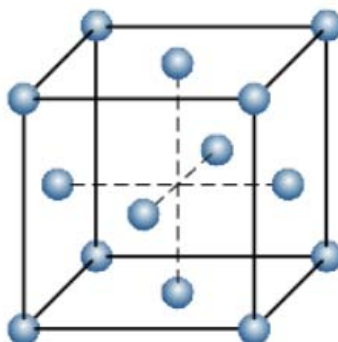


HW 3	Inorganic Materials Chemistry	Name:	
Points:	C7780	Date due:	December 17
Max. 100 points	Fall 2019		

1. (15 pts) In the manganese(II) oxide, the Mn^{2+} ions occupy the octahedral holes in the cubic close packed structure of oxides.

- Describe the splitting of the d-orbitals and assign symmetry labels (draw energy level diagram).
- Assuming the oxide ligand to be a weak field ligand, populate the d-orbitals with electrons.
- The total spin of the Mn^{2+} is _____ and its multiplicity is _____.

2. (15 pts) The unit cell for a cubic close-packed (ccp) metal is shown below. Label atoms A, B or C to identify the close-packed layers they belong to.

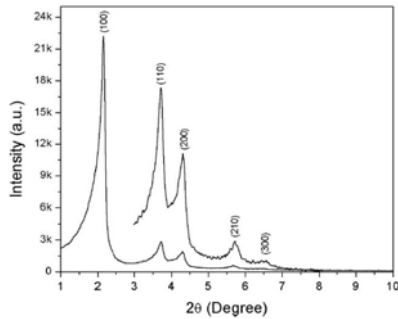


3. (15 pts) Zeolite A (LTA) displays a single peak in the ^{29}Si MAS NMR spectrum at 89 ppm and has a Si/Al ratio of 1. Explain these observations.

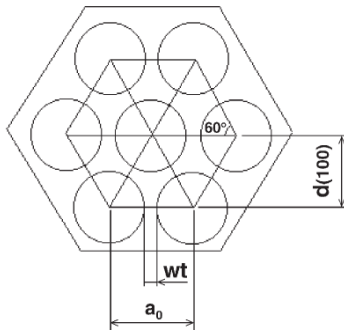
4. (15 pts) Zeolite A (Ca form), when loaded with platinum, has been found to be a good catalyst for the oxidation of hydrocarbon mixture. If the mixture contains branched chain hydrocarbons, these do not react. Describe a possible reason to explain these observations.

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

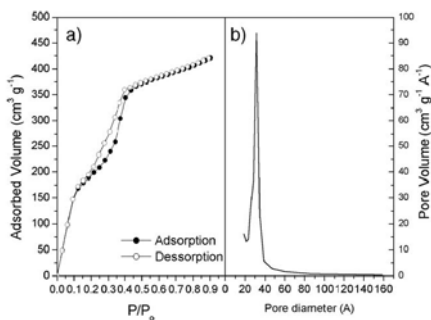
a) First, calculate the $d(100)$ = interplanar distance in the (100) plane from the XRD diffractogram. CuK α radiation was used with $\lambda = 1.542 \text{ \AA}$. Diffraction maximum was found at $2.14^\circ 2\theta$.



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 ($870 \text{ m}^2/\text{g}$) and total pore volume V_p ($0.683 \text{ cm}^3/\text{g}$). Assume cylindrical pores.



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