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ICH 501

**III Semester M.Sc. Degree Examination,
November/December 2019**

INDUSTRIAL CHEMISTRY

Spectroscopic Techniques

Time : 3 Hours]

[Max. Marks : 70

Instructions :

- (i) Answer any five subdivisions from Part A and any five questions from Part B.
- (ii) Figures to the right indicate marks.

PART - A

Answer **any five** questions :

(5 × 2 = 10)

1. (a) Sketch the Morse PE diagram for an anharmonic oscillator.
- (b) State and explain the rule of mutual exclusion.
- (c) Write the mathematical expression for the Beer-Lambert law and elaborate the terms.
- (d) How do electron withdrawing (-I) groups shift the position of the carbonyl frequency in IR spectroscopy.
- (e) Predict the structure of following molecule given data :

Molecular formula :

C_3H_7NO : ^1H NMR (400 MHz), δ ppm : 2.22 (s, 3H) ; 2.81 (s, 3H) ; 6.71 (bs, 1H)



ICH 501

- (f) Sketch the Karplus curve in ^1H NMR spectroscopy and highlight its importance.
- (g) Highlight the significance of the base peak in mass spectrometry.
- (h) Aromatic hydrocarbons normally exhibit their molecular ion peak as the base peak. Why?

PART - B

Answer **any five** full questions :

(5 × 12 = 60)

- 2. (a) With suitable example, discuss the effect of isotopic substitution in microwave spectroscopy.
- (b) Using Hooke's law, obtain an expression for the frequency of vibration for a diatomic molecule.
- (c) Outline the quantum theory of Raman effect. **(4 + 4 + 4)**
- 3. (a) Discuss the rotational spectra of polyatomic molecules with special reference to symmetric and asymmetric top molecules.
- (b) Give the quantum mechanical basis of the Frank-Condon principle.
- (c) How does the breakdown of the Born-Oppenheimer approximation effect the P and R branch line of the vibration-rotation spectrum of a diatomic molecule. **(4 + 4 + 4)**
- 4. (a) With the help of a neat diagram, discuss solvent effects prevalent in effecting the position of bands UV-visible spectroscopy.
- (b) Write an account of the Woodward-Fieser rules to predict the λ_{max} of conjugated dienes.
- (c) With suitable examples, illustrate how inter and intra molecular H-bonding may be differentiated by IR spectroscopy. **(4 + 4 + 4)**



5. (a) What are Fermi-resonance bands? Illustrate the usefulness of the bands in distinguishing aldehydes from ketons.
- (b) How are the following compounds distinguished by IR spectroscopy?
- (i) Phenol
 - (ii) Aniline and
 - (iii) Nitrobenzene
- (c) Predict the UV λ_{max} for the following aromatics :
- (i) 2-hydroxy benzaldehyde
 - (ii) 2-hydroxy benzoic acid and
 - (iii) 2-hydroxy acetophenone. (4 + 4 + 4)
6. (a) Briefly outline the principle and working of an FT-NMR instrument.
- (b) State and explain the first order splitting rules of ^1H -NMR spectroscopy.
- (c) Outline Pople's notation for spin-spin interactions. (4 + 4 + 4)
7. (a) Describe any two methods for the simplification of complex ^1H -NMR spectra.
- (b) Write an account on nuclear Overhauser effect.
- (c) Discuss the importance of 2D-NMR spectroscopy. (4 + 4 + 4)
8. (a) Describe any two methods for production of molecular ions of organic molecules.
- (b) Sketch the fragmentation pattern of (i) cyclohexene and (ii) 2-heptanone.
- (c) How are mono-chloro and mono-bromo-alkanes distinguished by EI-MS? (4 + 4 + 4)

ICH 501



9. (a) Citing suitable examples, state and explain the nitrogen rule.
- (b) Write short notes on :
- (i) α -cleavage and
 - (ii) McLafferty rearrangement in the mass spectral fragmentations of carbonyl compounds.
- (c) Deduce the structure of an organic compound from the following data and assign the values :

Molecular formula : C_7H_9NO

UV λ_{max} : 293 nm

IR : 3460, 3381, 2869, 2951, 2832, 1513, 1241 and 1045 cm^{-1}

^1H NMR : δ : 6.66 (m, 4H), 3.72 (s, 3H) and 3.45 (s, 2H)

^{13}C NMR : δ : 152.7, 140.2, 116.3, 114.6 and 55.7

MS : m/e (relative intensity) : 123 (100%), 108 and 80. **(4 + 4 + 4)**
