



Name :
Roll No. :
Invigilator's Signature :

**CS / M.TECH (MBIN) / SEM-1 / MBIN-101 / 2010-11
2010-11**

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 from the rest.

1. Answer any *ten* questions : 10 × 1

- i) The non-aromatic system contains $(4n + 2)\pi$ electrons
where n can have zero value. State True / False.
- ii) Choose the correct alternatives :

In *cis*-peptide bond Torsion angle between CO-NH is

- a) 90° b) 0°
c) 180° d) -90° .

A helix can be defined by symbol ' n_k ', where n determines the

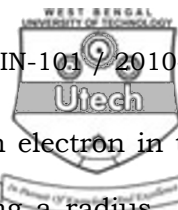
At equilibrium, ΔG of a reaction is

- v) Choose the correct alternative :

a) strong electrostatic b) covalent
c) van der Waal d) weak electrostatic.

 $\pi - \pi^*, \quad \sigma - \sigma^* \text{ and } n - \pi^* .$

viii) What is the magnitude of the angular momentum of an electron of mass m moving with uniform angular speed ν in an atomic orbit of radius r ?



- ix) What is the de Broglie wavelength of an electron in the ground state of a hydrogen atom having a radius of 0.52 \AA ?
- x) What is LCAO approximation in molecular orbital theory ?
- xi) Define π delocalization energy.
- xii) What is the angle between any two bonds in methane with sp^3 hybridized orbitals ?
2. a) In an electron microscope, a beam of free electrons is used. Show that the de Broglie wavelength of these electrons varies inversely as the square root of their energy E .
- b) Calculate the energy of an X-ray photon having a wavelength of 1.0 \AA . Express your result in electron-volts.

(Given : $h = 6.63 \times 10^{-34} \text{ J.s}$, $c = 3.0 \times 10^8 \text{ m/s}$,

$$1\text{eV} = 1.6 \times 10^{-19} \text{ J})$$

5 + 5



3. a) Solve Schrödinger equation to find the energy levels of an electron of mass m moving freely in a deep one-dimensional potential well of width L .

- b) In the linear conjugated part of a 'Vitamin A' molecule, 12.0 Å long, there are ten π electrons. Calculate the energy gap between the highest occupied and the lowest unoccupied levels in electron-volts.

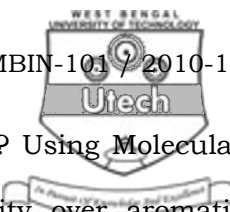
(Given : mass of electron $m = 9.1 \times 10^{-31} \text{ kg}$) 5 + 5

4. a) Calculate the reduced mass of a carbon monoxide molecule CO , given that the proton mass is $1.67 \times 10^{-27} \text{ kg}$ and the atomic weights of carbon and oxygen are 12 and 16 respectively.

- b) What is the frequency of microwave radiation emitted (in MHz) in a rotational transition from $J = 1$ to $J = 0$ for CO , whose bond length is 1.13 Å ? 3 + 7

5. a) From the Molecular Orbital concept, justify that H_2 is diatomic while He is monatomic.

- b) Can the amino acid 'His' show aromatic character ? Identify the site for protonation in histidine side chain.



- c) What is an antiaromatic compound ? Using Molecular Orbital concept, compare its stability over aromatic compound. 3 + 3 + 4

6. a) Define strength of an acid in terms of dissociation constant. What is 'isoelectric point' of an amino acid ? How does isoelectric point of an amino acid solution correlate with dissociation constant ?
- b) Draw the energy profile diagram of an α -helix formation from random coil, assuming that
- (i) it is a two state process,
 - (ii) it is a three state process where 3_{10} -helix is an intermediate and the intermediate state formation is the rate determining step.
- c) Starting from 100% *L*-configuration in a reaction an enantiomeric product mixture of 30% *D*- and rest amount of *L*- is formed. Calculate the amount of the enantiometric excess. 4 + 4 + 2



7. a) Draw the schematic representation of potential energy distribution of *n*-butane (using Newman projection) as function of angle of torsion about

(i) C1-C2 bond rotation and

(ii) C2-C3 bond rotation.

Identify the conformers in each case.

- b) Out of the two following amino acids in a peptide sequence

(i) $-\text{NH CH}_2 \text{CO}-(\text{Gly})$ and (ii) $-\text{NH CMe}_2 \text{CO}-(\text{Aib})$ which one has higher energy of torsion against the dihedral angle ϕ ? Also predict which amino acid has the higher allowed space in Ramachandran plot ?

- c) Define a 3 : 3 β -hairpin turn. 5 + 3 + 2

8. a) With the help of 'helical wheel' diagram of an α -helix and 3_{10} -helix consisting of *L*-amino acids only, justify that although 3_{10} -helix is kinetically favourable, α -helix is thermodynamically more preferred.



b) Draw the cartoon diagram of a 'Greek key motif' structure. Identify its secondary and supersecondary structures.

c) How do synthesize amino acid Ala from amino acid Gly ?

5 + 3 + 2

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