

Instructions for Rietica

1. Open data file
 - LFile
 - LOpen
 - change file type to *.xy
 - open file SrPr03_riet.xy
 - LPreferences
 - LMemory
 - Set the "Number of Data Points Per Histogram" to 20,000

At this point you should have a graph of the data. Do not be concerned if the graph only goes up to 50° in 2θ , it is a glitch in the program. You can zoom in on the graph using the mouse to click and drag over the region of interest. If you left click and drag you can scroll across the graph. Double clicking on the magnifying glass icon returns the graph to full range.

2. Create input files

- LFile
 - LNew
 - LOK
 - Create an input file name
- LModels
 - LGeneral
 - Make sure "Read data format" is set to "x,y"
 - Click desired "Output File Options" such as "Obs. & Calc. Intensities" and set "Bond Distances and Angles"
 - LPhase
 - Left click on "Phase 1" title
 - LRead Phase from CIF File
 - open the SrPrO3.cif file
 - Under "Phase 2," the CIF file will be loaded, however the file does not load perfectly so you need to delete atom 5. Left click on atom #5, and from the menu choose "Delete atom." Also, under "Type," you need to go through and select the appropriate ions.
 - There is no ICSD file for the second phase in this material (Sr_2PrO_4), so we must load it by hand. From the paper given (Fiscus, zur Loye, *J. Alloys and Compounds*, **306** (2000) 141-145) use the given data to fill in Phase 1 for Sr_2PrO_4 .
 - Set "B" thermal parameters, to "0.6" as an appropriate starting point.
 - Left click on # to "Add atom"
 - Left click on # and "Set all atoms to full occupancies", this sets "n" such the position has full occupancy, where $n = \text{site mult} / \text{gen mult}$.
- LHistograms
 - Set "Data min-max:" to 3 and 100
 - Set "Data step" to 0.005
- LSample
 - Start with "Pseudo-Voigt" for "Peak Shape"
 - Under "Instrument PeakShape," set $w = 0.03$, $\text{ASY1} = 0.02$, $\text{Gam0} = 0.1$, and $u, v, \text{Gam1}, \text{Gam2} = 0$ as generic start values
 - "Plot FWHM" to get an idea of what kind of peaks these values produce

LFile

LSave

3. Refine data

Indicate the number of refinement cycles and the specific parameters that will be refined. For example, to refine the "scale factor/phase scale."

LModels

LPhase

For each phase, checkmark next to the "Phase scale:" box. This tells the program that this is a parameter to refine.

LRIetveld

LRefine

In the "Refine" dialogue box, click "Dynamic Plotting" and "Watch Values" to see how the selected parameters are refining. Click "Start" and a starting graph will appear. Then click "Step" and a first iteration will be carried out. Continue to click on "Step" until the parameter being refined is stable. To update these values into your input file, check the "Update" box, and click "Finish."