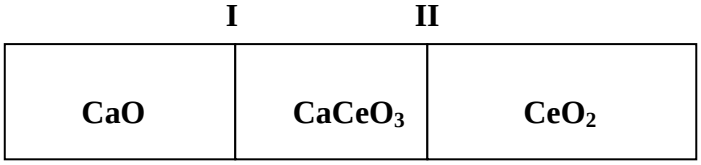
HW 2	**Inorganic Materials Chemistry**	**Name:**	
Points:	**C7780**	**Date:**	
Max. 100 points	**Fall 2014**	**A**	

1. (15 pts) Assume that CaO reacts with CeO_2 and forms $CaCeO_3$.
a) What could be the structure type of this compound? _____
b) Write balanced chemical equations for the reactions taking place at the interfaces (assume counter diffusion of both cations) and calculate the Kirkendall ratio for this process.



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 at .....of the cell which can be used for doping with a metal and hence varying the electrical and optical properties.
a) Draw a unit cell of Cu_3PdN.
b) Is this a primitive or centered cell?
c) What structure type it is?

3. (15 pts) Stishovite is a high-pressure modification of SiO_2 having the rutile structure.
a) What is the coordination number of Si .....and O.....?
b) Should it have <u>higher</u> or <u>lower</u> density then quartz?
c) Should it have <u>longer</u> or <u>shorter</u> Si–O bond lengths then quartz?
d) 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:

$ZnC_2O_4 + \quad Fe(OH)_3 \rightarrow \quad ZnFe_2O_4$

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 Å. Calculate the density in g cm^{-3} of the material.
N_A = 6.022141 10^{23} mol^{-1}, A_r(Zn) = 65.41, A_r(Fe) = 55.85, A_r(O) = 15,999.

6. (15 pts) Gibbs free energy change for nucleation ΔG_N is given by two terms – surface and volume. $\Delta G_N = 4\pi r^2 \gamma_{SL} + 4/3\pi r^3 \Delta G_V$

γ_{SL} = the solid/liquid interfacial energy
ΔG_V – the free energy change between the 'monomer' in solution and unit volume of bulk crystal $\Delta G_V = -\frac{RT \ln S}{V_m}$
S – supersaturation = the quotient (ratio) of the actual concentration and the concentration of the respective species at equilibrium conditions, indicates how far away from equilibrium the system is. V_m – molar volume of the bulk crystal, r – nucleus radius

a) Explain what is a critical radius of nuclei r_C – draw a graph of ΔG_N versus r.
b) Suggest a way how to control the critical nucleation radius r_C by changing some reaction parameter.

7. (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?

8. (15 pts) The binary phase FeSi can be crystallized by Vapor Phase Transport reactions with iodine. The transport takes places (T1→T2) with deposition temperatures between T1 = 700 °C and T2 = 1030 °C.

a) Complete the balanced chemical equation:

FeSi (s) + I_2 (g) ⇆

b) Is the transport reaction of FeSi with iodine exothermic or endothermic?

c) Does this scheme correspond the transport reaction of FeSi? Why?