Enrollment No._____

NAVRACHANA UNIVERSITY
a UGC recognized University

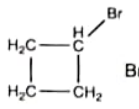
School: School of Science
Program/s: MSc Chemistry (Organic)
Year: 2nd **Semester:** 3rd
Examination: End Semester Examination
Examination year: December - 2022

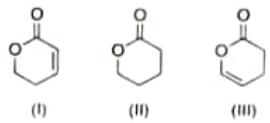
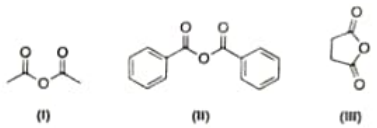
Course Code: CH221 **Course Name:** **Organic Spectroscopy**
Date: 02/12/2022 **Total Marks:** 40
Time: 14:30 to 16:30 **Total Pages:** 4

Instructions:

- *Write each answer on a new page.*
- *Use of a calculator is permitted/~~not permitted~~.*
- ** COs=Course Outcome mapping. # BTL=Bloom's Taxonomy Level mapping*

Q. No.	Details	Marks	COs*	BTL#
Q.1	**Choose the correct answer (s) from the followings.**	**10**		
	1. IR spectrum of an oxygen containing compound has shown three significant peaks at 2960 cm^{-1}, 1720 cm^{-1} and 750 cm^{-1}. The wavelength corresponding to the peak at 1720 cm^{-1} is... a. 5.81 µm b. 6.17 µm c. 5.81 nm d. 6.17 nm		CO2	BT3 BT4
	2. Enantiotropic protons are a. Chemically equivalent b. Magnetically equivalent c. Both (a) and (b) d. Does not give NMR signal		CO3	BT2
	3. The types of transitions possible in UV-visible region for a compound with molecular formula C_2H_4O are P. $n\rightarrow\pi^*$ Q. $\sigma\rightarrow\sigma^*$ R. $n\rightarrow\sigma^*$ S. $\pi\rightarrow\pi^*$ a. P, Q, R b. Q, R c. P, S d. P, Q, R, S		CO1	BT3 BT4
	4. Which of the following statement is false for mass spectroscopy? a. Mass spectroscopy is used to identify unknown compounds within a sample, and to elucidate the structure and chemical properties of different molecules b. Particle are characterized by their mass to charge ratios (m/z) and relative abundances c. This technique basically studies the effect of ionizing energy on molecules d. This technique can be used on all state of matter		CO4	BT3

	5. Which one of the following have weak parent ion (molecular ion) peak? a. Alcohols b. Amines c. Alicyclic compounds d. Aromatic compounds		CO4	BT3
	6. Chemical shifts originate from a. magnetic momentum b. electron shielding c. free induction decay d. scalar coupling (*J*-coupling)		CO3	BT2
	7. The Fourier transformation is a mathematical conversion of a. Time domain to frequency domain b. Frequency domain to time domain c. Time domain to concentration domain d. Concentration domain to time domain		CO3	BT1
	8. When the λ_{max} of a compound shift to a shorter wavelength on certain treatment, the compound is said to have undergone a. Hypochromic effect b. Hypsochromic effect (Blue shift) c. Bathochromic Shift (Red shift) d. Hyperchromic Shift		CO1	BT2
	9. How many numbers of peaks are possible in proton NMR spectra of the following cyclic compound?  Bromocyclobutane a. Two b. Three c. Four d. Five		CO3	BT3 BT4
	10. Separation of ions in mass spectrometer take place on the basis of which of the following? a. Mass b. Charge c. Molecular weight d. Mass to charge ratio		CO4	BT2
Q.2	**Answer the following questions.** ***(Any Four)*** (i) (a) Methyl chloride and Methyl bromide display in their mass spectra pairs of peaks ($M^{+\cdot}$ and M+2). Why? (b) What is the intensity (approx.) ratio of $M^{+\cdot}$: M+2 in methyl chloride and methyl bromide? (ii) Mass spectrum of *n*-hexane shows fragment ions at *m/z*= 71, 57, 43 and 29. Show the fragmentation of *n*-hexane corresponds to fragment ions at *m/z* = 71, 57, 43 and 29. (iii) Mass spectrum of 2-pentanone shows fragment ions at *m/z*=86, 71, 58 and 43. Show the fragmentation of 2-pentanone corresponds to fragment ions at *m/z*=86, 71, 58 and 43.	**8**	CO4	BT3 BT4

	(iv) Mass spectrum of methyl butanoate shows fragment ions at m/z=74, 71, 59 and 43. Show the fragmentation of methyl butanoate corresponds to fragment ions at m/z=74, 71, 59 and 43. (v) The mass spectrum of Anisole (methyl phenyl ether) shows peaks at m/z 93, 65, 78 and 77. Show the mass fragmentation of Anisole corresponds to above mentioned m/z values.			
Q.3	**Do as directed. *(Any Three)***	**6**		
	(i) The carbonyl stretching absorptions for the following lactones are 1760 cm^{-1}, 1745 cm^{-1} and 1720 cm^{-1}. Match the absorptions with the appropriate structure and justify your choice.  (I) (II) (III)		CO2	BT3 BT4 BT5
	(ii) Assign each of the following pairs of absorptions to one of the compounds below: (a) 1865 and 1780 cm^{-1} (b) 1815 and 1750 cm^{-1} (c) 1775 and 1720 cm^{-1} Justify your answer.  (I) (II) (III)		CO2	BT3 BT4 BT5
	(iii) For UV light of wavelength 315 nm, calculate (a) frequency of this light (b) the amount of energy absorbed by one molecule when it interacts with this light (c) the amount of energy absorbed by one mole of substance.		CO1	BT3 BT4
	(iv) An unknown compound is believed to have either structure A or B. Its UV-spectrum shows λ_{max} at 320 nm (ethanol). What could be its likely structure?  (A) (B)		CO1	BT3 BT4 BT5
Q.4	**Do as directed. *(Any Four)*** **Note: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, bs = broad singlet, dd = doublet of doublet**	**16**		
	(i) The proton NMR data of a compound with formula $C_6H_5NCl_2$ is given. The normal corbon-13 and the DEPT experimental results are tabulated. The infrared spectrum shows peaks at 3432 and 3313 cm^{-1} and a series of medium-sized peaks between 1618 and 1466 cm^{-1}. Draw the structure of this compound and justify. ^{1}H NMR (δppm): 4.4 (bs, 2H), 6.55 (t, 1H), 7.15 (d, 2H) Normal Carbon (ppm) / DEPT-135 / DEPT-90 118 / Positive / Positive 119.5 / No peak / No peak 128 / Positive / Positive 140 / No peak / No peak		CO3	BT3 BT4 BT5
	(ii) An organic compound, C_6H_8O shows the following spectral data: ▪ UV: λ_{max} 225 nm (ε = 10,000), 318 nm (ε = 40) ▪ MS: Molecular ion at m/z = 96, base peak at m/z = 68. ▪ IR: A strong band at 1690 cm^{-1} ▪ ^{1}H NMR (δppm): 1.54 (m, 2H), 1.94 (q, 2H), 3.16 (t, 2H) 5.9 (d, 1H), 7.0 (m, 1H) Propose the structure for this compound with explanation (explanation necessary).		CO3	BT3 BT4 BT5
	(iii) Following are the NMR data (^{1}H NMR (δppm)) of two isomeric compounds with the formula $C_7H_{14}O_2$. Provide structure for each. Compound A: 0.9 (d, 6H), 1.15 (t, 3H), 1.95 (m, 1H), 2.35 (q, 2H), 3.85 (d, 2H) Compound B: 1.1 (t, 3H), 1.45 (s, 9H), 2.2 (q, 2H)		CO3	BT3 BT4 BT5

(iv) The proton NMR data of a compound with formula $C_5H_{10}O$ is listed. The normal carbon-13 and the DEPT experimental results are tabulated. The infrared spectrum shows a broad peak at about 3340 cm-1 and a medium size peak at about 1651 cm-1. Draw the structure of this compound and justify.

CO3 BT3 BT4 BT5

^{1}H NMR (δppm): 1.75 (s, 3H), 2.15 (s, 1H), 2.3 (t, 2H), 3.7 (t, 2H), 4.8 (d, 1H), 4.9 (d, 1H)

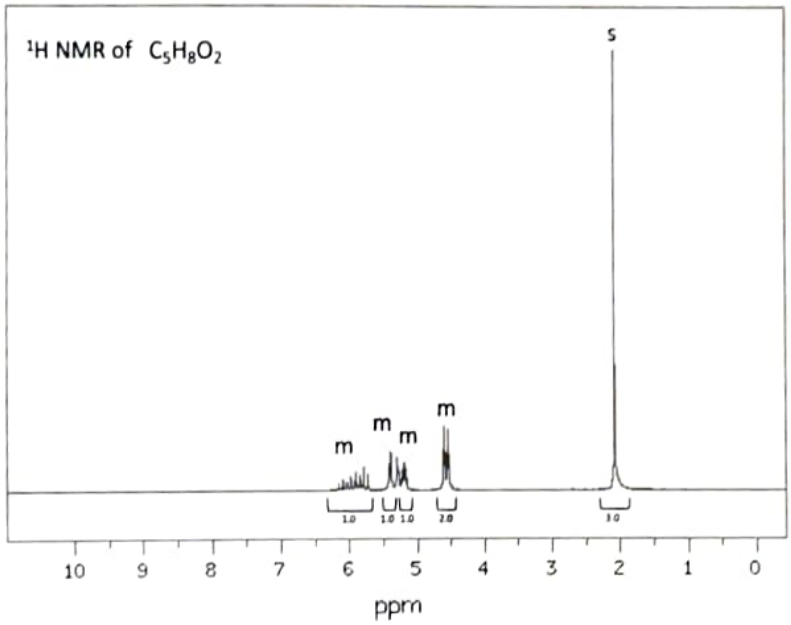
Normal Carbon (ppm)	DEPT-135	DEPT-90
22.2	Positive	No peak
40.9	Negative	No peak
60.2	Negative	No peak
112.5	Negative	No peak
142.3	No peak	No peak

(v) The proton NMR data, ^{1}H NMR spectrum and infrared spectra data for a compound with formula $C_5H_8O_2$ is given below. Draw the structure of this compound and justify.

CO3 BT3 BT4 BT5

^{1}H NMR (δppm): 2.1 (s, 3H), 4.5-4.6 (m, 2H), 5.1-5.25 (m, 1H), 5.25-5.5 (m, 1H), 5.75-6.25 (m, 1H)

IR spectrum has following bands (cm^{-1}): 3070, 2987, 2895, 1740, 1375, 1210, 1024, 990,910.



**********End of Question Paper**********