Take Home Assignment #3 Name______________________________

Mineral Chemistry and the Unit Cell

The ***unit cell*** of a mineral contains 1 or an integral multiple of chemical formula units. Most minerals do not have "molecules" per say but rather almost infinite three-dimensional repetitions of the unit cell (atomic scale, 5-15 Å, parallelepipeds) which form crystals. If the dimensions of the unit cell (determined by x-ray diffraction analysis (see our in-class discussions) and the density of the mineral are known then the unit cell content ("***Z***" the number of formula units in the unit cell) can be calculated. First let's warm up a little.

1. Calculate the density of the common lead ore, Galena (PbS) .
   Density (*G*) is the mass *(M)* per unit volume *(V)* of some material in grams per cubic centimeter (g/cm^3). This property is extremely important in all sorts of natural occurring Earth processes such as Earth's early density stratification, ocean thermohaline circulation, and atmospheric circulation.
   The unit cell of Galena has 4 formula units per unit cell (*Z=4*, as per our class discussion) and the dimensions of 5.94 Å on each cube side ($V = (5.94\ Å)^3$)

   G = (Z x M)/(A x V) A = Avogadro's number, 6.023×10^{23}
   (number of atoms of a substance in it's gram atomic weight
   1 Å = 10^{-8} cm
   207.2= atomic weight of Pb
   32.1= atomic weight of S

Show your calculations.

2. Let's look again at the chemical analysis of a sphalerite sample and ***calculate the Z number, the number of formula units in the unit cell*** (column 4 in the table below) given the density, G, is 3.92g/cc and the unit cell dimension, V, is $(5.41)^3$ (remember that sphalerite is isometric and the unit cell volume is a^3)

From the above simple formula, G = M/V, we can also determine M for a unit cell of a mineral:

$M = V \times G$.

Since the volume of a unit cell is given in Å we must convert to centimeters as above

$M = (V \times G \times 10^{-24})$ grams

If a mineral contains a weight percent (P) of a certain element X with an atomic weight of N the weight of this element in the unit cell of the mineral (X_m) equals

$X_m = (PM)/100$

The actual weight in grams of an atom of X equals

N/A (Avogadro's number) {btw; $1/A = 1.66 \times 10^{-24}$}

$= N \times (1.66 \times 10^{-24})$

The number of atoms of X in the unit cell, Z, is thus

$Z= (PM)/100(N \times (1.66 \times 10^{-24}))$

$Z= (P \times V \times G \times 10^{-24})/100(N \times (1.66 \times 10^{-24}))$

$Z= PVG/N(166.02)$

Element (N)	P (weight % of element N)	Atomic Proportions (P/N)	Z (atoms of element N per unit cell of the mineral)
Fe (55.85)	18.36		
Mn (54.9)	2.68		
Cd (112.4)	0.28		
Zn (65.4	44.92		
Total Metals			
S	33.68		
	100%		

Show your work on a separate sheet and attach to this one (or on the back).