M.Sc. (Part-II) (Chemistry) (CBCS Pattern) Sem-IV

PSCHT13 - Spectroscopy Paper-XIII

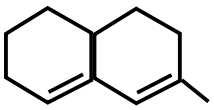
P. Pages : 3 **GUG/W/22/11448**

Time : Three Hours * 2 1 1 7 * Max. Marks : 80

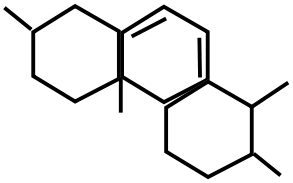
Notes : 1. All questions are compulsory.
2. All questions carry equal marks.
3. Use of calculator is allowed.

1. a) Explain the Fiesher Woodward rules for dienes. Also calculate the λ_{max} value of the following compounds. **8**

A)



B)



b) i) Explain the basic principle of photoelectron spectroscopy. **8**

ii) What is the basis for qualitative and quantitative analysis in ESCA technique?

OR

c) State and explain the Frank-Condon principle. **4**

d) Derive Beer Lamberts Law and give its limitations. **4**

e) State and explain Koopmans theorem. And also explain the basic idea about Auger electron spectroscopy. **4**

f) Discuss the various electronic transition in UV-visible spectroscopy. **4**

2. a) Define chemical shift. Explain the various factors affecting the chemical shift. **8**

b) i) Explain the theory of spin-spin interaction for an AMX and AX_2 type case. **8**

ii) A neutral compound with molecular formula $C_6H_{10}O_2$ shows the following signals in ^{13}C -NMR, suggest probable structure for the compound.
^{13}C – NMR δ : 6.3(q), 15.3(q), 71.1(t), 119.9(s), 168.4(d), 191.8(d).

OR

c) Describe the role of shift reagent in NMR spectroscopy. **4**

d) Explain the variation of coupling constant with dihedral angle. **4**

e) Explain the following in ^1H NMR spectroscopy. **4**
i) Resonance condition. ii) Spin-spin interaction.

f) Discuss the ^{19}F – NMR spectroscopy in detailed. **4**

3. a) Assign the structures of compound M and N on the basis of data given below; **8**

$$\text{compound M} \xrightarrow[\text{ii) } AlCl_3/CS_2 \\ \text{iii) Zn/Hg-HCl}]{\text{i) } PCl_5} \text{compound N}$$

Mol. Formula	Mol. Formula
$C_{11}H_{14}O_2$	$C_{11}H_{14}$
^1H – NMR δ : 1.22(s, 6H)	^1H – NMR δ : 1.21(s, 6H)
2.0(s, 2H)	1.85(t, J=6Hz, 2H)
7.0(s, 5H)	2.83(t, J=6Hz, 2H)
10.10(s, 1H. ex.)	7.02(m, 4H)

b) Explain the following terms, **8**
a) Quadrupole nuclei. B) Quadrupole moment.

OR

c) Discuss the advantages of FT-NMR. **4**

d) Explain the DEPT method with suitable example. **4**

e) Deduce the structure of compound having molecular formula C_3H_6O which give following spectral data, **4**
IR : 1200-1280 cm^{-1}, PMR : δ 1.32 (d, J=6Hz, 3H), 2.42(dd, J=3.5 & 2.5Hz, 1H), 2.72(dd, J=3.5 & 3.0Hz, 1H) 2.98(ddq, J=2.5, 3.0 & 6Hz, 1H) ppm.

f) Explain Nuclear overhausser effect. **4**

4. a) Give a brief account of Bragg's method used in the elucidation of crystal structure. What are the limitations of Bragg's method? **8**

b) Discuss the applications of electron diffraction technique. **8**

OR

c) Write a note on intensity in x-ray diffraction. **4**

d) Define and explain the term 'structure factor' used in XRD. **4**

e) Write Wierl equation and explain the terms involved in it. **4**

f) Give the application of neutron diffraction technique. **4**

5. a) Give the effect of solvent on $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transition in $\alpha,\beta-$unsaturated compound. **2**

b) A 1.0×10^{-5}M solution of a compound has a % transmittance of 50 at $\lambda_{max} = 280\,nm$ when a 1.0 cm cell is used. Calculate the ε_{max} of 280 nm. **2**

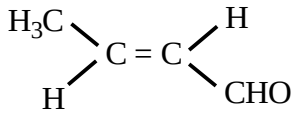
c) Why TMS is used as reference in NMR? **2**

d) Calculate the precessional frequency of a proton in a field of 1.8 T & factor for proton is 5.585. **2**

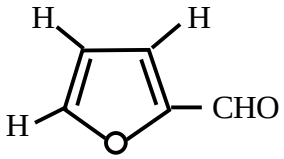
e) Write a short note on APT technique. **2**

f) Show the total number of signals in the following compound. **2**

i)



ii)



g) Calculate Miller indices of crystal planes which cut through the crystal axes of **2**
i) 2a, 3b, c ii) 2a, -3b, -3c.

h) Explain, magnetic scattering of neutron by a paramagnetic crystal in random one? **2**

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