

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

SUBJECT CODE: 11CH/PC/MS34
M.Sc. DEGREE EXAMINATION, NOVEMBER 2012
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:

- For a molecular species, which of the following terms are a function of concentration
(i) Absorbance (ii) Percent transmission (iii) Transmittance (iv) All
- A diene has λ_{\max} at 175nm. It may be
(i) 1,3-butadiene (ii) 1,3,5-hexatriene (iii) 1,4-pentadiene (iv) none
- Which of the following molecules is microwave inactive?
(i) H_2 (ii) HCl (iii) CO (iv) $CHCl_3$
- The Raman active vibrational mode of water molecule is
(i) symmetric stretching (ii) asymmetric stretching (iii) bending (iv) all
- Coupling constant reaches its maximum value for a dihedral angle of
(i) 90° (ii) 60° (iii) 80° (iv) 0°

II Fill in the blanks:

- Vibrational rotational spectra are found in _____ region.
- $n \rightarrow \pi^*$ transitions require _____ amount of energy among all transitions.
- _____ is the most widely used infra red detector.
- Water is a _____ top molecule.
- The high resolution of 2D NMR spectrum of H_2O consists of a _____.

III State whether the following statements are true or false:

- Radio waves have the shortest wavelength.
- Hydrogen bonding shifts the absorption towards shorter wave length.
- Number of vibrational degrees of freedom in CO_2 is 4.
- The presence of PR branch indicates that the molecule is non-linear.
- Enantiotopic protons have the same chemical shift and give only one NMR signal.

IV. Match the following:

- | | |
|------------------------|------------------------|
| 16. Base peak | (i) Coherent radiation |
| 17. NMR | (ii) IR spectroscopy |
| 18. Laser | (iii) UV spectroscopy |
| 19. Globar | (iv) Most intense peak |
| 20. Barrier-Layer cell | (v) TMS |

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COURSE : CORE
PAPER : MOLECULAR SPECTROSCOPY
TIME : 2½ HOURS

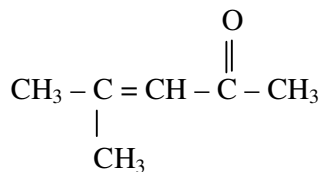
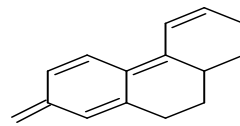
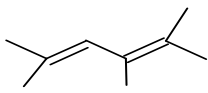
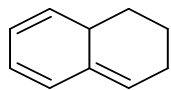
MAX.MARKS : 80

SECTION – B

(5 x 8 = 40)

Answer any five questions:

- (i) UV absorption peaks are broader than IR absorption peaks. Explain.
(ii) Why do amines absorb at a higher wavelength than alcohols?
- Derive an expression for J_{\max} of a rotational spectrum.
- Discuss the factors affecting chemical shift values in NMR.
- (i) Sketch the Morse curve for an anharmonic oscillator and explain.
(ii) Write a note on hot bands.
- (i) Discuss solvent effects of electronic spectra.
(ii) Explain Frank- Condon principle.
- (i) Write short notes on Stokes and Anti-Stokes lines.
(ii) Compare Raman and IR spectroscopy.
- Determine the λ_{\max} of the following compounds.



SECTION – C

(2 x 20 = 40)

Answer any two questions:

8. (i) Discuss McLafferty rearrangement
 (ii) State – Nitrogen rule
 (iii) Explain the NMR spectrum of pure and commercial ethanol
 (iv) Explain Nuclear Overhauser effect
 (v) Write a note on spin spin splitting. (5+3+5+5+2)
9. (a) How will you distinguish between the following compounds by IR spectral studies?
 (i) Phenol and cyclohexanol
 (ii) cis and trans – 2- butene.
 (b) Explain shielding and deshielding of a nucleus.
 (c) How will you distinguish between inter and intra molecular hydrogen bonding on the basis of ^1H NMR spectroscopy?
 (d) Predict the fragmentation pattern of diphenyl ether.
 (e) How will you distinguish among the three isomeric butanols on the basis of mass spectrometry? 1-butanol , 2- butanol and 2-methyl-2-propanol. (4+4+4+4+4)
10. (a) An organic compound containing C,H,O only showed abundant mass spectral peaks at $M^+(m/z\ 136)$, base peak ($m/z\ 91$) and fragment ion ($m/z\ 45$). Other spectral data are
 UV : $\lambda_{\text{max}} = 229\text{nm}$ and 257nm .
 IR : $\nu_{\text{max}}\ 1710\text{cm}^{-1}$
 ^1H NMR : $\delta 7.2$ (5H,s) and $\delta 3.5$ (2H,s).
 Deduce the structure of the compound and predict the principal ions in its mass spectrum.
 (b) Write a note on Fermi resonance.
 (c) Why R branch lines are closely placed at higher wave numbers and P branch lines are widely spaced at lower wave numbers? (12+4+4)

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