**CHEM 405 – Inorganic Chemistry**

**In Class Exercise – Crystal Structures**

In this exercise, you will use different size beads to explore the packing of hard spheres, as in a crystal. The exercise is set up in 4 different exercises. You will divide up into teams of two and move through the stations. Spend no more than 15 minutes on any one exercise.

In all cases, answer each question BEFORE moving on to the next. No skipping ahead!

Hints: It is easiest to get the spheres to pack tightly if you tilt the box down slightly toward one corner, especially for the flat-bottomed box. **Please be careful** not to spill the spheres/beads on the floor, or we will have a cleanup nightmare!

This exercise is modified from one written by Patrick Holland of Yale University.1

**Exercise 1 – Hexagonal Close Packed**

Using 8 mm beads of all one color (either white or gold), fill the bottom of a flat-bottomed box (purple) about ¾ full of beads. Tipping one corner of the box down slightly, gently shake the box.

1. Draw the structure formed by the beads below. Ignore any effects stemming from the edges. Draw only the regular structure formed.
2. How would you describe the pattern formed? What geometrical shape predominates in the pattern?

Find the red box that has the same pattern built into the bottom of it. Carefully add 8 mm beads to this box, so that you build a regular layer over the bottom of the box (do this starting in the center of the box, and avoid the edges). You may want to use a spatula or tweezers to help push or place the beads into place.

1. As you place beads in the box, they go into depressions in the layer below. What are the shape of these depressions? Draw a layer below, and show several beads in the next layer, including how they sit in their depressions.
2. Are all of the depressions filled with the layer of beads you are putting down? If not, what fraction of the depressions are filled?

Now, start building a second layer of beads on top of your first layer. As you build the second layer, you should note that there are voids in the structure, since spheres cannot pack perfectly. There are two types of voids formed, as shown below.



tetrahedral octahedral

1. In your supplies, you should have two triangles of 1” beads, one red, the other purple. If you align them as shown on the right, you should be able to see both kinds of holes. Identify on the picture on the right where there are tetrahedral and octahedral holes.
2. You have a variety of beads of different sizes in your supplies. Try putting different sized beads into each type of hole. What is the largest bead you can fit into each kind of hole without interfering with the lattice above?
3. What is the ratio of diameters between the largest bead you can fit and the 1” lattice? Be careful of your units here.
4. The number of other beads that one bead touches is known as the coordination number of the hole. What is the coordination number for the bead in each type of hole?

The octahedral holes correspond to a position where there is a gap in *two* adjacent layers, so you can see all the way through the structure. The tetrahedral holes are blocked, so you cannot see through them.

Go back to your structure in the red box. Carefully place a third hexagonal layer of 8 mm beads on your second layer (your third layer may only be a few spheres). You have two choices of where to put the third layer. You could put the layer on top of the tetrahedral holes. This will mean that all of the octahedral holes line up to form infinite columns of empty space in your structure. This is **hexagonal close packing** (hcp), and your 1st and 3rd layers are directly on top of one another. The repeating structure would continue with two alternating layers (ABAB…).

1. What is the coordination number of each sphere in the main lattice (not the holes)? In other words, how many other 8 mm beads does a single 8 mm bead touch? Don’t forget to count the beads in other layers.
2. The easiest repeating pattern to see in an hcp lattice is the hexagonal prism (it covers a total of three layers). How many atoms are in each layer of the hexagonal prism?
3. The actual unit cell for an hcp lattice is a rhombic prism (again, this prism covers three layers). How many atoms are in each layer of the rhombic prism?

**Exercise 2 – Cubic Close Packed (Face Centered Cubic)**

To get the hexagonal close packed lattice, you put the third layer directly above the first (ABAB…). The other option for building a third layer is to put the third layer over the octahedral holes. The fourth layer would then go over the first (ABCABC…).

This structure is known as cubic close packed. Each layer is identical to the hexagonal close packed layers, but the pattern of layers is different.

The resulting unit cell is known as face centered cubic. Seeing how the face centered cubic cell is generated from this pattern takes some work, however.

Using the red box with 8 mm beads in it, make sure the first layer of beads extends over most of the bottom of the box (but not touching the edges). Remove ONE bead from the center of the first layer. Replace that bead with an 8 mm bead of another color.



As you add layers, make sure they always align over the octahedral holes below, so that you maintain the ABCABC… structure. Add a second layer made up mostly of the original color of beads, but place beads of the second color in a triangle on top of the bead in the first layer.



Add a third layer made up mostly of the original color beads (succeeding layers will get smaller and smaller, but if your original layer was big enough, you should have room), but place six more beads of the other color in a triangle inverted above the triangle in the second layer.

Instead of adding a fourth layer, add a single bead of your second color to the center of the triangle in the third layer.

1. Very gently look at your structure from different angles. What shape is made by the 14 beads of the second color?

You can see this pattern using your triangles made up of six 1” beads. If you invert the triangles, as you did before, you can add a single 1” bead (either black or wooden) to the top and bottom. If you move this around, you should be able to see the face centered cube and how it relates to the hexagonal lattice layers.

There are interesting patterns along tilted planes in an fcc crystal: square, hexagonal (other than the horizontal one), etc. Find these in your remaining time.

When you are done, sort out the beads by color and return them to their containers.

**Exercise 3 – Primitive Cubic**

Go back to the purple flat-bottomed box. Use the 8 mm beads provided to make one layer of a cubic arrangement of beads, like that seen below.



This structure is relatively unstable, as if you shake the box slightly, it will revert to the hexagonal structure from before.

1. Which layer packs the atoms in more tightly, a hexagonal layer, or the cubic layer?

Switch to the white box with the cubic arrangement in the bottom. Build a second layer directly on top of the structure on the bottom of the box (NOT in the holes). Because this structure is less stable than the hexagonal structure, you will want to hold the box with one corner down slightly, and you will want to build all of your structures starting from that corner.

1. What is the coordination number of each atom in the lattice?
2. What is the smallest repeating (three-dimensional) structure in this lattice?
3. Draw the repeating pattern that you have created, and label the holes generated (the gaps between the beads).
4. What is the largest bead you can fit in one of these holes without disrupting the lattice layer above? What is the ratio of the diameter of the hole to the 8 mm beads making up the lattice?
5. What is the coordination number of these holes?

**Exercise 4 – Body Centered Cubic**

Empty out the white, cubic box. Using 8 mm beads, stack a layer of beads into the depressions of the box bottom. Fill the entire layer. Place a second layer of beads in the depressions of the first layer. Place the beads in carefully, so they don’t disrupt the layer below. Fill the layer, but don’t extend past the beads in the lower layer (this layer should be smaller than the bottom of the box). Build a third layer in the same manner along the edge of the box.

1. Are all the depressions in each layer filled? Draw two layers of the packing below.
2. What is the smallest repeating (three-dimensional) structure you can see in this structure?

Note that this repeating structure is not cubic. Technically, this is a tetragonal structure, because all angles are 90°, but the vertical dimension is longer than the other two, so this would be called body centered tetragonal.

1. What is the coordination number for the lattice sites in this structure?
2. Now, draw the structure you see at the edge of your structure (this should go up at an angle, as if you were building a pyramid). What shape do you see in this cut?

Interestingly, what you have done here is build a FCC cubic lattice, just held at a different angle (your first clue here is the coordination number, which matches that of the FCC and HCP lattices). If you look carefully, you should see that the hexagonal layers repeat in a ABCABC… pattern characteristic of the FCC lattice. This is not true of all body centered tetragonal lattices. It only occurs when the lattice vertical dimension is exactly .2

1. What would be required for the repeating tetragonal structure to become cubic (where a = b = c)?

Find the brown box and build several layers with 8 mm beads.

1. What kind of crystal packing do you observe? Draw at least two layers below.
2. What is the smallest repeating (three-dimensional) structure you can see in this structure?
3. What is the coordination number for the lattice sites in this structure? Be careful to only count those in direct contact.

Look between your top two layers for any holes present in the structure (NOT lattice sites that would extend the structure above, but holes in the completed lattice structure).

1. What is the coordination number of the holes you see? What shape do these holes have?
2. What is the largest bead you can fit in one of these holes, without disrupting the layer above? What is the ratio of that bead’s diameter to the 8 mm lattice beads?

When you are done, sort out the beads by size and return them to their containers.

Supplies:

1 Purple Box

1 Red Box

1 White Box

1 Brown or Yellow Box

2 1” 6-atom Triangles (1 Red, 1 Purple)

1 Tweezers

1 Spatula

Unit Cells

1 Hexagonal Close Packed

1 Face Centered Cubic

1 Primitive Cubic

1 Body Centered Cubic

Beads (Sizes are Diameters)

2 3 mm Silver

2 4 mm White

2 5 mm White

2 6 mm White

135 8 mm White or Gold

16 8 mm Colored

1 10 mm Wood

1 12 mm Wood

1 14 mm Wood

1 16 mm Wood

1 1/2” Wood

1 5/8” Wood

1 3/4” Wood

2 1” Black or Wood

**References**

1. Holland, P. Hands-On Experience with Close Packing. <https://www.ionicviper.org/class-activity/hands-experience-close-packing> (accessed April 8, 2025).

2. Dunlap, R. A., The Symmetry and Packing Fraction of The Body Centered Tetragonal Structure. *European Journal of Physics Education* **2017,** (3), 17-24.