

Name : .....

Roll No. : .....

Invigilator's Signature : .....

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

**2012**

**BIOMOLECULAR STRUCTURE & FUNCTION – I**

Time Allotted : 3 Hours

Full Marks : 70

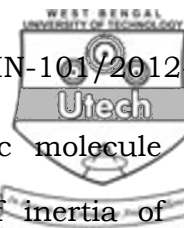
*The figures in the margin indicate full marks.*

*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 :  $10 \times 1 = 10$
- 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 ?
  - Atomic number of oxygen is 8. How many  $2p$  electrons are there in the ground state of an oxygen atom ?
  - What is the reduced mass of a hydrogen molecule in terms of the proton mass  $m$  ?
  - If  $\omega$  denotes the angular frequency of a harmonic oscillator, what is the zero-point energy of this oscillator in quantum mechanics ?
  - Atomic orbitals of carbon in  $\text{CH}_4$  are  $sp^3$  hybridized. What is the angle between any two C-H bonds in the molecule ?
  - Write the Schrödinger wave equation for an electron in 3D space.

- 10

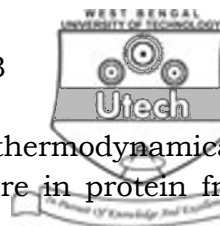


4. The rotational energy levels of a diatomic molecule are  $E = \frac{J(J+1)h^2}{8\pi^2 I}$ , where  $I$  is the moment of inertia of the molecule about its axis of rotation. Use this formula to calculate the bond length of the HCl molecule, if the rotational transition from  $J = 0$  or  $J = 1$  in 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  $\pi$  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  $n = 0, \pm 1, \pm 2, \dots, N/2$ ,  $\alpha = -13 \cdot 2 \text{ eV}$  and  $\beta = -2 \cdot 8 \text{ eV}$ . Calculate (a) all the bonding and the antibonding energy levels for a benzene molecule in terms of the parameters  $\alpha$  and  $\beta$  and (b) the delocalization energy per  $\pi$  electron in benzene. 7 + 3

6. a) Write the postulates of LCAO method and justify that Helium is monoatomic.  
 b) UV spectrum of 1, 3 butadiene can be obtained at ease while for Ethylene no normal UV spectrum can be obtained, although both contain  $\pi$ -electrons. Justify.  
 c) Draw the orbital representation of  $-\text{CONH}-$  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  $\text{C}_1-\text{C}_2$  bond. How the profile changes if the rotation occurs between  $\text{C}_2-\text{C}_3$  ? (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  $\alpha$ -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  $\beta$ -turn with 3-residue loop, show the location of dihedral angle ( $\phi, \psi$ ) of the three loop residues in Ramchandran plot.

Given,

$$\text{Planck's constant} = 6.63 \times 10^{-34} \text{ J.s}$$

$$\text{Speed of light} = 3.0 \times 10^8 \text{ m/s}$$

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

$$\text{Mass of electron} = 9.1 \times 10^{-31} \text{ kg}$$

$$\text{Mass of protein} = 1.67 \times 10^{-27} \text{ kg.}$$

3 + 4 + 3

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