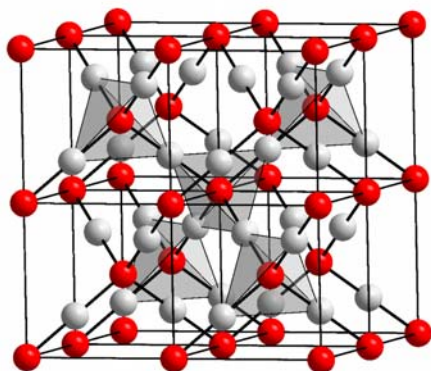


HW 2	Inorganic Materials Chemistry	Name:	
Points:	C7780	Date:	
Max. 100 points	Fall 2015	A	

1. (15 pts) Give the stoichiometric formula for a compound possessing the unit cell below. Atoms: red = O, silver = Cu (all Cu inside the unit cell).



2. (15 pts) Cu_3N has the cubic anti- ReO_3 structure, which is a rather open structure with Cu atoms occupying..... and the N atoms occupying.....of the cubic unit cell. It exhibits a large vacant site atof the cell which can be used for doping with a metal and hence varying the electrical and optical properties.

- Draw a unit cell of Cu_3PdN .
- Is this a primitive or centered cell?
- What structure type it is?

3. (15 pts) Stishovite is a high-pressure modification of SiO_2 having the rutile structure.

- What is the coordination number of Siand O.....?
- Should it have higher or lower density than quartz?
- Should it have longer or shorter Si–O bond lengths than quartz?
- Another phase of SiO_2 at extremely high pressure was predicted to have a pyrite type structure. Draw the unit cell. What is interesting about the oxygen bonding.

4. (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.

$N_A = 6.022141 \cdot 10^{23} \text{ mol}^{-1}$, $A_r(\text{Zn}) = 65.41$, $A_r(\text{Fe}) = 55.85$, $A_r(\text{O}) = 15,999$.

5. (15 pts) The cell parameter for cubic spinel ZnFe_2O_4 is $a = 8.42 \text{ \AA}$, for MnFe_2O_4 $a = 8.50 \text{ \AA}$.

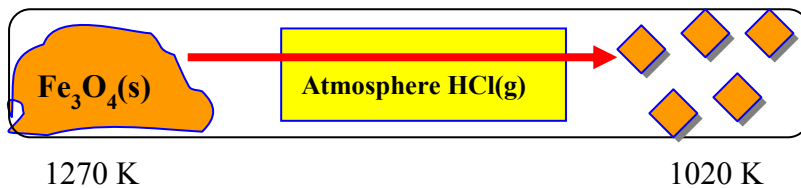
a) Suggest a reason for the difference.

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. (10 pts) It has been predicted that transition metal oxides at high pressures will experience so called “magnetic collapse”. Consider an octahedral coordination of the metal and based on your knowledge of the ligand field theory suggest whether the high spin or the low spin configuration of d electrons is more stable at high pressure?

7. (15 pts) Ferromagnetic magnetite can be crystallized by a vapor transport reaction under atmosphere of $\text{HCl}(\text{g})$ as a transport agent. Powder of Fe_3O_4 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? Explain.