



SCT 332-3 Materials Chemistry II

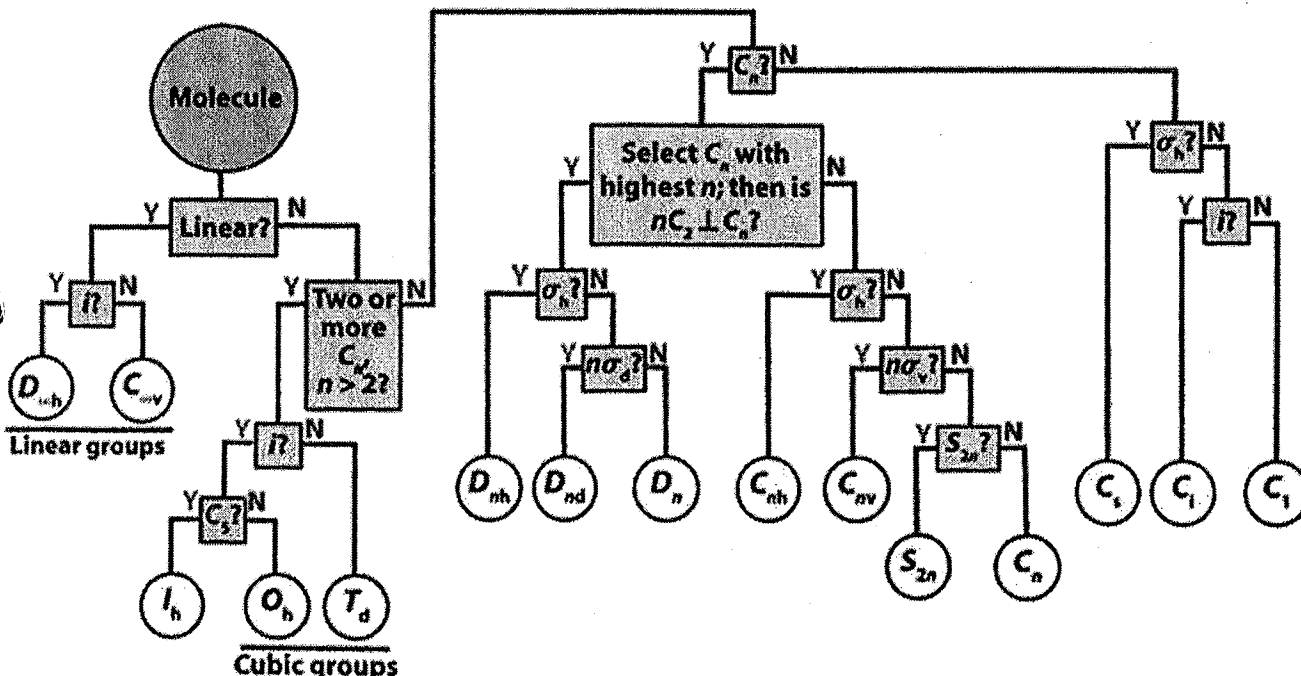
Number of questions: Seven (07)

Answer any six (6) questions only

Time allocation: Three (03) hours

Total marks allocated: 100

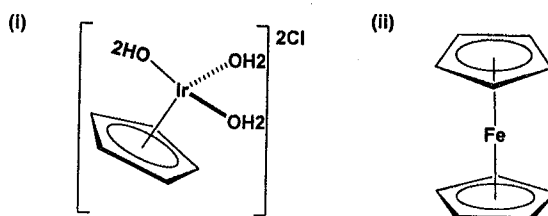
- a. What is a symmetry element? What is a symmetry operation? Explain the difference using a water molecule as an example.
- b. Find symmetry elements present in following molecules.
(i) B_2H_6 (ii) PCl_3 (iii) $POCl_2$ (iv) CO_2
- c. Use the decision tree below to find the point group of each molecule in part (b)



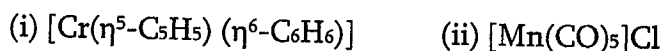
2. CH_2Cl_2 molecule belongs to the C_{2v} point group. The character table for C_{2v} point group is given below.

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

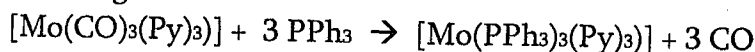
- Calculate the order of the group.
 - Find the reducible representation (Γ_{red}) for all symmetry operations.
 - Do the multiplication for each row using orthogonality theorem in order to find the irreducible representation (Γ_{irred})
 - Using irreducible representation, identify what type of orbitals will participate in bonding.
3. a. Name following organometallic complexes according to the IUPAC nomenclature.



- b. Use 'donor-pair' method to calculate the validity of 18e rule for following complexes. Show each step in this calculation.



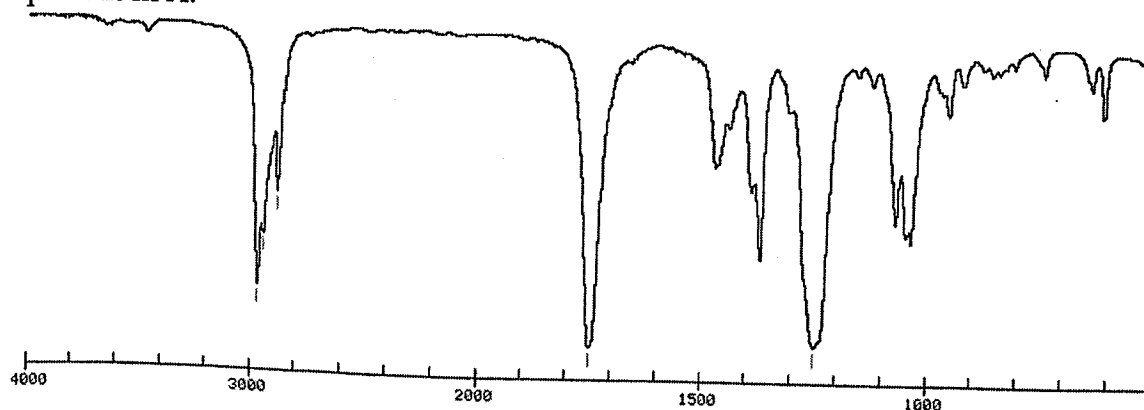
- c. How can you use CO-stretching frequencies in IR spectroscopy to detect products of the following reaction?



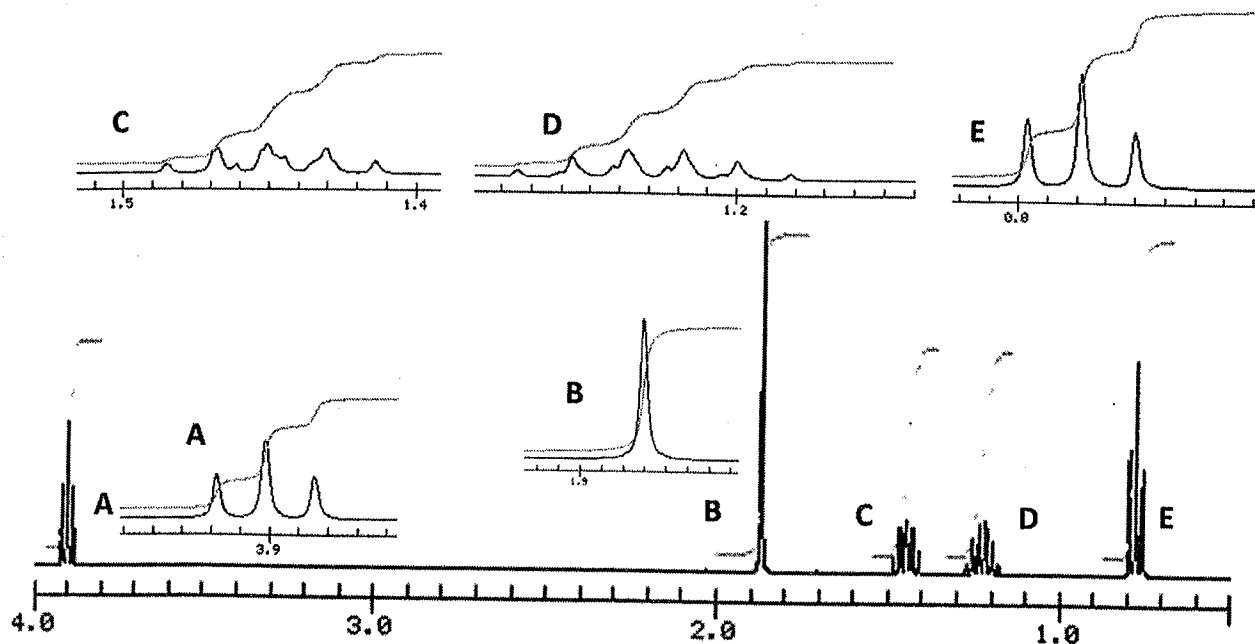
4. Compound A has a pleasant smell and hydrolysis products of A yielded acetic acid as one of the major products.

- a. Elemental analysis of Compound A contained C = 62.01% ; H=10.39%; O=27.53%. Calculate the elemental formula for this compound.

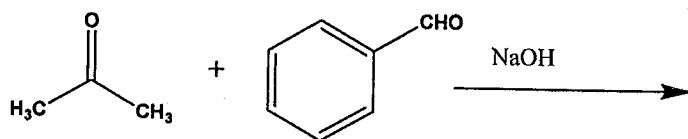
- b. FTIR Spectra for the Compound A is given below. Identify at least two major functional units present in A.



c. ^1H NMR of the compound A is given below. (i) How many different types of protons present in this compound? (ii) Identify structure for A (iii) Draw structure for A and assign ^1H NMR peaks.



5. a. Draw possible structures of Aldol-condensation products formed from a mixture of acetone and benzaldehyde?



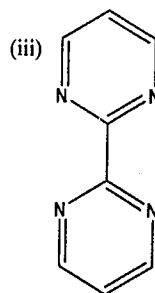
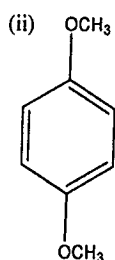
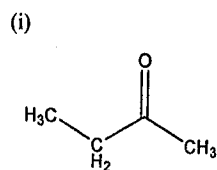
b. How do you setup experimental conditions (order of mixing of each reactant) to obtained product formed between acetone and benzaldehyde as the major product?

c. Draw the structures of acetone, benzaldehyde, and major product of part (b) and predict multiplicities expected for each proton in ^1H NMR spectroscopy.

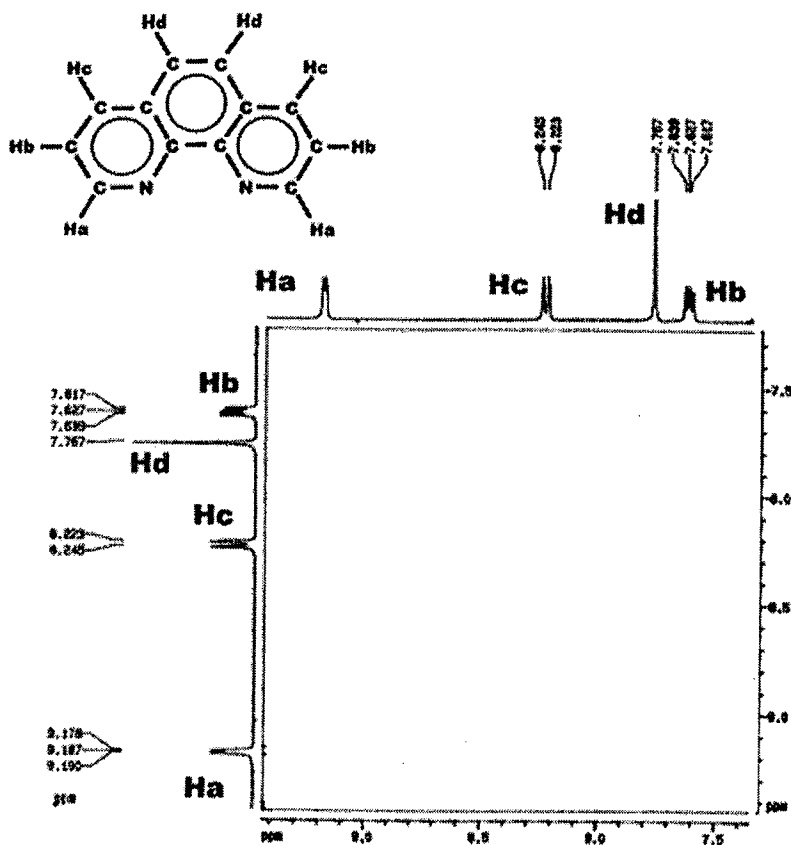
d. List two separation techniques you can use to isolate major product in part (b).

6. a. List three different types of 2D-NMR techniques available for structure identification and briefly explain what kind of NMR techniques were used as X and Y axis.

b. Predict multiplicities expected for following molecules in ^{13}C NMR.



c. Copy following COSY spectrum for 1,10 phenanthroline to your answer book and draw the signals expected.



7. a. Give examples for two Zn containing enzymes and draw the active site indicating coordination around Zn.
- b. Which enzyme is responsible for liver alcohol degradation and explain its function. Which conditions would lead to cirrhosis?
- c. Draw the structure of porphyrin and give mechanism for synthesis.