G-1/162/22   Roll No. ....

I Semester Examination, January, 2022

M.Sc.

CHEMISTRY

Paper IV

(Basics of Spectroscopy)

Time : 3 Hours]   [Max. Marks : 80

Note : *All questions are compulsory. Question Paper comprises of 3 Sections. Section A is objective type/multiple choice questions with no internal choice. Section B is short answer type with internal choice. Section C is long answer type with internal choice.*

SECTION A   **1×8=8**

(Objective Type/Multiple Choice Questions)

Choose the correct answer :

1. The energies of E_1 and E_2 of two radiations are 25 eV and 50eV respectively. The relation between their wavelength, i.e. λ_1 and λ_2 will be :

   (a) $\lambda_1 = \frac{1}{2}\lambda_2$ (b) $\lambda_1 = \lambda_2$

   (c) $\lambda_1 = 2\lambda_2$ (d) $\lambda_1 = 4\lambda_2$

P.T.O.

2. The rotational constant (B) of $H^{35}Cl$, $H^{37}Cl$ and $D^{35}Cl$ follows the order :

   (a) $H^{35}Cl > D^{35}Cl > H^{37}Cl$

   (b) $H^{35}Cl > H^{37}Cl > D^{35}Cl$

   (c) $D^{35}Cl > H^{35}Cl > H^{37}Cl$

   (d) $H^{37}Cl > H^{35}Cl > D^{35}Cl$

3. Highest occupied molecular orbital of HF is :

   (a) Bonding   (b) Antibonding

   (c) Ionic   (d) Nonbonding

4. The absorption at λ_{max} 279 nm in the UV spectrum of acetone is due to :

   (a) π-π^* transition   (b) n-π^* transition

   (c) a-a* transition   (d) π-a* transition

5. The spectroscopic ground state symbols and total number of electronic transitions of $\left[Ti(CH_2O)_6\right]^{2t}$ are :

   (a) ^3Tig and 2   (b) ^3Arg and 3

   (c) ^3Tig and 3   (d) ^3Arg and 2

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6. Choose the correct answer for binding energy (I) and Kinetic energy :

(a) Kinetic Energy = $Hv - I$

(b) Kinetic Energy = $Hv + I$

(c) Kinetic Energy = $\dfrac{hv}{I}$

(d) Kinetic Energy = $Hv \times I$

7. For a non-linear molecule like H_2O the number of vibrational modes are :

(a) 3   (b) 4

(c) 5   (d) 6

8. For CO_2 molecule :

(a) All the vibrational modes are either IR or Raman active

(b) The number of IR and Raman active vibrations will be the same

(c) All vibraions are IR active

(d) None of the above

SECTION B   6×4=24

(Short Answer Type Questions)

Note : *Answer the following questions in* **250** *words.*

Unit-I

1. Write notes on the following :

(a) Born-oppenheimer approximation

(b) Absorption of radiations

Or

The rotational constant for $H^{35}Cl$ is observed to be 10.5909 cm^{-1}. What are the values of B for $H^{37}Cl$ and $^2D^{35}Cl$?
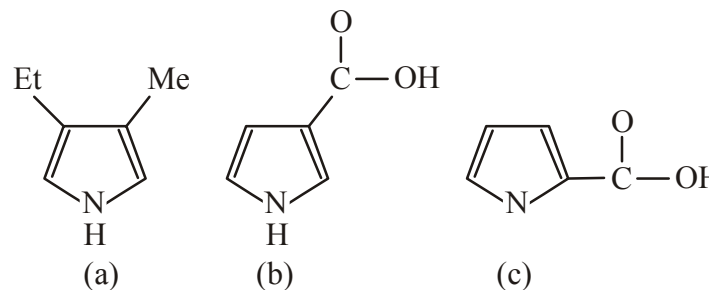
Unit-II

2. Write notes on the following :

(a) K and R bands

(b) Chromophores and Auxochromes

(c) Bathochromic and hypsochromic shifts.

Or

Explain the increasing order a → c of the λ_{max} for the following pyrrole derivatives :

(a)   (b)   (c)

Unit-III

3. Write notes on the following :

    (a) Frank-Condon Principle

    (b) Koopman's Theorem.

Or

Describe electronic Spectra of Polyatomic molecules with two examples.

Unit-IV

4. Discuss the factors which affect the IR Absorption frequency, band positions and intensities of functional group.

Or

What are the advantages of Raman spectroscopy over IR spectroscopy ?

SECTION C   12×4=48

(Long Answer Type Questions)

Note : *Answer the following questions in* **500** *words.*

Unit-I

1. (a) What is Selection Rule ? Write down the selection rule for rotational, vibrational and electronic energy levels transitions.

    (b) Explain effect of isotopic substitution on the transition frequency intensity in Microwave Spectroscopy by taking example of HCl and DCl.

Or

Explain the following terms :

    (a) Dispersion

    (b) Reflection

    (c) Polarization

    (b) Scattering.

Unit-II

2. Explain Woodward-Fieser rule for polyenes and α-β unsaturated carbonyl compounds with suitable examples.

Or

    (a) Calculate the molar absorptivity, ε for a solution containing 1.0×10^{-3} mole per liter of solute. When the absorbance of a 1 cm cell was 1.5.

    (b) Explain stereochemical Factors in electronic spectroscopy.

Unit-III

3. (a) Explain electronic spectra of polyatomic molecules with examples.

(b) Describe electronic spectra of Diatomic molecules and ions and draw MO diagram for homonuclear diatomic molecules.

Or

(a) Discuss basic principle, theory and application of photoelectron spectroscopy.

(b) Explain the following :

(i) Auger Electron Spectroscopy

(ii) Charge Transfer Spectra.

Unit-IV

4. (a) Write short notes on the following :

(i) P, Q, R branches in IR Spectroscopy

(ii) Morse Potential Energy.

(b) Write short note on Rotational Raman Spectra.

Or

(a) Discuss simple Harmonic Oscillator and Anharmonic Oscillator.

(b) Describe the Raman Spectroscopy in terms of :

(i) Classical Theory of Raman effect

(ii) Rule of Mutual Exclusion.

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