MODELING IONIC LATTICES

Introduction

The study of ionic lattices falls within the realm of inorganic chemistry. Much research is currently devoted to the areas of materials science and crystal engineering. In this lab you will become familiar with the most common ionic lattices. You will be required to build small-scale models and sketch a structure of each lattice. The structures to be studied are discussed in the following sections.

1. The Cesium Chloride Structure

The cesium chloride structure is the only structure discussed here that is not a close-packed structure. In the cesium chloride structure, the cesium atoms form a simple cubic and the chloride ions occupy the cubic holes (the hole at the center of a simple cubic). Models of the cesium chloride structure showing one and eight unit cells are shown in Figure 1. What is the coordination number of each ion in this structure?

2. The Halite Structure

Halite is the mineral name for sodium chloride. The halite structure is based on the face-centered cubic lattice. In this structure the chloride ions form a face-centered cubic and the sodium ions occupy all of he octahedral holes. Models of this structure are shown in Figure 2. What is the coordination number of each ion in this structure?

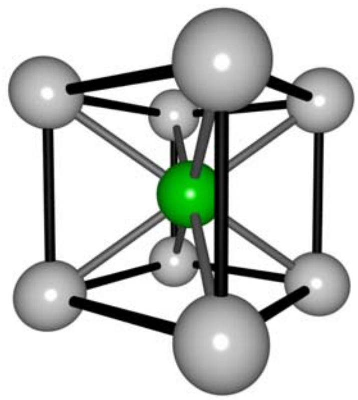
3. The Fluorite Structure

Fluorite is the mineral name for calcium fluoride. The fluorite srtucture, like the halite structure, is based on a face-centered cube. In this structure, the calcium ions form a face-centered cubic and the fluoride ions occupy all of the tetrahedral holes. Models of the fluorite structure showing one unit cell and eight unit cells are shown in Figure 3. Can you tell which represents calcium and which represents fluorine? What is the coordination number of each ion in this structure?

4. The Diamond Structure

There are two ways to visualize the diamond structure. First, diamond may be visualized as a face-centered cubic lattice with additional atoms in half of the tetrahedral holes. The two models of the diamond structure shown in Figure 4 are drawn from this perspective. The green cylinders show the outlines of the face-centered cell but cannot be cannot be represented with the current model set.

Figure 1. *Two models of the cesium chloride structure showing one unit cell (left) and eight unit cells (right). The black bonds outlining the cell cannot be represented with the model kits.*



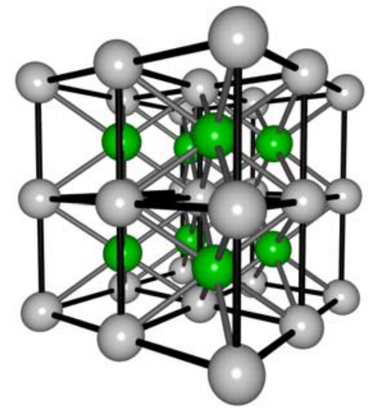


Figure 2. *A model of the halite structure.*

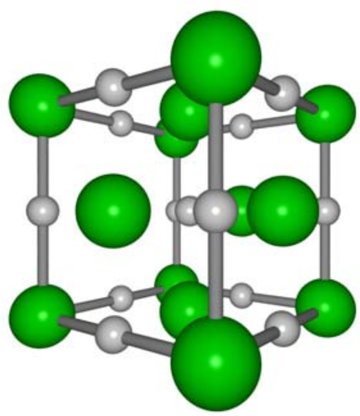
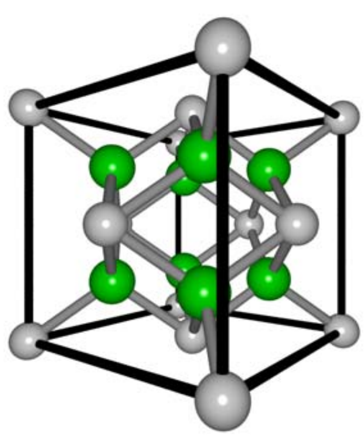


Figure 3. *Models showing one unit cell (left) and eight unit cells (right) of the fluorite structure. The black bonds outlining the cell cannot be represented with the model kits.*



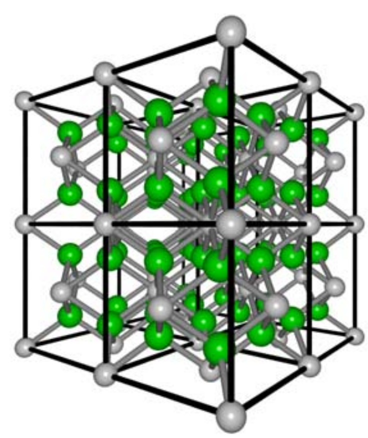
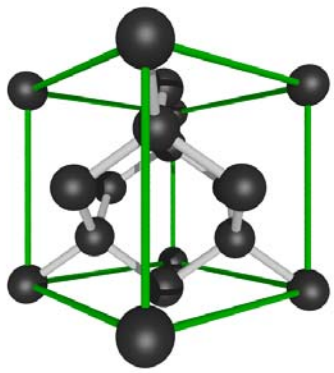
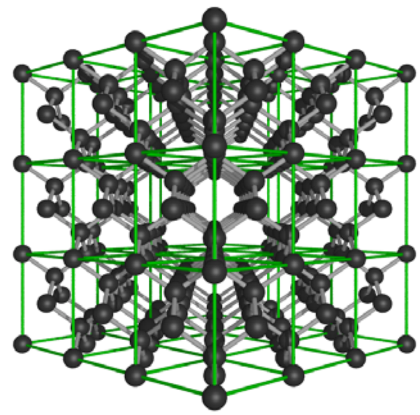


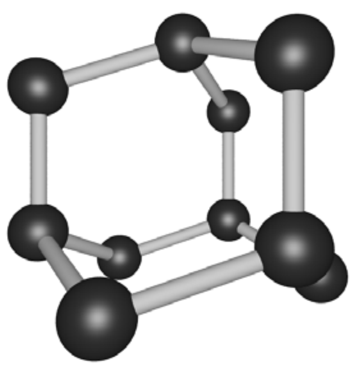
***Figure 4**. Two models of the diamond structure from the cubic perspective. The green bonds show the outline of the cell and cannot be represented with the models.*

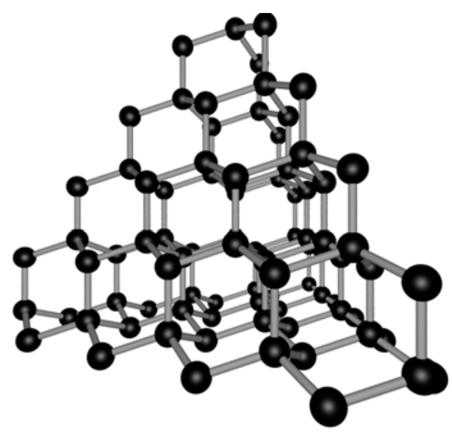




A second way of representing the diamond structure is shown in Figure 5. Shown on the left is a small piece of this structure. This is the same carbon skeleton as found in the hydrocarbon adamantane and consists of a six-membered ring “capped’ by the center atom above. Repetition of this carbon skeleton gives the larger model shown on the right.. When represented this way the diamond structure easier to compare to the lonsdaleite structure, which is discussed below. Just remember that there is only one diamond structure; ultimately these two ways of representing diamond are equivalent.

***Figure 5**. On the left, a model of the carbon cage from which the diamond structure can be constructed. On the right is a larger-scale model. Both the small-scale and large-scale models have tetrahedral symmetry owing to the tetrahedral geometry of the carbon atoms from which they were constructed.*

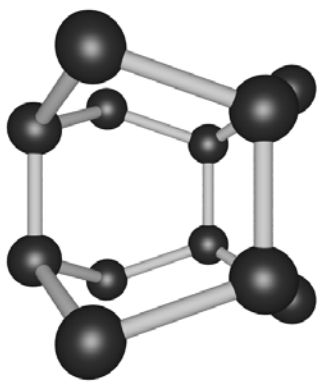


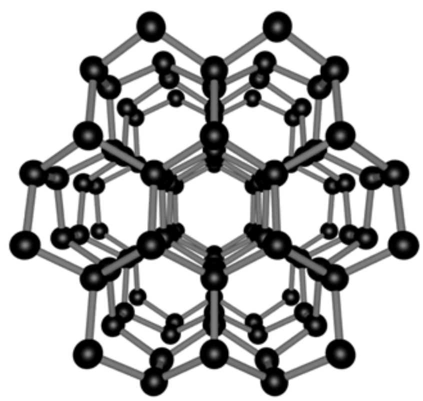


The Lonsdaleite Structure

Lonsdaleite is the hexagonal form of diamond; there is no way to visualize this structure as a cubic. Shown below are models of the lonsdaleite structure. On the left is the basic carbon skeleton of this structure. It is similar to the carbon skeleton of the diamond lattice in that it contains a six-membered ring. However, it is different that this ring is connected not to a "cap" atom but to a second six-membered ring. Repetition of this basic carbon cage gives a srtucture in which alternating layers of rings are equivalent, which can be described as hexagonal.

Figure 6. Models of the lonsdaleite structure. *On the left; a model of the basic carbon cage that serves as the building block of the lonsdaleite structure (as seen from the side). On the right, a larger model as seen from the top.*





Lattices Related to Diamond and Lonsdaleite

There are many structures related to diamond and lonsdaleite. For example, silicon lies in the same group as carbon and can substitute for carbon on the above structures. Two forms of silicon carbide are known, one analogous to diamond and the other analogous to lonsdaleite. In either structure, each carbon atom is connected to four silicon atoms and each silicon atom is connected to four carbon atoms.

The structures of sphalerite and wurtzite are completely analogous to the structures of diamond and lonsdaleite. Although diamond and lonsdaleite are network covalent solids and sphalerite and wurtzite are ionic solids, the physical arrangement and connectivity of the atoms are identical. By building the diamond and lonsdaleite models with alternating atoms, these models can also double for the sphalerite and wurtzite structures.

Figure 7. *Models of the diamond structure in which alternating carbon atoms have been replaced. This model could represent the cubic form of SiC or the cubic form of ZnS (sphalerite).*

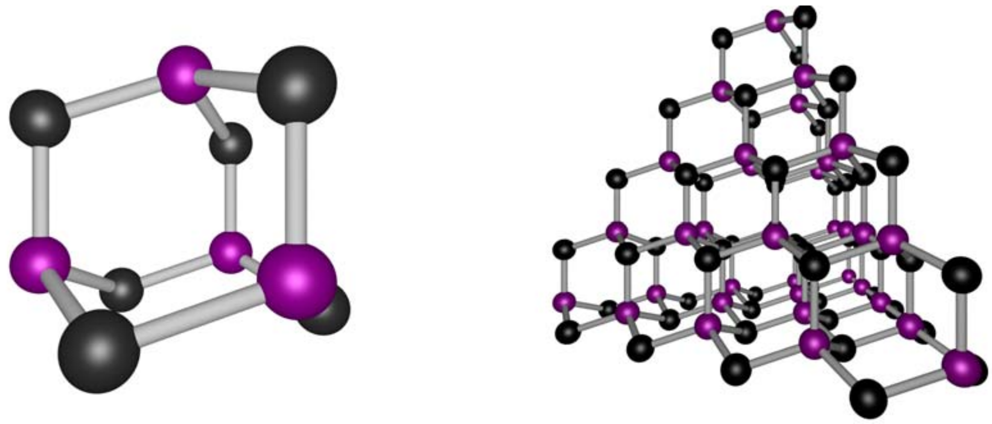
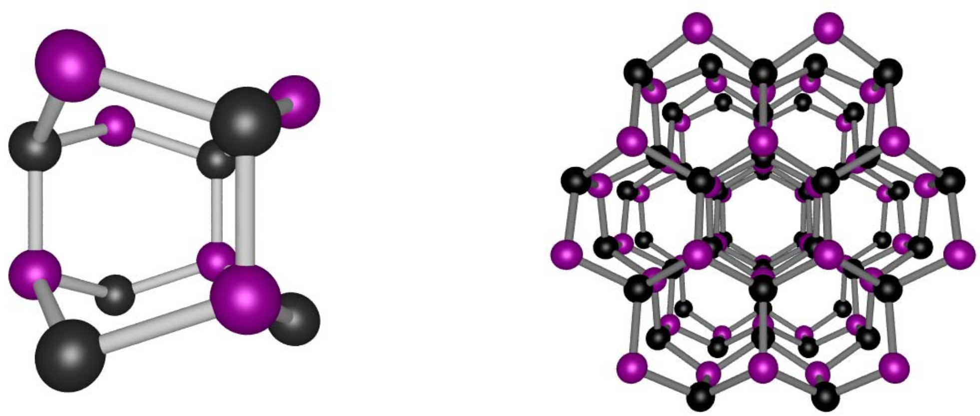


Figure 8. *Models of the lonsdaleite structure in which alternating carbon atoms have been replaced. This model could represent the hexagonal form of SiC or the cubic form of ZnS (wurtzite).*



The Experiment

In this experiment you will build small-scale models of the ionic lattices previously discussed. Atom centers with four, six, and eight prongs will be available as shown in Figure 9. You must decide which atoms centered to use for each structure. Two things should provide clues as to which atoms centers to use. The first of these is *coordination number*. The coordination numbers of the various structures should provide a clue as to which atoms centers to use. For example, structures which have a coordination number of 4:4 should be built with atom centers which both have four prongs. A second clue is *atom color*. Atom color should provide an additional guide; metal atoms are usually black or silver, carbon atoms are usually black, and chlorine atoms are usually green.

As you proceed you must make a sketch of each structure; do not go onto the next structure until your instructor has checked off the sketch and model.

Figure 9. *Atom centers with four, six, and eight prongs will be available*.

Eight-prong (silver and green)	Six-prong (black and green)	Four-prong (black and violet)

Ionic Lattices **Pre-Laboratory Exercise**	**Name:**

1. The model kits you will use will have four-prong, six-prong, and eight-prong atom centers. The coordination numbers of the various lattices will tell you which atom centers to use. Consult your textbook, and list the coordination number of each of the following ionic lattices.

a. Halite, NaCl

b. Fluorite, CaF_2

c. Sphalerite, ZnS

d. Wurtzite, ZnS

e. Cesium Chloride, CsCl

2. Why are two coordination numbers (4:4, 6:6, etc….) listed for ionic compounds? What does each number represent?

3. There are two forms of ZnS, sphalerite and wurtzite. What is the difference between these two forms?

Ionic Lattices **Report Page 1**	**Name:**

Sketch	**Instructor Initials**
Halite, NaCl	
Cesium Chloride, CsCl	
Fluorite, CaF_2	

Ionic Lattices **Report Page 2**	**Name:**

Sketch	**Instructor Initials**
Diamond / Sphalerite (refer to Figure *7 as a guide*)	
Lonsdaleite / Wurtzite (refer to Figure 8 as a guide)	