

M.Sc. DEGREE EXAMINATION, NOVEMBER 2014
BRANCH IV- CHEMISTRY
THIRD SEMESTER

REG.NO

COURSE : CORE
PAPER : MOLECULAR SPECTROSCOPY
TIME : 30 MINUTES


MAX.MARKS : 20

SECTION – A

(20x1=20)

Answer all the questions:

I. Choose the correct answer:

- The presence of M-15 or M-18 or M-31 peak confirms the presence of
a) Molecular ion peak b) CH₃ peak c) H₂O peak d) –OCH₃ peak
- How many signals do you get for the following compound in ¹³C NMR

a) 2 signals b) 3 signals c) 4 signals d) 5 signals
- The selection rules for Vibrational-Rotational spectra is
a) $\Delta J = 0, \Delta v = \pm 1$ c) $\Delta J = 0, \pm 2, \Delta v = \pm 1$
b) $\Delta J = 0, \Delta v = \pm 1, \pm 2$ d) $\Delta J = 0, \pm 2, \Delta v = \pm 1, \pm 2$
- In o-nitrophenol the O-H stretching frequency has a lower value than expected. This is due to
a) Weak O-H bond c) Strong electrostatic interaction
b) Exists in resonance hybrid d) All the three
- Benzene shows a B- band at 256 nm, ϵ_{\max} 200, whereas aniline shows B-band at 280 nm, ϵ_{\max} 1430. The change in ϵ_{\max} value is called
a) Bathochromic b) Hypsochromic c) Hyperchromic d) Hypochromic

II. Fill in the blanks:

- Methanol/ethanol is a good solvent for ----- spectroscopy.
- Raman active molecules should have -----.
- Molecular mass can be easily obtained in mass spectra by -----.
- In PMR shift reagents are very much useful for ----- signals.
- In Rayleigh scattering $\Delta J =$ ----- .

III. State whether true or false:

11. Frequency is the number waves passing through a point in a minute.
12. Acetone will not respond to UV-Vis region, since it is a solvent.
13. Meta stable peak is always broad in NMR.
14. Catalysts always change the λ_{\max} value not the ϵ_{\max} value.
15. Mass spectrograph M^+ ion peak is always the most intense peak.

IV. Match the following:

IR spectrum of methyl salicylate shows the following absorption bands, match them with their respective groups.

- | | |
|-------------------|-----------------------|
| 16. 10000 nm | 3300 cm^{-1} |
| 17. C=O | 2990 cm^{-1} |
| 18. CH_3 | 1700 cm^{-1} |
| 19. O-H | 1590 cm^{-1} |
| 20. aromatic ring | 1540 cm^{-1} |
| | 1000 cm^{-1} |

STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2011–2012 and thereafter)

SUBJECT CODE: 11CH/PC/MS34

M.Sc. DEGREE EXAMINATION, NOVEMBER 2014
BRANCH IV- CHEMISTRY
THIRD SEMESTER

COURSE : CORE

PAPER : MOLECULAR SPECTROSCOPY

TIME : 2½ HOURS

MAX.MARKS : 80

SECTION – B

(5 x 8 = 40)

Answer any FIVE questions:

1. a) What is effect of hydrogen bonding in UV absorption? (4)
b) How will you prove if an unknown molecule has a centre of symmetry? (4)
2. a) How will you distinguish inter- and intra- molecular hydrogen bonding with IR Spectroscopy. (4)
b) Water can be used as a solvent for Raman but not for IR why? (4)
3. a) List the factors affecting the coupling constant J. (4)
b) What is chemical shift and list the factors affecting it? (4)
4. a) Discuss nitrogen rule as applied to mass spectrometry. (4)
b) What is meant by M + 1 and M + 2 peaks in mass spectra? (4)
5. a) Differentiate base from parent peak. (4)
b) Explain the basic principle of mass spectroscopy. (4)
6. a) Deduce the structure of two isomeric compounds with the molecular formula with the given IR data i) 1710 cm^{-1} ii) 3300 cm^{-1} and 1640 cm^{-1} (4)
b) How is PMR useful in the detection of aromaticity? (4)
7. a) What is meant by fingerprint region in IR ? (4)
b) Explain the term 'Fermi resonance' (4)

SECTION – C

(2 x 20 = 40)

Answer any TWO questions:

8. a) Brief about lasers, their types and their role in electromagnetic spectroscopy? (5)
b) Explain Raman shift and Mutual exclusion principle. (5)
c) Give a explanatory note on spin-spin decoupling and nuclear overhauser effect. (5)
d) A hydrocarbon exhibits peaks at m/e 100 (M^+), 85, 71, 57, 43 (100 %), 41 and 29 in the mass spectrum. Deduce the structure of hydrocarbon and give its fragments. (5)

9. a) Calculate the number of fundamental vibrations possible in ethanol and oxygen? (6)
- b) A compound $C_{10}H_{13}Cl$ gave δ 1.57, singlet, 6H; δ 3.07, singlet, 2H;
 δ 7.27, singlet, 5H; – NMR data. Deduce its structure. (7)
- c) Outline the mode of fragmentation leading to the ions causing peaks at m/e in the mass spectra of pentanoic acid, at m/e 60 and diethylamine, at m/e 30. (7)
10. a) List the difference between Raman and fluorescence spectra. (5)
- b) Give an account of vicinal and germinal couplings in PMR spectra. (5)
- c) Account for the effect of deuterium substitution on CMR signals. (5)
- d) How will you distinguish 3-methylcyclohexane from 4- methylcyclohexane using mass spectroscopy? (5)
