

HW 2	Inorganic Materials Chemistry	Name:	
Points:	C7780	Date:	
Max. 100 points	Fall 2018	A	

1. (10 pts) Copper metal crystallizes with a cubic close packed (ccp or fcc) structure having a lattice parameter $a = 3.6147 \text{ \AA}$. Calculate the Cu-Cu distance (separation) between nearest-neighbor Cu atoms in the crystal. **Hint:** nearest-neighbor Cu atoms are any two within the same close-packed layer (plane).

2. (10 pts) Molybdenum metal crystallizes with a body-centered cubic (bcc) structure having a lattice parameter $a = 3.1469 \text{ \AA}$. Calculate the Mo-Mo distance (separation) between nearest-neighbor Mo atoms in the crystal. **Hint:** the nearest-neighbor atoms are aligned along the body diagonal of the bcc unit cell.

3. (10 pts) The compound AgCl exhibits the NaCl structure. Frenkel defects in AgCl result from placement of Ag^+ ions in T sites of the Cl^- sublattice. These displaced Ag^+ ions are associated with Ag^+ vacancies elsewhere in the crystal. Sketch a diagram of the AgCl structure that clearly depicts the environment around a Ag^+ ion in a T defect site. Describe the number and nature of cation and anion nearest neighbors about the interstitial Ag^+ ion. What characteristic or characteristics of the compound or crystal structure may stabilize such a defect?

4. (15 pts) Use the Born-Landé equation and the appropriate Shannon-Prewitt radii (provided below) to calculate lattice energies (L_0) for the following structures. Comment on results.

NaCl having the NaCl structure: $r_{\text{Na}^+}(\text{CN}6) = 1.16 \text{ \AA}$; $r_{\text{Cl}^-}(\text{CN}6) = 1.67 \text{ \AA}$

NaCl having the CsCl structure: $r_{\text{Na}^+}(\text{CN}8) = 1.32 \text{ \AA}$; $r_{\text{Cl}^-}(\text{CN}6) = 1.67 \text{ \AA}$ (CN8 not avail.)

5. (15 pts) a) Write balanced chemical equation for a solid state reaction:



b) What is the driving force in this reaction?

c) Cubic spinel ZnFe_2O_4 crystallizes with 8 formula units in the cubic unit cell. The cell parameter $a = 8.42 \text{ \AA}$. Calculate the density in g cm^{-3} of the material.

$N_A = 6.022141 \times 10^{23} \text{ mol}^{-1}$, $A_r(\text{Zn}) = 65.41$, $A_r(\text{Fe}) = 55.85$, $A_r(\text{O}) = 15.999$.

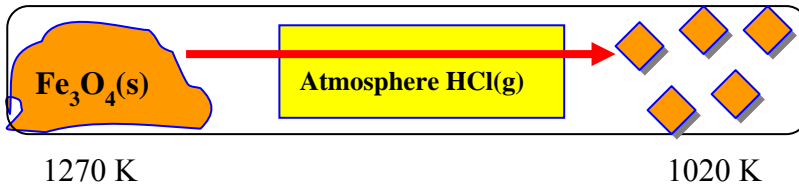
6. (15 pts) The cell parameter for cubic spinel ZnFe_2O_4 is $a = 8.42 \text{ \AA}$, for MnFe_2O_4 $a = 8.50 \text{ \AA}$.

a) Suggest a reason for the difference.

b) What would be the cell parameter for the mixed-metal phase $(\text{Mn}_x\text{Zn}_{1-x})\text{Fe}_2\text{O}_4$ when $x = 0.25$, 0.50 , and 0.75 .

6. (25 pts) Ferromagnetic magnetite can be crystallized by a vapor transport reaction under atmosphere of HCl(g) as a transport agent. Powder of Fe₃O₄ reacts with HCl at hotter end and crystallizes at cooler end.

a) Write and balance the VPT reaction:



b) Is the reaction endo- or exothermic?

Provide an explanation by using van't Hoff equation.

$$\ln K_2 - \ln K_1 = \ln \frac{K_2}{K_1} = \frac{\Delta H^0}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$