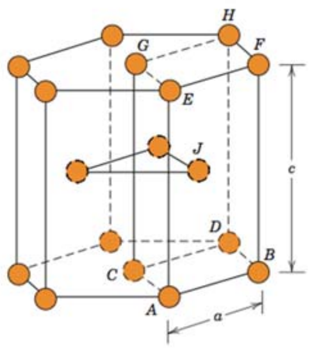
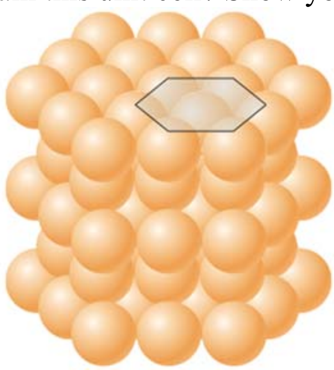
HW 3	**Inorganic Materials Chemistry**	**Name:**	
Points:	**C7780**	**Date due:**	
Max. 100 points	**Fall 2022**		

1. (15 pts) In the manganese(II) oxide, the Mn^{2+} ions occupy the octahedral holes in the cubic close packed structure of oxides.
a) Describe the splitting of the d-orbitals and assign symmetry labels (draw energy level diagram).
b) Assuming the oxide ligand to be a weak field ligand, populate the d-orbitals with electrons.
c) The total spin of the Mn^{2+} is _________ and its multiplicity is_________.

2. (15 pts) The unit cell for a hexagonal close-packed (hcp) metal is shown below.
a) Label atom layers A, B or C to identify the close-packed layers they belong to.
b) How many lattice points Z contain this unit cell? Show your work.



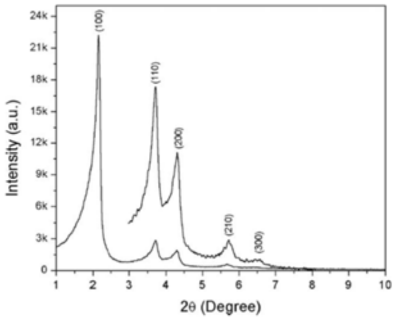


3. (15 pts) Zeolite A (LTA) displays a single peak in the ^{29}Si MAS NMR spectrum at 89 ppm and has a Si/Al ratio of 1. Explain these observations.

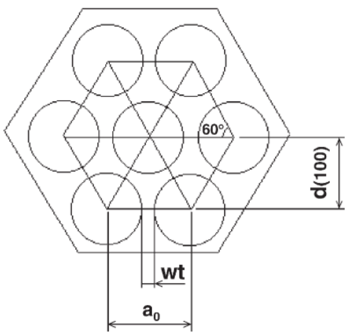
4. (15 pts) Zeolite A (Ca form), when loaded with platinum, has been found to be a good catalyst for the oxidation of hydrocarbon mixture. If the mixture contains branched chain hydrocarbons, these do not react. Describe a possible reason to explain these observations.

5. (40 pts) Calculate the wall thickness of a hexagonal MCM-41 mesoporous material, assume that it possesses cylindrical pores.

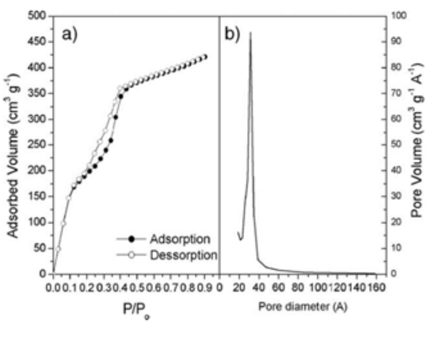
a) First, calculate the $d(100)$ = interplanar distance in the (100) plane from the XRD diffractogram. CuKα radiation was used with λ = 1.542 Å. Diffraction maximum was found at 2.14 °2θ.



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.