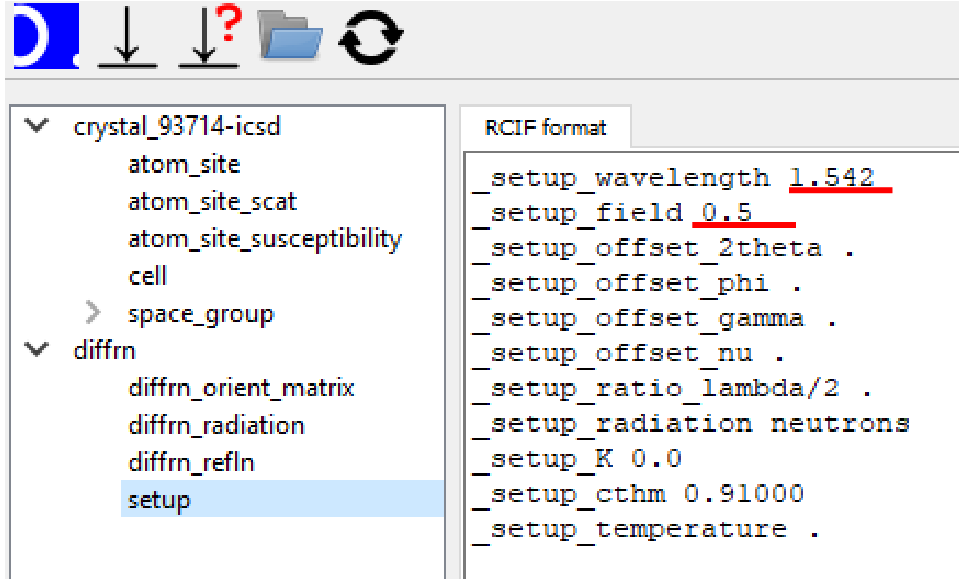
```
<?xml version="1.0" encoding="utf-8" standalone="no"?>
<!--UB Matrix Information-->
<ubmatrix>
  <time time="4/30/2024 12:12:38 AM" />
  <unitcell a="7.8394" b="7.8394" c="13.6131" alpha="90" beta="90" gamma="90" />
  <wavelength lambda="1.540" />
  <matrix matrix="-0.00542512776226676 0.0176855506166714 0.0728776258663485 0.0916792306496558 0.0885584368073539 -
0.0048753938807909 -0.0887956525319003 0.0903537814479214 -0.00948630667630885" />
</ubmatrix>
```

Step 1.2: Fill in the new .rcif fields

3. Fill in the polarization, wavelength and magnetic field information obtained from the experiment



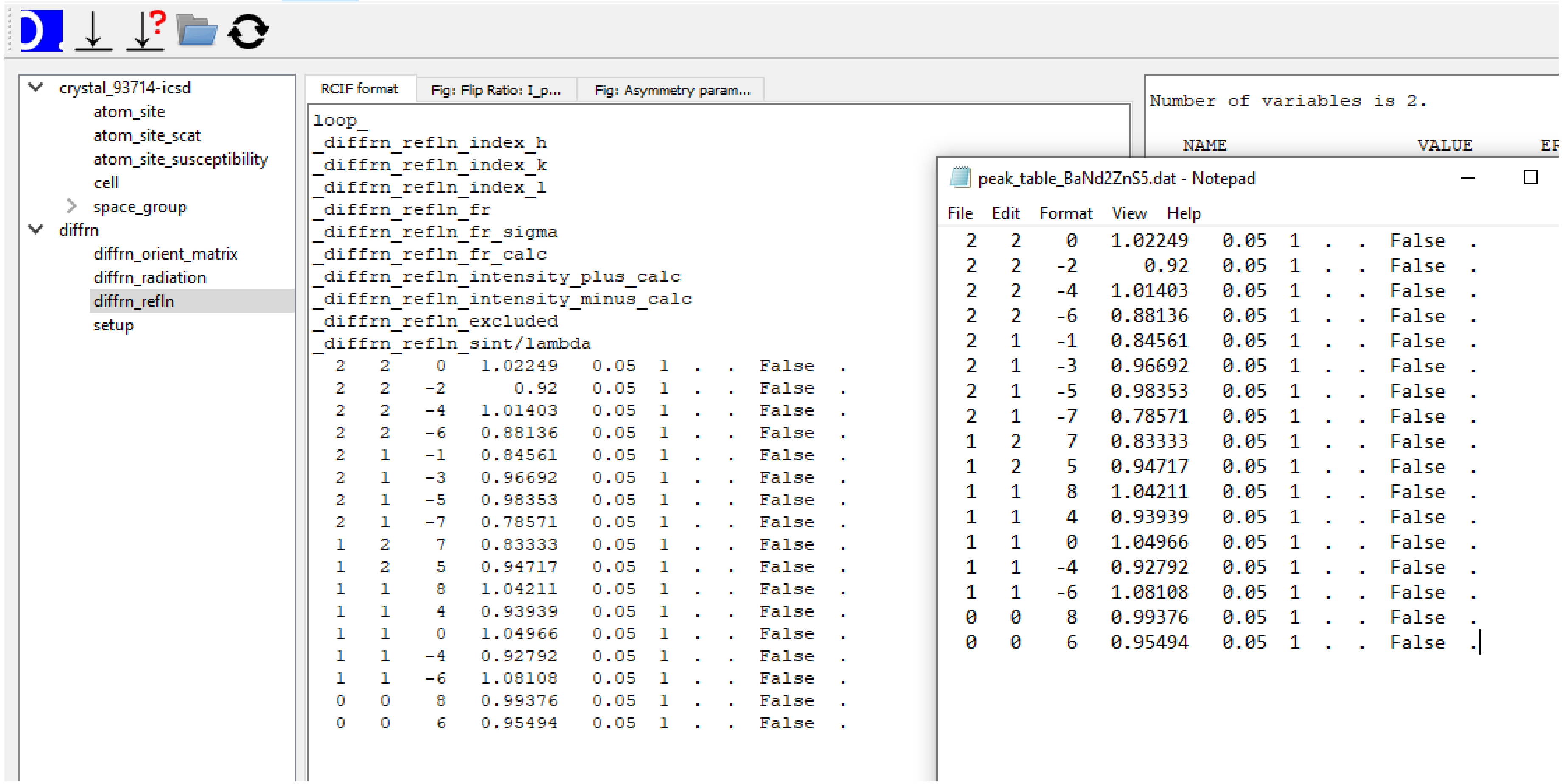
```
_diffrn_radiation_polarization -0.72
_diffrn_radiation_efficiency 1.0
```



```
_setup_wavelength 1.542
_setup_field 0.5
_setup_offset_2theta .
_setup_offset_phi .
_setup_offset_gamma .
_setup_offset_nu .
_setup_ratio_lambda/2 .
_setup_radiation neutrons
_setup_K 0.0
_setup_cthm 0.91000
_setup_temperature .
```

Step 1.2: Fill in the new .rcif fields

4. Fill in the **diffrn_refln** with the experiment-measured peak table with flipping ratio



```
loop_
_diffrn_refln_index_h
_diffrn_refln_index_k
_diffrn_refln_index_l
_diffrn_refln_fr
_diffrn_refln_fr_sigma
_diffrn_refln_fr_calc
_diffrn_refln_intensity_plus_calc
_diffrn_refln_intensity_minus_calc
_diffrn_refln_excluded
_diffrn_refln_sint/lambda
 2   2   0  1.02249  0.05  1  .  .  False  .
 2   2  -2     0.92  0.05  1  .  .  False  .
 2   2  -4  1.01403  0.05  1  .  .  False  .
 2   2  -6  0.88136  0.05  1  .  .  False  .
 2   1  -1  0.84561  0.05  1  .  .  False  .
 2   1  -3  0.96692  0.05  1  .  .  False  .
 2   1  -5  0.98353  0.05  1  .  .  False  .
 2   1  -7  0.78571  0.05  1  .  .  False  .
 1   2   7  0.83333  0.05  1  .  .  False  .
 1   2   5  0.94717  0.05  1  .  .  False  .
 1   1   8  1.04211  0.05  1  .  .  False  .
 1   1   4  0.93939  0.05  1  .  .  False  .
 1   1   0  1.04966  0.05  1  .  .  False  .
 1   1  -4  0.92792  0.05  1  .  .  False  .
 1   1  -6  1.08108  0.05  1  .  .  False  .
 0   0   8  0.99376  0.05  1  .  .  False  .
 0   0   6  0.95494  0.05  1  .  .  False  .
```

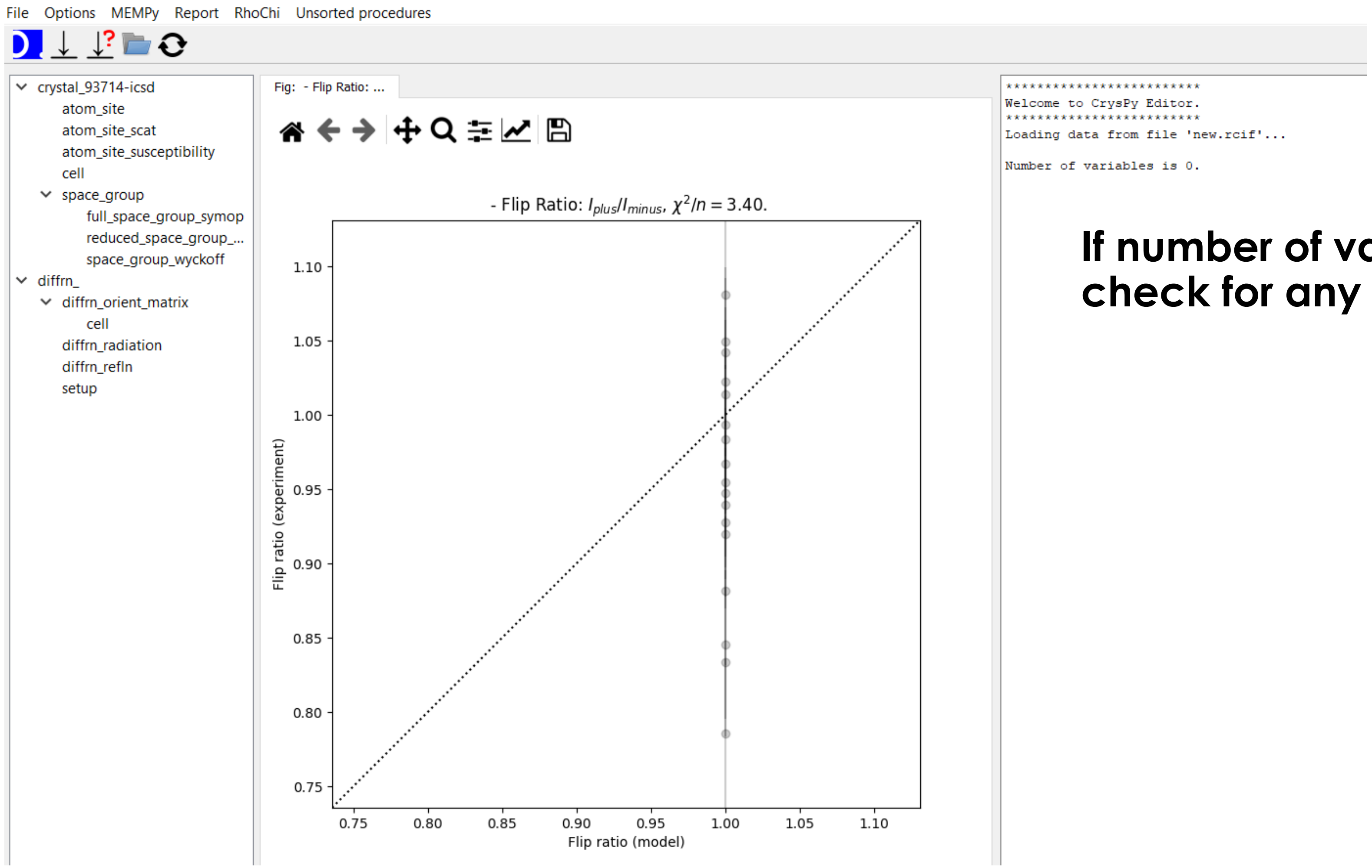
```
Number of variables is 2.

  NAME                VALUE      EF
```

```
2   2   0   1.02249   0.05   1   .   .   False   .
2   2  -2      0.92   0.05   1   .   .   False   .
2   2  -4   1.01403   0.05   1   .   .   False   .
2   2  -6   0.88136   0.05   1   .   .   False   .
2   1  -1   0.84561   0.05   1   .   .   False   .
2   1  -3   0.96692   0.05   1   .   .   False   .
2   1  -5   0.98353   0.05   1   .   .   False   .
2   1  -7   0.78571   0.05   1   .   .   False   .
1   2   7   0.83333   0.05   1   .   .   False   .
1   2   5   0.94717   0.05   1   .   .   False   .
1   1   8   1.04211   0.05   1   .   .   False   .
1   1   4   0.93939   0.05   1   .   .   False   .
1   1   0   1.04966   0.05   1   .   .   False   .
1   1  -4   0.92792   0.05   1   .   .   False   .
1   1  -6   1.08108   0.05   1   .   .   False   .
0   0   8   0.99376   0.05   1   .   .   False   .
0   0   6   0.95494   0.05   1   .   .   False   .
```

The .rcif file is now complete and ready for refinement!

Step 1.3: Refinement

1. Save the file as a new .rcif file, then open it again,

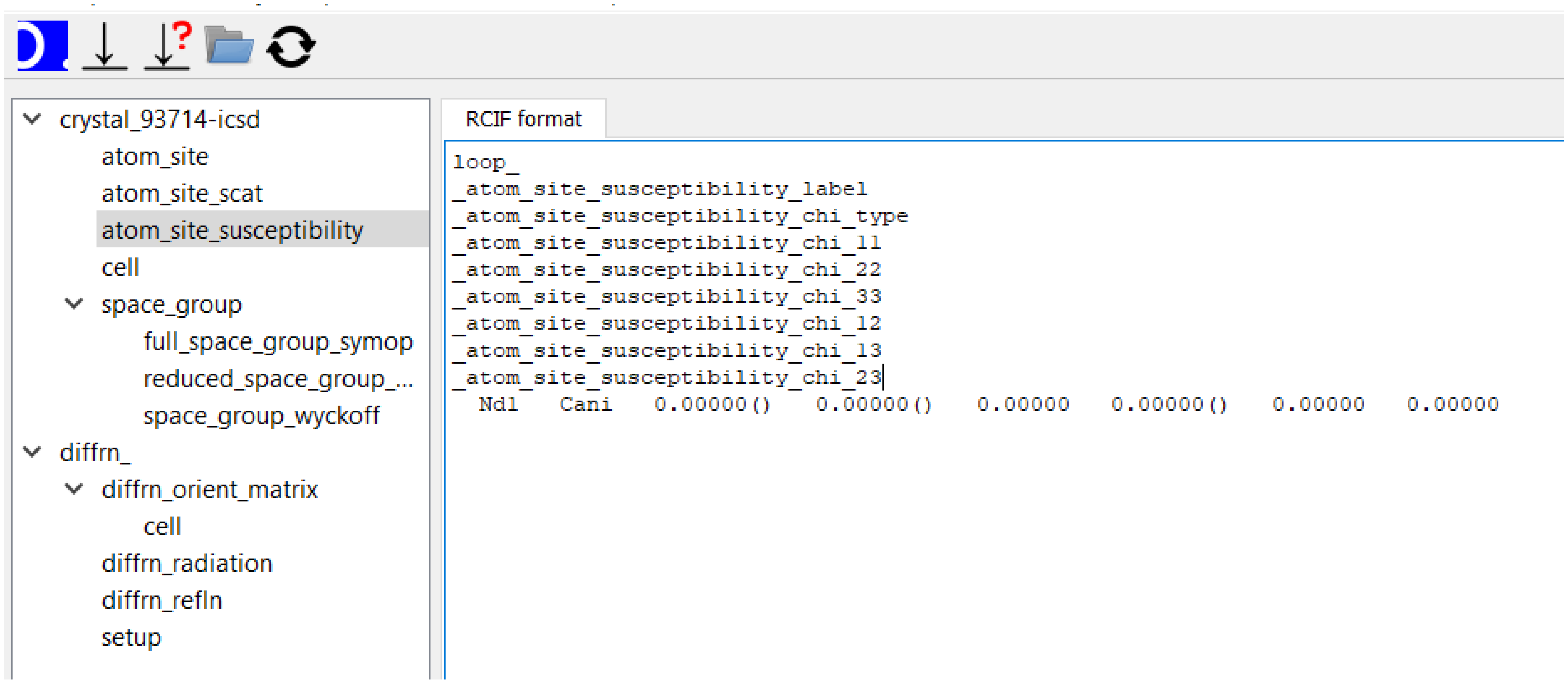


```
************************
Welcome to CrysPy Editor.
************************
Loading data from file 'new.rcif'...

Number of variables is 0.
```

If number of variables is not 0, check for any ()

Step 1.3: Refinement

2. Go to **atom_site_susceptibility**, use () to specify the refined parameters, and **play with the refinement!** (Rhochi→Rietveld Refinement (autorun)



```
loop_
_atom_site_susceptibility_label
_atom_site_susceptibility_chi_type
_atom_site_susceptibility_chi_11
_atom_site_susceptibility_chi_22
_atom_site_susceptibility_chi_33
_atom_site_susceptibility_chi_12
_atom_site_susceptibility_chi_13
_atom_site_susceptibility_chi_23
  Nd1    Cani    0.00000()    0.00000()    0.00000    0.00000()    0.00000    0.00000
```

Step 2: