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# Example of Jana refinement of magnetic structure on single-crystal data

**Zachary Morgan and Feng Ye**

Neutron Scattering Division

Oak Ridge National Laboratory

**Magnetic Structure Determination from Neutron Diffraction Data, October 3-7, 2022**

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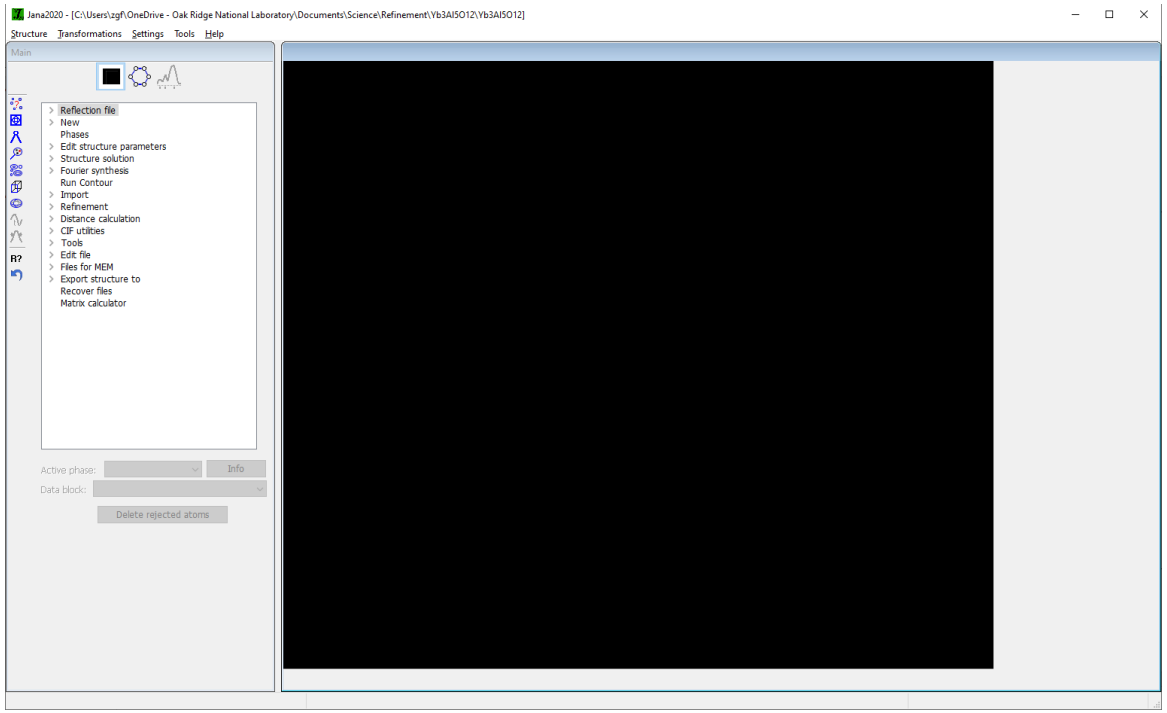
# Yb3Al5O12: Jana 2020 Single Crystal Refinement Tutorial

- Open Jana2020
- Structure > New
- Navigate to Yb3Al5O12
- Choose Yb3Al5O12_300K.hkl



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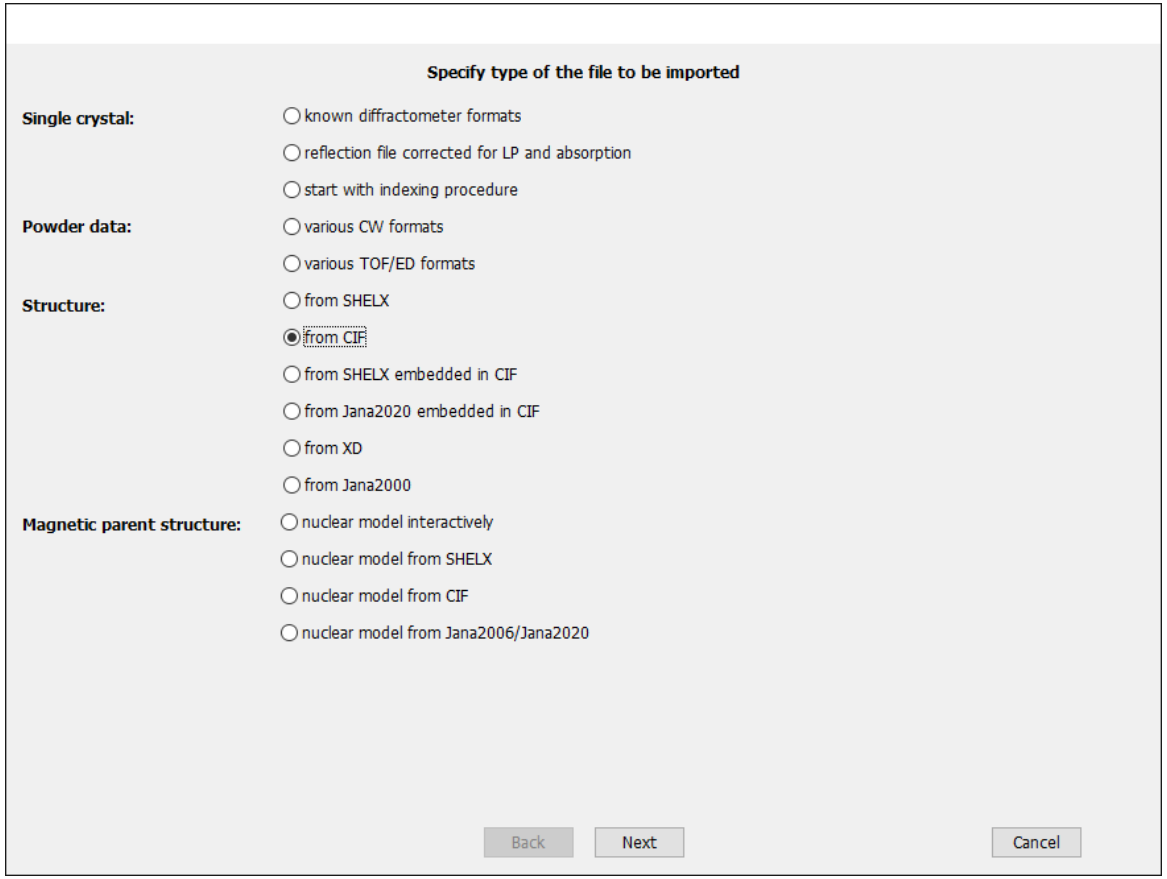
# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

- Choose Structure from CIF





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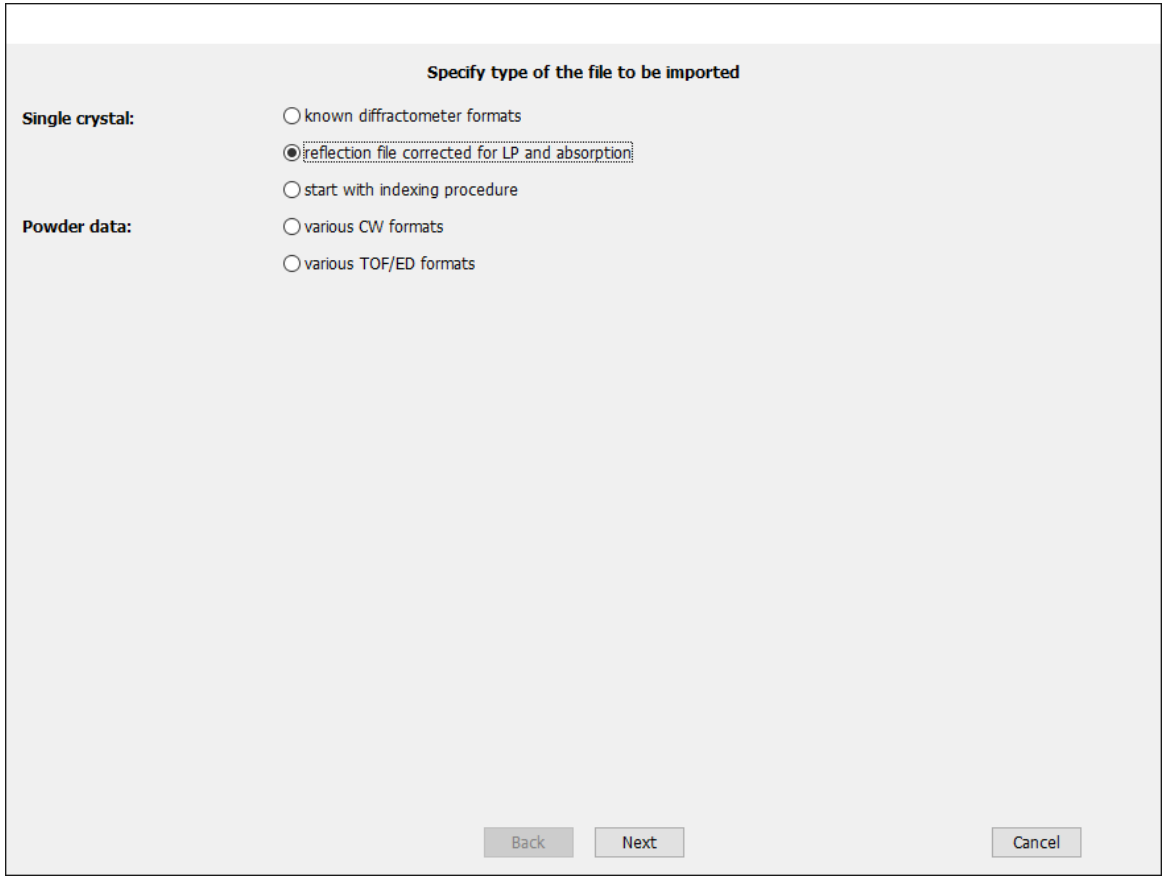
# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

- Choose Single Crystal reflection file corrected for LP and absorption





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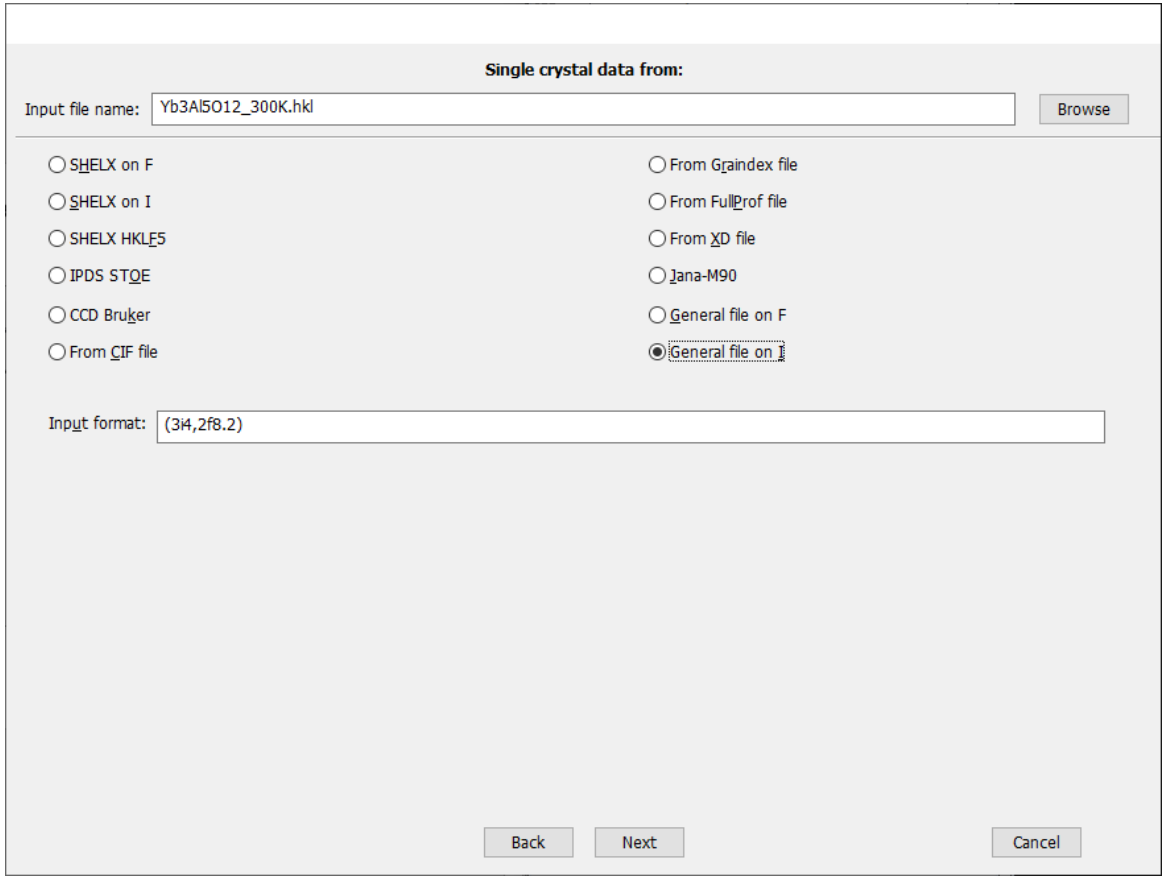
# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

- Input file name is Yb3Al5O12_300K.hkl
  - General file on I



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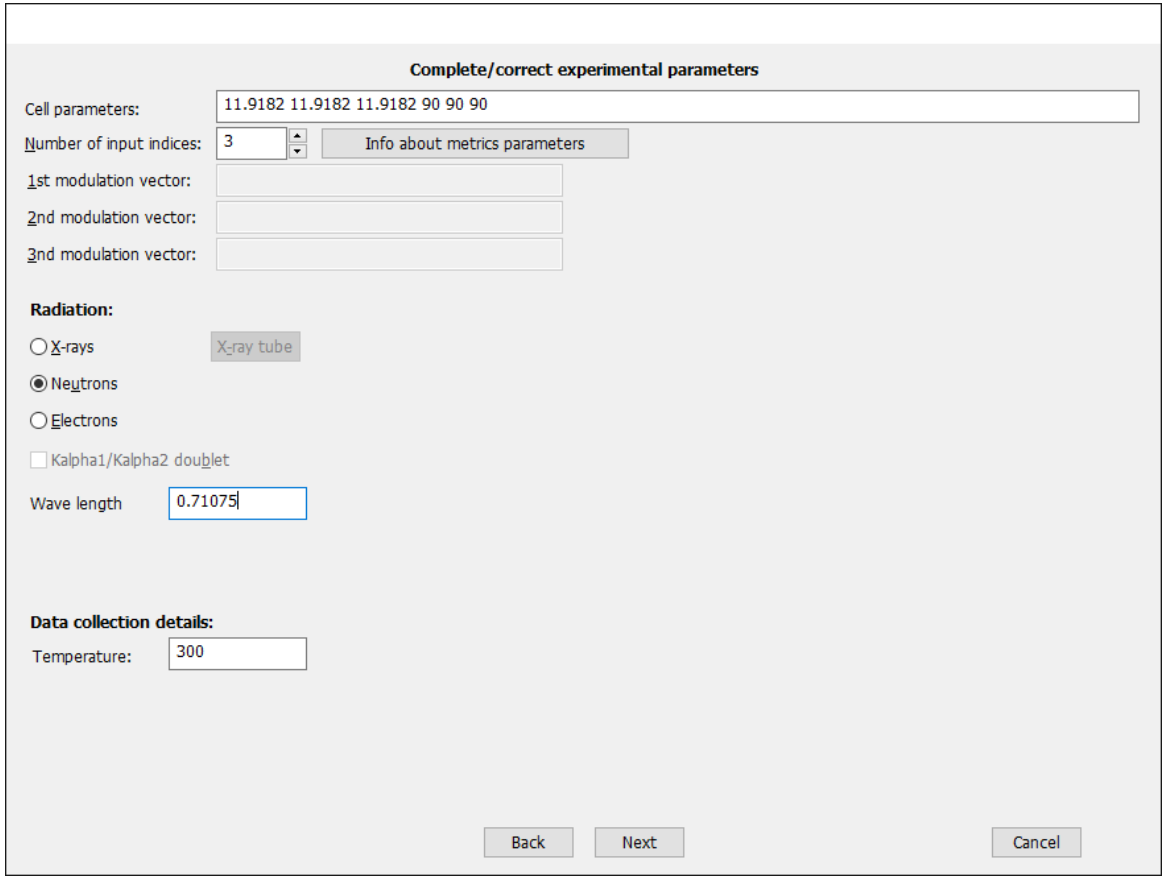
# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

- Choose Neutron
- Temperature is 300 K



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# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

- Run Refinement
  - Square button

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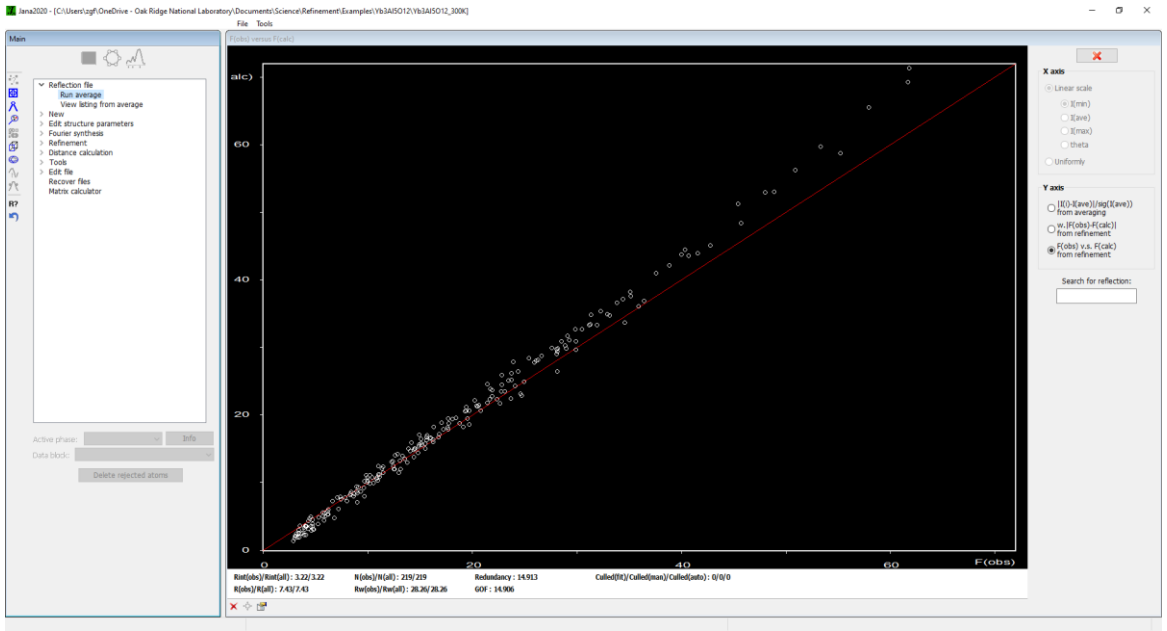
# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

- Reflection file > Manual culling
- Yaxis F(obs) vs F(calc) from refinement



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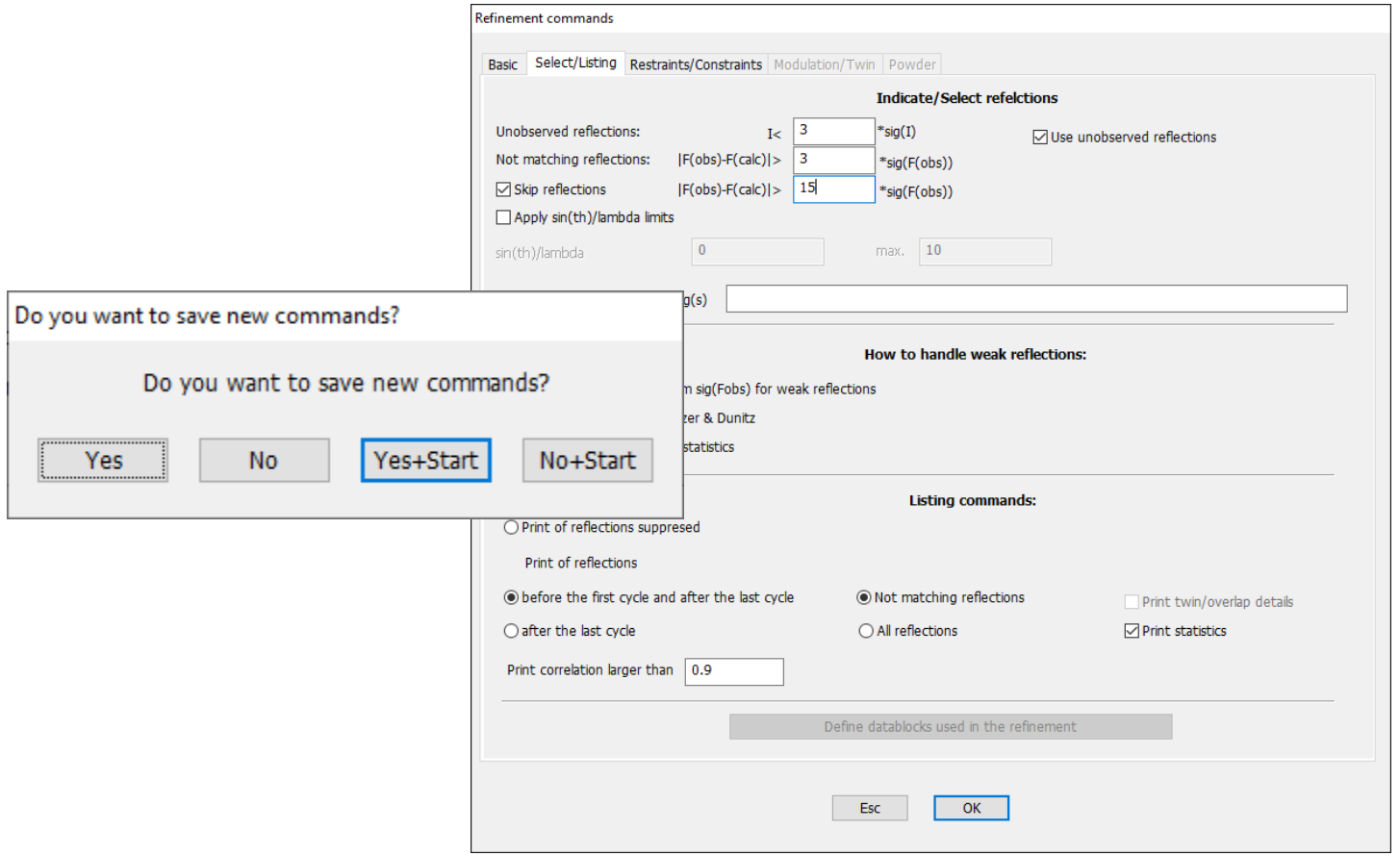
# $Yb_3Al_5O1_2$ : Jana 2020 Single Crystal Refinement Tutorial

**OPTIONAL:**

- Right click on refinement
- Select/Listing tab
- Skip reflections 15
- Yes+Start



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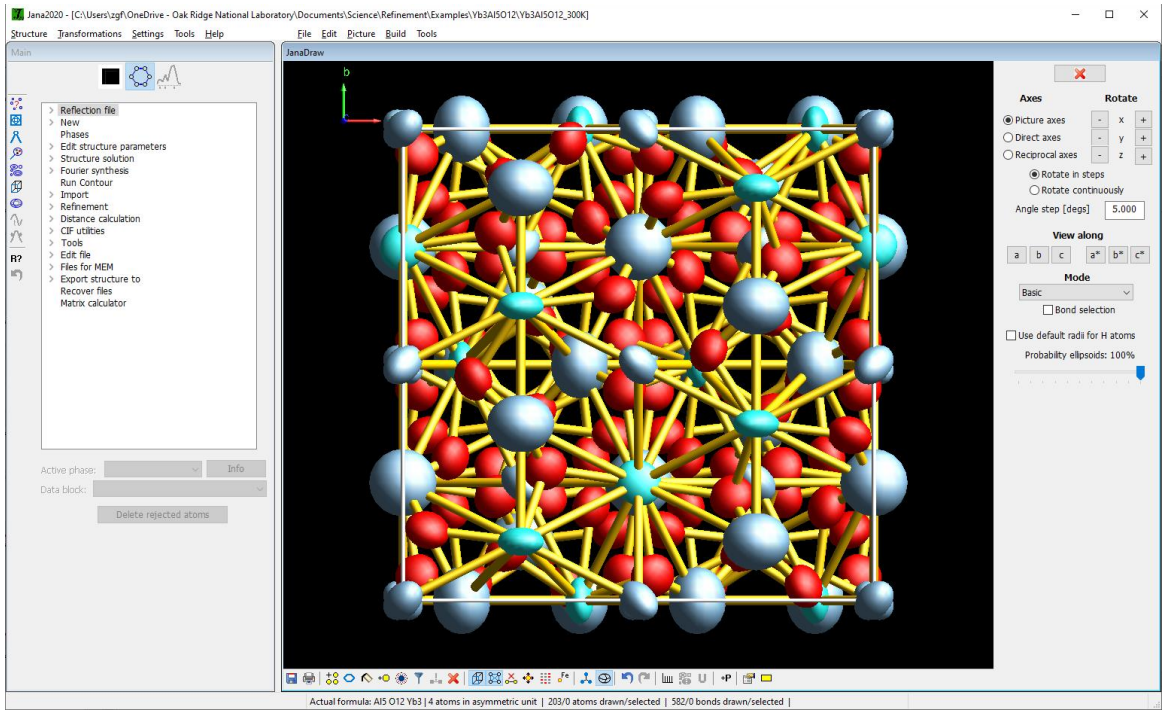
# $Yb_3Al_5O1_2$: Jana 2020 Single Crystal Refinement Tutorial

**OPTIONAL:**

- Draw only independent atoms
- Fill unit cell
- Draw ellipsoids > slider 99% probability



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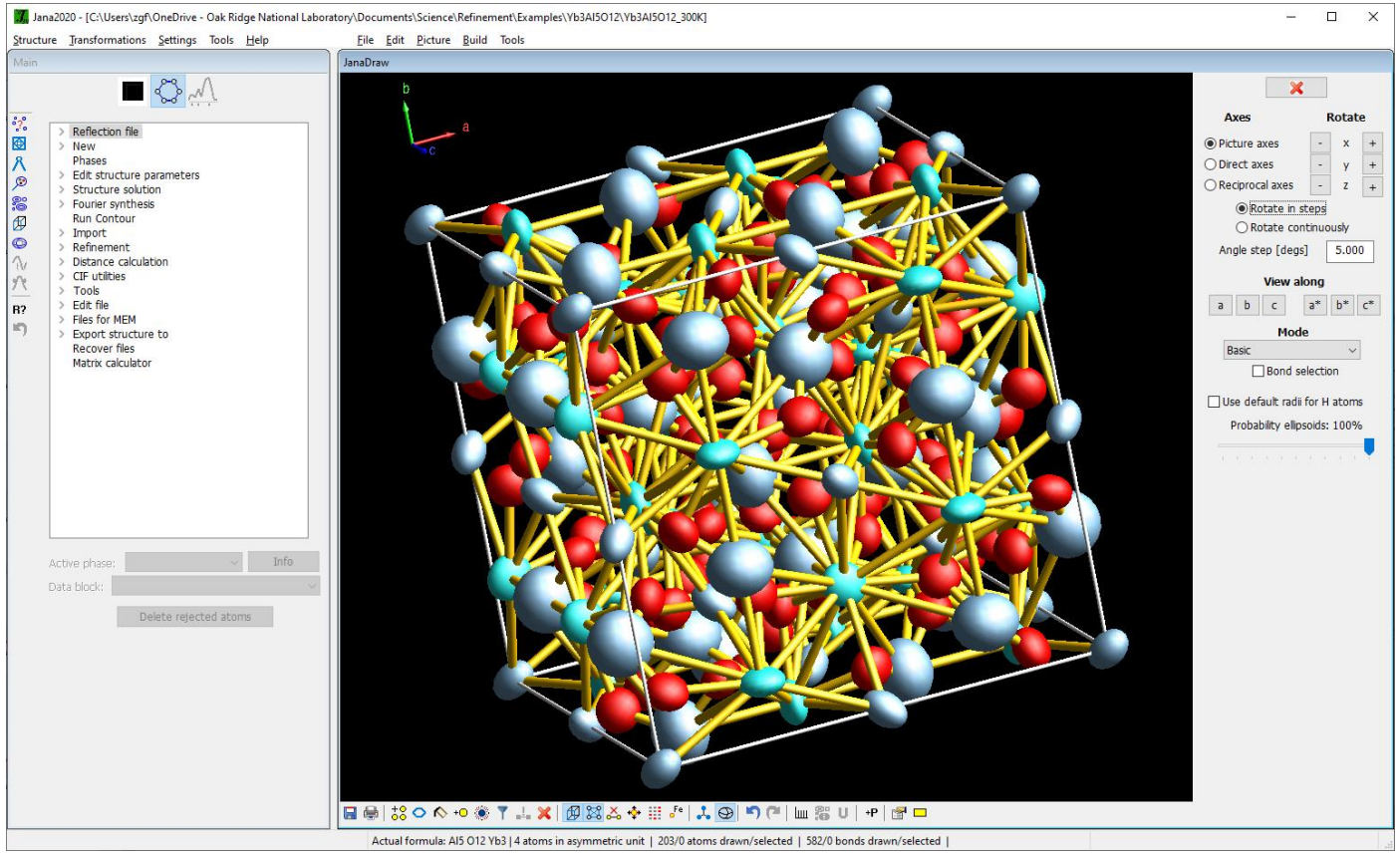
# Yb3Al5O12: Jana 2020 Single Crystal Refinement Tutorial



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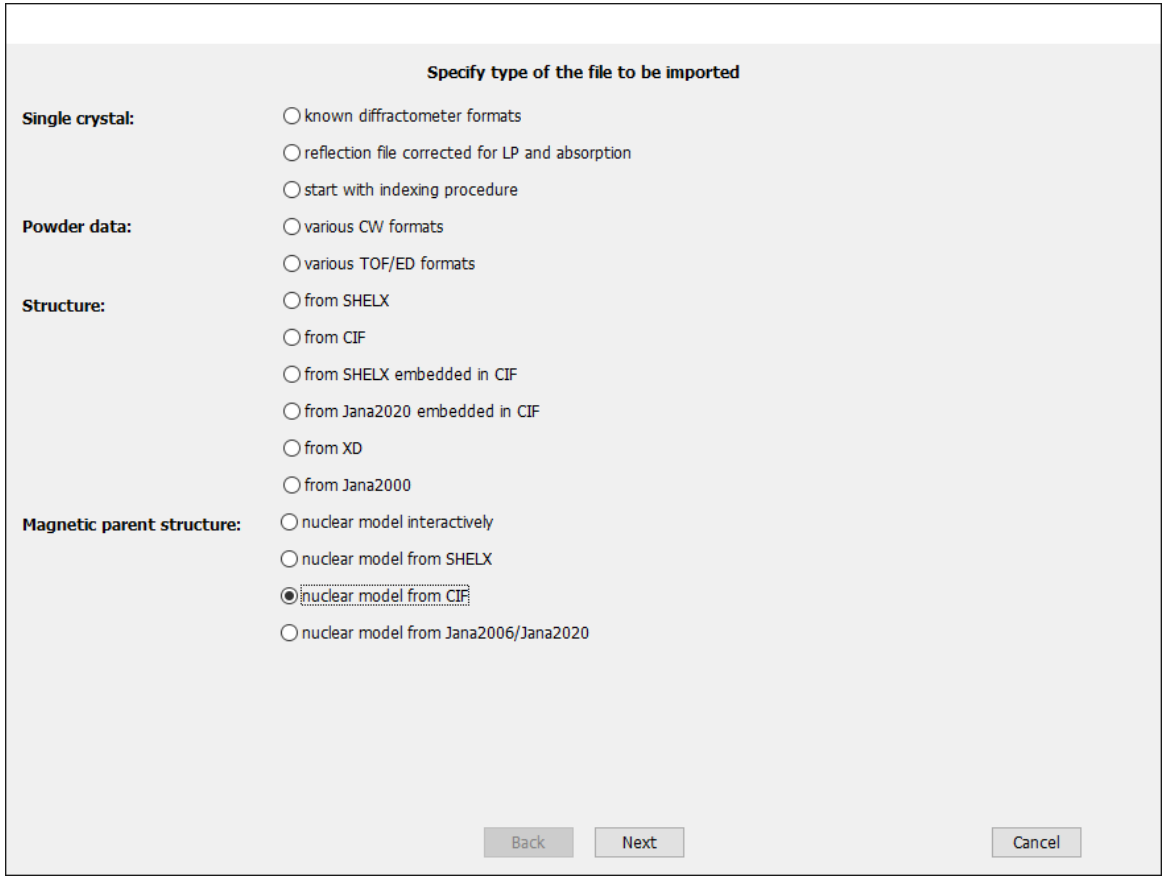
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Structure > New
- Navigate to Tb2Ir3Ga9
- Choose Tb2Ir3Ga9_007K.hkl
- Magnetic parent structure nuclear model from CIF
- Choose Tb2Ir3Ga9.cif





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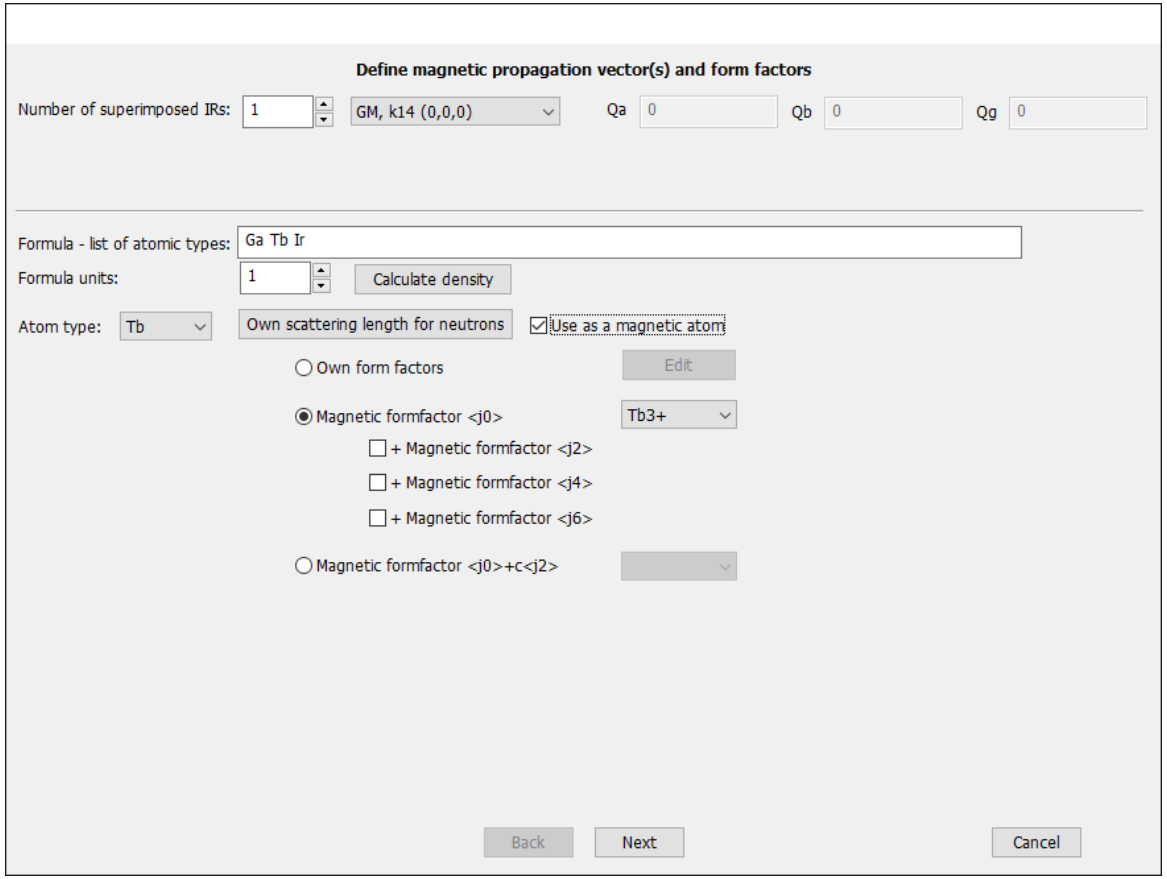
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Select Tb atom type
  - Use as magnetic atom
  - Magnetic form factor <j0>
- Number of superimposed IRs is 1
  - 0 0 0 propagation vector





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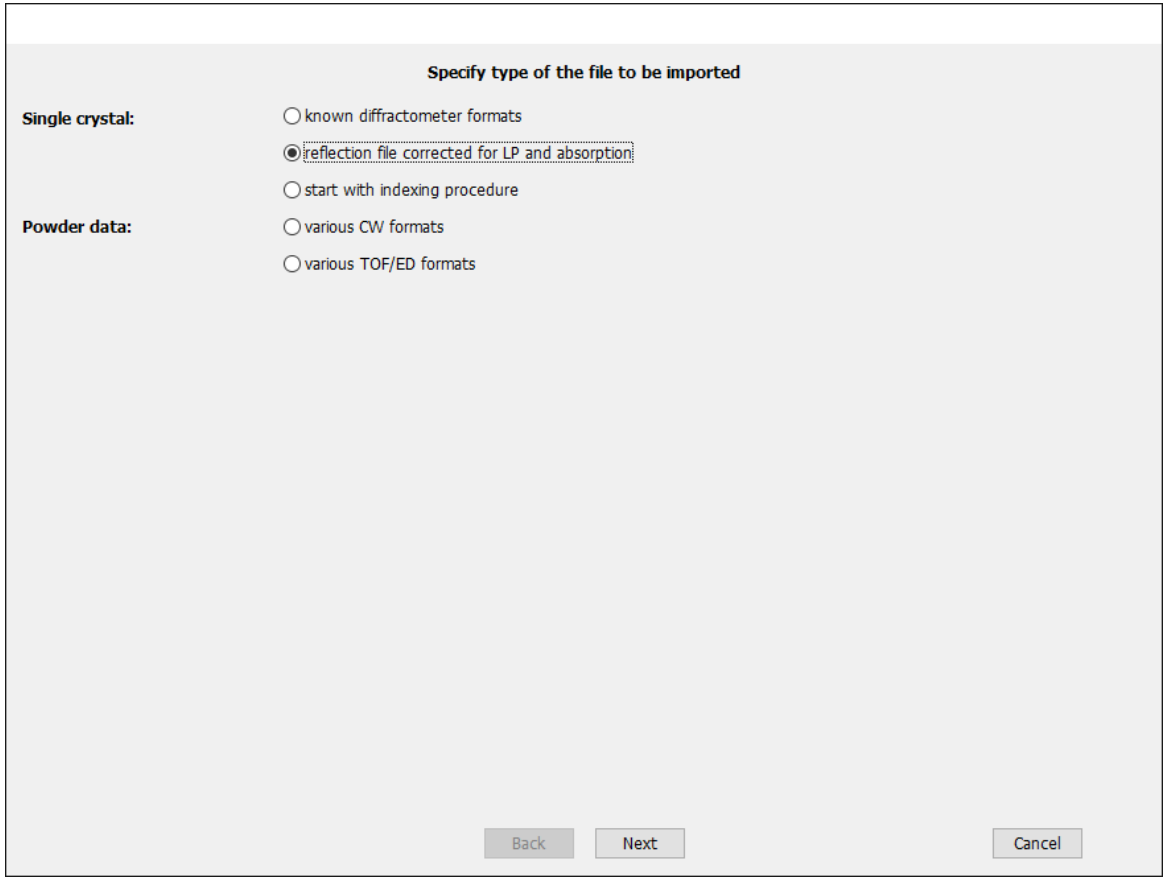
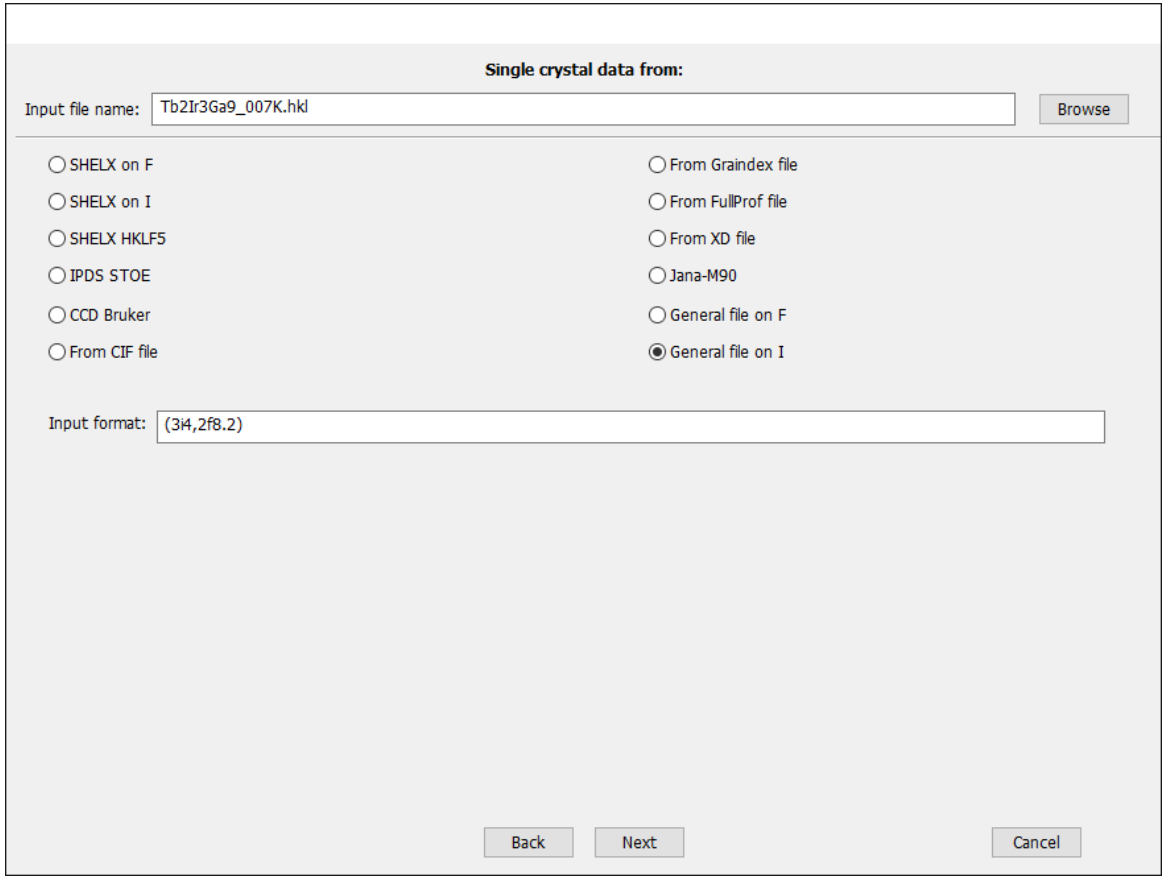
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial



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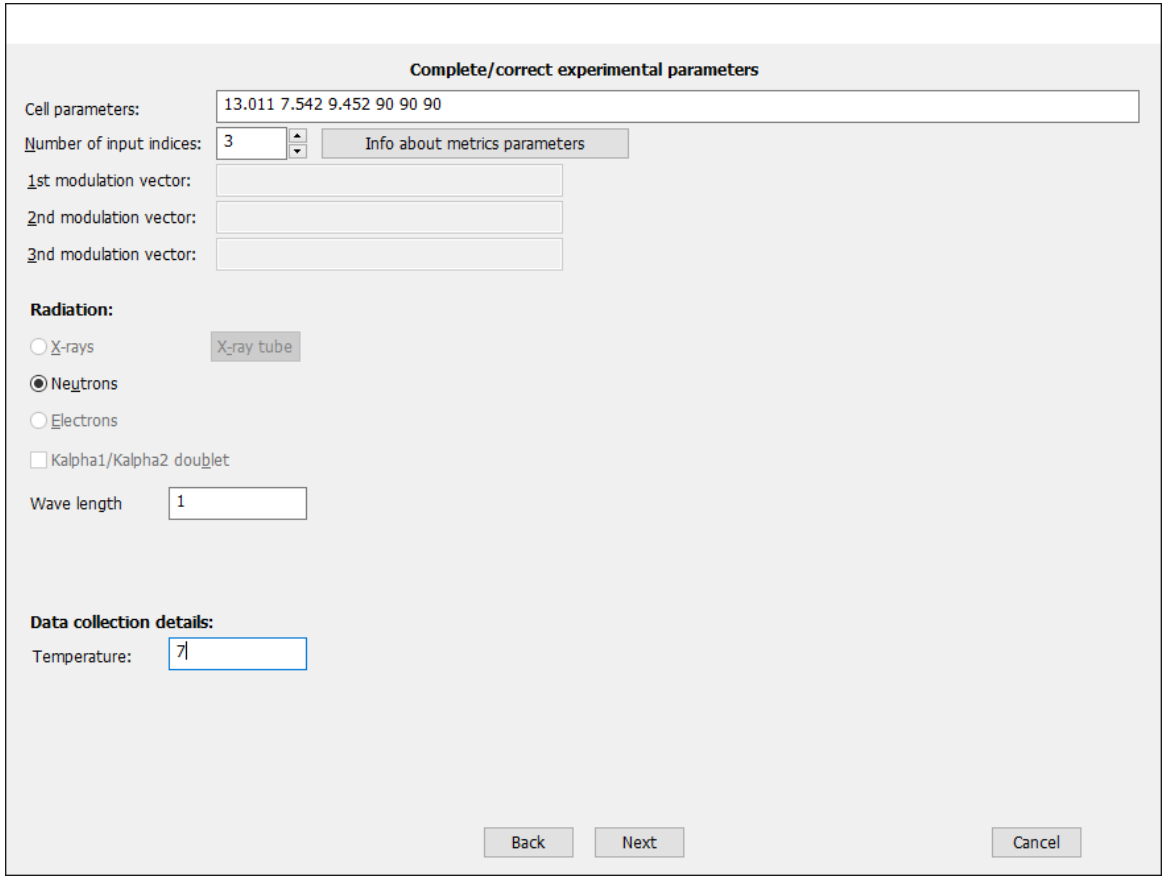
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Temperature is 7K



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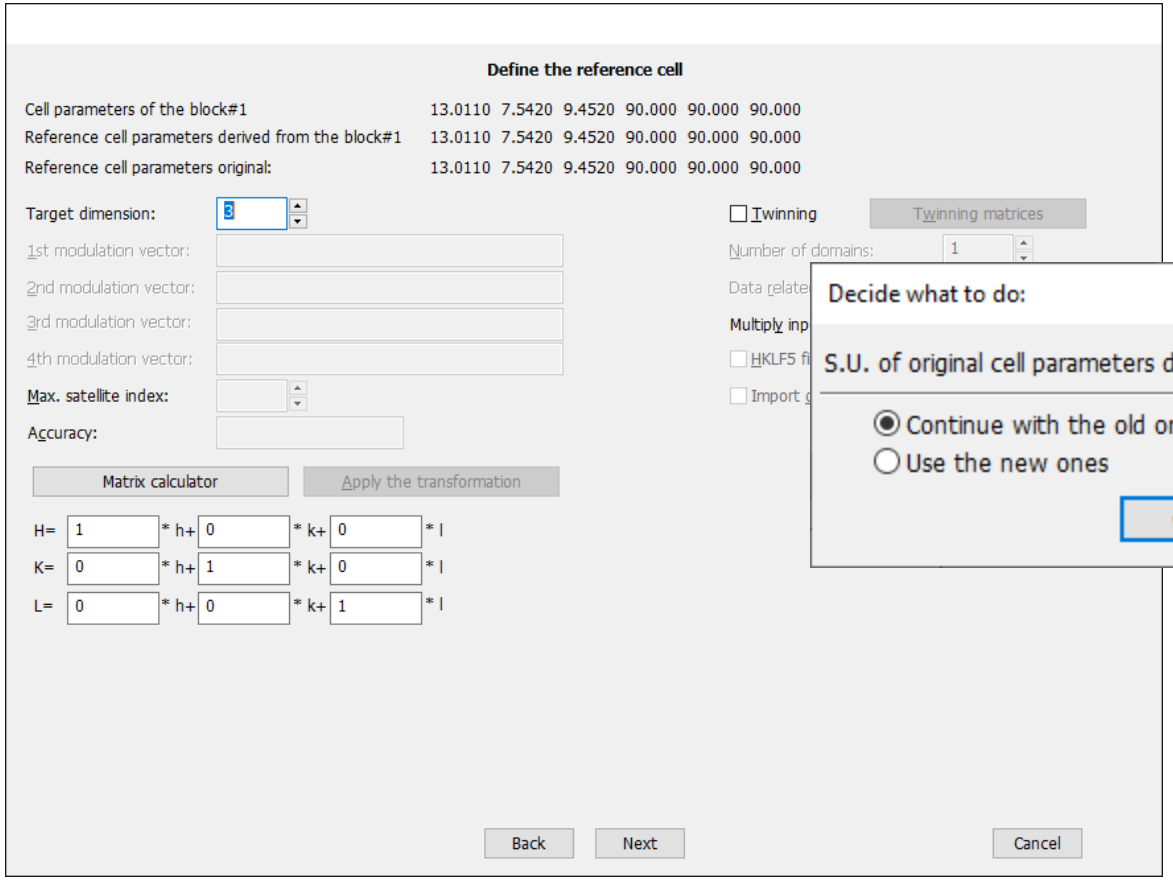
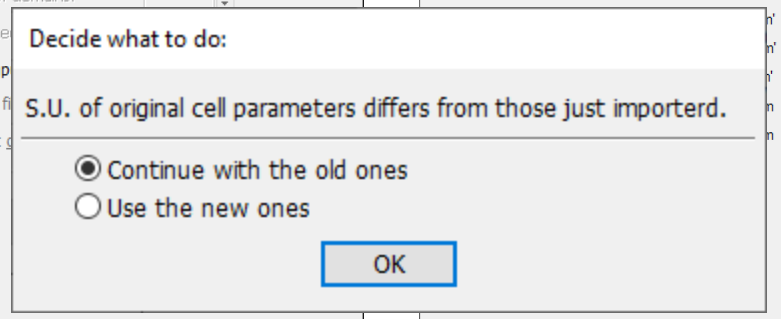
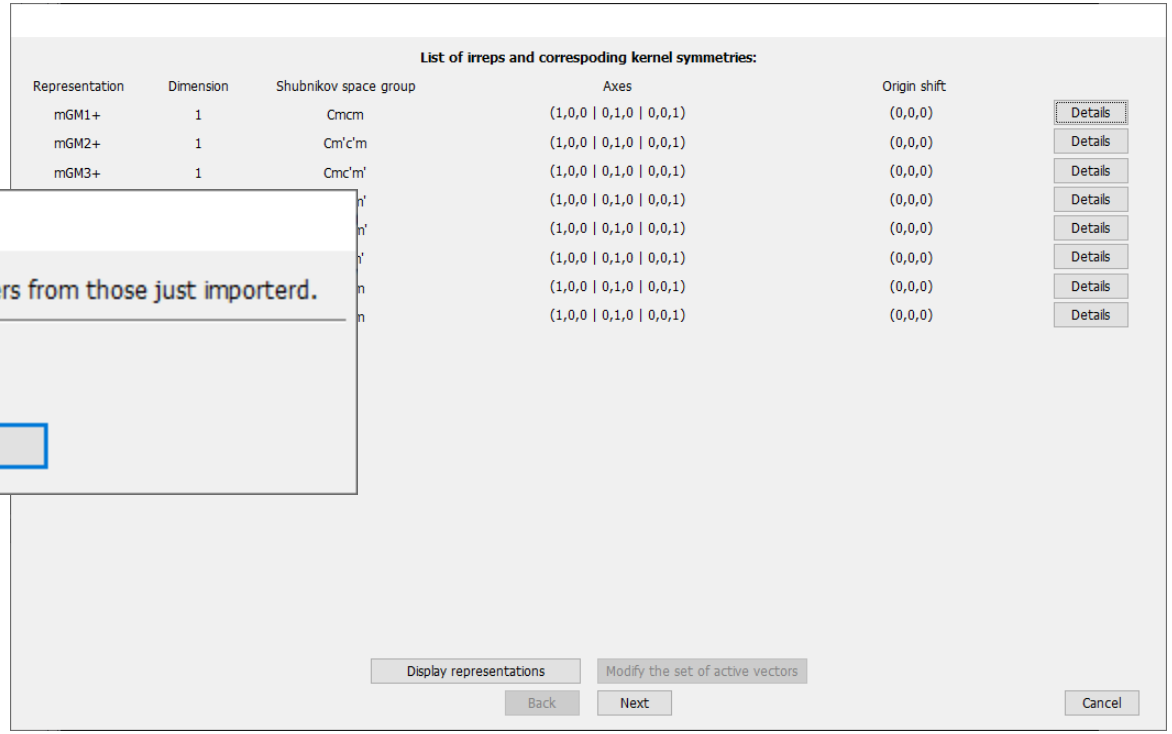
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial



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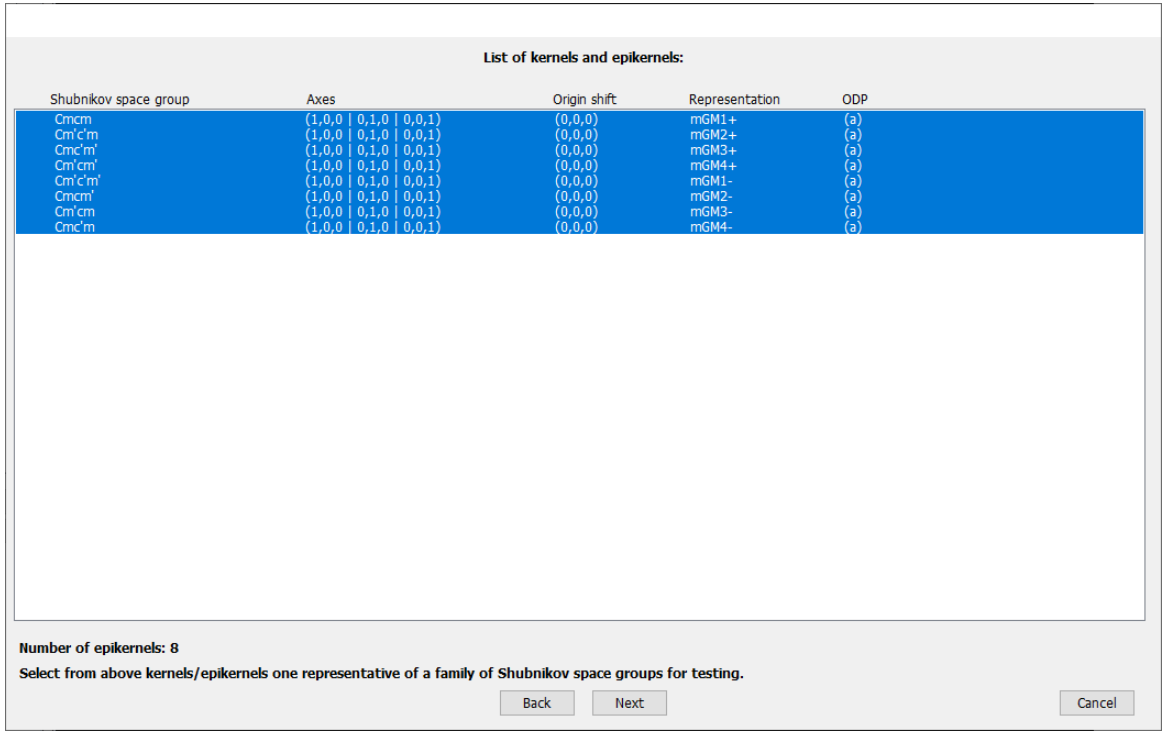
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- 8 Shubnikov groups selected
- Next



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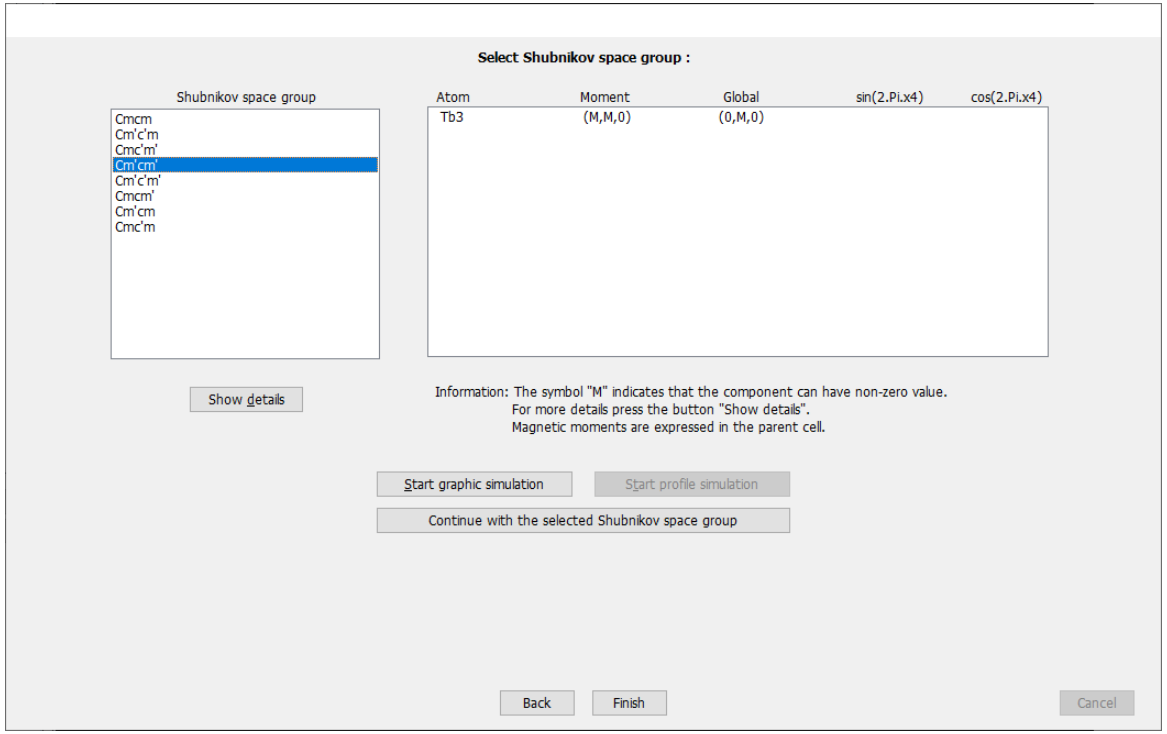
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Choose Cm'cm'
  - Moment is (M,M,0)
- Continue with the selected Shubnikov group
- Save with a different name than the parent space group
  - Tb2Ir3Ga9_007K_Cmpcmp.m50
- A new Jana2020 instance will be opened
- Run refinement





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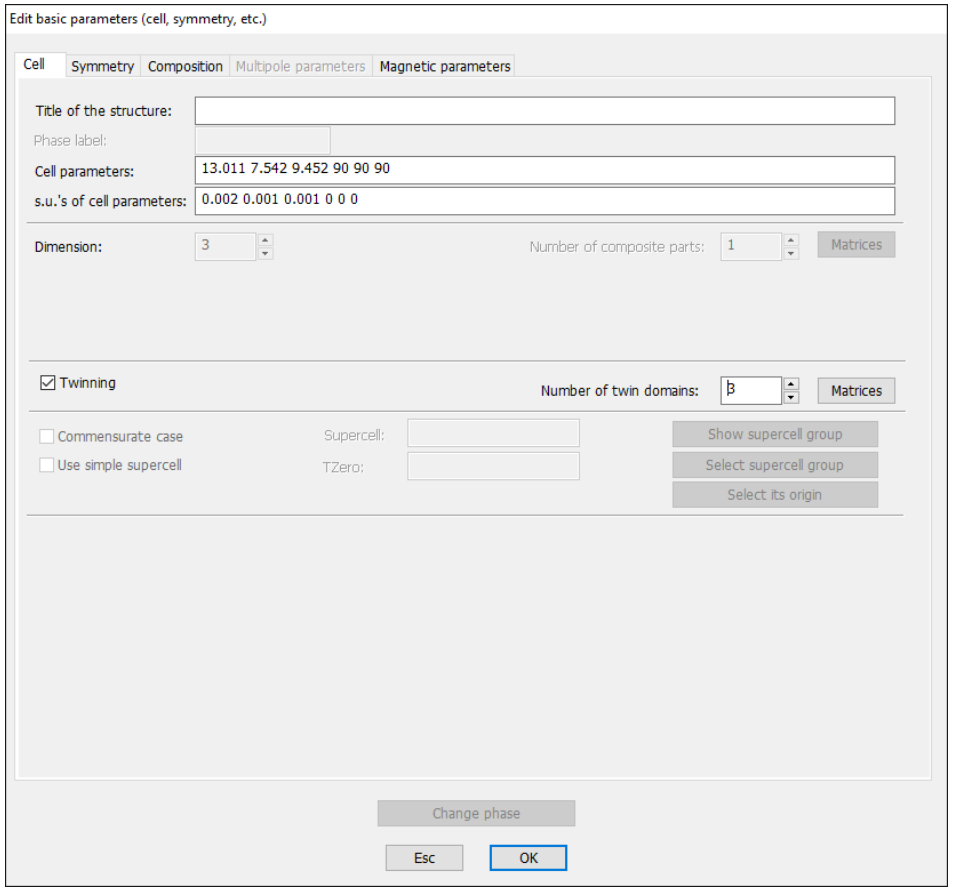
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Edit structure parameters > Edit basic parameters
- Check twinning (under cell tab)
  - Number of twin domains is 3
- Matrices



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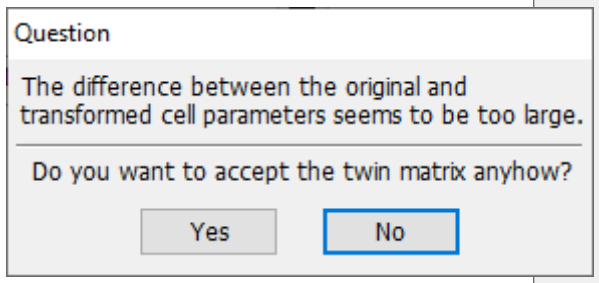
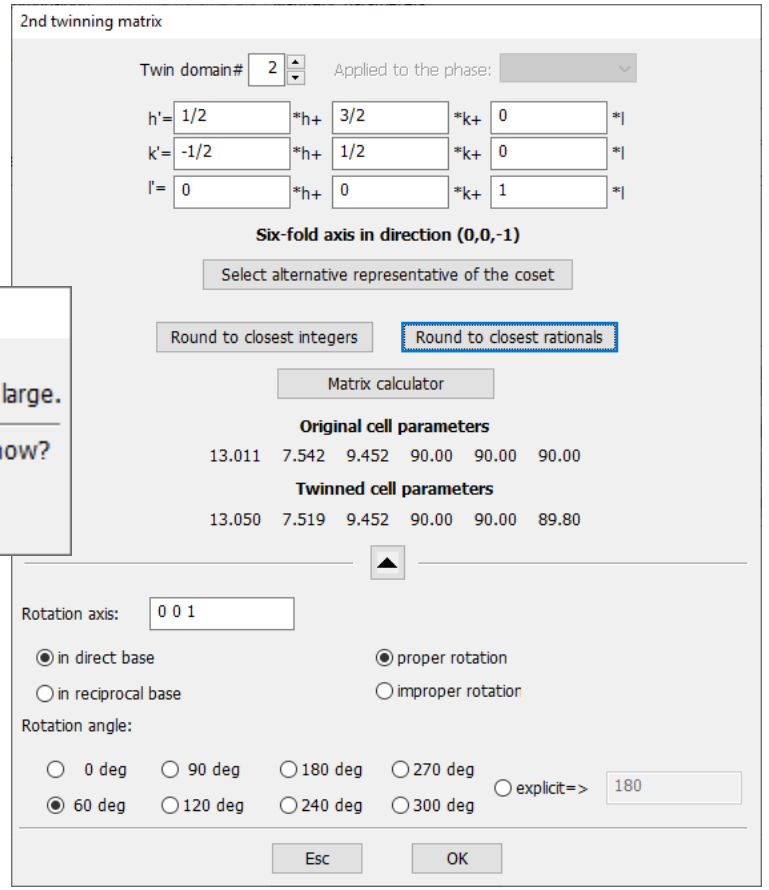
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Twin domain #2
  - 60 deg proper rotation in direct base about 0 0 1
  - Up arrow
  - Round to closest rational
- Increment to next domain
- Yes





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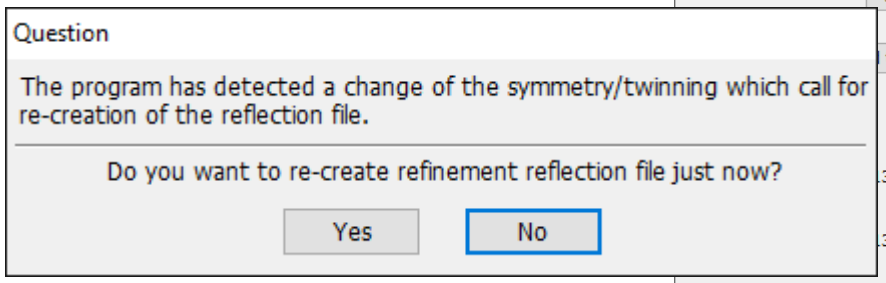
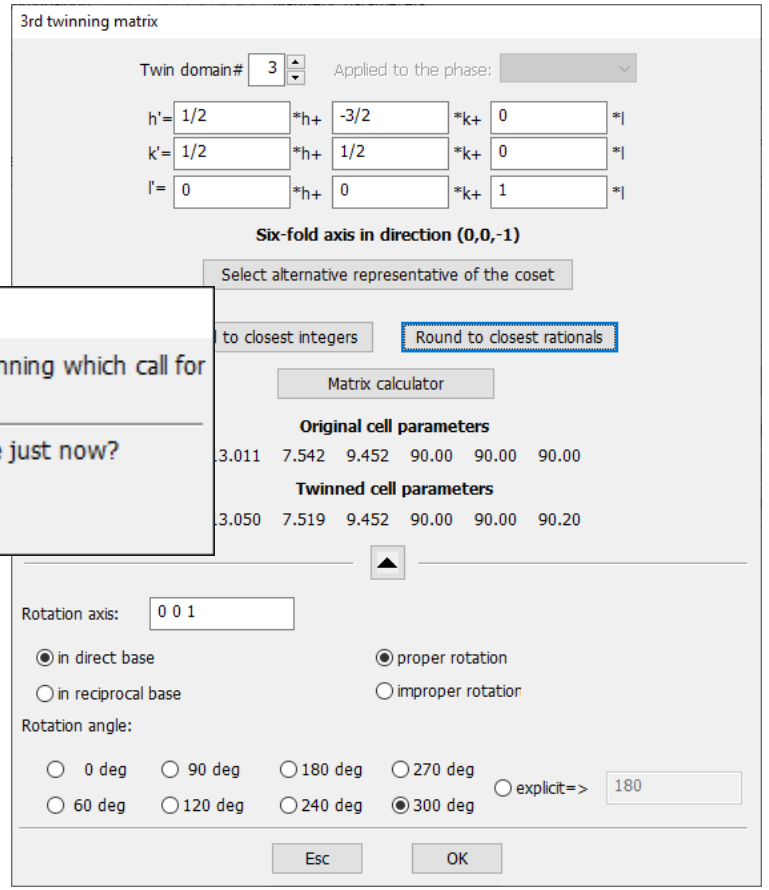
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Twin domain #3
  - 300 deg proper rotation in direct base about 0 0 1
  - Up arrow
  - Round to closest rational
- OK
- Yes
- Accept all defaults
- Re-run refinement





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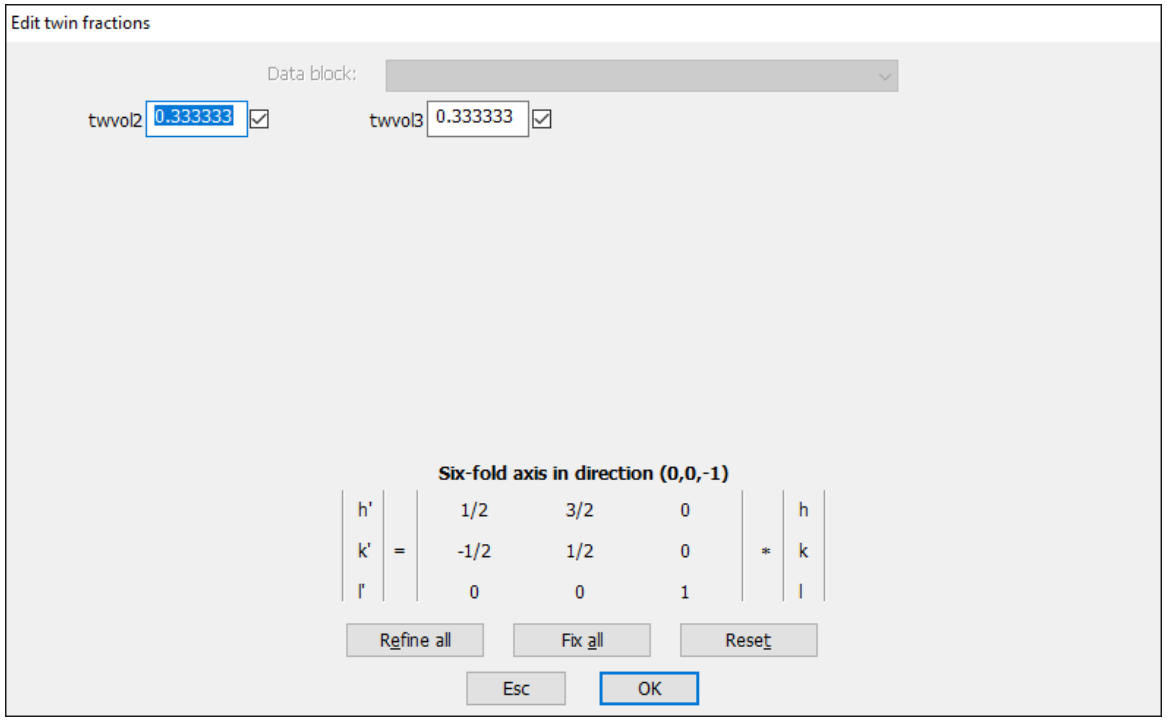
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Edit structure parameters > Edit twin phase/volume fractions
- Refine all



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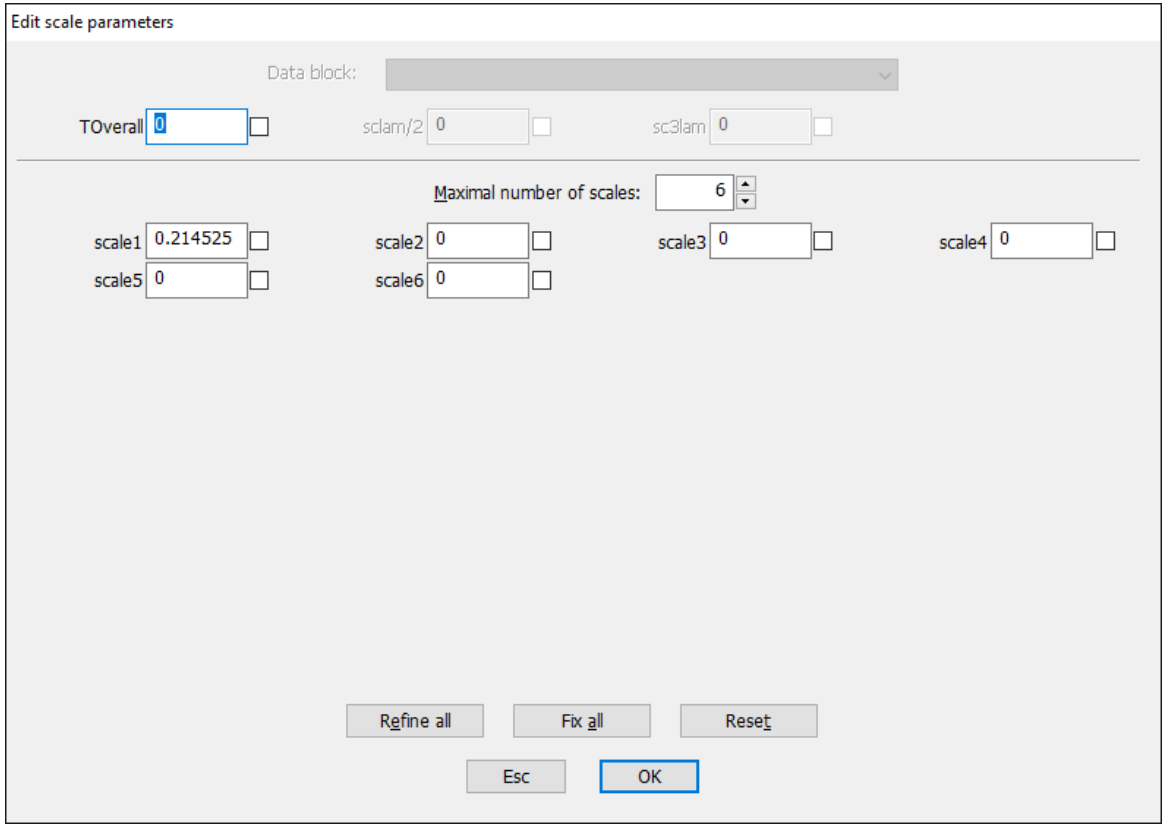
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Edit structure parameters > Edit scale parameters
- Fix all
- Re-run refinement



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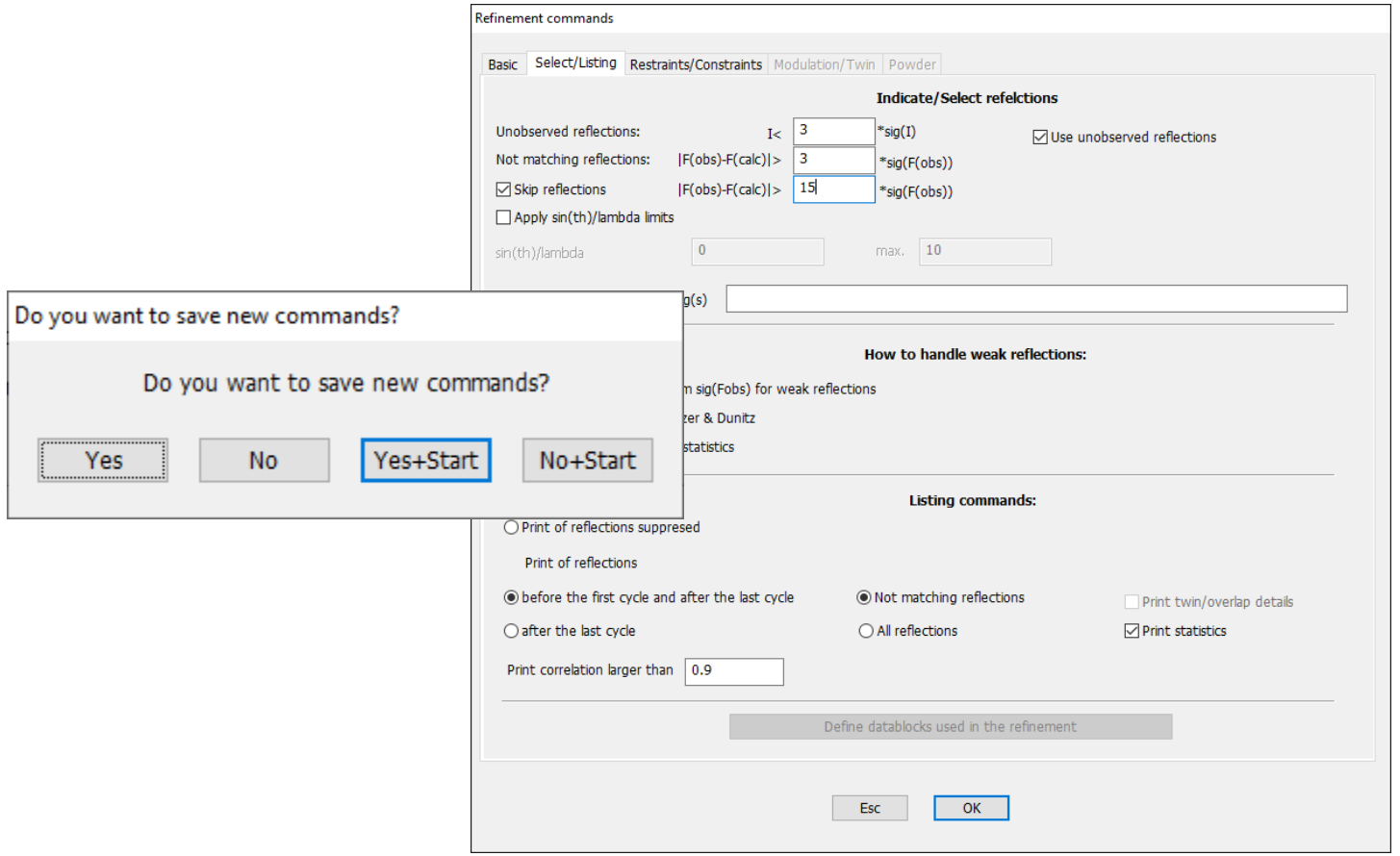
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

**OPTIONAL:**

- Right click on refinement
- Select/Listing tab
- Skip reflections 15
- Yes+Start



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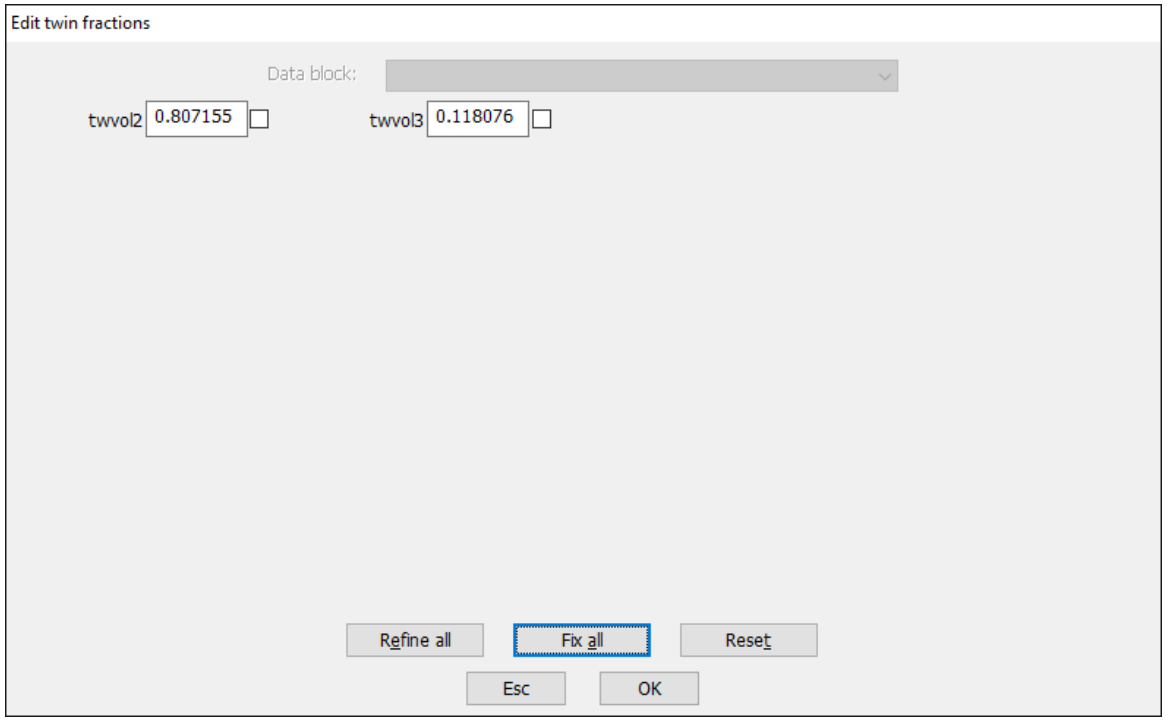
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

- Edit structure parameters > Edit twin phase/volume fractions
- Fix all
- Edit structure parameters > Edit scale parameters
- Fix all
- Re-run refinement





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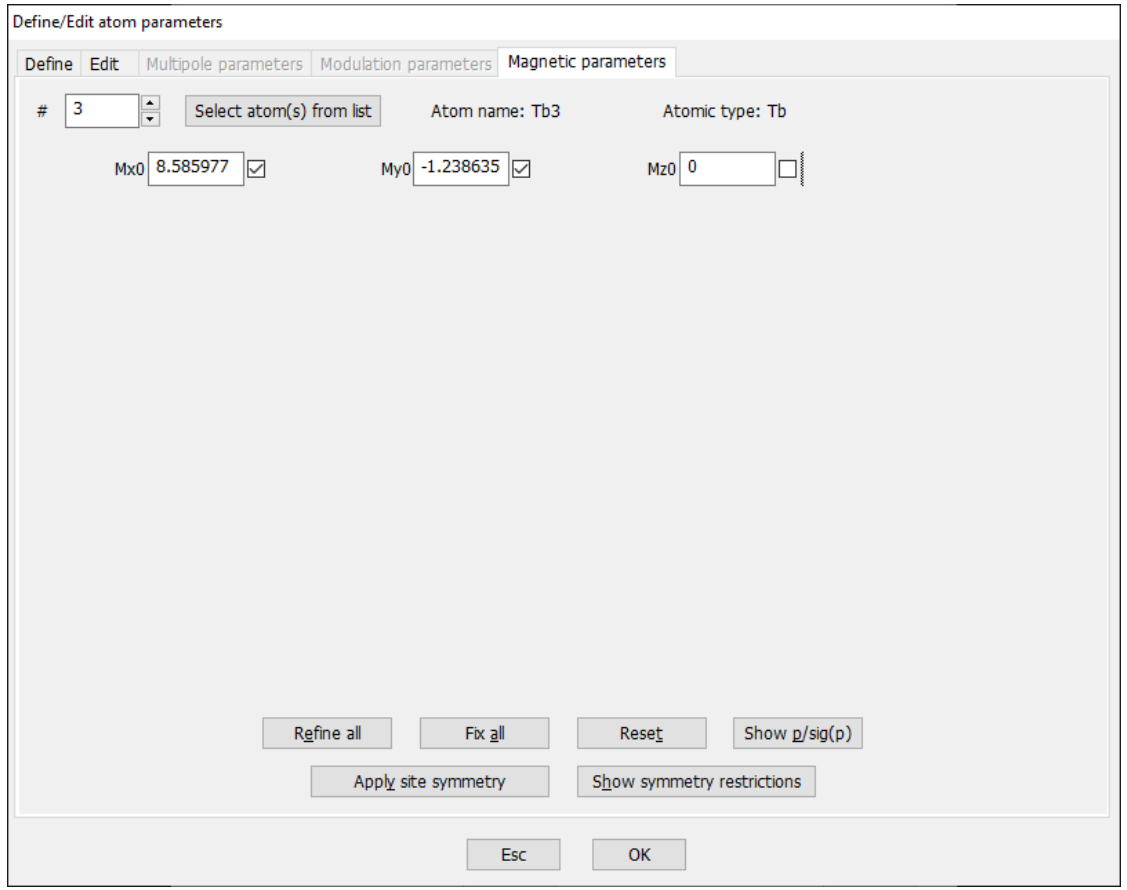
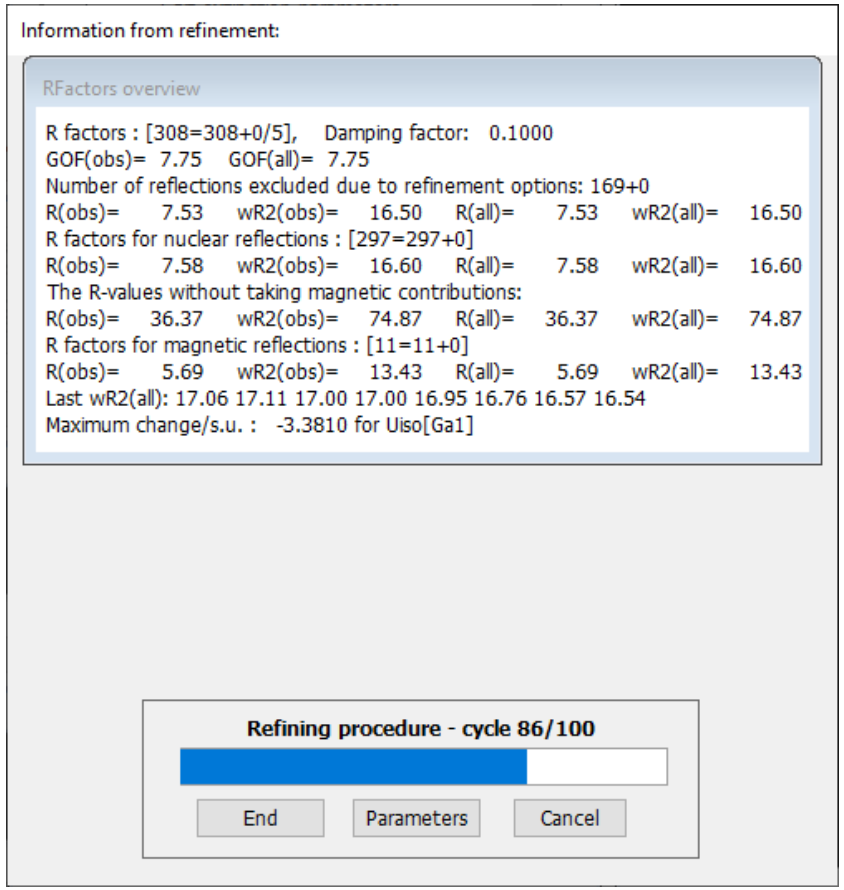
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial



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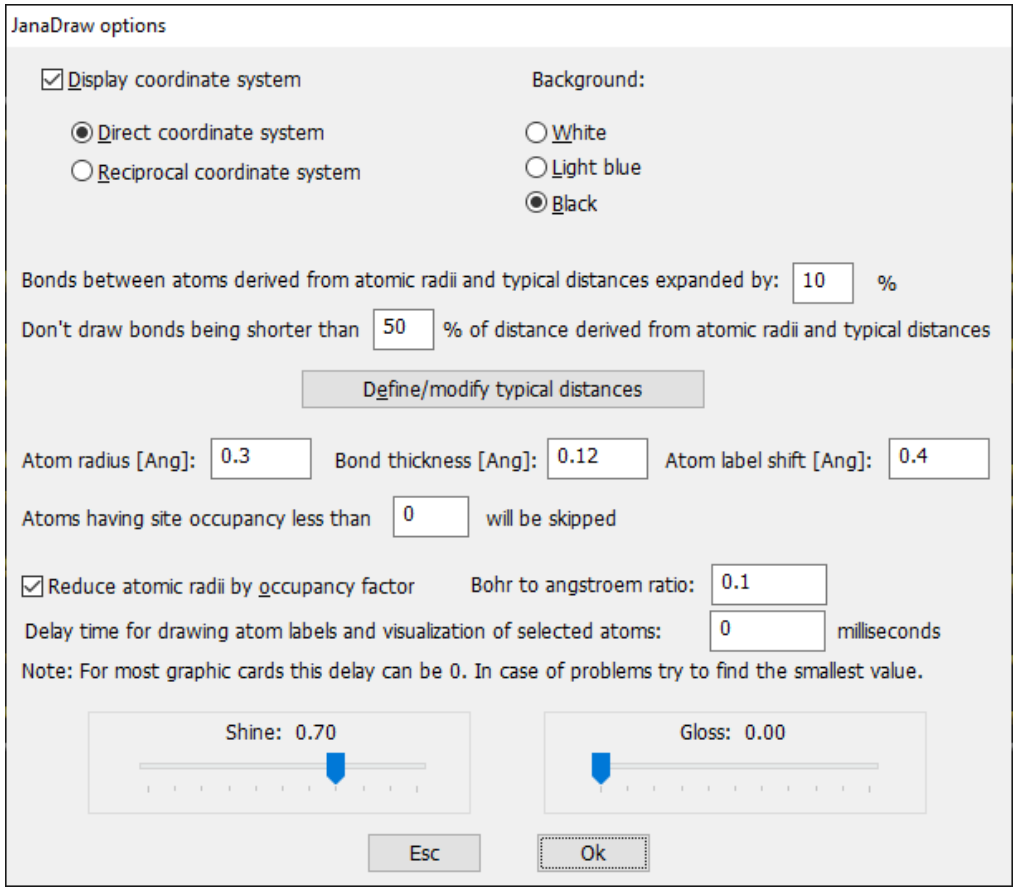
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial

**OPTIONAL:**

- Draw only independent atoms
- Fill unit cell
- JanaDraw options
  - Bohr to angstrom ratio is 0.1





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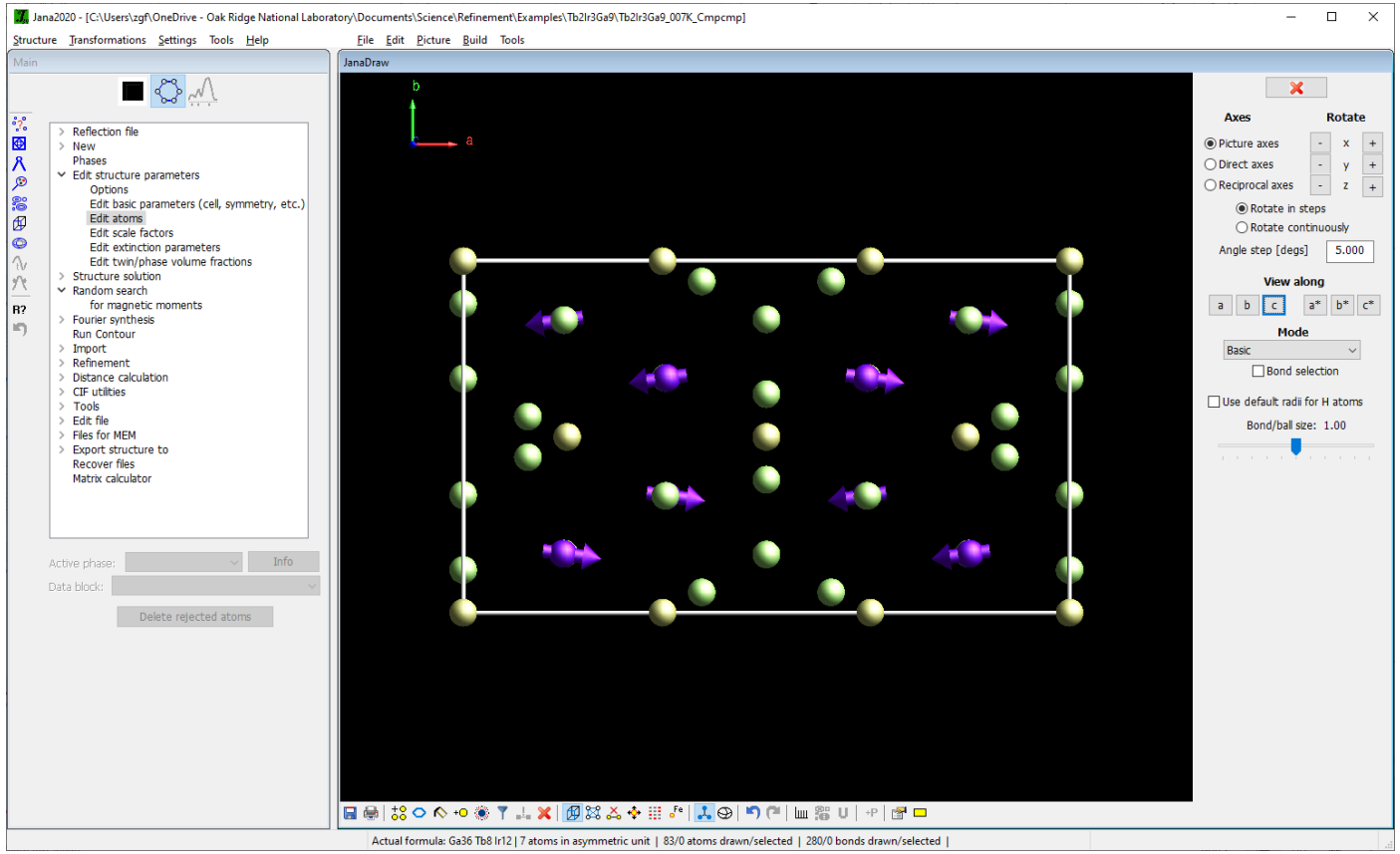
# $Tb_2Ir_3Ga_9$: Jana 2020 Single Crystal Refinement Tutorial



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