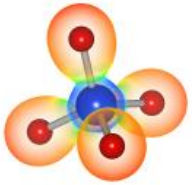
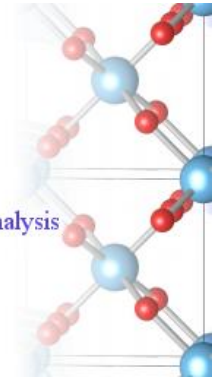


VESTA

Visualization for Electronic and STructural Analysis



VESTA installation and basic use

Installation of VESTA

- VESTA is a very versatile program for the visualization of crystal structures
- It runs on Windows, macOS, and Linux
- Let's first "install" VESTA on your computer (instructions for Windows 10)

1. MyCourses -> Solid State Chemistry -> Software -> VESTA
2. Download the **zip file** (macOS and Linux users: download from VESTA website)
3. Save the zip file anywhere you like (even Desktop is fine, that's easy to find)
4. Extract the zip file (for example by right-clicking and choosing **Extract All…**)
   - You will get a folder ***VESTA-x.y.z-win64,*** where *x.y.z* is the version
5. VESTA is now "installed"
6. Go to the VESTA folder and double-click ***VESTA.exe*** to start VESTA

Structures discussed on the lectures can be found in VESTA format from MyCourses -> Materials -> Data files for lectures

Using VESTA

- Short instructions for the basic use of VESTA now follow
- We focus on visualization, but VESTA also includes many crystallographic tools
- **File** -> **New structure** can be used to build structures from scratch
  - Convenient if a journal paper lists unit cell data, but the structure is not available in a structural database
- We will mainly work with CIF files downloaded from structural databases

- Let's use RbCl from Maija Ahtee (1969) as an example crystal structure (*Fm*-3*m*)
- Download the file **rbcl.cif** from http://www.iki.fi/ankarttu/ssc/rbcl.cif
- If for some reason the link above fails, the structure can be retrieved from COD with COD ID 9009736

Citation for using VESTA: "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data" K. Momma, F. Izumi *J. Appl. Crystallogr.* **2011**, *44*, 1272-1276.
VESTA web page: http://jp-minerals.org/vesta/en/

Opening a CIF file in VESTA

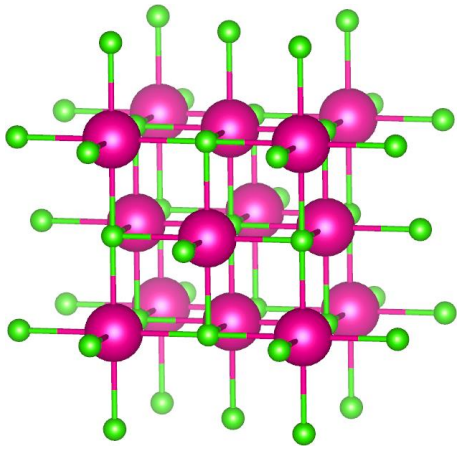


Figure: AJK

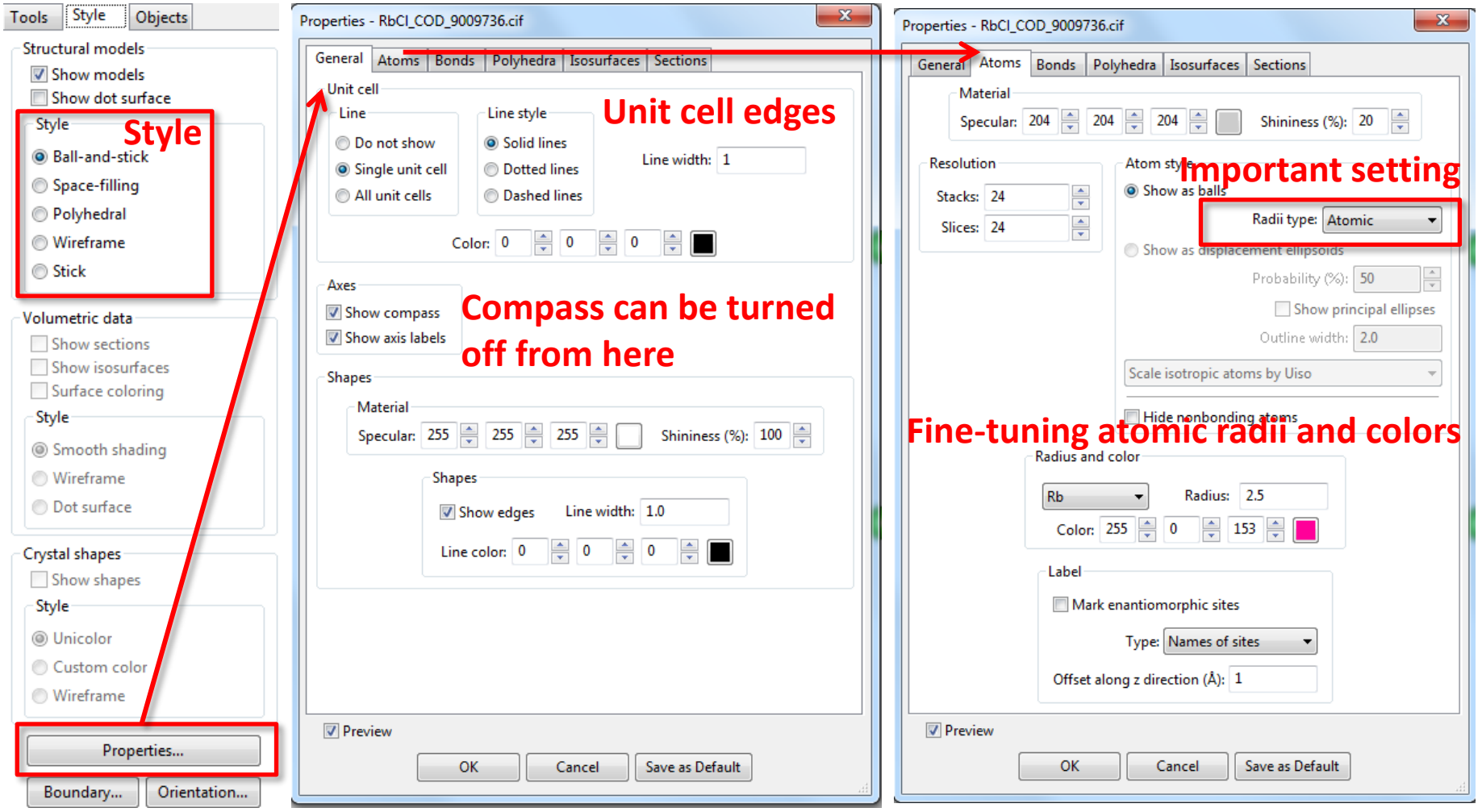
- Open the file **rbcl.cif** in VESTA
  - File -> Open
  - Or drag & drop the file to VESTA
- The structure should first look something like this:

- VESTA draws the bonds automatically
  - If you have a very old version of VESTA, it does not draw them. Please update.
  - If necessary, the automatic bond search can be turned off from Edit -> Preferences -> Bond search

- Try moving the structure:
  - Hold left mouse button to ***rotate***
  - Use mouse wheel to ***zoom***
  - Enter ”t” to ***translate*** with the left mouse button (”r” returns to ”rotate”)
  - Shift + left button selects atoms or bonds

Changing properties

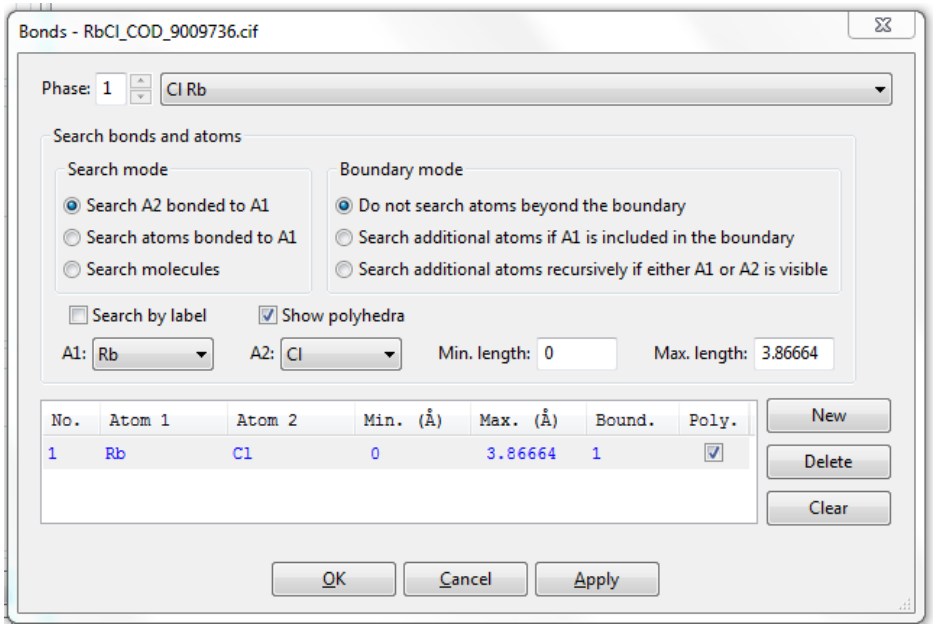
Several important settings are under ”Properties…”:

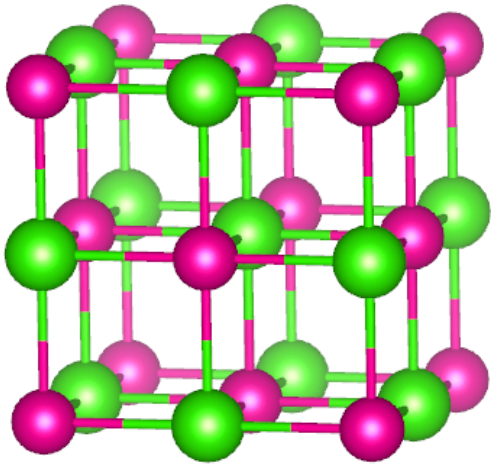


Figures: AJK

Changing bonds

- Change **Radii type** in Properties -> Atoms to ”Ionic”
- Close Properties dialog with OK and go to Edit -> Bonds… (**Ctrl + B**)
- Choose Rb-Cl ”bonds” from the list, change **Boundary mode** to ”Do not search atoms beyond the boundary”, and click ”Apply”
- The structure should look like below
- The Bonds dialog is very important for the final appearance of the structure
- Here we chose to show only one crystallographic unit cell (face-centered cubic)

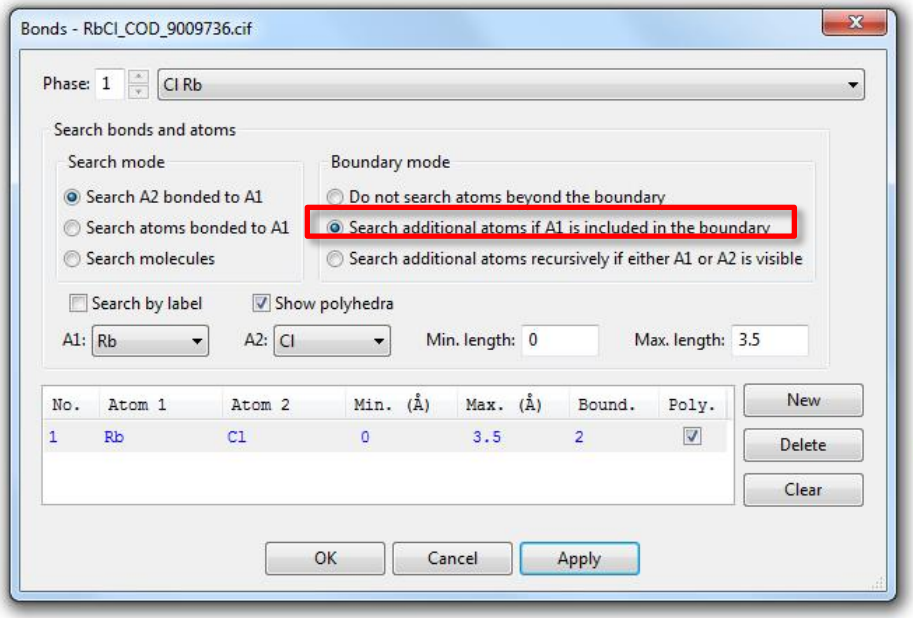


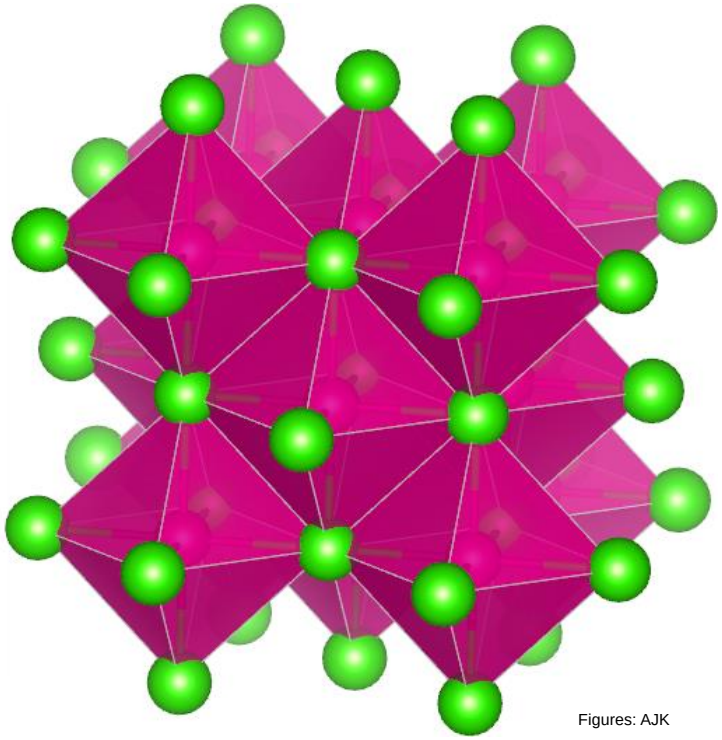


Figures: AJK

Polyhedral style

- The Bonds dialog also determines how coordination polyhedra are drawn
- Choose the ”Search additional atoms if A1…” Boundary mode in the **Bonds** dialog
- Change **Style** from the main window to **Polyhedral**
  - The resulting figure should look like below:
- Octahedral coordination polyhedra around Rb (Cl in the corners of the octahedra)

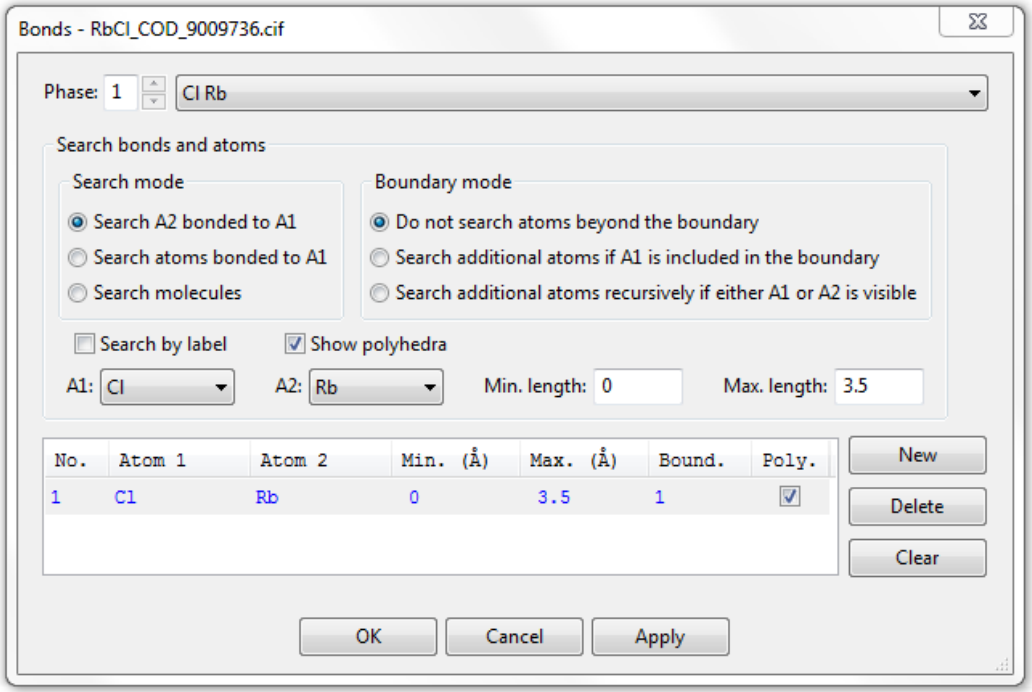


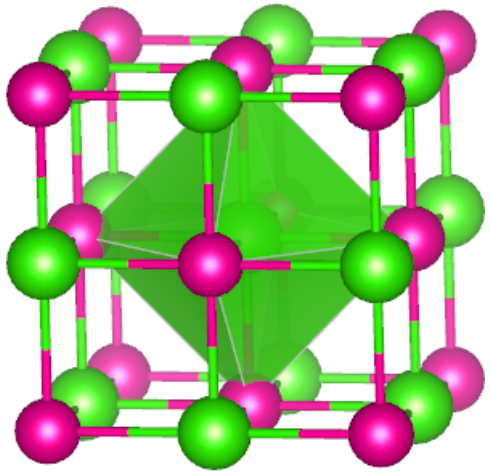


Figures: AJK

Set central atom for polyhedra

- The order of the atoms in the Bonds dialog determines the central atom in the polyhedron.
- Delete the automatically determined Rb-Cl bond and make a new bond with A1 = Cl; A2 = Rb
- Change the Boundary mode to ”Do not search atoms…”. The result should look like the following:

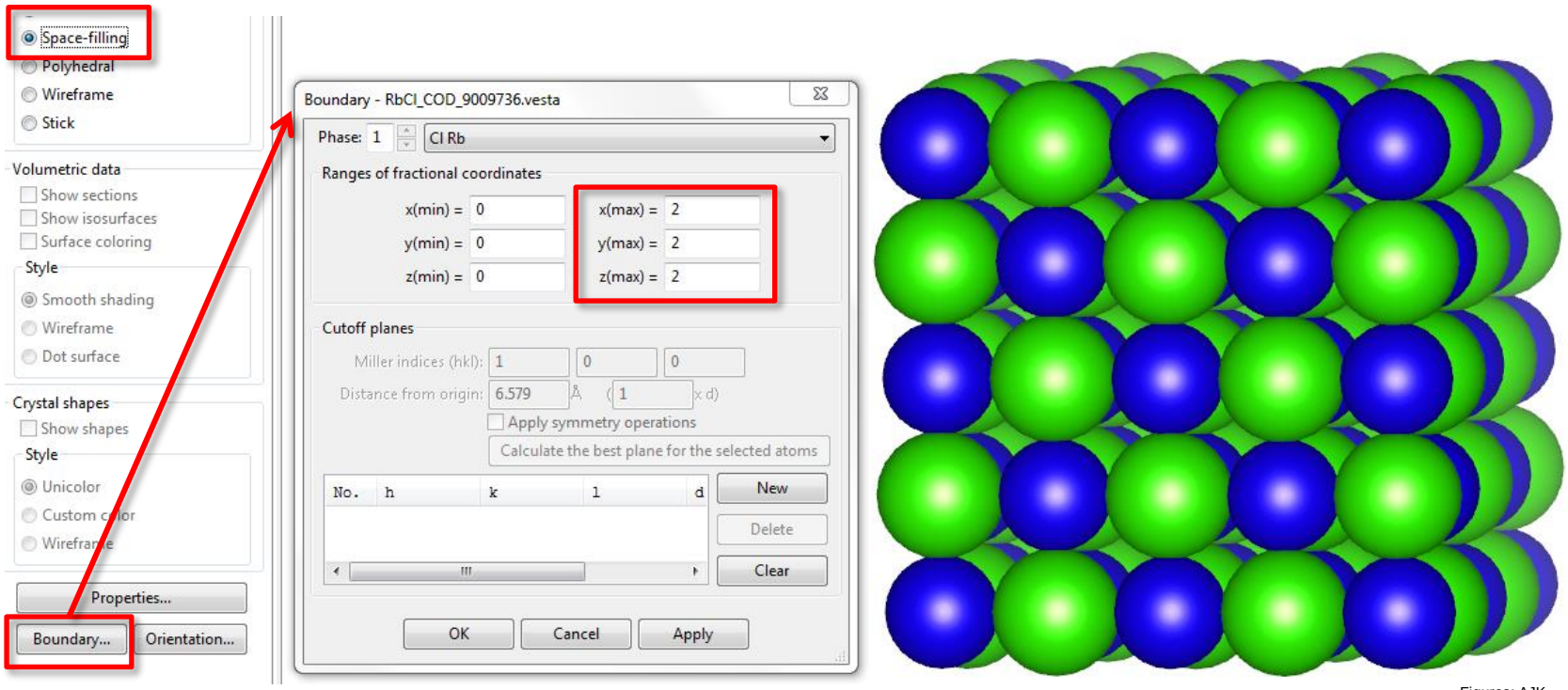




Figures: AJK

Supercells and space-filling style

- If you want to show more than just one unit cell, click ”Boundary” and enter the dimensions of the ***supercell***
- Below, a 2x2x2 supercell of RbCl is drawn with a **space-filling** style
  - The color of Rb atoms has been changed to blue from Properties -> Atoms



Figures: AJK

Fine-tuning the appearance

- VESTA offers a vast number of options for tuning the appearance of the structures
- Go through the various options in the Properties dialog and try to make the structure look as close to the figure below as possible
  - Blue = Rb, green = Cl
  - Black polyhedral edges, more transparent polyhedron
  - Unicolor bond style

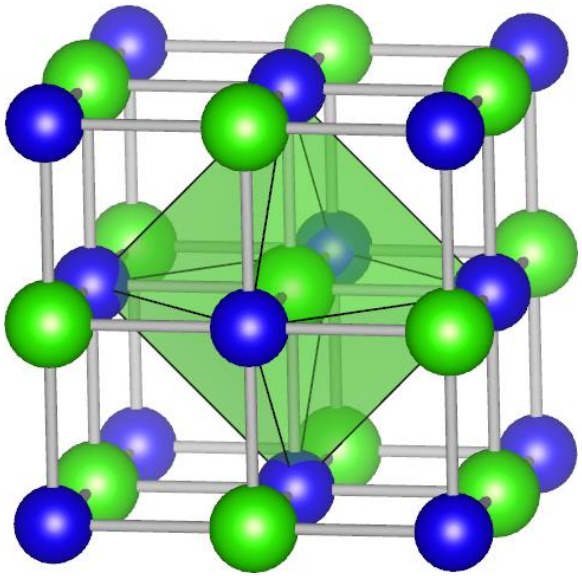
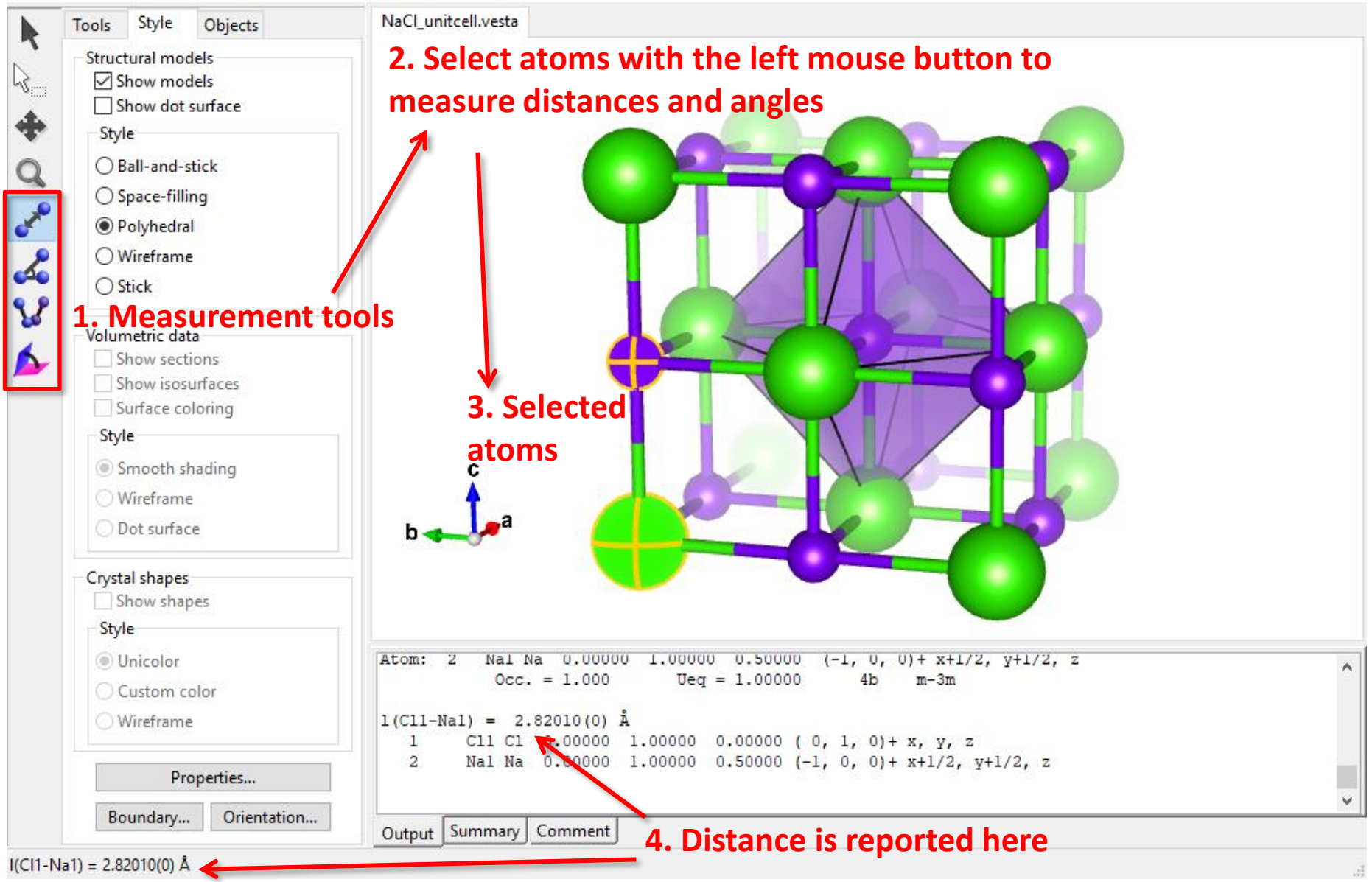


Figure: AJK

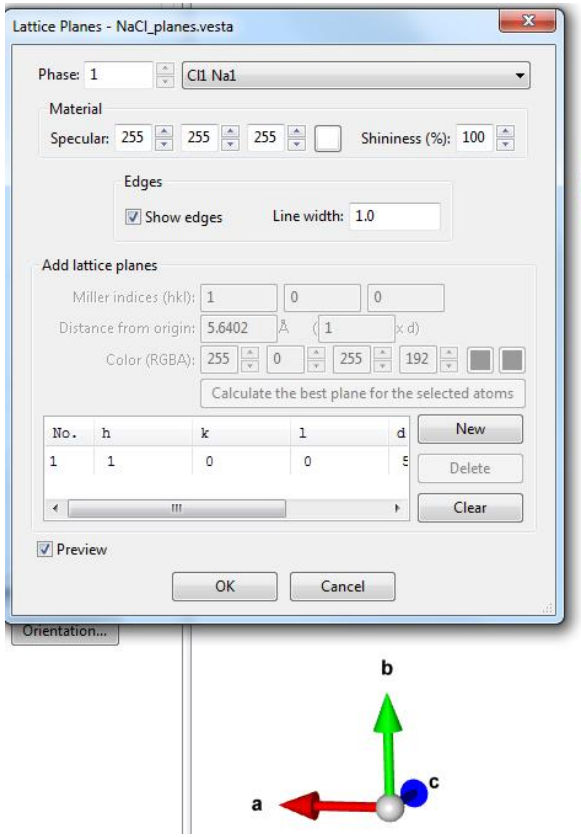
Measurements with VESTA



Advanced VESTA topics (starting from Lecture 7)

Lattice planes with VESTA

- Edit -> Lattice planes -> New -> Choose the Miller index and distance from origin)
- Usually ”**Distance from origin**” = (1 x d) is the best starting point for visualization
- If you want to orient the crystal exactly, use Objects -> Orientation



NaCl (*Fm*-3*m*), lattice plane (001)

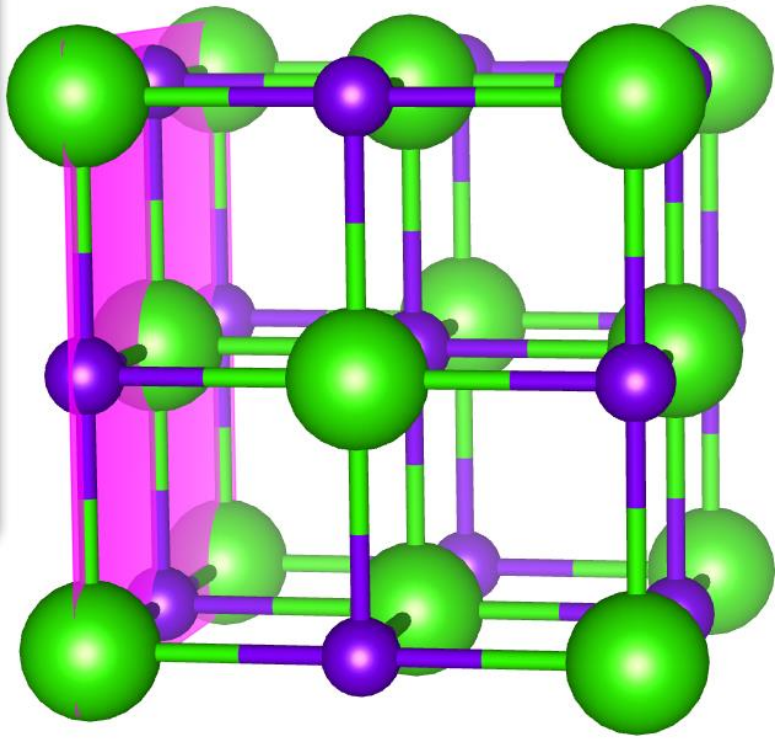


Figure: AJK

XRD powder patterns with VESTA

- VESTA has built-in tools for XRD powder pattern simulation
- Go to Edit -> Preferences and make sure that the RIETAN text box is empty
- Open a CIF file
- Go to Utilities -> Powder Diffraction Pattern
- Open **Conditions** tab and set only one wavelength (here Cu-Kα)
- Click **Calculate** to simulate the pattern (see **Plot**)
- **Reflections** tab shows a peak listing
- You can also simulate mixtures by adding phases from Edit -> Edit Data -> Phase