[This question paper contains 4 printed pages.]

Your Roll No. 2022

Sr. No. of Question Paper : 1005 C

Unique Paper Code : 32171501

Name of the Paper : Organic Chemistry IV: Biomolecules

Name of the Course : **B.Sc. (Hons)**

Semester : V

Duration : 3 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **6** questions. **All** Questions carry equal marks.

1. (a) (i) β- D-Glucose and α-D-Glueose have different specific rotations. When either anomer is dissolved in water, their rotations change until a fixed value results. Name the term used to describe this change and discuss the mechanism. (3)

   (ii) Draw Fisher projection of β-D-glucose, convert it to Haworth structure and then to the chair conformation. (3)

(b) A pentapeptide X having an empirical composition, Lys, Phe, Thr, Leu, Asp, gave DNP-Thr on treatment with DNFB followed by hydrolysis. Treatment of X with Carboxypeptidase released Asp. Treatment of X with Trypsin gave a tripeptide, (Lys, Leu, Thr) and a dipeptide (Asp, Phe). Elucidate the sequence of amino acids in X. What products are obtained on treatment of X with Chymotrypsin? (6.5)

2. (a) Differentiate between nucleosides and nucleotides. Draw the structure of Cytidine. (4)

(b) Define acid value and saponification value of an oil. Calculate the saponification value of glyceryl tripalmitate. (4.5)

(c) When D-Glucose is treated with dilute aqueous alkali, a mixture of D-Mannose, D- Fructose and D-Glucose is obtained. Explain the mechanism of this reaction. What is the name of this reaction? 4

3. (a) Outline significant differences between catabolism and anabolism. (3)

(b) Which steps in glycolysis consume ATP and which ones produce ATP? How many molecules of ATP are obtained from each molecule of glucose that is metabolized to pyruvate? (3.5)

(c) What is transcription. Explain. (6)

4. (a) Give the structure of disaccharide maltose. How was the nature of linkage between its two monosaccharide units established? (3)

(b) Give the reaction catalysed by the following enzymes. To which class of enzymes do they belong according to enzyme commission

(i) Phosphofructokinase

(iii) Fumarase (4)

(c) Explain the principal of electrophoresis. How can it be used to separate a mixture of Alanine, Lysine and Glutamic acid? (3.5)

(d) Give the structure of NAD+. (2)

5. (a) Explain oxidative rancidity in oils and fats giving an example. Suggest a method to prevent it. (4)

(b) Explain the term hardening of oils by taking a suitable example. (4)

(c) Explain the process of replication? (4.5)

6. (a) Discuss the effect of substrate concentration on the activity of an enzyme. (4.5)

(b) Give the products from the reaction of methyl α-D-Glucopyranoside with HIO_4. (2)

(c) Discuss the various steps involved in the TCA cycle giving the names of enzymes and structures of intermediates. (6)

7. (a) (i) Explain the use of dicyclohexylcarbodiimide (DCC) in peptide synthesis. Use chemical reactions to illustrate. (3)

(ii) Outline the synthesis of either Methionine or Proline using any method. (3.5)

(b) A carbohydrate **X** with molecular formula $C_{12}H_{22}O_{11}$ gives a positive test with Benedict reagent, it forms an osazone and undergoes mutarotation. Hydrolysis with aqueous acids or by emulsin produces only D-Glucose. Methylation of X gives an octamethyl derivative which on hydrolysis affords 2,3,4,6 tetra O-methyl D-Glucose and 2,3,4 tri-O-methyl D-Glucose. Workout the structure of X. (6)

8. (a) Give the reactions involved in Killiani -Fischer synthesis starting with D-arabinose.
What is the stereochemical relationship between the aldohexoses obtained? (4)

(b) What is allosteric inhibition? Explain using an example. (4.5)

(c) What are the different types of RNA? Explain the role of any one of them. (4)

[This question paper contains 8 printed pages.]

Your Roll No. 2022

Sr. No. of Question Paper : 1041 C

Unique Paper Code : 32171502

Name of the Paper : Physical Chemistry V: Quantum Chemistry & Spectroscopy

Name of the Course : **B.Sc. (Hons) Chemistry**

Semester : V

Duration : 3 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt **six** questions in all, **three** questions each from Sections **A** and **B**.
3. Attempt all part of a question together.
4. **All** questions carry equal marks.
5. Use of a non-programmable scientific calculator is allowed.

P.T.O.

Physical constants

Atomic mass unit	$=1.66 \times 10^{-27}$ kg
Planck's constant	$= 6.626 \times 10^{-34}$ J s
Velocity of Light	$= 3 \times 10^{8}$ m s^{-1}
Boltzmann constant	$= 1.381 \times 10^{-23}$ J K^{-1}
Mass of Electron	$= 9.1 \times 10^{-31}$ kg
Avogadro's number	$= 6.023 \times 10^{23}$ mol^{-1}
Nuclear magneton	$= 5.05 \times 10^{-27}$ J T^{-1}
Bohr magneton	$= 9.274 \times 10^{-24}$ J T^{-1}

SECTION A

(Quantum Chemistry)

1. (a) Discuss the postulates of quantum mechanics.

   (b) Write the complete Hamiltonian operator for Li atom explaining all the terms. Write the modified Hamiltonian operator after applying Born Oppenheimer approximation.

   (c) Show that the eigenvalues of a Hermitian operator are always real. (4.5,4,4)

2. (a) A particle of mass m, in a one-dimensional box of length a can be represented by the function, $\psi_n = \sin\frac{n\pi x}{a}$ $(n = 1,2,3...)$ Normalize the given function ψ_n and find whether it is an eigen function of (i) $\widehat{p_x}$ (ii) $\widehat{p_x^2}$.

(b) A particle of mass, m, in a one-dimensional box of length a can be represented by the following normalized trial wave function where N is the normalization constant.

$$\psi_{trial} = N\{x(a-x)\}$$

(i) Calculate the expectation value of energy, (E), of this particle in the ground state using the trial wave function.

(ii) Compare this energy with the actual energy. Calculate the percentage error.

(iii) Is the trial wave function acceptable? Explain on the basis of variation theorem.

(4.5,(4,2,2))

3. (a) Plot the radial functions and radial probability distribution functions for an electron in hydrogen atom for all wave functions having n = 2. Write the number of nodes in each case.

(b) Evaluate the expectation value of the radius, $\langle r \rangle$, at which the electron in the ground state of Hydrogen atom (Z=1) is found. Given the wave function for this state is

$$\psi_{1,0,0} = \frac{1}{\sqrt{\pi}}\left(\frac{z}{a_o}\right)^{\frac{3}{2}} e^{\frac{-Zr}{a_o}}$$ where a_o is the Bohr radius

and $\int_0^\infty r^n e^{-ar}\, dr = \frac{n!}{a^{(n+1)}}$.

(c) Giving reason, state which of the following are acceptable wave functions in the indicated interval.

(i) $\sin x$ $(0, 2\pi)$

(ii) e^{-x} $(-\infty, \infty)$

(iii) $\frac{1}{x}$ $(0, \infty)$

(iv) $\sin^{-1} x$ $(-1, 1)$ (4.5,4,4)

4. (a) By applying the procedure of separation of variables on the following Schrodinger equation for an electron in a hydrogen atom, derive three equations, one dependent on variable, r, second dependent on variable, θ and third dependent on variable, ϕ. In this equation ψ(r, θ, ϕ) is the function of three independent variables r, θ and ϕ. Considering ψ(r, θ, ϕ) = R(r) * Θ(θ) * Φ(ϕ),

$$\left[-\frac{h^2}{8\pi^2\mu r^2}\left\{\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)+\frac{1}{\sin^2\theta}\frac{d^2}{d\varphi^2}\right\}-\frac{z e^2}{r}\right]\psi = E\psi$$

(b) Set up the Hamiltonian operator for a particle oscillating about a mean position (a simple harmonic oscillator). Explain the significance of zero-point energy of a simple harmonic oscillator.

(c) Starting from the expression for total energy of a rigid rotator, setup the Schrodinger equation for the system in Cartesian coordinates.

(4.5,4,4)

SECTION B

(Spectroscopy)

5. (a) Chlorine gas is microwave and infra-red inactive but Raman active. Explain.

(b) How will the microwave spectrum of HCl^{35} change if Cl^{35} is replaced by Cl^{37}?

(c) The rotational spectrum of $^{79}Br^{19}F$ shows a series of equidistant lines 0.71433 cm^{-1} apart. Calculate the rotational constant, B, the moment of inertia and bond length of the molecule. (4.5,4,4)

6. (a) How do the P, Q and R branches arise in the Vibrational-Rotational spectrum. Why is Q branch not observed for most of the heteronuclear diatomic molecules?

(b) What is the ratio of the number of protons in each spin state at temperature 300 K, given that the ^1H NMR spectrometer is operating at 60MHz and $g_n = 5.585$ for the ^1H nucleus.

(c) The fundamental and first overtone transitions of $^{14}N^{16}O$ are centered at 1876.06 cm^{-1} and 3724.20 cm^{-1}, respectively. Calculate the equilibrium vibration frequency and anharmonicity constant.

(4.5,4,4)

7. (a) A molecule AB_2 has the following Infrared and Raman spectra :

v (cm^{-1})	Infrared	Raman
519	Active (PQR)	Active (Polarized)
1151	Active(PQR)	Active (Polarized)
1367	Active(PQR)	Active (Depolarized)

Predict the geometry of the molecule with justification and assign the observed wavenumbers to the specific vibration mode.

(b) What is Raman effect? Explain the origin of Stokes and Anti-Stokes line.

(c) Arrange the following groups in increasing order of their absorption frequencies: Give Justification

(i) CF, CCl, CBr, CH

(ii) C-C, C≡C, C=C (4.5,4,4)

8. (a) A ^1H NMR spectra of an organic compound with the molecular formula $C_3H_6Br_2$ gives three signals (p1, p2 and p3) with their respective intensity ratios as follows: 1(sixtet): 2 (doublet): 3(doublet) (δ values are in the order p1>p2> p3). Write the probable structure and justify your answer.

(b) Write short notes on any **two** of the following :

(i) Difference between internal conversion and intersystem crossing.

(ii) Factors affecting the intensity of transition.

(iii) Larmor precession. (4.5,4,4)