MASTER'S DEGREE (C.S.S) EXAMINATION, NOVEMBER 2024
2023 ADMISSIONS REGULAR
SEMESTER III - CORE COURSE CHEMISTRY
CH3C12TM20 - Spectroscopic Methods in Chemistry

**Time : 3 Hours**   **Maximum Weight : 30**

Part A

I. Answer any Eight questions. Each question carries 1 weight   **(8x1=8)**

1. Identify possible electronic transition for the following compounds a. Cyclopentene b. Acetaldehyde c. Dimethyl ether.

2. Explain axial haloketone rule.

3. Discuss types of vibrations in IR spectroscopy.

4. Explain briefly the functional group region and finger print region in IR spectroscopy.

5. Explain virtual coupling with an example.

6. Draw the ^{1}H NMR spectrum for each of the following compounds:
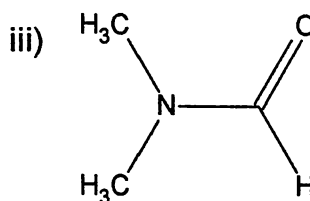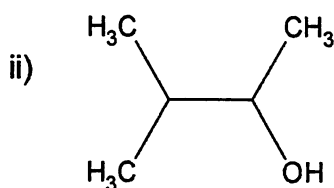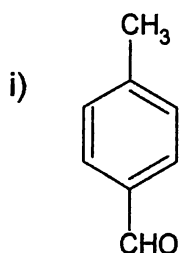
7. Describe Retro-Diels Alder reaction and its significance in mass spectrometry.

8. The mass spectrum of 2-butenal shows a peak at m/z 69 that is 28.9% of as intense as the base peak. Propose atleast one fragmentation route to account for this peak and explain why this fragment would be reasonably stable.

9. The compound that gives the following NMR spectrum has the formula $C_3H_6Br_2$. Draw the structure.
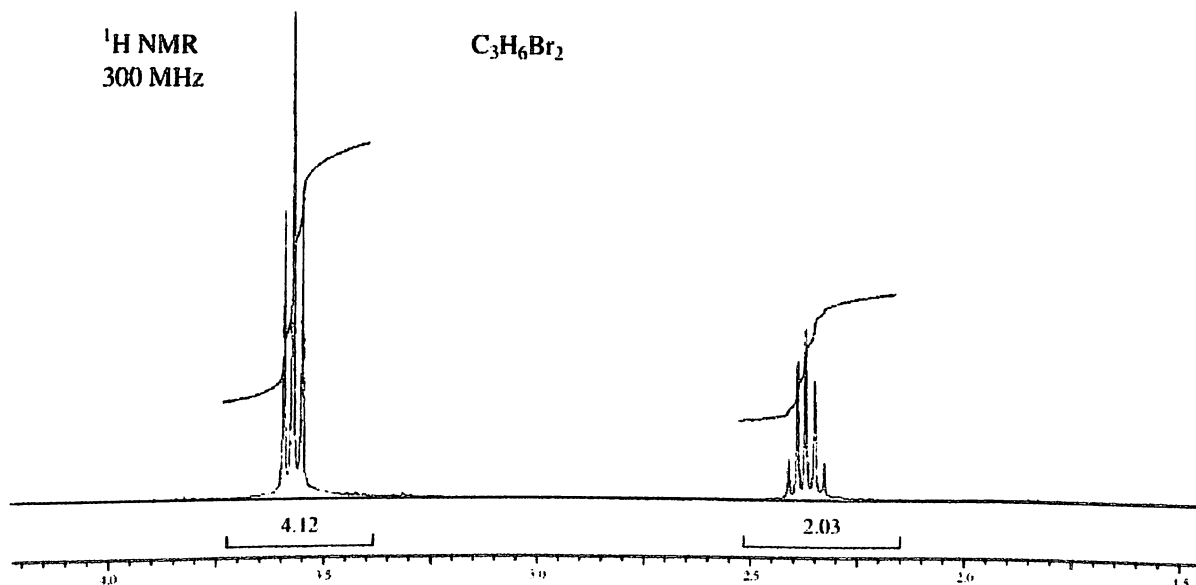
10. The position of the OH resonance of phenol varies with concentration in solution. On the other hand, the hydroxyl proton of ortho-hydroxyacetophenone appears at 12.05 ppm and does not show any great shift upon dilution. Explain.
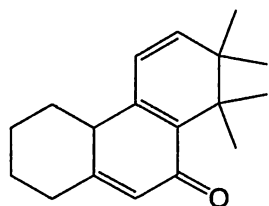
Part B

11. Using Woodward Fieser rule calculate the λ_{max} for the following structure.

a)

b)
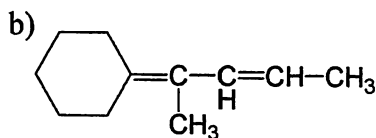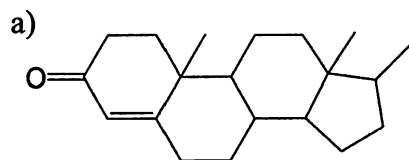
12. a) Calculate the λ_{max} for the following structure by using Woodward Fieser rules.

b) Using Fieser-Kuhn rules calculate λ_{max} for the following structures.
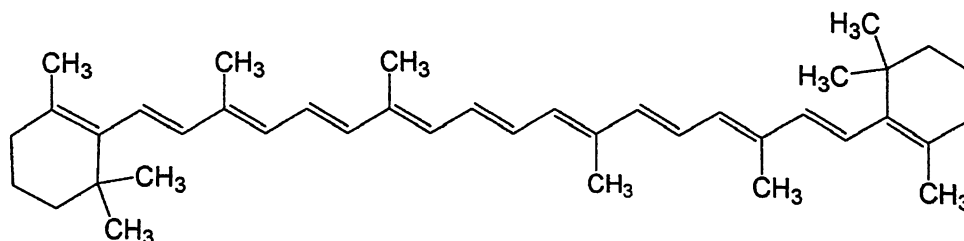

13. Illustrate IR spectra of C=O stretching in carbonyl compounds with the help of spectral data of carbonyl compounds.

14. Explain influence of substituents on the IR spectra of a compound.

15. Discuss the origin of NOE.

16. Below is the mass spectrum of 2-methylhexane. What is the m/z value of the M+ peak and of the base peak? Give possible structures of the fragments giving rise to the large peaks at m/z = 85, 57, and 43.
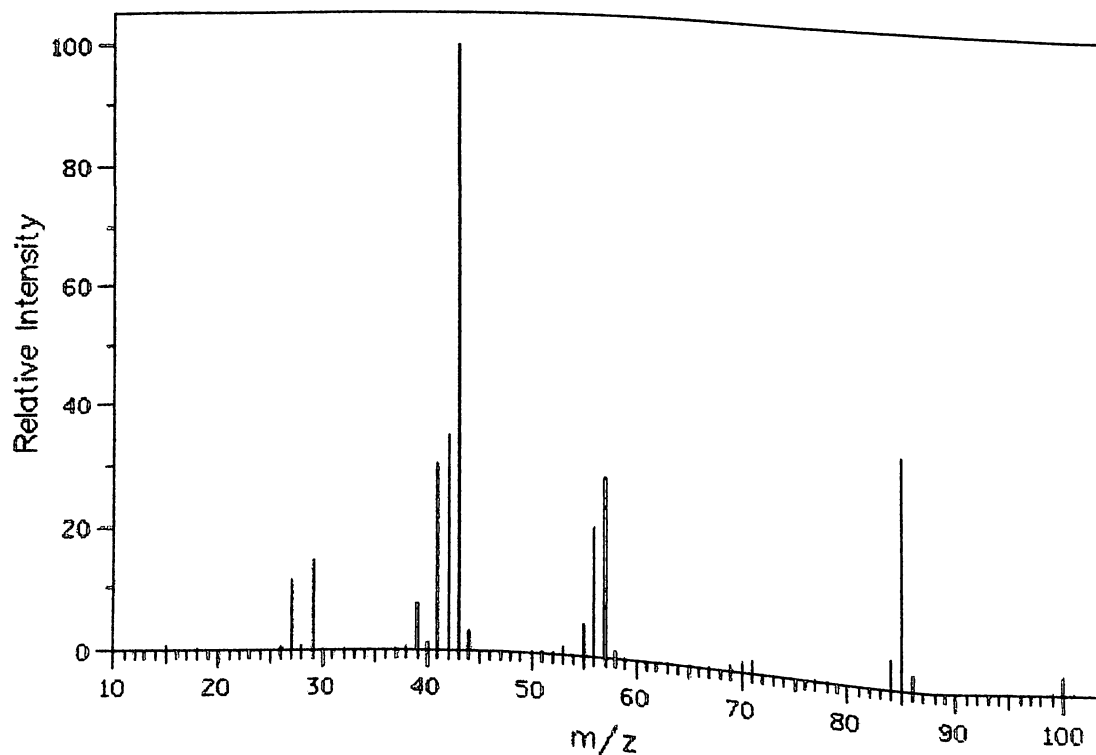
17. Describe the fragmentation pattern of aromatic hydrocarbons with suitable examples.

18. An organic compound dissolves in sodium hydroxide to form a yellow coloured solution. It gives brisk effervescence with sodium bicarbonate solution. Its infrared spectrum exhibits the following absorption bands:
i) 3060-3110 cm^{-1} ii) 3000-2520 cm^{-1} iii) 1602,1510,1420 cm^{-1} iv) 1620,1375(s) cm^{-1} and 830 cm^{-1}.
Deduce the structure of the compound.

Part C

III. Answer any Two questions. Each question carries 5 weight   (2x5=10)

19. Explain Effect of solvent on UV visible absorption spectroscopy.

20. (i) The proton NMR spectrum for a compound with formula C_8H_{18} shows only one peak at 0.86 ppm. The carbon-13 NMR spectrum has two peaks, a large one at 26 ppm and a small one at 35 ppm. Draw the structure of this compound.

(ii) The proton NMR spectrum for a compound with formula $C_5H_{12}O_2$ is shown below. The normal carbon-13 NMR spectrum has three peaks. The DEPT-135 and DEPT-90 spectral results are tabulated. Draw the structure of this compound.

Normal Carbon	DEPT-135	DEPT-90
15 ppm	Positive	No peak
63	Negative	No peak
95	Negative	No peak

Proton spectrum

$C_5H_{12}O_2$

2.07   4.03   5.93
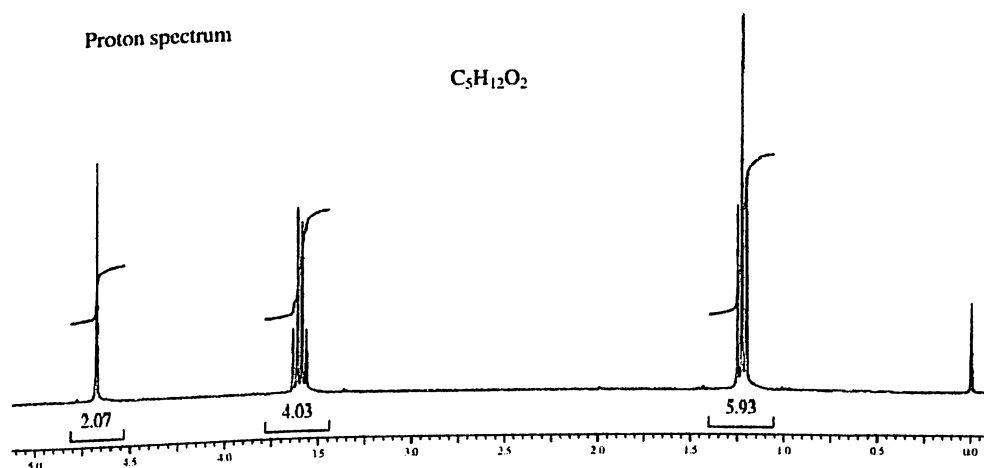
21. Describe the GC-MS technique.

22. Discuss the spectral analysis of i) Benzil-benzilic acid rearrangement ii) Fries rearrangement