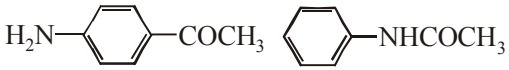
(b) How would you distinguish between the following on the basis of IR : **12**

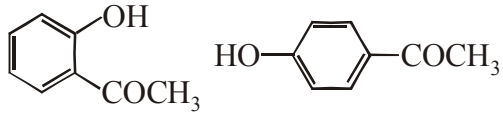
(i) Ester and carboxylic acid

(ii) Ethylbenzene and o-xylene

(iii) Cis and Trans Stilbene.

(iv) 

(v) 

(vi) 

4. (a) Taking suitable examples, discuss briefly the effect of hybridization on the C-H stretch of hydrocarbons and aldehydes. **5**

(b) Explain basic theory and instrumentation including FTIR infrared spectrum. **8**

(c) What is Fermi resonance ? Giving suitable examples explain its usefulness in interpreting IR spectra. **4**

(d) α, β-unsaturated ester absorbs at lower frequency as compared to its saturated analogue. Explain. **3**

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CC-297

M. Sc. EXAMINATION, May 2017

(Third Semester)

(Re-appear Only)

(CHEMISTRY)

CH-613-B

Organic Chemistry Special-I

(Organic Spectroscopy)

Time : 3 *Hours*] [*Maximum Marks :* 100

Before answering the question-paper candidates should ensure that they have been supplied to correct and complete question-paper. No complaint, in this regard, will be entertained after the examination.

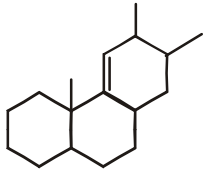
Note : Attempt *Five* questions in all, selecting at least *one* question from each Unit. All questions carry equal marks.

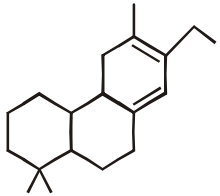
Unit I

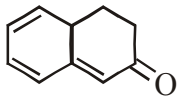
1. (a) What is an auxochrome ? Explain how an auxochrome exerts abathochromic shift on a chromophore such as ethylenic bond ? **5**

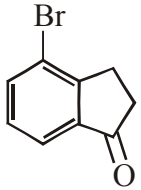
(b) Discuss the effect of steric hindrance to complanarity in UV spectra. **5**

(c) Calculate λ_{max} for the following compounds : **10**

(i) 

(ii) 

(iii) 

(iv) 

2. (a) Discuss the applications of UV spectroscopy in organic molecules : **10**

(i) Study of tautomerism

(ii) Study of geometrical isomerism

(iii) Identification of chromophore (functional group).

(b) Define the terms bathochromic shift and hypsochromic shift. What structural feature may produce a bathochromic shift or hypsochromic shift in an organic compound ? **5**

(c) Draw structural formulas that are consistent with the following observations : **5**

(i) An acid $C_7H_4O_2C_{l2}$ shows a UV maximum at 242 nm

(ii) An aldehyde $C_8H_{12}O$ absorbs in UV with λ_{max} = 244 nm

Unit II

3. (a) Describe the factors influencing vibrational frequencies in the IR spectra. **8**

Unit III

5. (a) Explain the anisotropic effects in acetylene, ethylene and benzene. **5**

(b) Explain briefly the following :

(i) Sheilding and Desheilding of nucleous

(ii) Vicinal coupling and Karplus equation curve

(iii) First order and second order spectrum.

(c) Deduce the structure of the following compound from the given NMR data. Molecular formula : $C_9H_{10}O_3$. **4**

^{1}H NMR : δ3.37(S, 2H), 3.77(S, 3H), 6.94(d, 2H), 7.26(d, 2H), 11.83(S, 1H) ppm

(d) $CDCl_3$ exhibits a triplet at δ 76, 77 and 78 in its 13C-NMR spectrum. **2**

6. (a) What do you understand by relaxation process in NMR ? Explain its significance. **8**

(b) How can the two isomeric hydrocarbons with molecular formula C_3H_4 be distinguish by ^{13}C-NMR ? **4**

(c) Write short notes on following : **8**

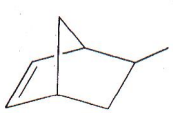
(i) Double resonance

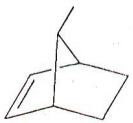
(ii) Nuclear overhauser effect.

Unit IV

7. (a) Explain the Mclafferty rearrangement and write down its mechanism with an example. **5**

(b) Which of the following compounds would be expected to undergo retro-Diels Alder to yield and intense ion at m/z = 66 ?

(i) 

(ii)  **4**

(c) Compare the advantage and disadvantage of electron ionization and chemical ionization methods used in mass spectrometry. **5**

(d) Comment upon salient features of the mass spectra of compounds containing two chlorine and one bromine atoms. Do fluorine and iodine containing compounds display the same feature in their mass spectra ? Give reasons. **6**

8. (a) How molecular weight and molecular formula of an organic compound can be determined using mass spectrometry ? **5**

(b) Predict the fragmentation in the following compounds from their molecular ions :

(i) Benzyl acetate

(ii) 2-Ethylphenol

(iii) 1-phenylethanol.

(c) How can you use the information of ortho effect to explain the formation of ion m/z = 149 in the esters of phthalic acid ? **4**

(d) What is octane rule ? What information can be obtained by its application to cyclohexanone ? **5**