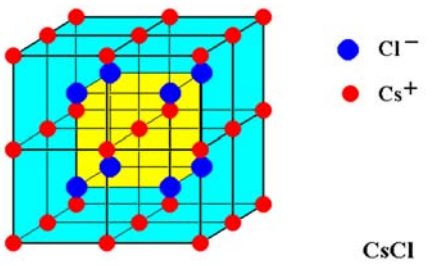
HW 2	Inorganic Materials Chemistry	Name:	
Points:	**C7780**	**Due date:**	**23.11.2022**
Max. 100 points	**Fall 2022**	**A**	

1. (10 pts) Copper metal crystallizes with a cubic close packed (ccp or fcc) structure having a lattice parameter a = 3.6147 Å. 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 Å. 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. (20 pts) Derive the first three terms of the series to calculate the Madelung constant for CsCl. Use interionic separation d ($d = r_{Cs^+} + r_{Cl^-}$) as the distance parameter in the Coulomb equation.



CsCl

4. (10 pts) Should it be possible to convert β-cristobalite to some of the other modifications by applying high pressure?

Modification of SiO_2	**Density / g cm^{-1}**
α-quartz	2.65
β-quartz	2.53
β-tridymite	2.27
β-cristobalite	2.33
Vitreous	2.20

5. (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) The cell parameter for cubic spinel $ZnFe_2O_4$ is a = 8.42 Å, for $MnFe_2O_4$ a = 8.50 Å.
a) Suggest a reason for the difference.

b) What would be the cell parameter for the mixed-metal phase $(Mn_xZn_{1-x})Fe_2O_4$ when x = 0.25, 0.50, and 0.75.

7. (20 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.