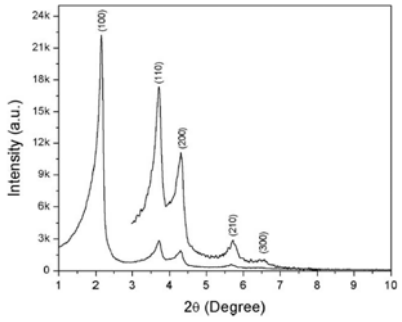
HW 3	Inorganic Materials Chemistry	Name:	
Points:	**C7780**	**Date due:**	**Dec. 21, 2016**
Max. 100 points	**Fall 2016**		

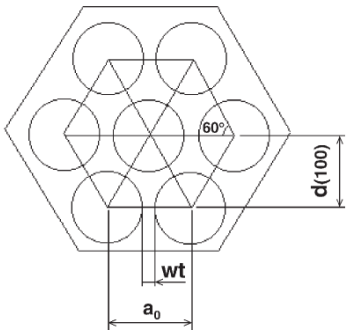
1. (30 pts.) Use the ligand field theory to explain why Mn_3O_4 is a normal spinel while Fe_3O_4 is an inverse spinel. Hint: draw diagrams of energy levels of d-electrons for ions in tetrahedral and octahedral sites, use approximation $\Delta_T = 4/9\ \Delta_O$, consider all MO_4 and MO_6 moieties as 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. (50 pts.) Calculate the wall thickness of a hexagonal MCM-41 mesoporous material, assume that it possesses cylindrical pores.

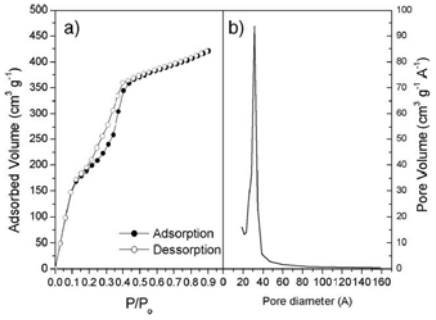
a) First, calculate the *d*(100) = interplanar distance in the (100) plane from the XRD diffractogram. CuKα radiation was used with λ = 1.542 Å. Diffraction maximum was found at 2.14 °2θ.



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.

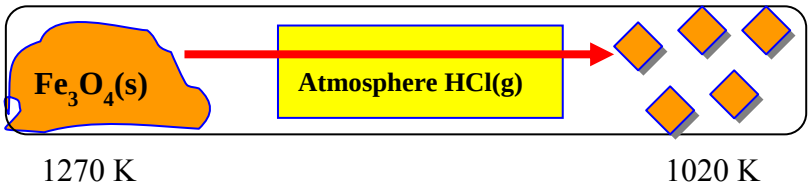


d) Finally, calculate the wall thickness (*wt*) of MCM41 material.

3. (20 pts.) Ferromagnetic magnetite can be crystallized by a vapor transport reaction under atmosphere of HCl(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:

Fe_3O_4(s) + HCl (g) ⇄



b) Is the reaction endo- or exothermic?