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

PSCCHT13 / PSCHT13 - Spectroscopy Paper-XIII

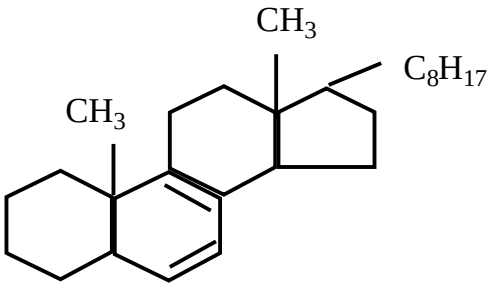
P. Pages : 3 **GUG/S/18/20148**

Time : Three Hours * 3 0 2 7 * Max. Marks : 80

Notes : 1. All questions are compulsory.
2. All questions carry equal marks.

1. a) i) Give applications of Auger electron spectroscopy. **8**

ii) Calculate λ_{max} for the following compound.



b) i) Derive Beers Lambert law & give it's limitations. **8**

ii) The λ_{max} for ethylene is about 185 nm while for 1,3 butadiene is 217 nm, Explain using energy level diagram.

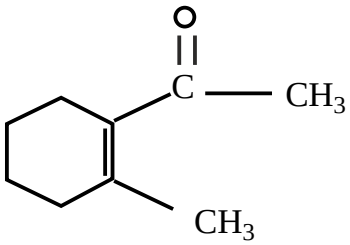
OR

c) Give the short note on photoelectron spectroscopy. **4**

d) For 1.0×10^{-4} m solution of compound in hexane λ_{max} & $\in_{max}$ are 220 nm & 14,500 respectively. Calculate % transmission. **4**

e) Explain the term Bathochromic shift. Why benzene show λ_{max} at 203 nm and phenol at 235 nm. **4**

f) Calculate λ_{max} for ethanolic solution in the given compound. **4**



2. a) i) Give the splitting pattern for AMX and AX_2 type of molecule. **8**

ii) Predict the structure of compound from the following PMR Data, mol. Formula ($C_9H_{10}O$) PMR :

δ 2.3 (S, 3H)

δ 2.5 (S, 2H)

δ 7.5 (M, 5H)

b) i) The PMR spectrum values of 2, 2, trifluoroethanol are given below : **8**

i) δ 3.38 (S, 1H) Disappeared on D_2O

ii) 3. 93 (q, 2H) J = 9 H_2

Account for only these peak in PMR spectrum.

ii) The 400 MHz PMR spectrum of an organic compound exhibit doublet. The two lines are at δ2.35 & 2.38 calculate the coupling constant 'J'.

OR

c) Define chemical shift. Explain the factors affecting the chemical shift. **4**

d) Predict the structure of compound from ^{13}C NMR having molecular formula - **4**
$C_3H_5Cl_3$ & ^{13}C NMR Data

δ 32 q, (quarlet)

δ 54 t (triplet)

δ 87 s (singlet)

e) Deduce the structure of organic compound having PMR Data **4**
δ in PPM : – 3.4 (S, 3H)

6.6 (d, 2H)

7.5 (d, 2H)

9.5 (S, 1H)

Molecular formula is $C_8H_8O_2$.

f) Write a note on shift reagent. **4**

3. a) An organic compound $C_9H_{10}O_2$ gives the following spectral data : **8**

UV : λ_{max}, 257 nm

IR : Significant absorption band at 3040, 2950, 1740, 750, 700 cm^{-1}

PMR : δ(1.96) (S, 3H)

5.00 (S, 2H)

7.22 (S, 5H)

m/ s : m/ e 150 (M^+) , 108, 91, 77

Deduce the correct structure.

b) i) Write note on DEPT ^{13}C spectra.

ii) Write note on quadrupole nuclei & quadrupole moment. **8**

OR

c) Explain cos Y technique with suitable example. **4**

d) Give the structure of the compound having following spectral results mol. Formula **4**
$C_{10}H_{14}O$

PMR : δ in PPM 1.21 (6H, d, J = 7Hz)
2.83 (1H, septate J = 7Hz)
3.72 (3H, S)
6.74 (2H, d J = 9Hz)
7.18 (2H d J = 9Hz)

Show the peak at m/e 43.

e) Give the advantages of FT - NMR. **4**

f) Discuss the APT technique in brief. **4**

4. a) Give the application of Electron diffraction techniques. **8**

b) Derive Bragg's equation. How it is useful for structure identification of unit cell. **8**

OR

c) Explain the term magnetic scattering. **4**

d) Write a note on Wierl equation. **4**

e) Give Laue method for identification of unit cell. **4**

f) Write a note on Ramchandran diagram. **4**

5. a) Define with suitable examples. **2**
i) Chromophore
ii) Auxochrome

b) Give the effect of solvent on $\pi - \pi^*$ and $n - \pi^*$ transition in α, β-unsaturated compound. **2**

c) Compare ^{13}C-NMR spectroscopy with ^{1}H NMR spectroscopy. **2**

d) Write a note on geminal coupling constant. **2**

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

f) Write a note on nuclear overhauser effect. **2**

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

h) Compare scattering intensity vs scattering angle. **2**

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