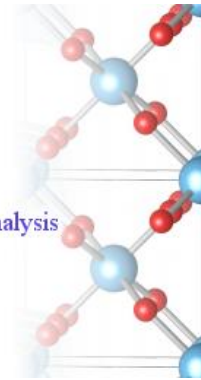


VESTA
Visualization for Electronic and Structural Analysis



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-3m*)
- 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

- 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

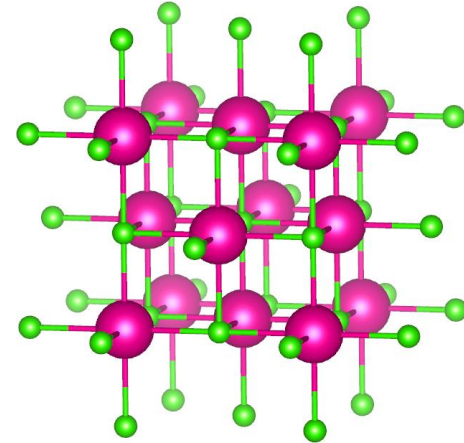


Figure: AJK

Changing properties

Several important settings are under "Properties...":

Style

- Ball-and-stick
- Space-filling
- Polyhedral
- Wireframe
- Stick

Unit cell edges

Line style: Solid lines, Dotted lines, Dashed lines

Line width: 1

Compass can be turned off from here

Axes: Show compass, Show axis labels

Important setting

Atom style: Show as balls, Show as displacement ellipsoids

Radii type: **Atomic**

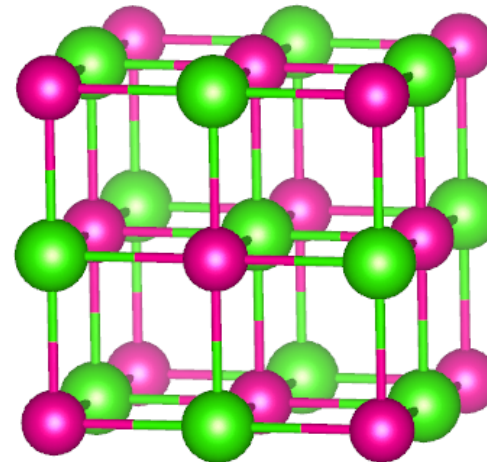
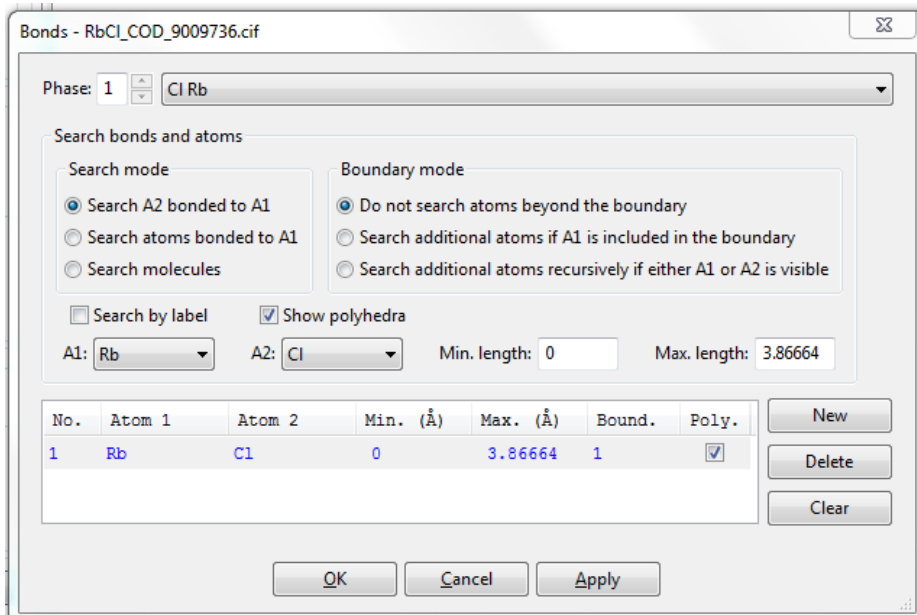
Fine-tuning atomic radii and colors

Radius and color: Rb, Radius: 2.5, Color: 255, 0, 153

Properties...

Changing bonds

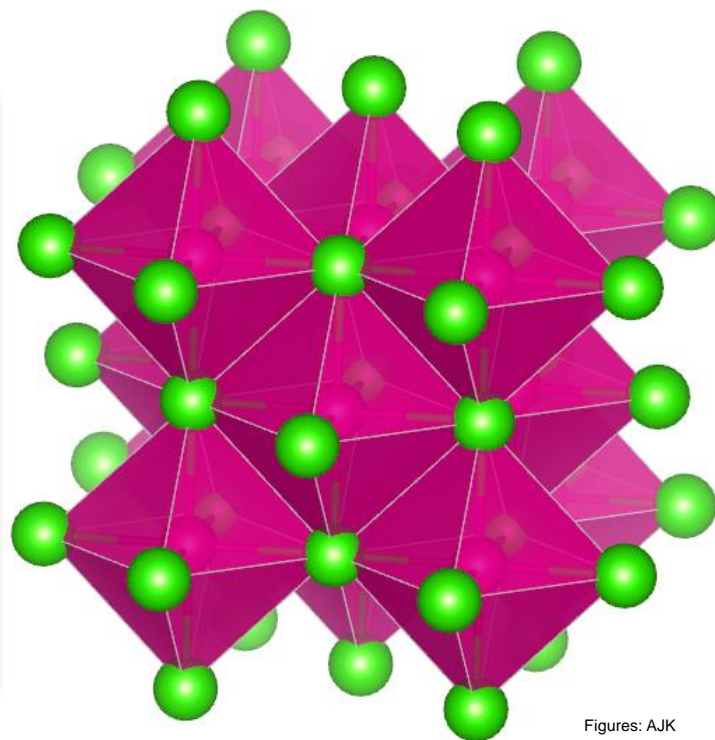
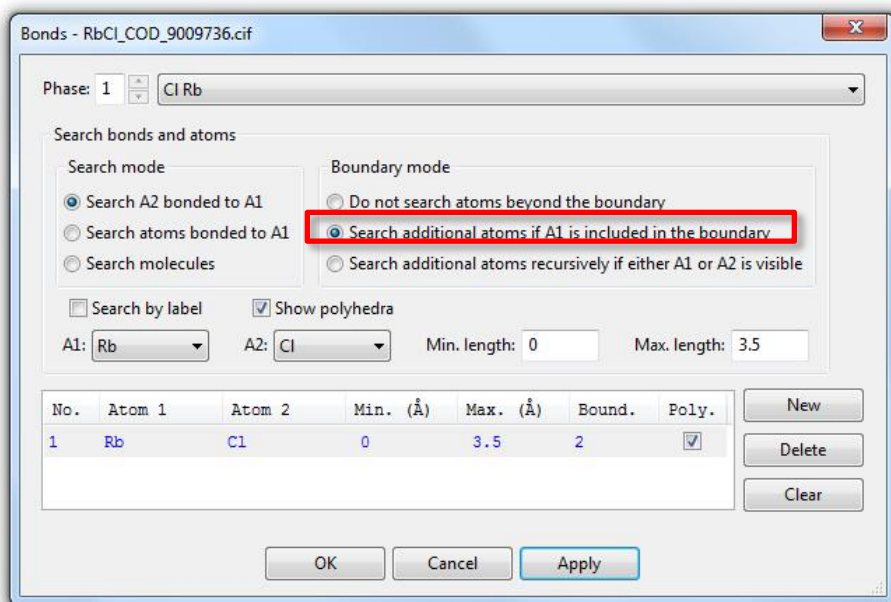
- Change **Radii type** in Properties -> Atoms to "Ionic"
- Close Properties dialog with OK and go to Edit -> Bonds... (**Ctrl + B**)
- Choose Rb-Cl "bonds" from the list, change **Boundary mode** to "Do not search atoms beyond the boundary", and click "Apply"
- The structure should look like below
- 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

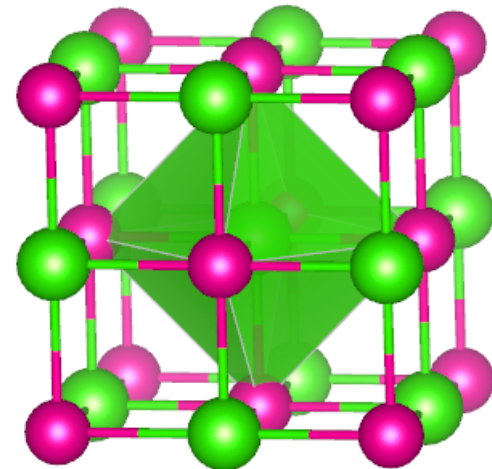
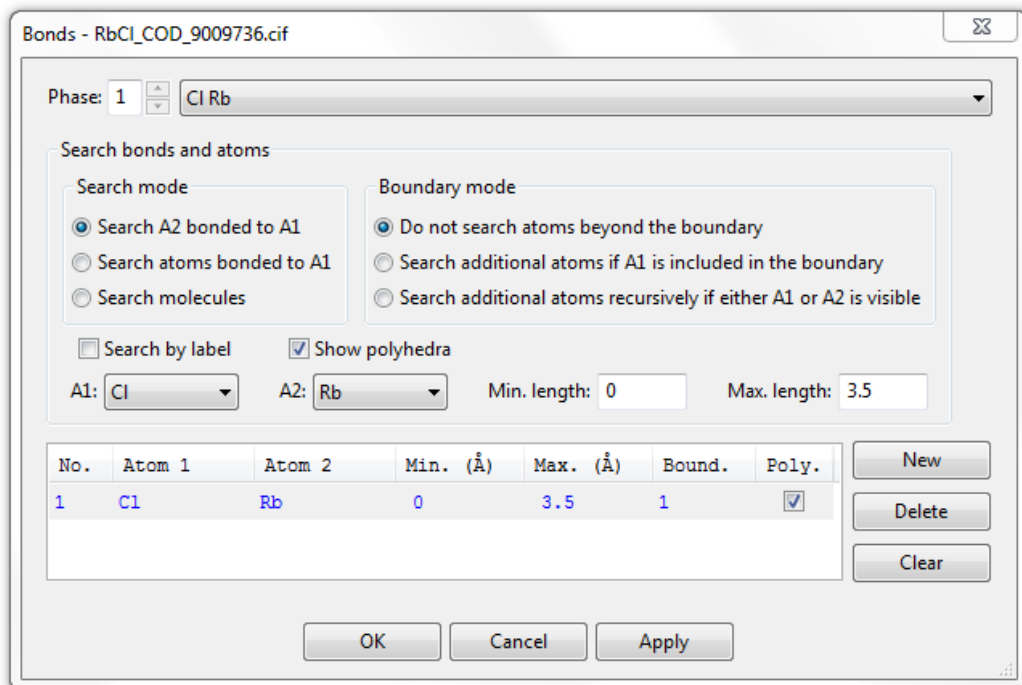
- The Bonds dialog also determines how coordination polyhedra are drawn
- Choose the "Search additional atoms if A1..." Boundary mode in the **Bonds** dialog
- Change **Style** from the main window to **Polyhedral**
 - The resulting figure should look like below:
- Octahedral coordination polyhedra around 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

The image shows a software interface for visualizing crystal structures. On the left, a sidebar contains several panels: 'Style' with 'Space-filling' selected, 'Volumetric data', and 'Crystal shapes'. A red box highlights the 'Space-filling' option. Below the sidebar, a 'Boundary...' button is also highlighted with a red box. A red arrow points from this button to a central dialog box titled 'Boundary - RbCl_COD_9009736.vesta'. The dialog box has a 'Phase' dropdown set to '1' and 'Cl Rb'. Under 'Ranges of fractional coordinates', the 'x(max)', 'y(max)', and 'z(max)' fields are set to '2' and are highlighted with a red box. The 'Cutoff planes' section shows Miller indices (1 0 0) and a distance of 6.579 Å. At the bottom of the dialog are 'OK', 'Cancel', and 'Apply' buttons. To the right of the dialog is a 3D visualization of a 2x2x2 supercell of RbCl, where Rb atoms are represented by blue spheres and Cl atoms by green spheres in a space-filling style.

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

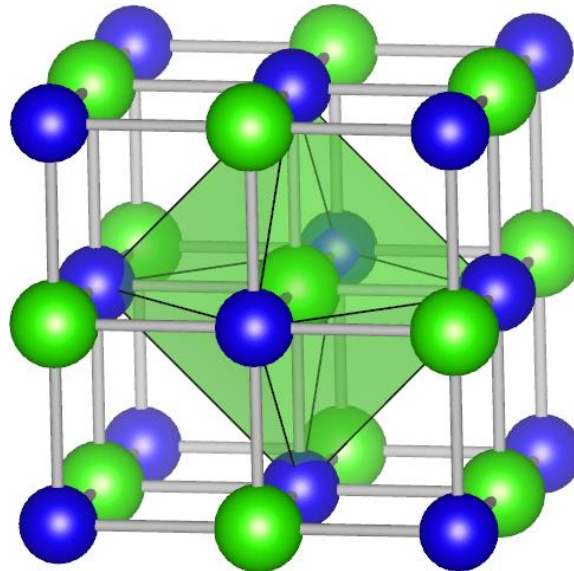


Figure: AJK

Measurements with VESTA

The screenshot displays the VESTA software interface for a NaCl unit cell. The left sidebar contains various tool categories: Structural models, Volumetric data, Style, and Crystal shapes. The 'Style' section is active, showing options for 'Ball-and-stick', 'Space-filling', 'Polyhedral', 'Wireframe', and 'Stick'. The 'Polyhedral' option is selected. A red box highlights the 'Measurement tools' icon in the top-left toolbar. The main window shows a 3D model of a NaCl unit cell with green spheres for Cl atoms and purple spheres for Na atoms. Two atoms are highlighted with yellow circles and orange crosses, indicating they are selected. A red arrow points from the text '3. Selected atoms' to these atoms. A red arrow points from the text '2. Select atoms with the left mouse button to measure distances and angles' to the measurement tool icon. A red arrow points from the text '4. Distance is reported here' to the 'Output' tab in the bottom-right panel. The 'Output' panel shows the following data:

```
Atom: 2 Na1 Na 0.00000 1.00000 0.50000 (-1, 0, 0)+ x+1/2, y+1/2, z
      Occ. = 1.000      Ueq = 1.00000      4b      m-3m

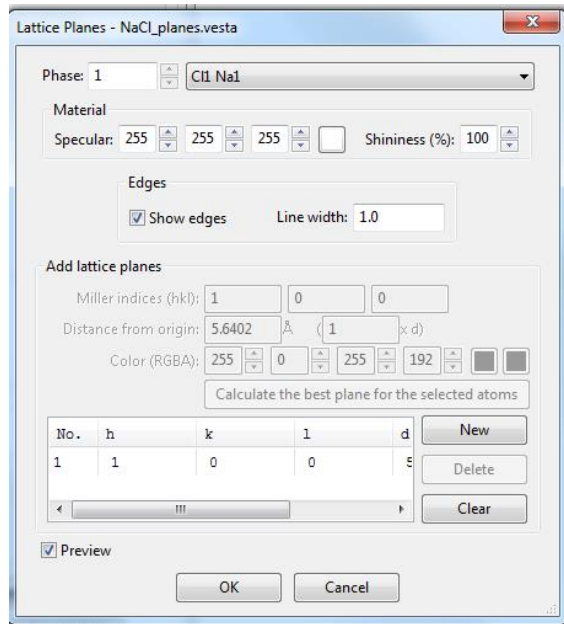
1(C11-Na1) = 2.82010(0) Å
  1 C11 Cl 0.00000 1.00000 0.00000 ( 0, 1, 0)+ x, y, z
  2 Na1 Na 0.00000 1.00000 0.50000 (-1, 0, 0)+ x+1/2, y+1/2, z
```

At the bottom left of the interface, the distance is reported as: $l(\text{Cl1-Na1}) = 2.82010(0) \text{ \AA}$

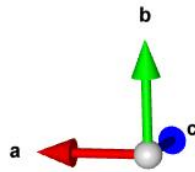
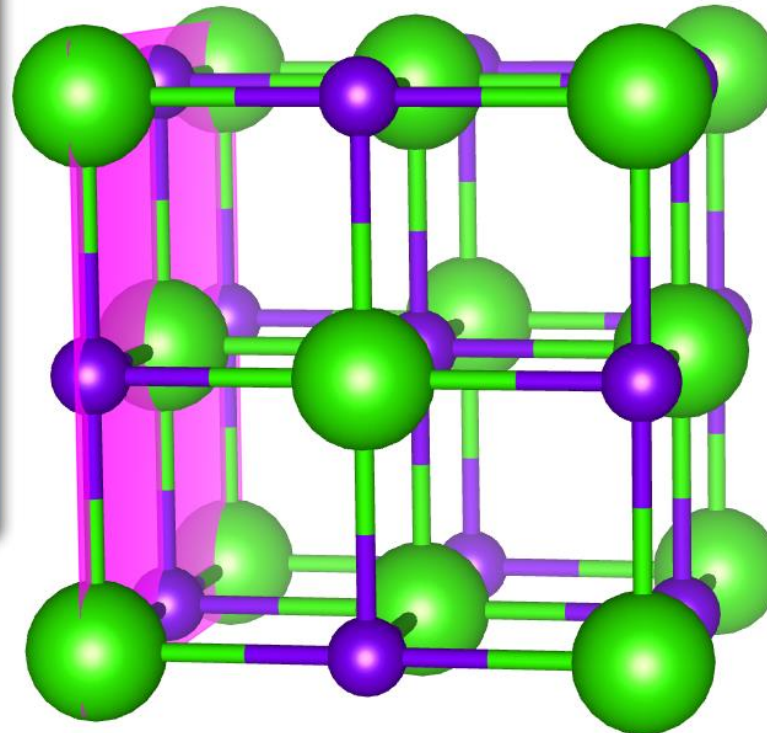
Advanced VESTA topics (starting from Lecture 7)

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-3m*), lattice plane (001)



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-K α)
- 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

