HW 3	**Inorganic Materials Chemistry**	**Name:**	
Points:	C7780	**Date due:**	
Max. 100 points	**Fall 2018**		

1. (30 pts.) Use the ligand field theory to explain why Mn_3O_4 is a normal spinel while Fe_3O_4 is an inverse spinel. Hint: draw diagrams of energy levels of d-electrons for ions in tetrahedral and octahedral sites, use approximation $\Delta_T = 4/9\ \Delta_O$ for ligand field splitting energy, consider all MO_4 and MO_6 moieties as high spin complexes, calculate ligand field stabilization energy in terms of Δ_O for both normal and inverse arrangement of ions, compare them and find which is more stable.

2. (30 pts) Mixed metal oxides could be prepared by sol-gel reactions from aqueous solutions of metal salts.

a) Order these ions Al^{3+}, Ba^{2+}, Cs^{+}, H^{+}, Li^{+}, Mg^{2+} according to the increasing value of hydration enthalpy: $M^{z+} + n\ H_2O \rightarrow [M(H_2O)_n]^{z+}$ $\Delta H_{hydration}$

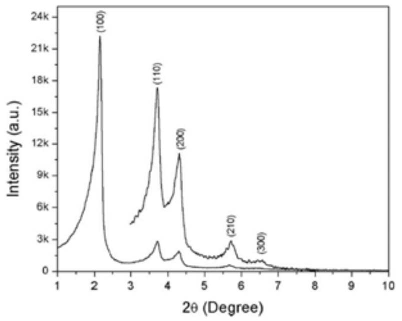
b) For a hydrolytic reaction $[M(H_2O)_N]^{z+} + h\ H_2O \rightarrow [M(OH)_h(H_2O)_{N-h}]^{(z-h)+} + h\ H_3O^+$

$\Delta H^{\circ} = (75.2 - 9.6\ z)$ kJ mol^{-1} and $\Delta S^{\circ} = (-148.4 + 73.1\ z)$ J K^{-1} mol^{-1}

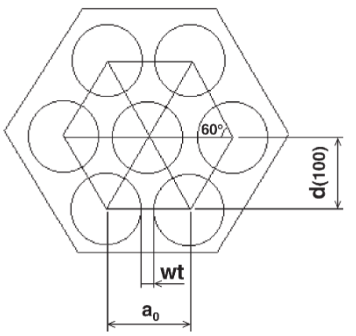
Write equation that gives a measure of spontaneity of reaction (= write a formula relating this state function to ΔH° and ΔS°). Calculate, for which of the above listed ions is this reaction spontaneous?

3. (40 pts.) Calculate the wall thickness of a hexagonal MCM-41 mesoporous material, assume that it possesses cylindrical pores.

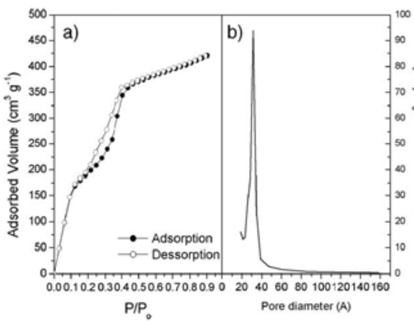
a) First, calculate the $d(100)$ = interplanar distance in the (100) plane from the XRD diffractogram. CuKα radiation was used with λ = 1.542 Å. Diffraction maximum was found at 2.14 °2θ.



b) Now, derive the formula relating the interplanar distance $d(100)$ to the hexagonal mesoporous parameter a_0 and calculate its value.



c) Derive the formula relating the diameter D_p of a pore to specific surface area SA (870 m^2/g) and total pore volume V_p (0.683 cm^3/g). Assume cylindrical pores.



d) Finally, calculate the wall thickness (wt) of MCM41 material.