a short tour through VESTA

VESTA is a free viewer for cif files, that is rather popular in the computational community. It runs on Windows, Mac and Linux. After having downloaded and installed VESTA on your computer (see elsewhere in the course site for instructions how to do that), you can go through the following straightforward tasks to make yourself familiar with the basic features of VESTA.

We assume you have a cif file stored on your computer, for instance the cif file for NaCl in the rocksalt structure that you find in the COD database at http://crystallography.net/cod/9003308.cif .

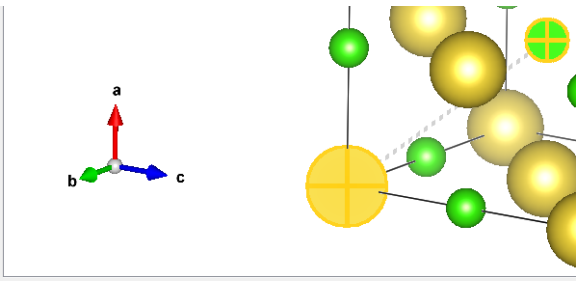
After opening VESTA, choose File/Open to open the cif file. You'll see a 3D drawing at once. With the left mouse button, you can rotate the crystal in any direction. You can use the top bar to orient the crystal along (reciprocal) axes, or shift and rotate it in a controlled way – try out every button:

The mouse wheel or the magnifying glass at the left-hand column bar are other ways to magnify the picture.

In the text box under the crystal picture, you can read some information about the crystal, which can be useful:

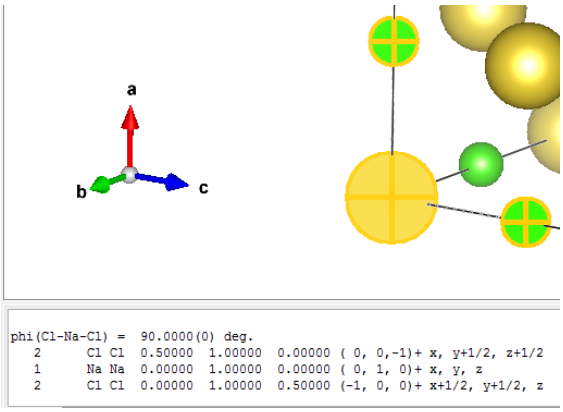
```
================================================================================
Title               Cl Na

Lattice type        F
Space group name    F m -3 m
Space group number  225
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.64010  5.64010  5.64010  90.0000  90.0000  90.0000

Unit-cell volume = 179.415687 Å^3

Structure parameters

                        x          y          z          Occ.     B     Site    Sym.
   1 Na  Na          0.00000    0.00000    0.00000    1.000    1.000    4a    m-3m
   2 Cl  Cl          0.50000    0.50000    0.50000    1.000    1.000    4b    m-3m
================================================================================
```

The toolbar at the left is a useful one. By default, the black arrow is selected. This is the normal operation mode, where you can rotate and displace the crystal. If you select the two balls connected by a double arrow (4th item on the bar), then you can measure distances between atoms. Do that, click then on a Na and on a Cl atom, and you'll see the distance between both in the text window under the crystal.

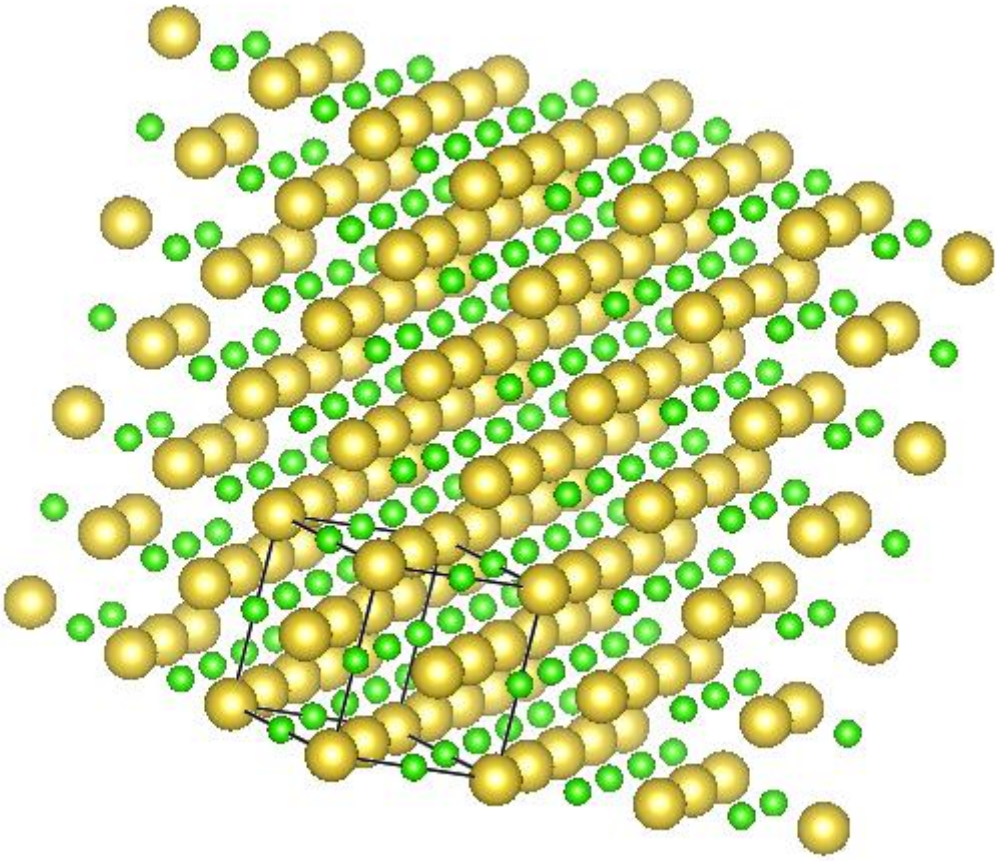



```
1(Na-Cl) =  4.88447(0) Å
   1      Na Na  0.00000  1.00000  0.00000 ( 0, 1, 0)+ x, y, z
   2      Cl Cl  0.50000  0.50000  0.50000 ( 0, 0, 0)+ x, y, z
```

Take the button with 3 atoms on it, to measure angles. Now you should click on any three atoms, and you'll see the angle spanned by that triangle (obviously 90 degrees in the example you see at the right).



With Objects/Boundary, you can draw extended (or reduced) sections of the infinite lattice that is defined by the unit cell. For instance, if you select x(min)=y(min)=z(min)=0, and x(max)=y(max)=z(max)=3, you get a 3x3x3 extension of the initial unit cell. This can help to get a better feeling of the threedimensional crystal:



Examine what happens if you change to x(min)=y(min)=z(min)=0.1. With the 'cut-off planes' that you see in the same dialogue box, you can erase parts of the crystal using planes specified by Miller indices (useful to draw specific surfaces, for instance).

The Edit/Bonds menu can be used to decide which pairs of atoms you connect by sticks, and which not (this doesn't change any physics or chemistry, but it can help viewing). Try to draw all bonds between Na-Cl nearest neighbor pairs, or all bonds between Na-Na nearest neighbor pairs.

With the Edit/Lattice Planes menu, you can give the Miller indices of a specific plane that will be drawn into the picture (in contrast to the cut-off planes discussed above, no atoms will be erased).

There is much more VESTA can do, but this gives you a start. Just remind: there is no DFT involved here, it's only for viewing and analysis.