

Report Form for Experiment 7: Solid State Structures

Note: Many of these questions will not make sense if you are not reading along in the laboratory handout! Please use the handout to help answer these questions, not just the answer sheet!

Station 1. Simple Cubic Lattice

1. How many unit cells share an atom located on a corner of the unit cell? _____
2. Based on your answer to the previous question, what fraction of a corner atom lies within each individual unit cell? _____
3. How many nearest neighbors does each atom have in a unit cell (we call this the atom's coordination number)? _____
4. How many total atoms make up one unit cell (consider only the fraction of each atom completely inside this particular unit cell)? _____
5. What kind of hole occupies the center of the simple cubic lattice? _____
6. How many of this type of hole are in a unit cell? _____
7. Express the length of the unit cell, a , in terms of the radius of an atom, r . Give your answer in the form of an equation, such as $a = 1.5 \times r$. You may assume that the atoms in the unit cell touch each other. Show your work!

Station 2. Face-Centered Cubic Lattice

1. How many atoms are in this unit cell (count only the fraction of each atom contributing to the unit cell)? _____
2. How many complete (totally within the unit cell) octahedral holes are in this unit cell? _____
3. How many complete tetrahedral holes are in this unit cell? _____
If you are having trouble seeing the tetrahedral holes, take a look at the unit cell for fluorite on the computer (Station 8) which has cations in these holes.
4. How many octahedral holes are partially contained (shared with other unit cells) in this unit cell? _____
5. Express the length of the unit cell, a , in terms of the radius of an atom, r . Give your answer in the form of an equation, such as $a = 1.5 \times r$. Show your work!
6. Consider the simple cubic unit cell and the fcc unit cell. Assuming that the anions in each are of the same size, which unit cell's holes can best accommodate a larger cation?

Station 3. Body-Centered Cubic

1. Along what line in the bcc lattice do you find spheres touching each other? _____
2. What is the coordination number of each sphere in the unit cell? _____
3. What is the length of the body diagonal in terms of r ? _____
4. Express the length of the unit cell, a , in terms of the radius of an atom, r . Give your answer in the form of an equation, such as $a = 1.5 \times r$.? Show your work!
5. What is the ratio of corner spheres to center spheres in the unit cell? Be sure to consider only the fraction of each atom in the unit cell.
6. What kind(s) of holes are in this unit cell, including partial holes shared with other unit cells, and how many complete holes are there?

Station 4. Closest Packed

1. Using the available pennies and box, arrange a single layer of pennies using the simple cubic unit cell. How many pennies did you fit in the box? _____
2. Using the available pennies and box, arrange a single layer of pennies using a closest packing arrangement of pennies. How many pennies did you fit in the box? _____
3. Using the diagram from the lab handout, what is the area of the two-dimensional cross-section through the simple cubic unit cell? What percentage of this area is empty? Show your work!
4. Using the diagram from the lab handout, what is the area of the two-dimensional cross-section through the closest packed unit cell? What percentage of this area is empty? Show your work!
5. What is the packing pattern for hexagonal closest packing? _____
6. What is the packing pattern for cubic closest packing? _____
7. Are any of the structures from the first three stations examples of closest packing? If so, which one(s)? _____

Station 5. NaCl

1. What type of lattice do the Na^+ ions form? _____
2. What is the coordination number for the Na^+ ions? _____
3. What is the coordination number for the Cl^- ions? _____
4. In what types of holes do you find the Cl^- ions? _____
5. What percentage of these holes are occupied by Cl^- ions? _____
6. Verify by counting atoms and partial atoms that the number of Na^+ ions is the same as the number of Cl^- ions. Show your work!

Station 6. CsCl

1. What type of lattice do the Cl^- ions form? _____
2. In what kind of holes are the Cs^+ ions located? _____
3. What is the coordination number for Cs^+ ? _____
4. What is the coordination number for Cl^- ? _____
5. Verify by counting atoms and partial atoms that the number of Cs^+ ions is the same as the number of Cl^- ions. Show your work!

Station 7. Zinc Blende Structure

1. What type of lattice do the S^{2-} ions form? _____
2. In what type of holes are the Zn^{2+} ions located? It may help to examine the computer model for zinc blend that shows only two layers of Zn^{2+} and S^{2-} ions. _____
3. What percentage of these holes contain a Zn^{2+} ion? _____
4. Verify by counting atoms and partial atoms that the number of Zn^{2+} ions is the same as the number of S^{2-} ions. Show your work!

Station 8. Fluorite Structure

1. What type of lattice do the Ca^{2+} ions form? _____
2. In what type of holes are the F^- ions found? _____
3. What percentage of these holes are occupied by a F^- ion? _____
4. How many total Ca^{2+} ions and F^- ions are in the unit cell? Does your answer make sense. Show your work and explain your reasoning!
5. What kind of forces hold the fluorite structure together (be sure to give more than just listing the type of bonding)?

Station 9. Wurtzite Structure

1. What type of lattice do the S^{2-} ions form? _____
2. In what type of holes are the S^{2-} ions located? _____

Station 10. Rutile Structure

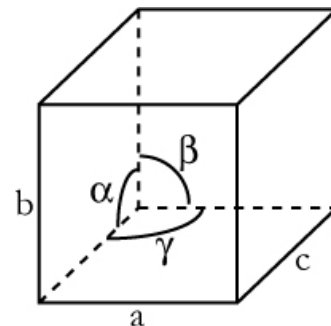
1. How many titanium atoms and how many oxygen atoms are in the unit cell. What does this suggest about the simplest chemical formula for rutile? Show your work and explain your reasoning.
2. Given your answer to the previous question, what is the oxidation state for titanium?
3. What is titanium's coordination number? _____
4. What is oxygen's coordination number? _____

Station 11. Diamond

1. The computer model of diamond's unit structure suggests that some carbon atoms make up the lattice and some carbon atoms occupy holes within the lattice. What type of lattice makes up the unit cell?
2. In what type of holes are the other carbon atoms located? _____
3. What percent of these holes are occupied? _____
4. What forces hold this solid together (try to go beyond just the type of bonding, though you can mention that!)

Station 12. Calcite Structure

1. The unit cell for calcite is quite different from those you have considered thus far. Using the diagram to the right as a guide, are the three sides of equal length? If not, which side(s) are longer?
2. Examine the angles α , β , and γ in the unit cell for calcite and describe each as $> 90^\circ$, $< 90^\circ$, or equal to 90° .
3. What forces hold this solid together (be as specific as possible about different parts of the solid!)?



Station 13. Bonus: There are several samples of real minerals that correspond to structures for which you've looked at the unit cell: sodium chloride, fluorite, and calcite. By just looking at the samples, try to match them with the appropriate mineral samples. Describe each sample and say which mineral it is matched with. Provide your reasoning!

Supplement to Lab 6: Solid State Synthesis of Spinel

Solid State Structure Visualization

You and your partner will be provided with two types of structural files (based on real X-ray crystallography data!) for each of the four compounds. The *.cif files are the raw crystallographic information files and the “pretty” *.cmdf files are files to bring directly into the CrystalMaker program.

To investigate the unit cell parameters, open the *.cif file as a text file using the TextEdit program on the Mac (use files I have sent you via email). Click the file and select “Open with” from the file menu, and select TextEdit to open the file. If you scroll past the initial information at the top of the page, you will eventually come to the unit cell parameters. These will have labels like a, b, and c for the side lengths and α , β , and γ . Use those cell parameters to answer the appropriate question on the lab handout.

- Examine the unit cell parameters. These represent the size of the “box” for these structures. Are the box size variations consistent with size differences for these ions. Why or why not?

To answer the questions about the coordination number (nearest neighbors) of the ions in the CoAl_2O_4 and ZnCr_2O_4 structures, open the *.cmdf file from within the File Menu in CrystalMaker. Focus on atoms near the center of the structure since these are significantly more complicated structures and it can be hard to see how many neighbors the atoms on the edge of the unit cell have.

- Examine the different ions in the structure. How many other ions are bound to each type of ion, i.e. give coordination number for each ion in structure?