Instructions (example):

1. go to http://www.crystallography.net/cod/search.html

2. Search for BaZrO3:
   a) in field "1 to 8 elements" field enter Ba, Zr, O
   b) in field "number of distinct elements min and max" enter 3 and 3

3. Press "Send"

4. Choose structure for which you wish to import data (In this case choose file 1532743)

5. Click on "COD ID"

6. In the new window, click on
Coordinates 1532743.cif
This will download to your computer a .cif file with atomic coordinates of the compound that can be read by Vesta.

7. Open downloaded file with Vesta
   7a. On the left side bar, click Style/Polyhedral and you will see Polyhedra around Ba atoms. This is too easy (this file had all information needed already in) but you see only polyhedra around Ba, but not about Ti. So, we will now do something else which will help you use Vesta.

8. First, identify atoms. In the side bar on the left, choose "Objects" on the top of the menu, then press Atoms.

9. Now go back to "Style" of the side bar and press "Properties" at the bottom. A new window will open with the following tabs/buttons: "General, Atoms, Bonds, Polyhedra, Isosurfaces, Sections"

10. Press "Atoms".

11. Choose Radii "ionic". In section "Radius and colors" check atoms one by one and change color and radius. Choose any color you wish, and for radius choose: **O** 1.26, **Ba** 1.75, **Zr** 0.86. (find radii at: http://www.knowledgedoor.com/2/elements_handbook/shannon-prewitt_crystal_radius.html). Press OK.

12. Press "Polyhedra" and choose colors of polyhedra for each atom. It is a good idea to choose color of polyhedra that is similar to that of the atom. Press OK.

13. On the side bar under "Styles", at the bottom, press "Boundary". Change x(max) to 0.5, y(max) to 0.5 and z(max) to 0.5. Press Apply then OK.

14. Now you should see one polyhedron around the remaining Ba atom and one around Zr atom. (If you do not see polyhedral and only sticks, go to the side bar under “Style” and press “Style/Polyhedral”).
What observations can you make? How are two polyhedra connected?
In Boundaries, change z(max) to 1. How are cuboctahedra connected?

15. Go to boundaries and change x(max) and y(max) to 1.

16. Let's assume that the file was not as complete as this one was. Let's try to see how we can build this from the beginning. Go to “Edit/Bonds” in the main top menu (or press Crtl+B). Erase bonds for **Ba-O** and **Zr-O**. Click Apply/Ok. Now you see only some of the atoms, without bonds.

17. Go back to “Edit/Bonds”. Now define new Bonds that you want to see. First press “New”. Chose A1 and A2 atoms between which you wish to see bonds. Choose A2 as **O**, and for A1 choose **Ba**. Press “New” again and now choose **Zr-O** bond, with **Zr** as A1 atom and **O** as A2. Change Max bond length for both Zr and Ba to **3.5**. Mark the “Poly.” block to activate it for both atoms. Press Apply and OK.

18. To show **only** atoms and bonds within the unit cell go to “Edit/Bonds”. Now under “Boundary mode” you can select “Do not search atoms beyond the boundary”. Click this option for the **Ba-O** bonds. Now you only see atoms and bonds within the unit cell.

19. Go back to “Edit/Bonds”. Deselect “Poly.” for either **Zr** or **Ba**. Press Apply and OK. You should see polyhedra for either **Zr** or **Ba**.

20. Go back to “Style/Boundary” and choose xmax, ymax, zmax=0.5. You should see one polyhedra for Ba and one for Zr.

21. To visualize Lattice planes or Axes go to “Edit” and then “Lattice planes” or “Vectors” respectively.

22. To create a new lattice plane click “New”. By playing with the “Miller indices (hkl)” and “Distance from origin” (in absolute distance or unit cell dimensions) you can move the plane and align it with certain symmetry elements.

23. For displaying axes go to “Edit/Vectors”. On the right side under “Vector” press “New”. In “Latice vector notation” you set the direction of the vector axis. Choose (0, 0, 1). Press OK. On the left side click on “Individual Atoms”. Choose the atom you are interested in (you can see which one you selected). Now press “Set” to apply the vector to the position of the selected atom.

24. To export picture of the structure to a jpg, tiff,… file which you can import into a Word or another document, go to File/Export raster image….
(If you wish, You can remove compass arrows by going to Properties/General/Show compass…).