

Today: solids of all kinds

November 22nd

Sunday: Problem club w/ Kendall

Monday: (11/25) class does NOT meet

Next week: continue to get ready for final exam 12/10/19

↳ checklist for CK5

↳ * see items 17 + 22 in syllabus

↳ * Dr. Mattson is in his office Monday & Tuesday

Solids

* all ionics are solids

* metals are (usually) solids

* covalent molecular

5 } (I₂)

2 } H₂O

3 } NH₃

IMF

(inter-molecular forces)

* graphite

* network covalents

↳ ex: graphite

↳ ex: diamond (sp³)

↳ 3D network of covalent bonds

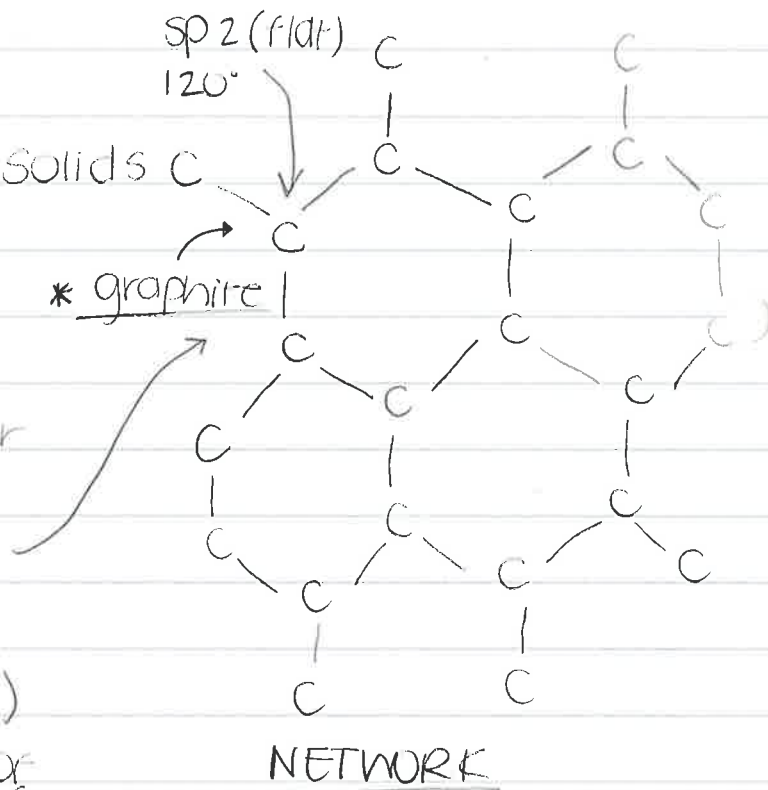
↳ ex: silicon carbide (SiC)

↳ diamond structure

→ carbon dioxide covalent, gas

→ silicon dioxide (sand) network covalent

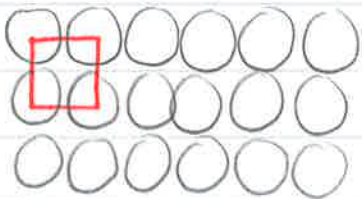
sp² (flat)
120°



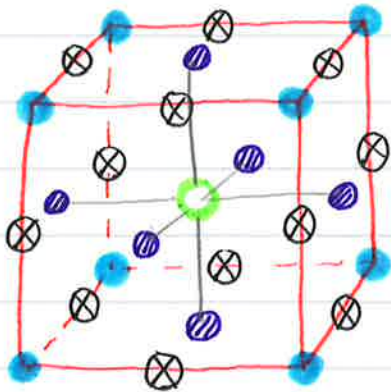
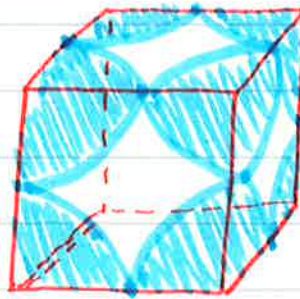
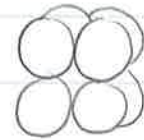
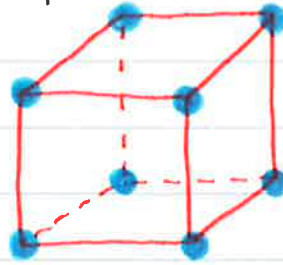
Metals

November 22nd

unit cells — simplest repeating pattern



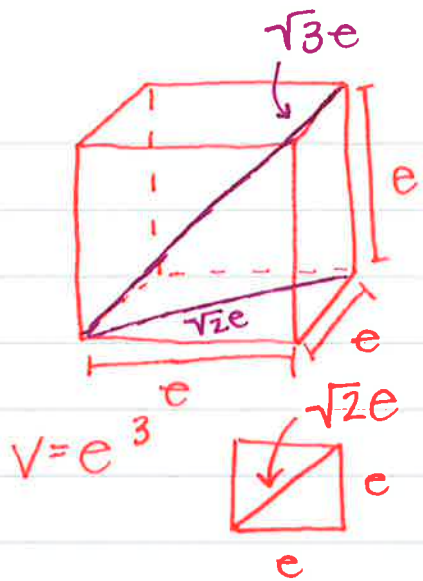
Simple cube unit cell.



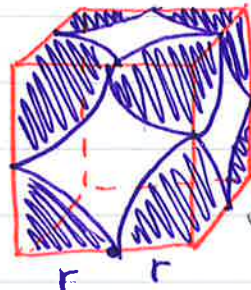
Position names within a cube.

- = corners, 8, each is $\frac{1}{8}$ inside the cube
- = body centered position, one per cube
- (hatched) = face-centered positions, 6, each $\frac{1}{2}$ inside the cube
- ⊗ = edge-centered positions, 12, each $\frac{1}{4}$ inside (small ions use these)

November 22nd



Simple cube:



unit cell has ONLY one atom per unit cell!

$$8 * \frac{1}{8} = 1$$

$$e = 2r$$

$$d = \frac{m}{V}$$

$$e \rightarrow V = \frac{m}{d} \rightarrow e \rightarrow r$$

1 atom/unit cell
 $e = 2r$

Polonium exists as a simple cubic unit cell with density = 9.4 g/cm^3 . Calculate the atomic radius of Po.

$$V = \frac{m}{d} = \frac{1 \text{ Po atom} / 209 \text{ g}}{1 \text{ mol} / 6.02 \times 10^{23} \text{ atoms}} \cdot \frac{1 \text{ cm}^3}{9.4 \text{ g}} = 3.7 \times 10^{-23} \text{ cm}^3$$

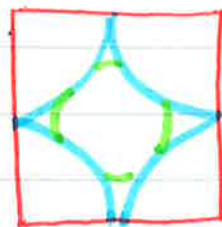
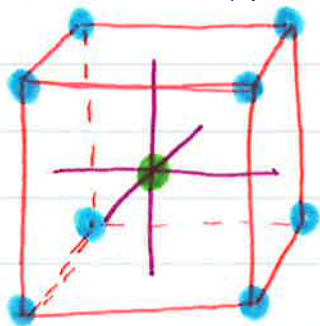
$$e = 3.3 \times 10^{-8} \text{ cm}$$

$$r = 1.7 \times 10^{-8} \text{ cm} \rightarrow 170 \text{ pm}$$

Body centered unit cell \rightarrow (2 atoms/unit cell)

* atoms at all 8 corners ($8 * \frac{1}{8} = 1 \text{ atom}$)

* one atom at body-centered position



* atoms contact along unit cell diagonal

$$4r = \sqrt{3}e$$

$$d \rightarrow V \rightarrow e \rightarrow r$$

Tungsten forms bcc unit cells with $e = 317$ pm, NOVEMBER 22nd
 What is the density & atomic radius
 of tungsten?

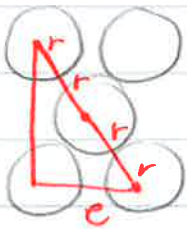
$$d = \frac{m}{V} = \frac{2 \overset{\text{Tungsten}}{\text{atoms}} | 183.8 \text{ g} | 1 \text{ mol}}{\text{mol} | 6.02 \times 10^{23} \text{ atoms} | 3.19 \times 10^{-23} \text{ cm}^3} = \boxed{19.14 \text{ g/cm}^3}$$

$$e = 317 \text{ pm} \rightarrow 3.17 \times 10^{-8} \text{ cm}$$

$$V = (3.17 \times 10^{-8} \text{ cm})^3 = 3.19 \times 10^{-23} \text{ cm}^3$$

face-centered cubic (fcc) \rightarrow 4 atoms/unit cell
 (packed as closely as possible)
 atoms at all 8 corners (\Rightarrow 1 atom)
 + atoms at all 6 face-centers ($6 * \frac{1}{2} = 3$)

*one face



$$\boxed{4r = \sqrt{2}e}$$

Aluminum exists with a face centered cubic unit cell and a density of 2.699 g/cm^3 .
 What is the atomic radius of Al?

$V = \frac{m}{d}$
 $d \rightarrow V \rightarrow e \rightarrow r$

$$V = \frac{4 \text{ Al atoms} | 26.9 \text{ g} | 1 \text{ mol}}{1 \text{ mol} | 6.02 \times 10^{23} \text{ atoms} | 2.699 \text{ g}} = 6.62 \times 10^{-23} \text{ cm}^3$$

$$V = e^3 \rightarrow e = 4 \times 10^{-8}$$

$$\hookrightarrow 4r = \sqrt{2}e$$

$$\hookrightarrow r = \frac{\sqrt{2}(4 \times 10^{-8})}{4} \rightarrow r = 1.4 \times 10^{-8} \text{ cm}$$

140 pm

Chapter 11-12 Day 3 (Sections 12.1, 12.3)

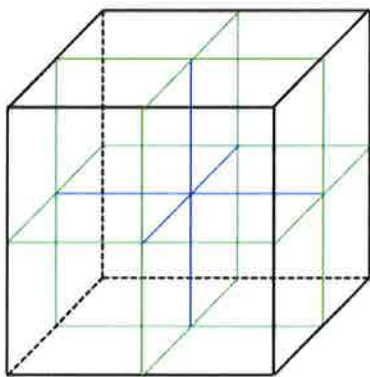
22 November 2019

Now we extend what we've learned about metal atom locations within various unit cells to include ionic substances. Most ionic substances with simple one-atom ions use the same sort of unit cells. (Ionic compounds that contain polyatomic ions, can be considerably more complicated.) The larger ion, usually the anion, can occupy the same locations as the metal atoms did in the previous worksheet. The smaller ions, usually the cations, will occupy specific holes created by the bigger ions.

1a. Write the letter **C** on each corner position in the unit cell below. How many corner positions are there?

_____ What fraction of each corner position is located within each unit cell? _____

It is common that there are ions located at the corner positions in an ionic unit cell lattice – but not necessary! An ionic substance may not have any ions at the corner positions. Nevertheless, the position still has a name, corner, even if there are no ions present.



1b. Write the letter **B** on the body-centered position in the unit cell above. How many body-centered positions are there? ? _____

1c. Write the letter **F** on the face-centered position in the unit cell above. How many face-centered positions are there? _____ What fraction of each face-centered position is located within each unit cell? _____

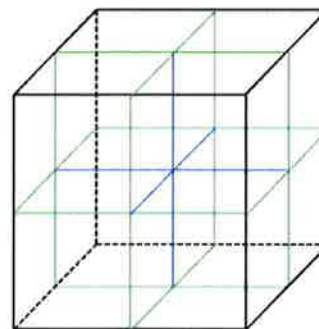
I used letters in this question so you don't automatically think there is an ion present there. There may well be. Knowing the names of the positions within a unit cell is useful when discussing ionic compounds. This is not a problem when discussing metals like we did on the previous worksheet.

1d. Ionic compounds need for us to know about three more positions. We can draw the first one on the unit cell above. That position, is midway along each of the 12 edges in the unit cell. Write the letter **E** at each of the 12 edge-centered positions in the unit cell pictured above. There are 12 edge-centered positions. What fraction of each edge-centered position is located within each unit cell? _____

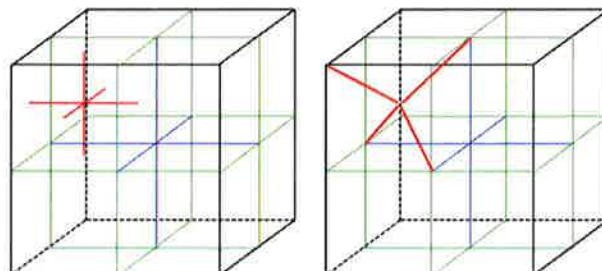
2a. For many simple ionic compounds, the large ion takes one of the familiar positions described earlier, simple cubic, body-centered cubic or face-centered cubic. The simple cube is commonly encountered in ionic compounds. Specifically, one states that the large ions form a **simple cube sublattice**. Don't worry about the sub part. The smaller ions are then located at the center of the large hole (called a cubic hole) created by big ions at the eight corners. At what position (location name) within the unit cell are the small ions located?

2b. If an ionic compound exists with the anions in a simple cubic sublattice and the cations at the body-centered position, what is the formula of the ionic substance? For example, An_2Cat_3 . Answer: _____

3. Face-centered ionic lattices have their own set of very important holes the **octahedral** or **tetrahedral** holes. *Again, this is only for the fcc unit cell.* Octahedral holes in the fcc sublattice are located at all of the edge-centered positions as well as the body-centered position. How many net octahedral holes are present in each unit cell? _____ Locate the octahedral holes in this unit cell sketch and mark the with an **O**.



4. Face-centered sublattices of large ions also feature **tetrahedral holes**, as shown in these diagrams. The figure on the left shows just one tetrahedral hole in a fcc unit cell. The figure on the right shows why they are called tetrahedral holes: A tiny ion located in a tetrahedral hole has four near neighbors ions of opposite charge. The four include three from face-centered positions and one corner position.



How many tetrahedral holes are present in each unit cell?