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CS/M.TECH/MBIN/SEM-1/MBIN-101/2012-13

2012

BIOMOLECULAR STRUCTURE & FUNCTION – I

Time Allotted : 3 Hours *Full Marks* : 70

The figures in the margin indicate full marks.

Candidates are required to give their answers in their own words as far as practicable.

Answer Q. No. 1 and any *six* questions of the remaining.

1. Answer briefly any *ten* of the following : $10 \times 1 = 10$

   i) Bohr radius in a hydrogen atom is about 0·05 nm. What is the de Broglie wavelength of the electron in the ground state of this atom ?

   ii) Atomic number of oxygen is 8. How many $2p$ electrons are there in the ground state of an oxygen atom ?

   iii) What is the reduced mass of a hydrogen molecule in terms of the proton mass m ?

   iv) If ω denotes the angular frequency of a harmonic oscillator, what is the zero-point energy of this oscillator in quantum mechanics ?

   v) Atomic orbitals of carbon in CH_4 are sp^3 hybridized. What is the angle between any two C-H bonds in the molecule ?

   vi) Write the Schrödinger wave equation for an electron in 3D space.

vii) Free radicals are formed from ..... cleavage. (Fill in the blank)

viii) Write the full form of CATH.

ix) ..... reagent is used for cleavage of Fmoc group during its deprotection in peptide synthesis. (Fill in the blank)

x) HOMO of antiaromatic compounds are bonding/ antibonding MO (Find the correct answer)

xi) Except ..... all the amino acids give the identical product in Ninhydrin test. (Choose the correct one.)

a) Gly b) Ala

c) Pro d) Lys.

xii) n_k is used to designate a helix. Describe the term n_k.

2. The electron of a hydrogen atom in its ground state is knocked off by an incident photon having energy 14·6 eV.

a) What is the wavelength of the incident photon ?

b) If the ionization potential of the hydrogen atom is 13·6 eV, what is the de Broglie wavelength of the ejected electron ? 5 + 5

3. The energy levels of an electron in a deep rectangular potential well are $E_n = \frac{n^2h^2}{8mL^2}$, where L is the width of the potential well and n is a positive integer. Use this formula to calculate the absorption wavelength for an electronic transition from HOMO to LUMO in a linear conjugated molecule consisting of 10 carbon atoms (each contributing one π electron to the molecule) with average bond length = 0·14 nm. 10

4. The rotational energy levels of a diatomic molecule are $E = \frac{J(J+1)h^2}{8\pi^2 I}$, where I is the moment of inertia of the molecule about its axis of rotation. Use this formula to calculate the bond length of the HCl molecule, if the rotational transition from $J = 0$ or $J = 1$ in this molecule is found to occur at $3 \cdot 2 \times 10^5$ MHz and the atomic weight of chlorine = 35. 10

5. Assuming that the π electronic energy levels for a closed conjugated molecule consisting of N carbon atoms are given by the formula

$$\varepsilon_n = \alpha + 2\beta \cos \frac{2n\pi}{N}$$

when $n = 0, \pm 1, \pm 2, \ldots N/2$, $\alpha = -13 \cdot 2$ eV and $\beta = -2 \cdot 8$ eV. Calculate (a) all the bonding and the antibonding energy levels for a benzene molecule in terms of the parameters α and β and (b) the delocaliztion energy per π electron in benzene. 7 + 3

6. a) Write the postulates of LCAO method and justify that Helium is monoatomic.

   b) UV sprectum of 1, 3 butadiene can be obtained at ease while for Ethylene no normal OV spectrum can be obtained, although both contain π-electrons. Justify.

   c) Draw the orbital representation of –CONH– group found in protein and justify its stereochemistry in terms of torsion angles. 3 + 4 + 3

7. a) Draw the conformational landscape in terms of conformational energy of butane with respect to rotation between C_1–C_2 bond. How the profile changes if the rotation occurs between C_2–C_3 ? (Use Newman projection formula)

   b) Can 'His' be considered as aromatic ? Predict the structure of 'His' at pH1.

c) How do you rationalize the thermodynamically favourable formation of helix structure in protein from coil structure ?

d) Why is 3_{10}-helix found in short stretches while α-helices are comparatively long in sequence ?

3 + 3 + 2 + 2

8. a) Write the strategic plan for synthesis of peptide Ala-Lys-Ala-Lys. Between Stepwise Synthesis and Convergent fragment condensation Synthesis which one will you prefer for this peptide sequence and why ?

b) What is dissociation constant for an amino acid ? Elucidate the relation between isoelectric point (pI) and the dissociation constants(pK) of Lys.

c) What is 'supersecondary structure' of protein ? For a reverse β-turn with 3-residue loop, show the location of dihedral angle (ϕ, ψ) of the three loop residues in Ramchandran plot.

Given,

Planck's constant = $6 \cdot 63 \times 10^{-34}$ J.s

Speed of light = $3 \cdot 0 \times 10^{8}$ m/s

1 eV = $1 \cdot 6 \times 10^{-19}$ J

Mass of electron = $9 \cdot 1 \times 10^{-31}$ kg

Mass of protein = $1 \cdot 67 \times 10^{-27}$ kg. 3 + 4 + 3

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