Chem 1515.001 - 006
Problem Set #4
Spring 2002

Name_____

TA's Name _____

Sec _____

ALL work must be shown to receive full credit. **Due in lecture at 8:30 a.m. on Friday, February 14, 2002.**

PS4.1. Indicate the type of crystal (molecular, metallic, extended covalent, or ionic) each of the following would form upon solidification:

a) CS_2 ; **molecular**

b) $C_{(diamond)}$; **extended covalent**

c) Si ; **extended covalent**

d) Na_2SO_4 ; **ionic**

e) Fe ; **metallic**

f) Br_2 ; **molecular**

g) CsCl ; **ionic**

h) H_2O_2 ; **molecular**

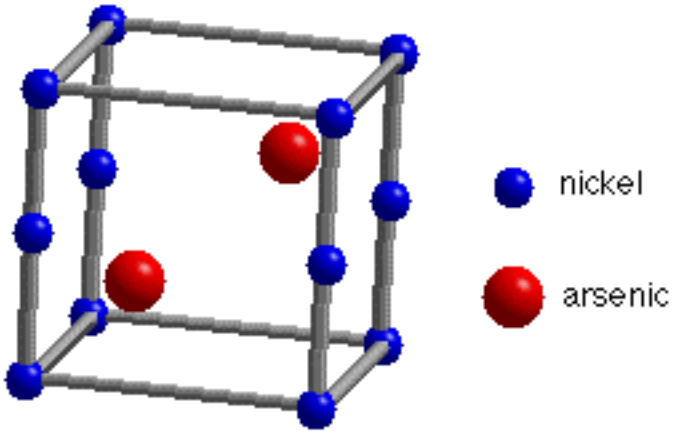
i) HCN ; **molecular**

j) Pb ; **metallic**

k) SF_6 ; **molecular**

l) $CaCO_3$. **ionic**

PS4.2. A cell of nickel arsenide is shown below. If this cell contains the unit cell for this compound, determine the correct formula for nickel arsenide. (NOTE: The arsenic atoms are completely inside the unit cell.)



There is 1 nickel atom per unit cell as a result of the $\frac{1}{8}$ contributions from each of the eight corner nickel atoms. There is one nickel atom per unit cell as a result of the $\frac{1}{4}$ contributions from each of the four edge-centered nickel atoms. The 2 atoms of arsenic are completely contained within the unit cell. Formula is NiAs. There are two formul units of NiAs per unit cell.

PS4.3. Perovskite is a mineral containing calcium, titanium and oxygen. Two different cells are shown below. Support or refute whether or not the two structures contain the same number of atoms?

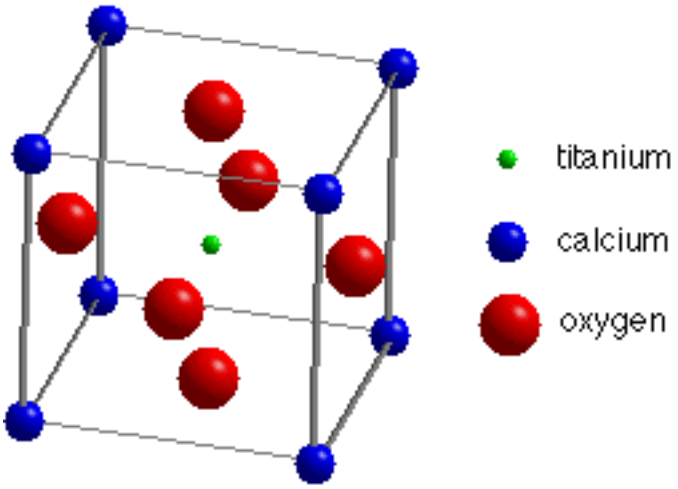


Figure I.

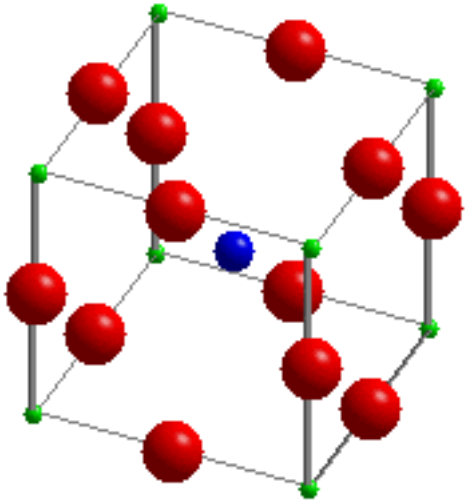


Figure II.

Explanation:

The cell in Figure I. has; one titanium atom located in the center of the cubic cell; one calcium atom from the eight $\frac{1}{8}$ contributions from each of the eight corner atoms. three oxygen atoms from the six $\frac{1}{2}$ contributions from each of the six face centered atoms. $CaTiO_3$	**The cell in Figure II. has; one titanium atom from the eight $\frac{1}{8}$ contributions from each of the eight corner atoms. one calcium atom located in the center of the cubic cell; three oxygen atoms from the twelve $\frac{1}{4}$ contributions from each of the six face centered atoms. $CaTiO_3$**

PS4.4. A particular solid has a structure in which W atoms are located at cube corners, O atoms at the centers of the cube edges, and Na atoms at cube centers. The cube edge is 3.86 Å.

a) What is the formula of this material? (Show some work.)

one tungsten atom from the eight $\frac{1}{8}$ contributions from each of the eight corner atoms.
one sodium atom located in the center of the cubic cell;
three oxygen atoms from the twelve $\frac{1}{4}$ contributions from each of the six face centered atoms.

$$\mathbf{NaWO_3}$$

b) What is its theoretical density?

$$\text{density} = \frac{\text{mass in the unit cell}}{\text{volume of the unit cell}}$$

$$= \frac{\frac{1 \text{ formula unit of } NaWO_3}{\text{unit cell}} \cdot \frac{1 \text{ mol}}{6.023 \times 10^{23} \text{ formula units}} \cdot 255 \frac{\text{g } NaWO_3}{1 \text{ mol}}}{(3.86 \times 10^{-8} \text{ cm})^3}$$

$$= \frac{4.23 \times 10^{-22} \text{ g}}{5.75 \times 10^{-23} \text{ cm}^3} = 7.36 \frac{\text{g}}{\text{cm}^3}$$

PS4.5. Iridium metal crystallizes in a body-centered cubic unit cell. The atomic radius of an iridium atom is 1.33×10^{-10} m. Calculate the density of iridium.

Body centered cubic unit cell has 2 atoms of iridium per unit cell.

The mass of the unit cell is;

$$\text{2 Ir atoms}\left(\frac{\text{1 mol}}{6.023 \times 10^{23}\ \text{atoms}}\right)\left(\frac{192\ \text{g}}{\text{1 mol}}\right) = 6.38 \times 10^{-22}\ \text{g}$$

The volume of the unit cell is;

$$\text{edge length (l)} = \frac{4r}{\sqrt{3}} = \frac{4 \cdot 1.33 \times 10^{-8}\ \text{cm}}{\sqrt{3}} = 3.07 \times 10^{-8}\ \text{cm}$$

$$\text{Volume} = (3.07 \times 10^{-8}\ \text{cm})^3 = 2.90 \times 10^{-23}\ \text{cm}^3$$

$$\text{Density} = \left(\frac{\text{mass}}{\text{volume}}\right) = \left(\frac{6.38 \times 10^{-22}\ \text{g}}{2.90 \times 10^{-23}\ \text{cm}^3}\right) = 22.0\ \frac{\text{g}}{\text{cm}^3}$$

PS4.6. Chromium metal crystallizes in a face-centered cubic unit cell. The density of chromium is $7.19\ \frac{\text{g}}{\text{cm}^3}$. Calculate the edge length of the unit cell and the atomic radius of chromium.

Face centered cubic unit cell has 4 atoms of chromium per unit cell.

The mass of the unit cell is;

$$\text{4 Cr atoms}\left(\frac{\text{1 mol}}{6.023 \times 10^{23}\ \text{atoms}}\right)\left(\frac{52\ \text{g}}{\text{1 mol}}\right) = 3.45 \times 10^{-22}\ \text{g}$$

The volume of the unit cell is;

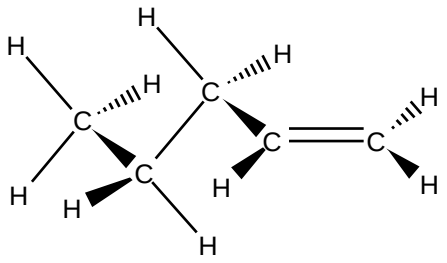
$$3.45 \times 10^{-22}\ \text{g}\left(\frac{1\ \text{cm}^3}{7.19\ \text{g}}\right) = 4.80 \times 10^{-23}\ \text{cm}^3$$

$$\text{edge length} = \sqrt[3]{4.80 \times 10^{-23}\ \text{cm}^3} = 3.64 \times 10^{-8}\ \text{cm}$$

$$r = \frac{\text{edge length (l)}}{2\sqrt{2}\cdot} = \frac{3.64 \times 10^{-8}\ \text{cm}}{2\sqrt{2}\cdot} = 1.29 \times 10^{-8}\ \text{cm}$$

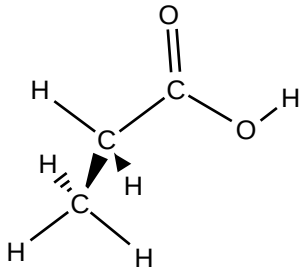
PS4.7. Draw the Lewis structure and name the following compounds;

a) $CH_3CH_2CH_2CHCH_2$



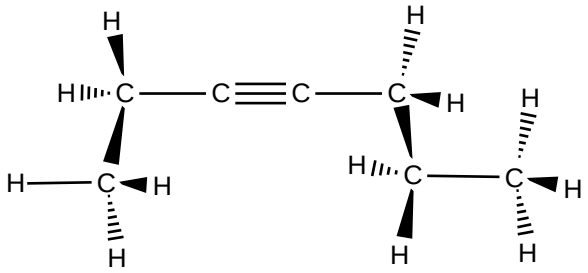
1-pentene

b) CH_3CH_2COOH



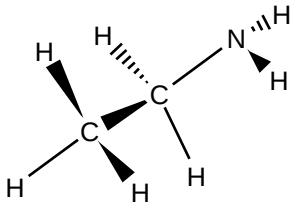
propionic acid

c) $CH_3CH_2CCCH_2CH_2CH_3$



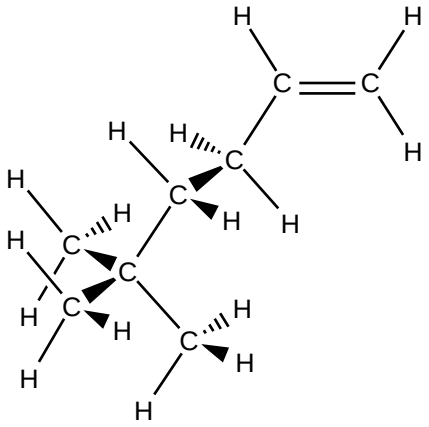
3-heptyne

d) $CH_3CH_2NH_2$



ethylamine

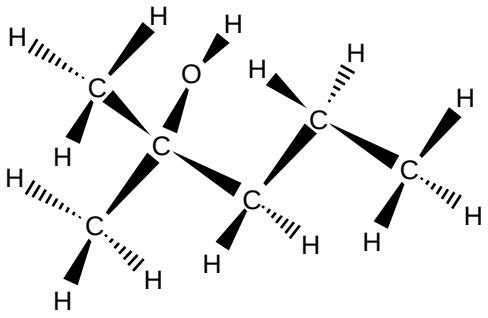
e) $CH_3C(CH_3)_2CH_2CH_2CHCH_2$



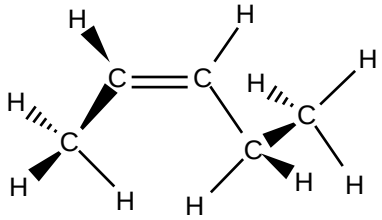
5,5-dimethyl-1-hexene

PS4.8. Draw the structure which corresponds with each of the following names.

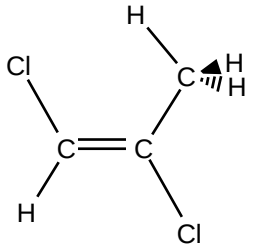
a) 2-methyl-2-pentanol



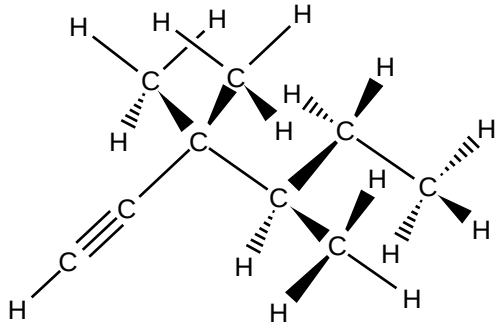
b) cis-2-pentene



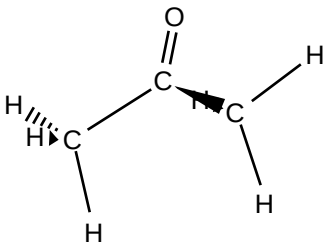
c) trans-1,2-dichloropropene



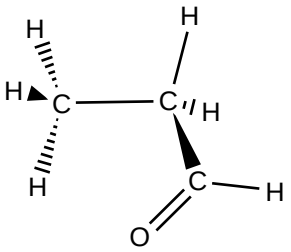
d) 3,3,4-trimethyl-1-hexyne



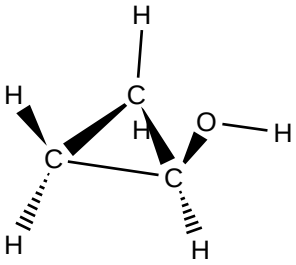
PS4.9. Draw the structural formula (Lewis structure) for five compounds with the formula C_3H_6O. Identify the name of each oxygen containing functional group used in each formula. Be sure you have at least three different functional groups in your five compounds.



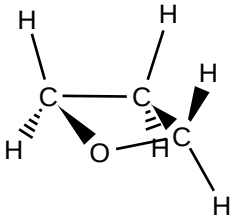
ketone



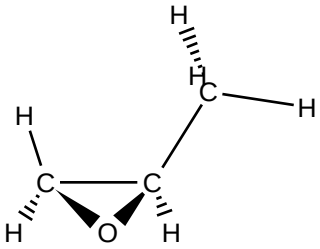
aldehyde



alcohol



ether



ether

PS4.10. Urea has the formula $(NH_2)_2CO$. Draw a Lewis structure for urea. Draw several molecules of urea and show (clearly label) at least two ways it can hydrogen bond in the liquid phase.