1 Cognitive reasoning in the chemical sciences 5.8

1. **Crystals** are solids which repeat the same motif, the *unit cell*, over and over again (think of a brick wall: the bricks are the unit cell, the wall is the solid.) Crystal skills required in freshman chemistry are primarily:

   (a) Identifying the number of atoms in the unit cell.
   (b) Based on the unit cell, deducing the density of the solid and vice-a-versa.
   (c) Identifying the volume of space occupied by the atoms in the unit cell.

I am a crystallographer. I feel keenly the need to profess two more skills:

   (a) Master the skill of making a orthographic projections indicating exactly where all the atoms in the unit cell are located.
   (b) Identify the number of bonds an atom makes based on this diagram.

2. The figures below show the unit cells of Fe and Cu. A perspective drawing, a space filling ball model, and the scientific orthographic projection are shown for both of the two structures.

(a) How many atoms are there in each of the two unit cells?
(b) How many bonds does each Fe atom make in its structure?
(c) How many bonds does each Cu atom make in its structure?
(d) Which of these structures is face-centered-cubic, i.e., there is an atom in the center of each square face of the cube?
(e) Which of these structures is body-centered-cubic, i.e., there is an atom in the center of the body of the cube?
(f) What % volume of the unit cell is occupied by the Fe atoms?
(g) What % volume of the unit cell is occupied by the Cu atoms?

3. **Diamond and NaCl**

(a) Shown below are perspective drawings of NaCl and diamond. Please draw orthographic projections for the two structures.

(b) How many atoms are there in each of the two cells?
(c) How many bonds does each carbon atom make?
(d) How many bonds does each Na atom make?
(e) How many bonds does each Cl atom make?
(f) What % volume of the unit cell is occupied by the carbon atoms?

4. **Connecting crystals to macroscopic density**

(a) The density of iron is 7.9 g/mL. Fe is body-centered-cubic. What is the Fe-Fe bond length?
(b) The density of iron is 7.9 g/mL. Iron atoms can be thought of as spheres. In iron these spheres occupy 68% of space, with the remaining 32% of space being taken up by the crevasses between atoms. What is the radius of a single Fe atom, measured in Å?
(c) Gold bond lengths are 3.00 Å. Au crystallizes in the face-centered cubic structure. What is gold’s density in g/mL?