IV. SOLIDS

Name _____ Section _____

For this activity, all of the file labels will begin with a Roman numeral IV.

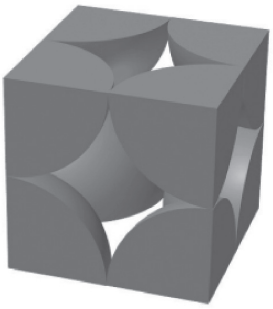
A. In Jmol, open the SCS file in IV.A.1. Click the Bounding Box and Axes function keys. Use the atom size and bond size slider bars to adjust the view so that the bounding box and axes can be easily seen. Move the figure around to a position that shows the 3-D orientation of the spheres and draw the figure below.

B. This figure is the basis for some solid compounds and ions. This particular structure is called a Simple Cubic packing Structure (SCS) and is one way atoms, ions, or molecules are arranged in a three-dimensional matrix (called a lattice). Polonium, Iridium, and Ruthenium are examples of the few elemental solids that utilize the SCS arrangement. The Jmol figure is the simplest unit of the SCS structure. A sample of a solid substance would be represented by adding spheres in the x, y, and z planes to make a large matrix. Describe the orientation of the spheres to each other in this matrix.

Taking the continuous nature of the lattice into account, how many nearest neighbors does each sphere have? _____ This number is called the coordination number.

The Bounding box defines what is called the Unit Cell for the structure. The lattice can be constructed by repeating unit cells in the x, y, and z directions. Only the spheres or partial spheres that are inside of the bounding box are considered to be in the unit cell (see figure).

How many spheres are contained in the SCS unit cell? _____



C. Adjust the sizes of the spheres using the atom size slider bar until the spheres just touch each other. The space between the spheres (called a Hole) can be occupied by other atoms, ions, or molecules depending on their sizes. As an example, if the spheres showing in the Jmol figure are the anions of an ionic salt, the hole could contain the cation.

If all of the holes in an SCS lattice were filled, what would be the ratio of cations to anions?_____

Estimate the relative maximum sizes of the cations and anions in an SCS lattice.

D. Calculate the density (packing efficiency) of the SCS packing arrangement. (Hint: Calculate the volume of the spheres [the sum of all the parts] contained in the unit cell and divide that by the total volume of the unit cell. The dimensions can be determined from the bond lengths.)

E. Another solid packing structure is the body centered cubic packing or BCC. In Jmol, open the BCC file (IV.A.2). Use the atom size and bond size slider bars to adjust the view so that only the spheres are showing. The alkali metals are examples of the elemental solids that utilize the BCC arrangement. Draw this unit cell structure and describe the orientation of the spheres to each other. Why is this structure called body centered cubic?

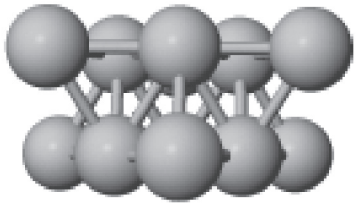
F. Use the same procedure that you used for the SCS structure to answer the following questions.

What is the coordination number for BCC packing? _____

How many spheres are contained in the BCC unit cell? _____

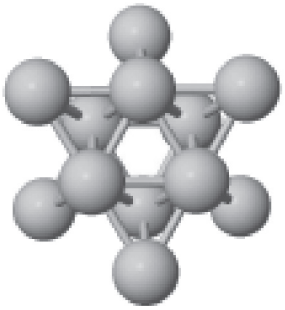
Calculate the density (packing efficiency) of the BCC packing arrangement. (When you adjust the size of the spheres, make them as large as possible without overlapping the boundaries of any of the spheres.)

G. In Jmol, open the CP file (IV.A.3). Adjust the atom and bond sizes. This kind of packing is called a closest packing structure. It is called a closest packing arrangement because the spheres are packed together as close as they can be. Manipulate the model until you can see two layers of spheres viewed from the side.



How is this packing arrangement different from the SCS and BCC packing?

Rotate the structure to view it from the top.



If you were to place a third layer on top of this structure you have two choices. Describe how these two structures would be different from each other. (Hint: One would have what is called an *abab* orientation and the other would have an *abcabc* orientation. What do you think this means?)

H. One of these two possible closest packing arrangements is called face centered cubic packing (FCC). In Jmol, open the FCC file (IV.A.4). Adjust the atom and bond sizes. Al, Ni, Cu, and Ag are examples of elemental solids that utilize the FCC arrangement. This arrangement is also called Cubic Closest Packing or CCP. It is called a closest packing arrangement because the spheres are packed together as close as they can be. Draw this unit cell structure and describe the orientation of the spheres to each other. Manipulate the model so as to convince yourself that this cube comes out of a closest packing structure. Draw this structure. Which of the two orientations, *abab* or *abcabc*, is this?

I. Use the same procedure that you used for the SCS and BCC structures to answer the following questions.

What is the coordination number for FCC packing? _____

How many spheres are contained in the FCC unit cell? _____

Calculate the density (packing efficiency) of the FCC packing arrangement.

J. The second of the two possible closest packing arrangements is called hexagonal closest packing (HCP). In Jmol, open the HCP file (IV.A.5). Adjust the atom and bond sizes. Unlike FCC, SCS, and BCC, this arrangement does not form a cube. Co, Zn, and Cd are examples of elemental solids that utilize the HCP arrangement. Draw this unit cell structure and describe the orientation of the spheres to each other. Manipulate the model so as to convince yourself that it comes out of a closest packing structure. Which of the two orientations, *abab* or *abcabc*, is this?

K. Use the same procedure that you used for the SCS and BCC structures to answer the following questions.

What is the coordination number for HCP packing? _____

In Jmol, open the HCPuc file (IV.A.6). Use the HCPuc file to help define the unit cell. How many spheres are contained in the HCP unit cell? _____

Optional: Calculate the density (packing efficiency) of the HCP packing arrangement.

L. Although it's not obvious why different elemental metals are found in different packing arrangements, there are some that can be rationalized. How does the packing arrangement for the alkali metals, which are soft enough to be cut with a knife, explain differences with metals such as copper and silver, which are harder and cannot be cut with a knife?

M. In Jmol, open the NaCl.LM file (IV.B.1). In a separate window, open the NaCl file (IV.B.2). This lattice represents NaCl. What packing arrangement is used by the Na^+ ions? Describe the orientation of the holes that contain the Cl^- ions.

N. In Jmol, open the CsCl.LM file (IV.B.3.CsCl). In a separate window, open the CsCl file (IV.B.4.CsCl). This lattice represents CsCl. What packing arrangement is used by the Cs^+ ions? What packing arrangement is used by the Cl^- ions?

Since both Na and Cs are alkali metals, what can account for the differences in their packing structures?

O. In Jmol, open the Diamond file (IV.B.5). In a separate window, open the Graphite file (IV.B.6). Compare the atomic makeup of these two compounds. How are they similar? Compare the structures of the two compounds. Graphite is used as a dry lubricant. Diamond is used on saw blades. How do the solid crystal structures account for the different physical properties of graphite and diamond?