QUICK START TUTORIAL

CREATING A PROJECT STEP-BY-STEP

Welcome! We assume that you have successfully installed Pintar ***VirtuaLab***$_{TM}$ Molecule on your computer. You are now ready to inspect your very first virtual molecule using the powerful Pintar VirtuaLab Molecule. Inspecting a molecule with Pintar VirtuaLab Molecule allows you to perform with ease tasks that otherwise you will not be able to perform in your school lab!

In this tutorial, we shall do a couple of small experiments. For a novice user, the quickest way to become familiar with Pintar ***VirtuaLab***$_{TM}$ Molecule is to follow this step-by-step tutorial. Throughout this tutorial, you will find quick references to the detail description, as indicated by the ? symbol.

This tutorial assumes that you possess a working knowledge of windows 9x, NT, ME, 2000 or XP. Certain words used to describe operations in this tutorial have procedural meaning.

Click	Press once on the mouse button.
Select	Click once on a specified object.
Drag	Click on a specified object. While holding down the mouse button on the object, drag the mouse. Let go the mouse button when you have dragged the object to the intended location.
Type	Press on one or more specified keys on the keyboard.
Draw (place)	Select a tool from the Tool bar. Move the cursor to a location on the Workbench where you want to 'draw' the object, and click once
Choose	Click on a menu item in a menu.

Launching Pintar VirtuaLab$_{TM}$ Molecule

We assume that you have successfully installed the Pintar ***VirtuaLab***$_{TM}$ Molecule. In the Molecule folder, double-click on the icon labeled MOLE.EXE.

EXPERIMENT 1

OBJECTIVE:

To compare the distances of carbon atoms in diamond and graphite.

PROCEDURES:

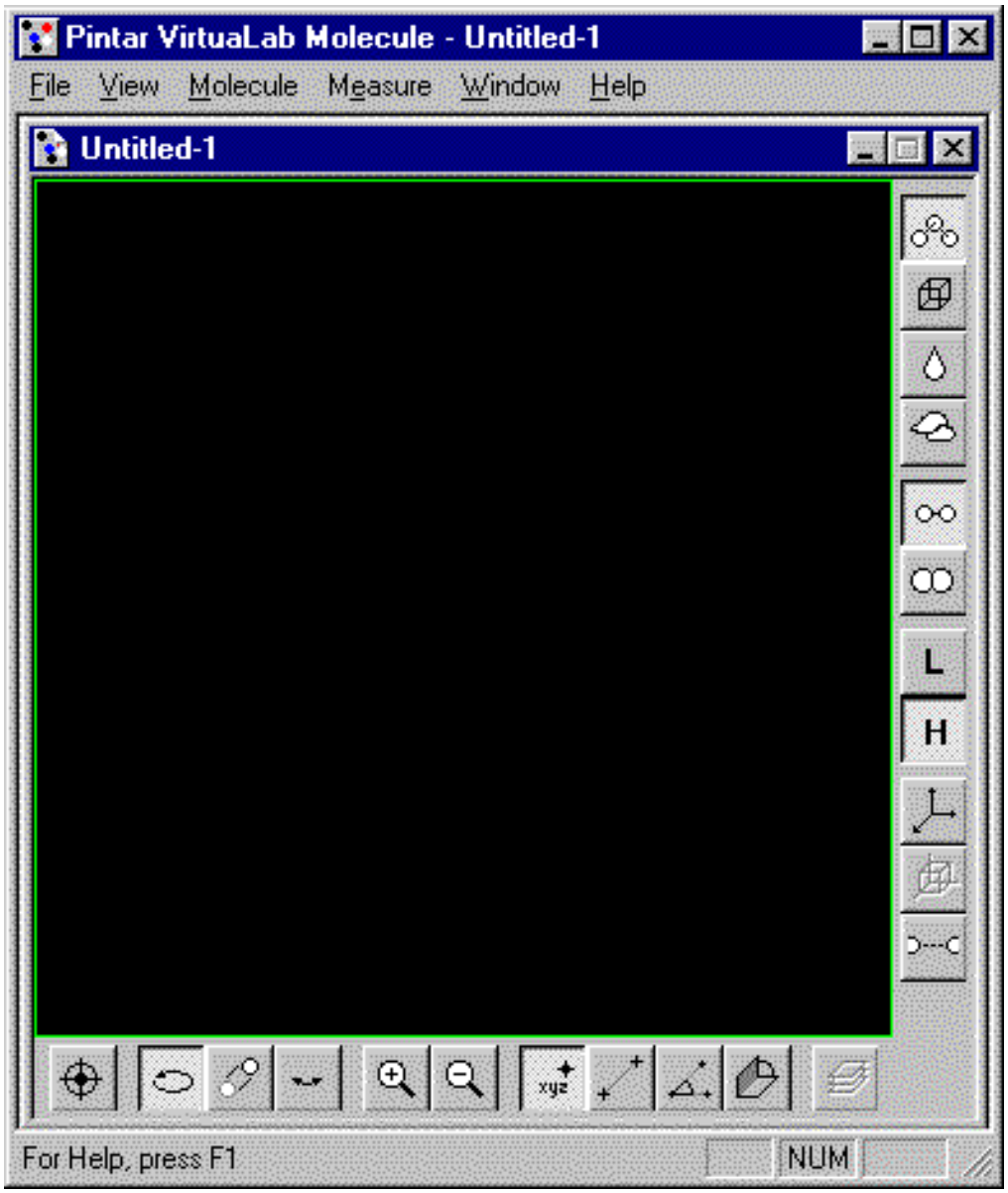
1. Starting a new experiment

Begin a new experiment by setting up a clean Workbench, on which a molecule can be placed for inspection.

a. Choose 'New...' from the File menu. This command will create a new, blank Workbench. The new Workbench will have the default name of "Untitled-1", and uses the default settings.

? • **New** (File menu command)

? • **Default Settings**



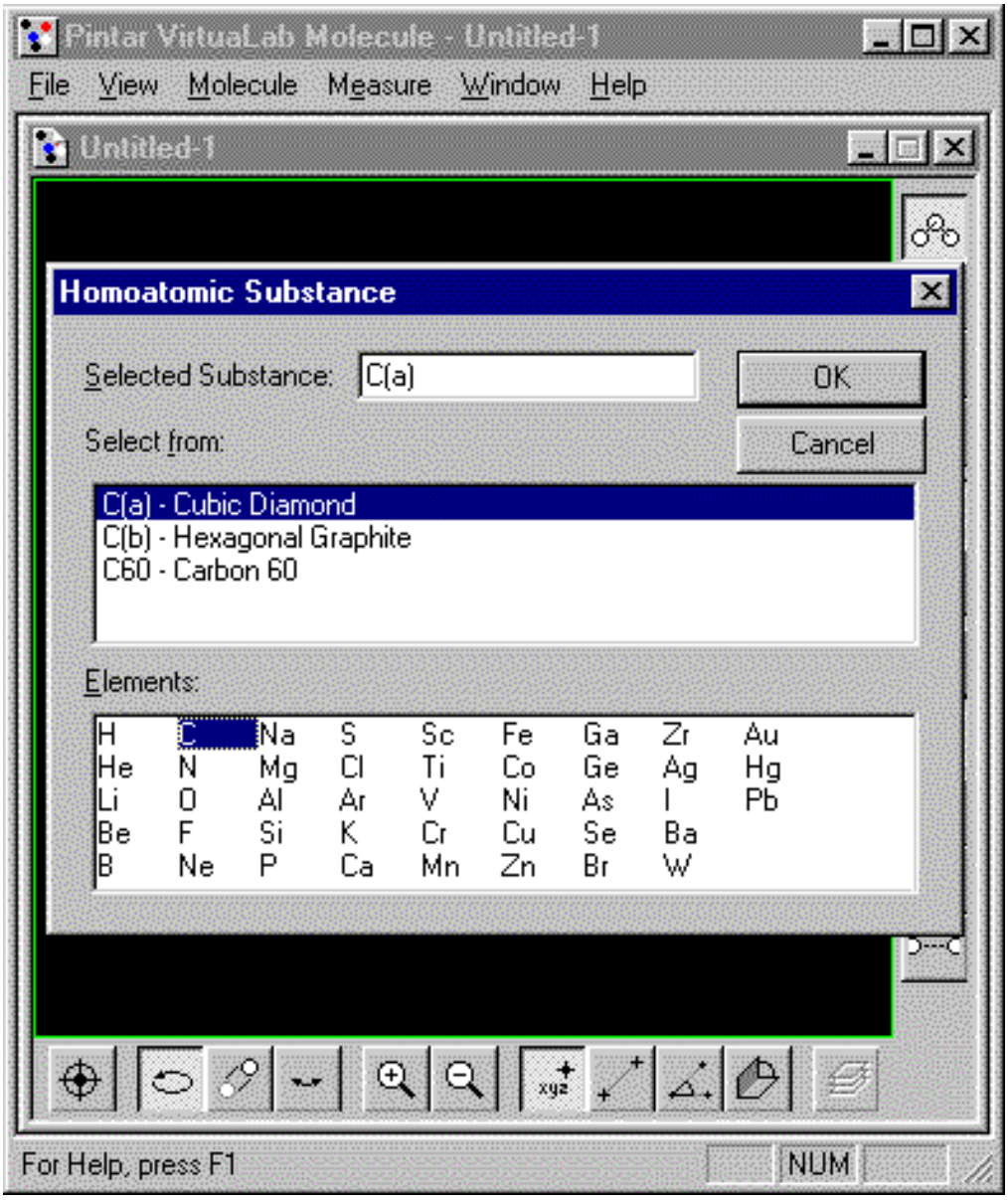
2. Selecting the homoatomic carbon for inspection

a. Choose 'Homoatomic...' from the Molecule menu. The Homoatomic Substances dialog panel appears. In the lower section of the dialog panel is a list of elements.
b. Select 'C' (carbon). The three allotropes of carbon in the Pintar ***VirtuaLab***$_{TM}$ Molecule database appear in the space under the heading 'Select from:'
c. From this list, select 'C – Cubic diamond'. The name of this selected substance is displayed in the 'Selected Compound:' text box.
d. Click OK.

Note: When a molecule is selected for display on the Workbench, it is represented in the default 'chemical unit' state. A chemical unit is the smaller structural unit that constitutes the chemical substance. It may be an atom, a group of atoms, ions or a molecule.

? • **Homoatomic...** (Molecule menu command)

? • **Chemical Unit**



3. To view the diamond unit in its crystalline solid state

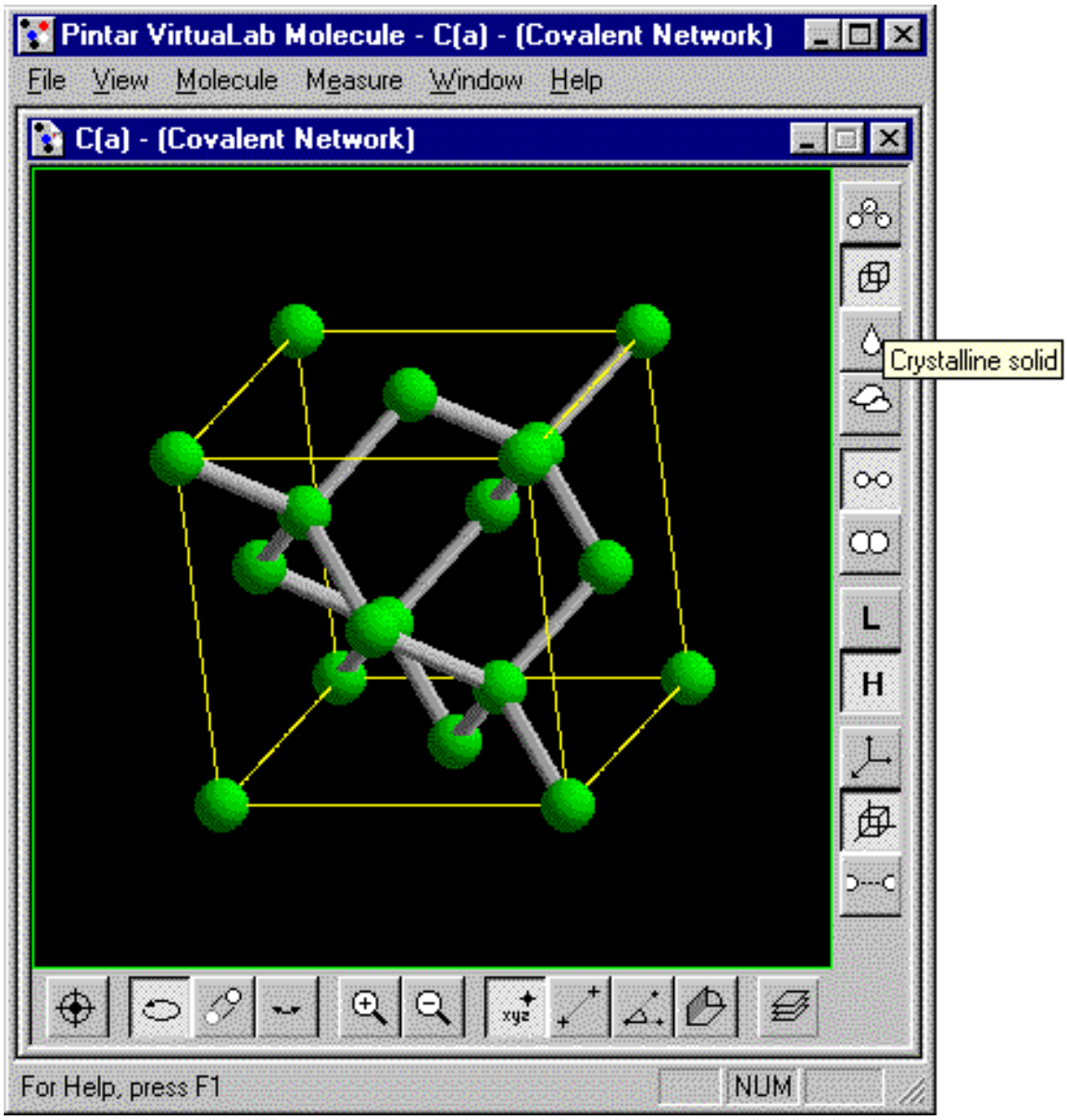
Now we wish to view the diamond in its crystalline solid state.

a. Click on the 'Crystalline Solid State' tool  in the Tool bar, or choose Crystalline Solid State from the sub-menu Display Structure in the View menu.

A yellow (for easy identification) wire frame demarcates the unit cell. The unit cell is the smaller parallelepiped that can be used to generate the entire crystal lattice by simple translation.

? • **Crystalline Solid State**

? • **Unit Cell Frame**



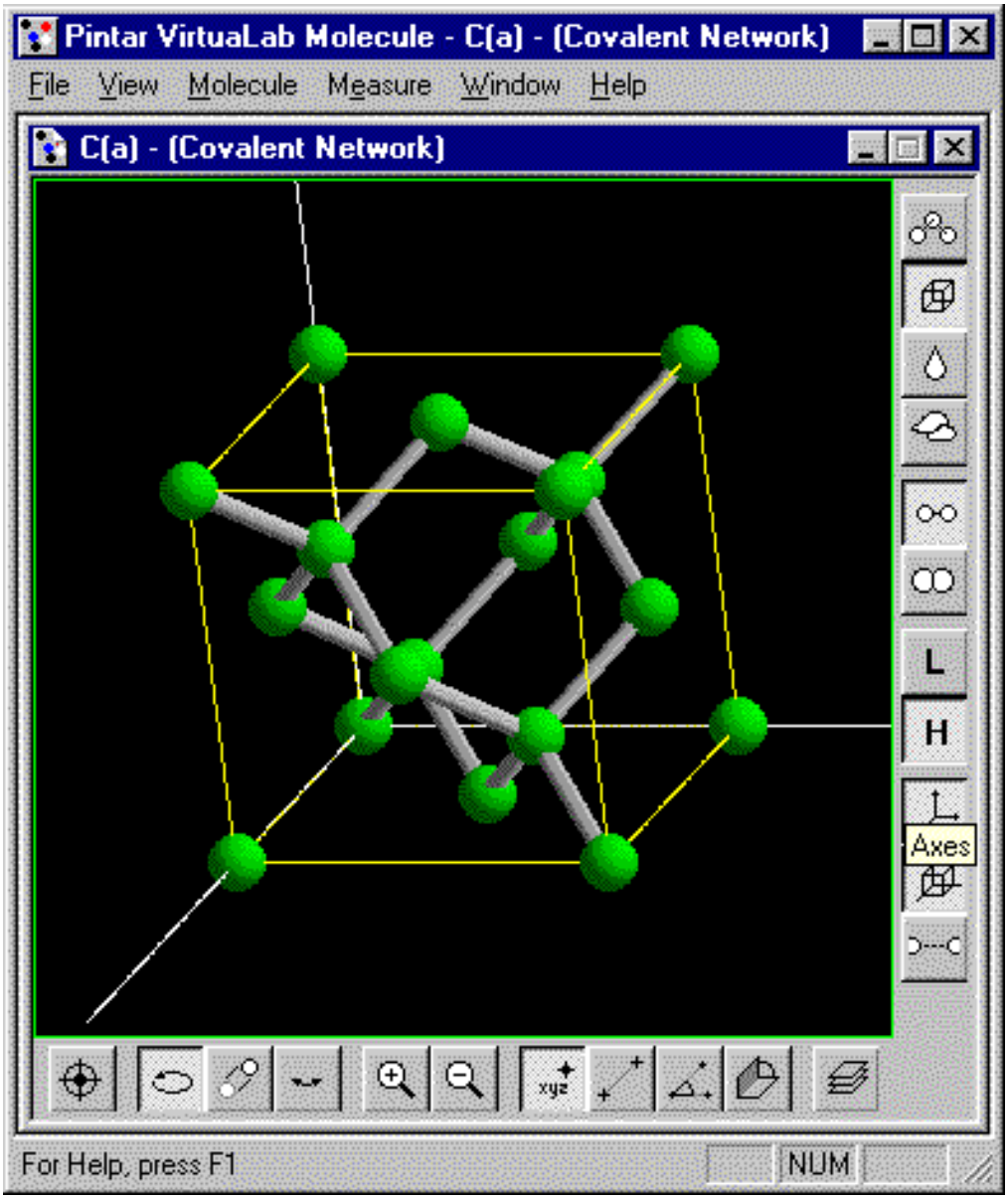
4. Showing the orientation of the crystal with the help of the axes

The orientation of a molecule is fixed to the axis. When you rotate a molecule, the axes rotate with it. The axes provides a frame of reference especially when comparing two similar molecules or different orientations of the same molecule.

a. Click on the Axes tool  or choose XYZ Axes from the View menu. To identify each of the three axes, place the cursor over an axis line. A label indicating the axis appears.

Note: The axes are parallel to the unit cell edges of cubic and rectangular cells but not so for oblique cells.

? • **Axes**


Pintar VirtuaLab Molecule - C(a) - (Covalent Network)
File View Molecule Measure Window Help
C(a) - (Covalent Network)
L
H
Axes
xyz
For Help, press F1
NUM

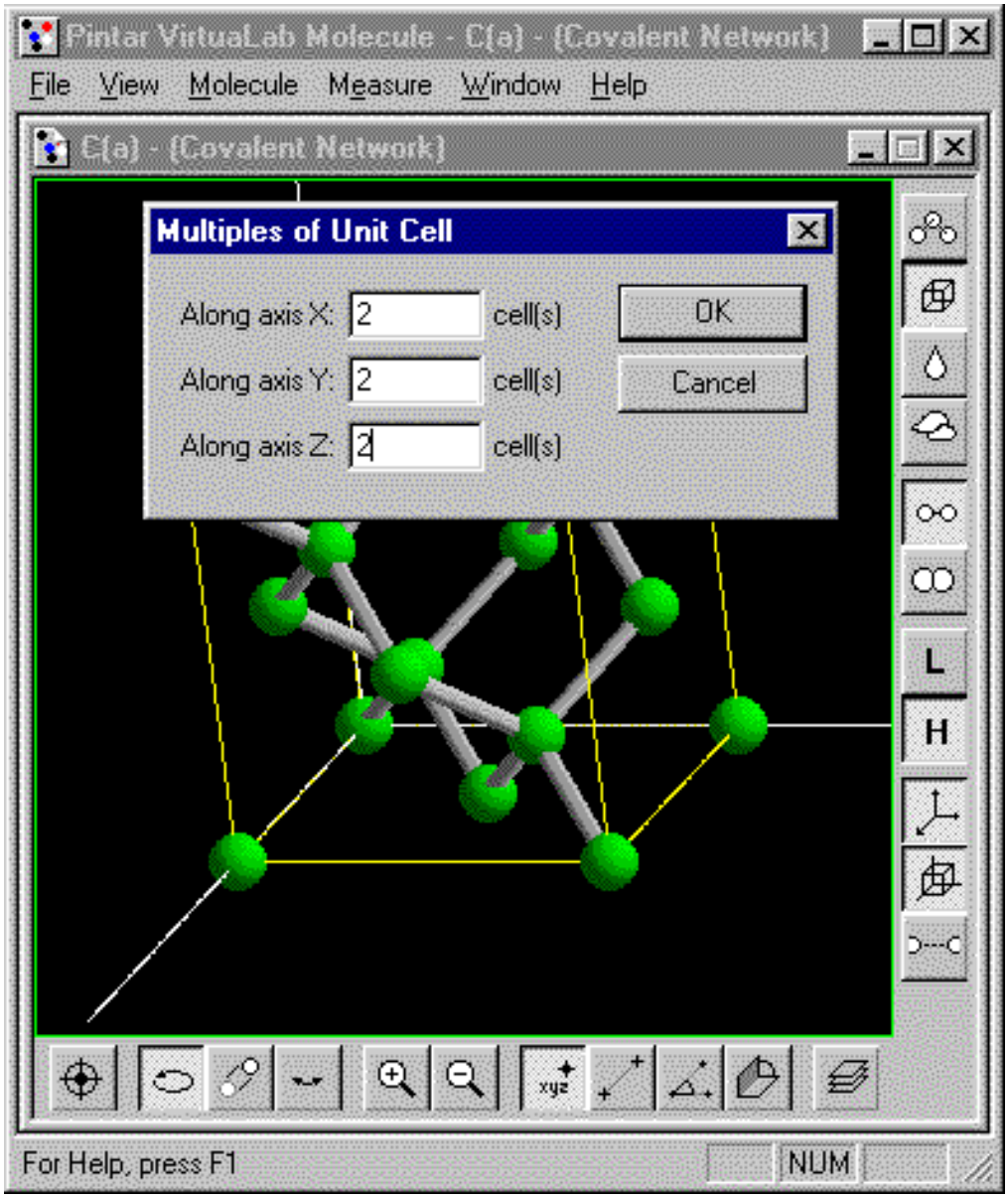
5. Multiples Of Unit Cell

Substances in nature normally exist as, simple multiples of chemical units which may or may not be complete in a unit cell. Therefore, to see how unit cells stack up into a larger crystal:

a. Click on the Multiples of Unit Cell tool  . A dialog panel titled 'Multiples of Unit Cell' appears. Here, we can specify the number of unit cells to 'stack' along each of the three axes.
b. Enter X = 2, Y = 2, and Z = 2 into the respective text entry boxes.
c. Click OK or type the return key.

A chemical substance may pack in different ways depending on the physical conditions (such as temperature and pressure) during crystallization. Hence, many modifications may exist for a single chemical substance.

? • **Multiples of Unit Cell**



6. Save your experiment

At this point, it is a good idea to save the experiment that you have created thus far.

IMPORTANT: If you are using a free trial version of Pintar ***Virtua*Lab**$_{TM}$ Molecule, you will not be able to save your experiment because this feature has been disabled. Continue with Step 7.

a. Choose 'Save As...' from the File menu.
b. Name the project, "Diamond".

7. Open a new file

8. Select another carbon allotrope, graphite, for comparison

Allotropes are substances that have the same chemical constituents but different structures. Diamond has an equally famous sister allotrope by the name graphite. The difference in structure between the two results in drastically different properties. Diamond is clear and is the hardest natural substance known on earth. On the other hand, graphite (pencil lead) is black and is soft enough to mark paper.

Repeat steps 1 to 4, except that this time you choose graphite from the 'select from:' list. For Multiples of unit cell, repeat step (a), enter X = 3, Y = 3, and Z = 2 for step (b), followed by step (c). Save the experiment as "Graphite".

9. Rotate the molecule

Rotate both the diamond and graphite molecules so that the layers of carbon atoms can be clearly visible. To rotate a molecule:

Choose the Rotate tool  in the horizontal tool bar (actually, the Rotate tool is selected by default).

a. Click and drag the molecule on the Workbench. The molecule will rotate in the direction you drag.

? • **Rotate**

10. Distance between atoms

Our next task is to compare the distance between carbon atoms in diamond and graphite. For each, we need to:

a. measure the distance between carbon atoms in the same layer, and
b. the distance between two layers of carbon atoms.

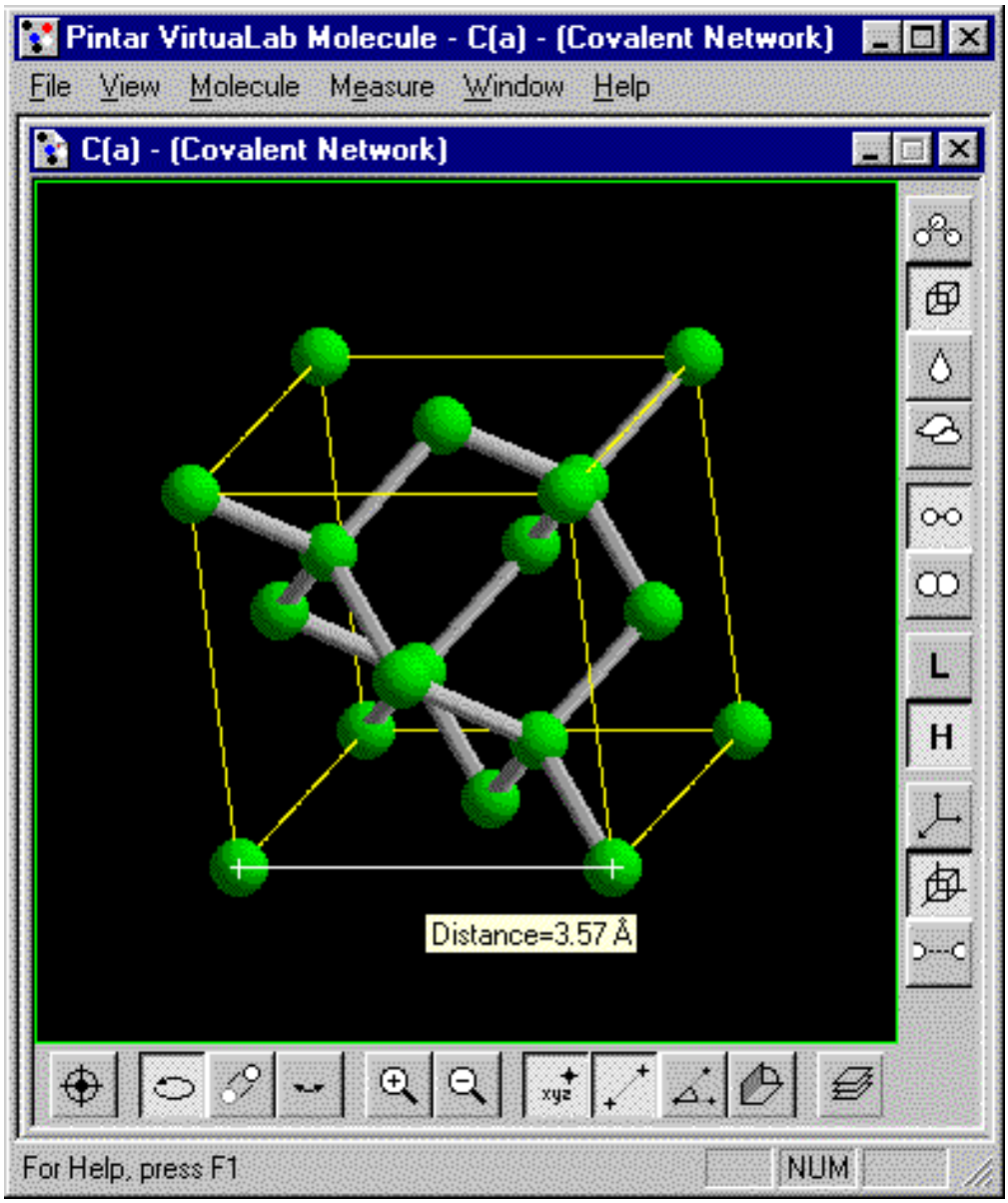
To read the distance between two atoms in a molecule:

a. Choose the Distance tool  .
b. First, click on one atom in the molecule. A small white cross is left on the atom you just clicked.
c. Move your cursor to the second atom and click. Another small white cross is left on this atom.

A white line connects the two crosses. When the cursor is over the white line the distance readout appears. The unit of measurement is in angstrom.

The readout will disappear after three seconds. To view the readings again, move the cursor away from the white connecting line and back over it.

? • **Distance**



11. Ending your work session

Are we having fun yet?

a. Go directly to Experiment 2, or
b. Choose 'Quit' from the File menu if you wish to call it a day.

EXPERIMENT 2

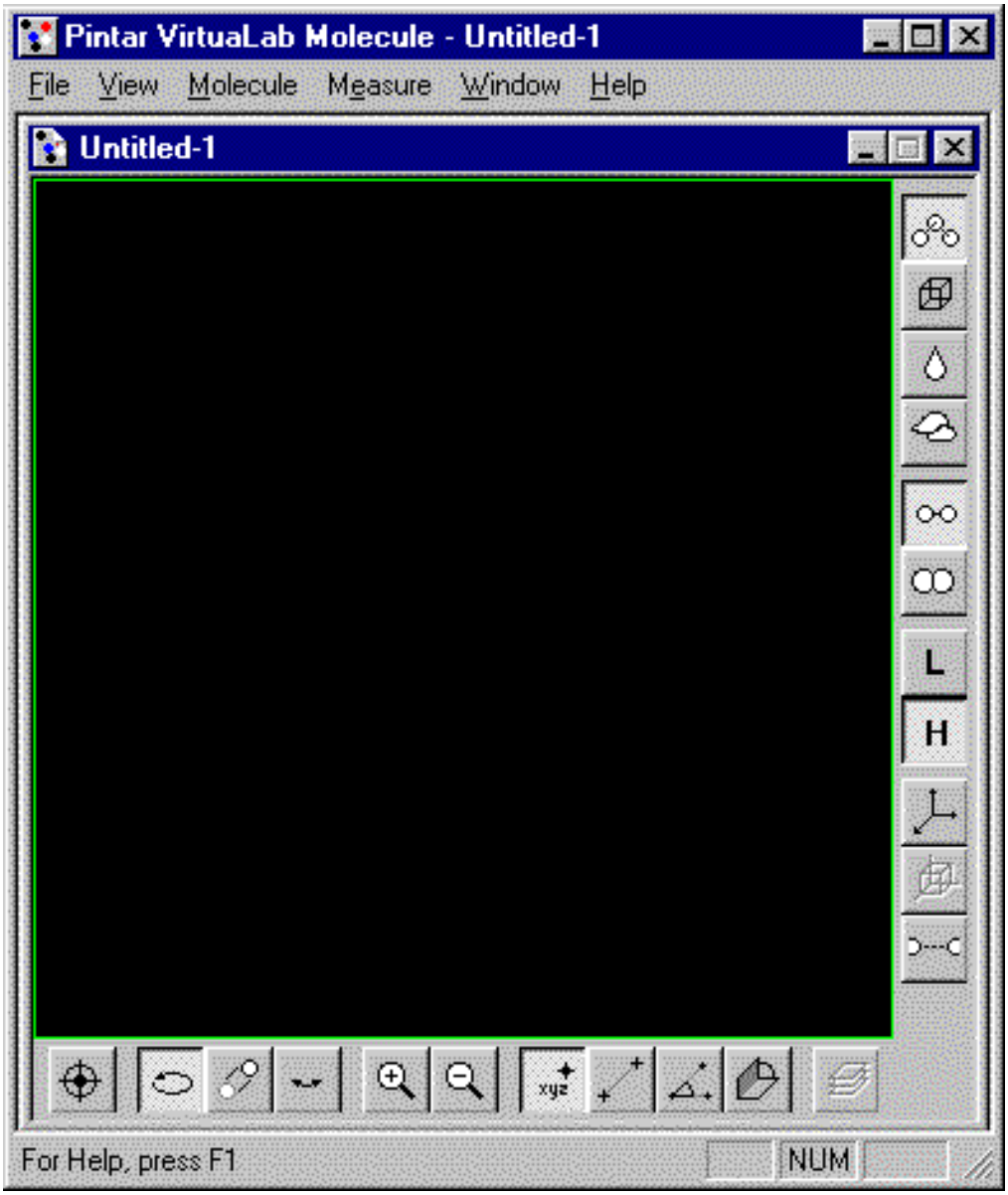
OBJECTIVE:

To view a metallic compound.

PROCEDURES:

1. Starting a new experiment

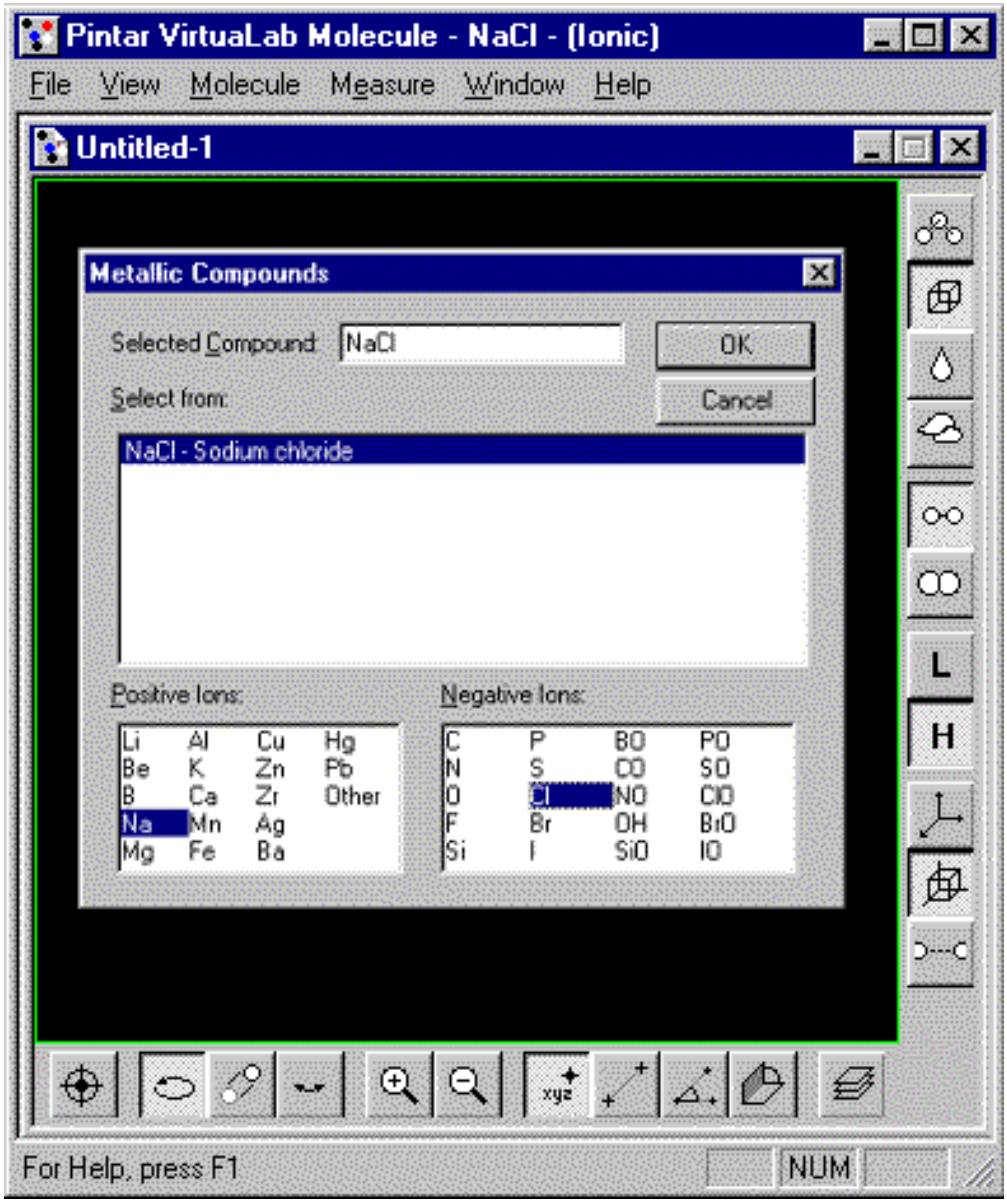
Begin a new experiment by opening a new Workbench



2. To select a metallic compound for viewing

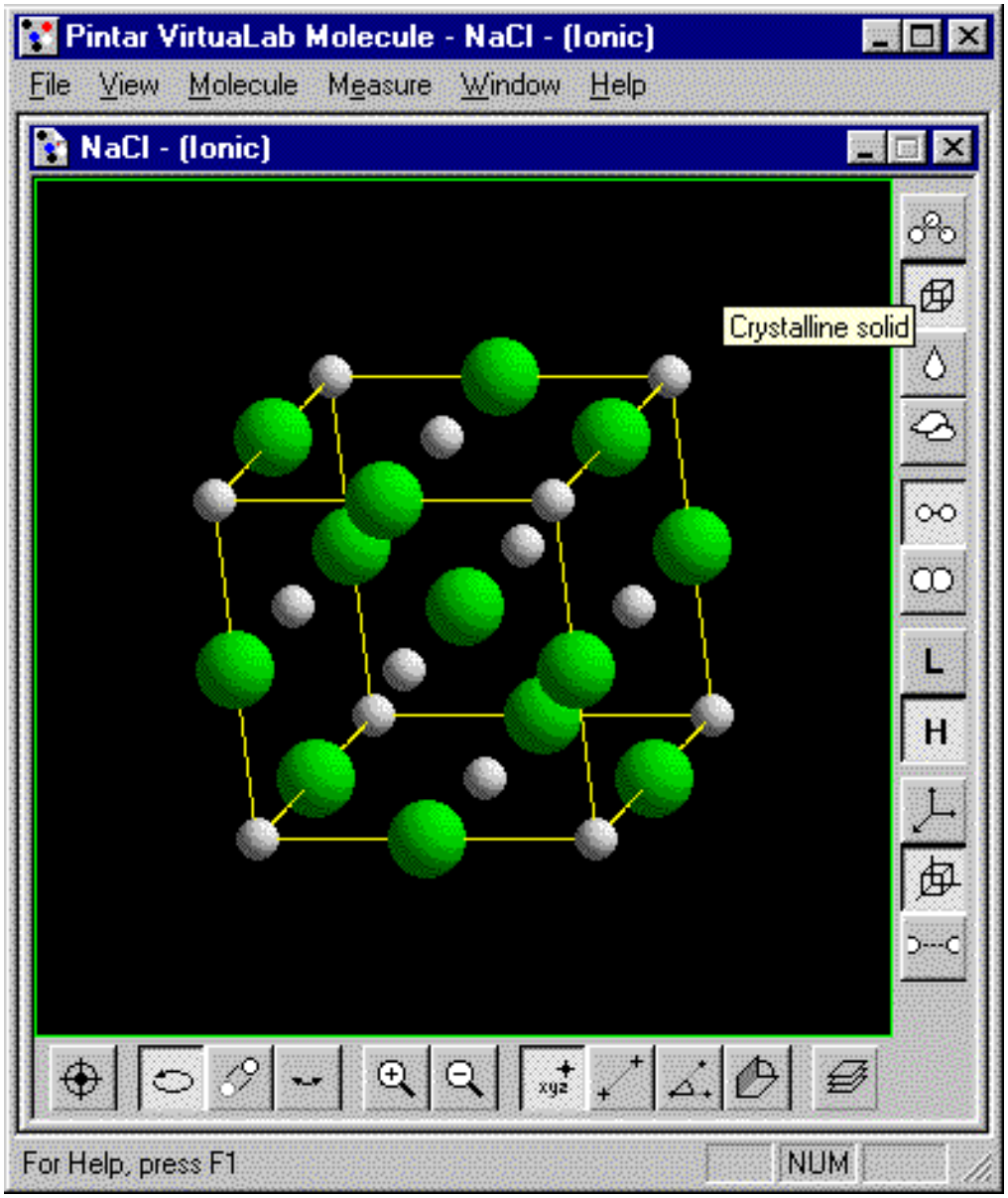
a. Choose 'Metallic Compounds...' from the Molecule menu. The Metallic Compounds dialog panel appears. In the lower section of the dialog panel are two groups of ions – positive and negative.
b. Choose 'Na' from the positive ion group, and 'Cl' from the negative ion group.
c. Click OK.

? • **Metallic**



3. To view the crystalline solid state

Next, display the sodium chloride compound in its 'crystalline solid' state.



4. Position of atoms

Identify and determine the position of the sodium atom in the sodium chloride structure:

a. Choose the position tool 

.
b. Move the cursor onto a white atom in the molecule. A string of data appears that looks something like: Na 1 (5.64, 5.64, 5.64) R = 0.98A

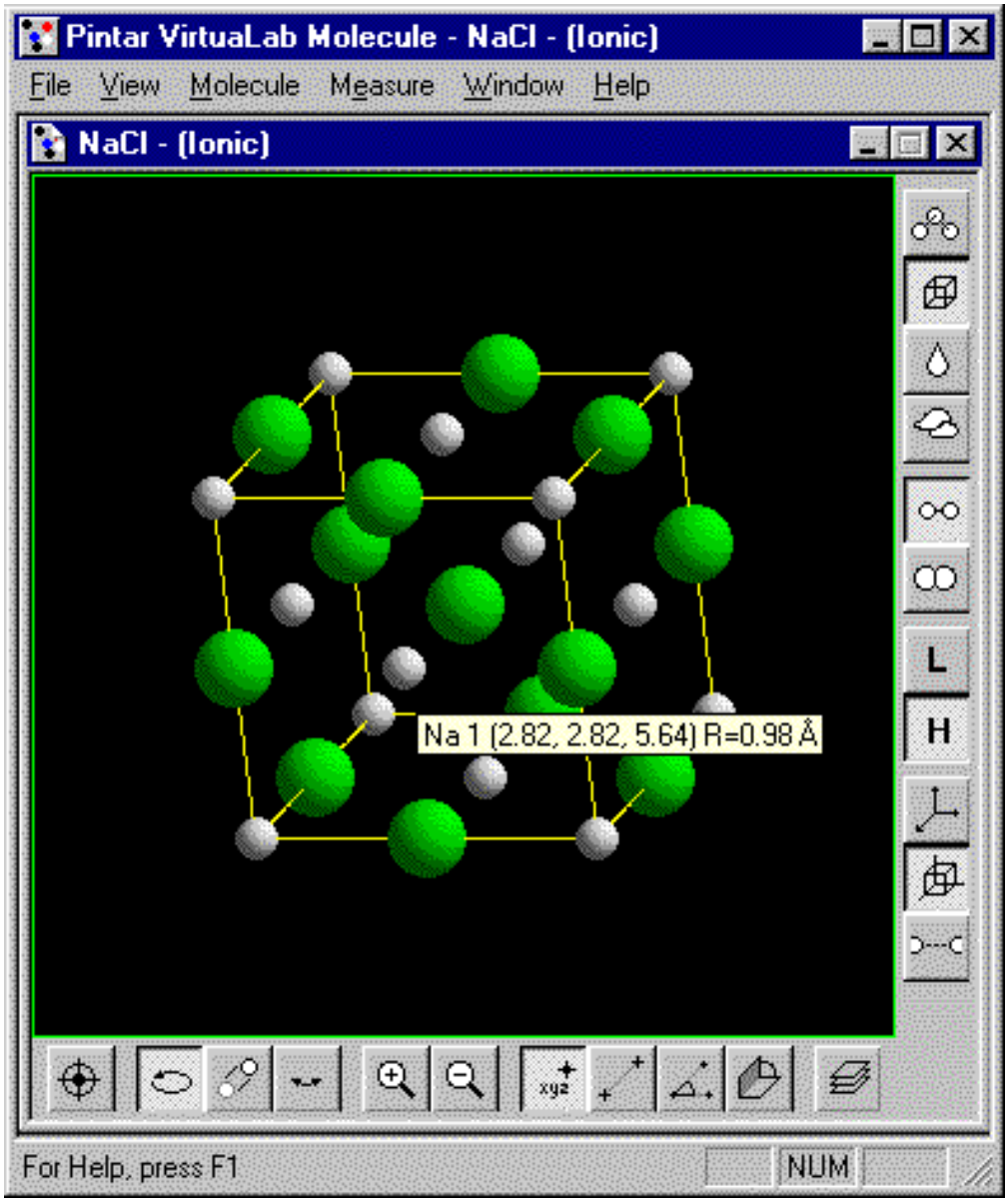
The first piece of data, Na, tells us that the atom is sodium. The integer 1 is the valency of the element.

The data within brackets indicate the position of the atom (measured in angstrom) with respect to the origin of the XYZ axes. The final piece of data is the radius of the atom, again measured in angstrom.

Do the same for the chlorine atom.

The read-out will disappear after three seconds. To view the readout again, move the cursor away from the atom and back over it.

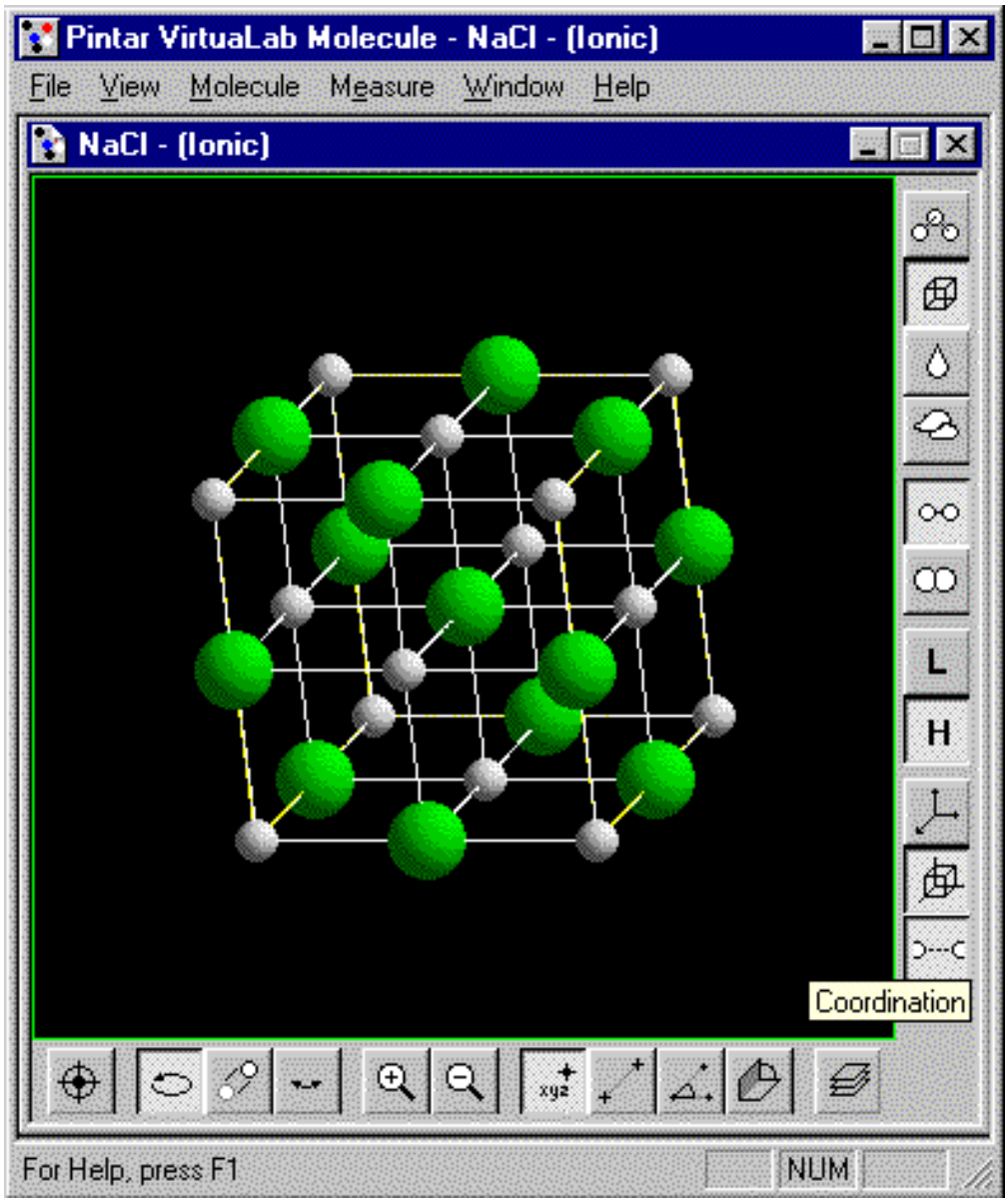
? • **Position**



5. Coordination number

The coordination number of an atom in a molecule is the number of closest neighbours around it . Determine the coordination number of the sodium atom, and then do the same for the chlorine atom. You may need to increase the number of unit cell along one axis.

You will find it easier to count the neighboring atoms if you click on the 'Coordination' button in the Tool bar  . Electrostatic attractions between oppositely-charged ions in ionic structures are also indicated by a single white line joining the cations with the anions.



6. Rock the molecule

We perceive depth with the aid of depth cues such as size difference, movement, overlap, brightness, etc. The Pintar ***VirtuaLab***$_{TM}$ Molecule employs parallel projection instead of perspective in constructing the 3D model of a molecule. Therefore, an atom that is further away does not decrease in size. To enhance depth perception, overlapping and movement (rocking) are used.

To rock a molecule, click on the Rock tool  in the horizontal Tool bar. Sit back and enjoy as the molecule pans by 12 degrees to either side.

? • **Rock**

7. Open a new file

Repeat step 2 to step 5 for CsCI (which may be selected from "other" under the positive ion). Compare the packing density of the two group 1 metal halides by clicking on the space filling button  .

? • **Space-filling**

8. Ending your work session

Although this experiment is coming to an end, your learning adventure with the Pintar VirtuaLab Molecule is just beginning.

If you wish, you may save your experiment.

a. Choose ‘Save As...’ from the File menu.
b. Name the project, "MyMolecule". You may want to save your project in the Examples folder.

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