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A-44

SEAT No. _____

No of printed pages : 04 + 06

SARDAR PATEL UNIVERSITY

M.Sc. SEMESTER-IV (Organic Chemistry) Examination

22/10/2018, Monday

Spectroscopy-II [PS04CORC01]

Time: 02:00 p.m. to 05:00 p.m.

PS04 CANCO.1
PS04 C.I.PC01

Total Marks: 70

Q.1 : Answer the following multiple choice questions.

[08]

- 1) Finger print region in IR is observed at -----
a) 1200-1500cm⁻¹ b) 1000-1500cm⁻¹ c) 900-1500cm⁻¹ d) 650-1500cm⁻¹
- 2) In UV, electronic transition shown by methanol is _____.
a) n → π* b) n → σ* c) π → π* d) σ → π*
- 3) In PMR spectrum of mesitylene ____ signals are obtained.
a) 4 b) 3 c) 2 d) 1
- 4) The pople notation for the protons in ethyl chloride is _____.
a) A₂M₃ b) A₃M₂ c) A₃B₂ d) A₃X₂
- 5) In ¹³C-NMR spectrum p-benzoquinone will give ____ signals.
a) 4 b) 6 c) 2 d) 3
- 6) The DEPT-90 spectrum will show only ____ signals.
a) -CH b) -CH₂ c) -CH₃ d) None
- 7) In Mass spectra, the ionization in MALDI technique is done by---
a) Xenone beam b) Laser beam c) high electric voltage d) chemical reaction
- 8) As the degree of branching decreases , the relative height of molecular ion peak ____
a) remains constant b) becomes zero c) decreases d) increases

Q.2 : Answer the following . (Any seven)

[14]

- 1) In UV spectra ethylene absorbs at 165 nm while 1,3-butadiene absorbs at 217 nm. Explain.
- 2) Explain the Fermi resonance in IR.
- 3) Write and explain all types of vibrations observed in IR spectroscopy.
- 4) Sketch the ¹H-¹H COSY spectra for ethyl chloride using approximate δ value.

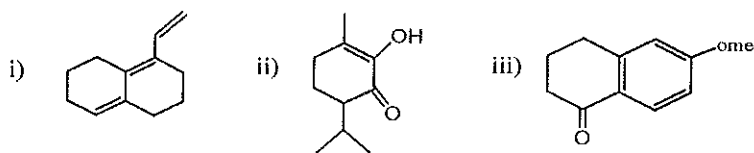
①

(P.T.O.)

- 5) Discuss the germinal coupling with example.
- 6) Sketch the proton coupled and proton decoupled ^{13}C -NMR spectra for n-pentane.
- 7) How will you differentiate o, m & p-dinitrobenzene using ^{13}C -NMR spectroscopy.
- 8) Write a note on chemical ionization method used in mass spectroscopy.
- 9) Predict the fragmentation pattern of diphenyl ether having molecular ion at m/z -170.

Q. 3 : Answer the following questions.

- A) i) Discuss the important IR absorptions shown by alcohol and phenol. [03]
 ii) Write a short note on chromophore and Auxochrome. [03]
- B) Calculate the λ_{max} for the following compounds. [06]

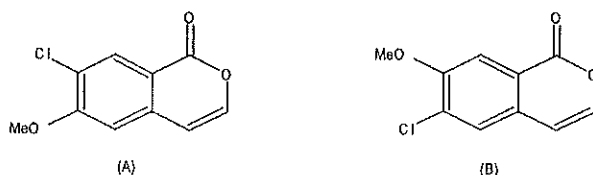


OR

- B) Discuss the important characteristics vibrations observed in the IR spectra of acids and amides. [06]

Q. 4 : Answer the following questions.

- A) i) What is coupling constant in PMR? Discuss Long range and Vicinal couplings in detail. [03]
 ii) Explain nuclear Overhauser effect in PMR. How will you differentiate following isomers using NOE PMR spectra? [03]



- B) i) Write a short note on D_2O exchange in PMR. [03]

- ii) A compound has a molecular formula $C_9H_{10}O_2$. It gives the following signals in PMR spectrum. Assign the structure of the compound by interpreting PMR data. [03]

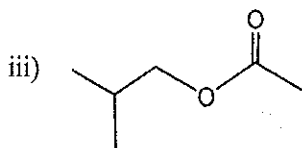
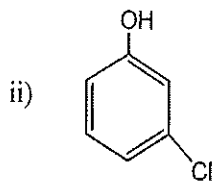
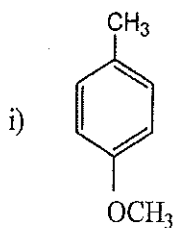
Signal position δ	Multiplicity	Protons
3.55	Singlet	2H
3.60	Singlet	3H
7.35	Singlet	5H

OR

- B) i) Sketch the expected PMR spectrum for pure ethanol and show that it is an AMX system with two different coupling constants. [03]
- ii) List the methods used for simplification of PMR spectra. Discuss the use of shift reagent in detail. [03]

Q. 5 : Answer the following questions.

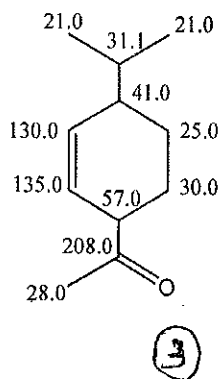
- A) Do the ^{13}C NMR Chemical shift calculation for the following molecules. [06]



- B) i) Calculate the chemical shift values for each carbon signals and sketch the proton coupled and decoupled ^{13}C NMR spectra for p-methoxy benzaldehyde. [03]
- ii) Sketch the HMBC spectrum for 3-heptanone by taking approximate δ -value for each signal. [03]

OR

- B) i) Sketch proton decoupled ^{13}C NMR DEPT 45° , DEPT 90° and DEPT 135° spectra for following compounds. (δ values for each carbon is assigned in the structure) [03]



(P.T.O)

- ii) A compound with molecular formula $C_5H_{10}O_2$ shows following signals in its proton coupled ^{13}C NMR. Interpret the data and assign the structure of the compound. [03]

20.4 δ (Quartet)

21.4 δ (Quartet)

66.8 δ (Doublet)

170 δ (Singlet)

Q. 6 : Answer the following questions.

- A) Do the mass fragmentation for the following molecules. [06]

i) 2-methyl pentane ii) Benzamide iii) 2-pentanone

- B) i) Write a short note on McLafferty rearrangement. [03]

ii) Discuss the Fast atomic bombardment (FAB) and Electron spray ionization techniques used in Mass spectroscopy. [03]

OR

- B) A compound has molecular formula $C_7H_{12}O_3$. It gives the following spectral data. [06]

Interpret spectral data and determine the structure of the compound.

IR(cm^{-1}) : 2960, 1725, 1160 and 1030.

1H NMR :

Signal δ	Multiplicity	Protons
1.25	triplet	3H
2.20	singlet	3H
2.55	triplet	2H
2.75	triplet	2H
4.10	quartet	2H

^{13}C NMR :

^{13}C (δ)	Multiplicity
14	+ ve
28	- ve
29	+ ve
37	- ve
60	- ve
172	-
208	-

Mass (m/z) (% r.a.): 144(5%), 129(20%), 116(2%), 101(20%), 99(50%), 74(20%), 55(15%), 43(100%).

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(4)