

STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted during the academic year 2015-16 & thereafter)

SUBJECT CODE: 15CH/MC/SP64

B.Sc. DEGREE EXAMINATION, APRIL 2018
BRANCH IV - CHEMISTRY
SIXTH SEMESTER

COURSE : MAJOR – CORE
PAPER : SPECTROSCOPY
TIME : 3 HOURS

MAX. MARKS : 100

SECTION – A

ANSWER ALL THE QUESTIONS.

(30x1=30)

I Choose the correct answer:

- The molecule which is an example of symmetric rotator is
a) CO₂ b) CH₄ c) CHCl₃ d) H₂O
- The peak intensity ratio of quartet signal in ¹H NMR is _____.
a) 1:1:1:1 b) 1:2:2:1 c) 1:3:3:1 d) 1:4:4:1
- Which of the following statements is incorrect?
a) mass spectrometry gives information about fragmentation patterns.
b) parent ions are not always observed in the mass spectra of compounds
c) isotopic distribution patterns are observed in mass spectra
d) mass spectrometry provides direct structural data
- Which statement is incorrect about CO₂?
a) CO₂ has 2 stretching modes of vibration
b) The IR spectrum of CO₂ shows 4 absorptions
c) CO₂ has two degenerate bending modes of vibration
d) CO₂ is linear
- In which region of the electromagnetic spectrum does an absorption at 600 nm come?
a) near UV b) Vacuum UV c) Infra red d) visible
- The ¹³C NMR spectrum of a compound A contains two signals and in the ¹H NMR spectrum there is a singlet. Which compound is consistent with these data?
a) ethanol b) dichloroethane c) bromoethane d) acetone
- In the mass spectral analysis m/e value of tropylium cation observed at _____.
a) 91 b) 44 c) 100 d) 60
- The number of types of protons that are present in propyl bromide is _____.
a) 2 b) 3 c) 4 d) 5
- Which among the following cannot be used as a solvent in NMR spectral analysis?
a) CCl₄ b) CS₂ c) CDCl₃ d) C₆H₆
- Which of the following nuclei will cause absorption in the NMR spectroscopy?
a) C¹³ b) O¹⁶ c) H² d) C¹²

II Fill in the blanks:

11. In the case of chloro compounds, M^+ and $[M^+ + 2]$ peaks are formed with the intensity ratio _____.
12. The spectral technique that is used in astrophysical applications is _____.
13. The theoretical number of fundamental vibrations of CO_2 molecules is _____.
14. The number of spin states of 1H is _____.
15. The peak arising out of reaction that occur outside the ionization chamber but before magnetic analyser of the mass spectrometer is known as _____.
16. For a nucleus with nuclear spin quantum number $I=1/2$, the value/s of m_I is/are _____.
17. A source used in UV-Visible spectrometer is _____.
18. The characteristic stretching vibrations of $C=O$ group in aldehyde is observed at _____ cm^{-1} .
19. The interaction of magnetic fields of two or more nuclei is called _____.
20. The radiations scattered with a frequency higher than the incident beam is called _____.

III State whether true or false:

21. Homonuclear diatomic molecules are microwave active.
22. The λ_{max} value of aniline shows hypsochromic shift in acidic medium than in neutral solvent.
23. Water is a good solvent for recording IR spectra of water-soluble compounds.
24. Chemical shifts are larger when shielding effects are greater.
25. A conventional mass spectrometer employs high energy UV radiation.

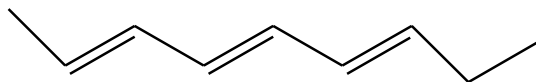
IV Answer briefly in one or two lines:

26. What is an electromagnetic spectrum?
27. Define mutual exclusion principle.
28. What are Stokes lines?
29. What is coupling constant and how does it influence the NMR peak of 1-bromopropane?
30. What is a metastable peak?

SECTION – B**ANSWER ANY FIVE QUESTIONS:****(5X6=30)**

31. The microwave spectrum of $^{12}C^{16}O$ shows lines spaced 3.8626 cm^{-1} apart. Calculate the moment of inertia and the C-O bond length.
32. a) Between acetylenic and aromatic protons which will be observed at a higher chemical shift value (δ). Why? (3)
 b) Compounds with molecular formula C_5H_{12} and C_8H_{18} show only one signal in the NMR spectrum find their structure. (3)

33. Distinguish between 1-pentene and 2-pentene using Mass spectroscopic technique.
 34. How many signals CH_3CHO have in ^1H NMR and ^{13}C NMR spectra?
 35. Differentiate between IR and Raman Spectroscopy.
 36. Draw the block diagram of a double beam UV- visible spectrophotometer and explain its parts.
 37. a) Estimate the λ_{max} for the compound shown:



- b) What are the effects of conjugation and aromaticity on UV-Vis absorption spectroscopy?

SECTION – C

ANSWER ANY TWO QUESTIONS:

2X20=40

38. a) What type of absorption shift is observed when aniline is in less polar solvent and HCl?
 b) What are the various types of absorption and intensity shifts in electronic transition?
 c) State Frank Condon principal.
 d) Draw Jablonskii diagram and mention various processes involved in it.
 e) Explain Nitrogen rule. (4+4+4+5+3)
39. a) Discuss the factors affecting chemical shift
 b) What is the moment of inertia, I_B , of $^1\text{H}^{79}\text{Br}$ if the bond distance is 142 pm? Atomic masses are: $^1\text{H} = 1.008$, $^{79}\text{Br} = 78.92$.
 c) Write the expected IR band values for the following compounds:
 (i) acetone (ii) ethanol
 d) Discuss the sampling technique used in IR spectrometry. (7+3+4+6)
40. a) Mention the significances of isotopic peaks in mass spectral analysis .
 b) Give the fragmentation pattern and m/e values of $\text{CH}_3\text{CH}_2\text{COCH}_3$ under mass spectral condition.
 c) An organic compound of molecular formula $\text{C}_8\text{H}_8\text{O}$ shows the following spectral data:
 UV: λ_{max} 238 nm (ϵ 10,000) 318 (ϵ 40)
 IR: sharp bands at 1400, 1500, 1600 cm^{-1} and a intense band at 1725 cm^{-1}
 Mass spectra: base peak m/e 43, another peak at 105
 ^1H NMR: δ 7.5 (5H, m); δ 3.5(3H, s)
 Predict the structural characteristics of the given spectral data and elucidate the structure of the compound. (5+5+10)

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