



Name :

Roll No. :

Invigilator's Signature :

**CS/M.TECH (MBIN)/SEM-2/MBIN-201/2012
2012**

BIOMOLECULAR STRUCTURE & FUNCTION-II

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 **Group-A** and any six questions from the other three **Groups-B, C and D** taking at least one from each Group.

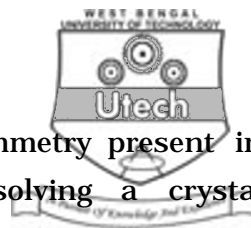
**GROUP - A
(Objective Type Questions)**

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

A) Choose the correct answer :

i) The vector $G_{hkl} = ha^* + kb^* + lc^*$ is

- a) parallel to the Bragg planes with Miller indices (hkl)
- b) perpendicular to the Bragg planes with Miller indices (hkl)
- c) $\Delta k = \frac{1}{|G_{hkl}|}$
- d) $|G_{hkl}| = d_{hkl}$



- ii) The maximum point group symmetry present in the crystal is exploited in solving a crystal structure to
- a) reduce the volume of the cell
 - b) select a primitive cell
 - c) reduce the number of molecules in the cell
 - d) reduce the volume of the asymmetric unit.
- iii) Combination of a 2 fold rotation with a mirror reflection (the mirror plane being perpendicular to the 2-fold axis of rotation) gives
- a) another 2-fold axis parallel to the original two fold axis of rotation
 - b) another mirror plane parallel to the original mirror
 - c) a centre of inversion at the intersection of the two fold axis and mirror
 - d) another mirror parallel to the original two fold axis of rotation.

B) Fill in the blanks :

- iv) Noe is related to the distance (r) of interacting nuclei. The relation is : $\text{Noe} \propto \dots\dots\dots$.
- v) In 2D NMR appearance of $\dots\dots\dots$ & $\dots\dots\dots$ Noe cross-peaks act as the signature of helical structure.



C) Write *True / False* for the following :

- vi) For taking *CD* spectra the amount of sample required is much higher than that required for taking *NMR* spectra.

D) Answer very briefly :

- vii) Why phosphorescence is a slow process compared to fluorescence ?
- viii) Calculate the value of RT in kcal/mole at $T = 300$ K, taking $R = 2$ cal/K/mole.
- ix) What is the approximate energy needed to break a hydrogen bond in kcal/mole ?
- x) Define Gibbs Free Energy.
- xi) Why are the peptide bonds rigid ?
- xii) Does the entropy increase or decrease when a random coil protein folds ?

GROUP - B

2. a) 100 moles of a perfect monatomic gas in a cylinder expands rapidly and adiabatically against a weightless piston. As a result, the gas cools down from 1000 K to 500 K. Calculate the work done by the gas in this expansion, taking $R = 8.3$ J/K/mole.
- b) If the same amount of the perfect gas expands isothermally to 10 times its original volume, what is the change in entropy ?

5 + 5



3. a) A molecular system consists of three non-degenerate energy levels, each separated from the previous one by an energy gap of 1.2 kcal/mole. Taking $R = 2$ cal/K/mole, what percentage of the molecules will populate the first excited state at $T = 300$ K ?
- b) Assuming that there are 3 equally probable rotational isomers for each of the two torsion angles ϕ and ψ in a 'random coil' protein molecule, what is the estimated amount of nucleation energy required to initiate a α -helix at $T = 300$ K ? 5 + 5
4. a) Energy needed to twist a molecule about its C - C single bond by an angle 20° from the original *trans* form ($\phi = 0$) is 0.75 kcal/mole. How much energy is needed to twist the molecule by 40° ? Assume energy $U(\phi) = \left(\frac{1}{2}\right) U_0 (1 - \cos 3\phi)$, where U_0 is the maximum energy barrier for the rotation.
- b) Lennard-Jones potential $U(r) = \left[\left(\frac{A}{r^{12}}\right) - \left(\frac{B}{r^6}\right) \right]$ operates between a given pair of non-bonded neutral atoms separated by a distance r , where the parameters A and B are constants for the pair. Find the contact distance for this pair of atoms (sum of van der Waal radii) in terms of A and B . 5 + 5

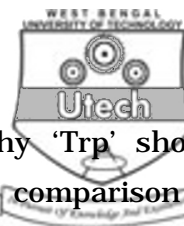


GROUP – C

5. Which pulse gives the maximum signal intensity in NMR spectroscopy? Draw the 1D NMR pulse sequence and justify the role of relaxation time in the pulse program. How do you measure longitudinal relaxation T_1 ? How do you identify whether two protons are scalar coupled or dipolar coupled in NMR spectra? 1 + 2 + 2 + 3 + 2

6. a) NMR spectra of a short peptide sequence (AC) Ala-Gly (NH_2) is taken initially in H_2O and then in D_2O . What changes do you expect both in 1D spectrum and 2D TOCSY spectrum of the peptide sequence during this solvent shift? [Given : Chemical shift values (δ in ppm) of Ala : NH (8.2) $\text{C}\alpha\text{H}$ (4.32) CH_3 (1.37) and Gly : NH (7.98) $\text{C}\alpha\text{H}$ (3.96)].

- b) Draw the carton representation of chemical shift index (CSI) value for $\text{C}\alpha\text{H}$ using ^1H and ^{13}C NMR spectra of a short seven residue peptide sequence (A-B-C-D-E-F-G) when its B-C-D-E-F segment undergoes a transition from an alpha helical conformation to beta strand conformation under thermal melting. 6 + 4



7. a) What is an intrinsic fluorophore ? Why 'Trp' shows higher fluorescence quantum yield in comparison to 'Phe' ? How protein folding can be studied using 'Trp' fluorescence ?
- b) What is Cotton effect ? How do you resolve plane polarized light into 'RCP' and 'LCP' ?
- c) A short helical peptide is treated with varying concentration of GnCl to study the unfolding process. Using CD spectroscopy how do you monitor this 'helix-coil transition' and correlate its thermodynamic parameter for transition ?

4 + 2 + 4

GROUP - D

8. Protein X is a tetramer which crystallizes in the space group $P222$ with cell parameters $a = 56.4$, $b = 73.2$, $c = 35.1$ Å, $\alpha = \beta = \gamma = 90^\circ$, with equivalent positions

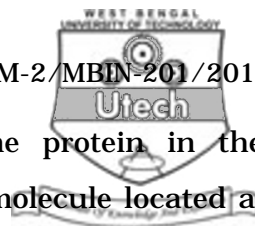
(x, y, z) , $(-x, -y, z)$, $(x, -y, -z)$ and $(-x, y, -z)$.

- a) Consider a protein atom with Cartesian coordinates :

$$20.564i + 33.216k + 10.097k$$

Generate all the equivalent positions of this atom in the cell in fractional coordinates.

- b) What is the volume of the asymmetric unit ?
- c) If there are three molecules of protein X in the asymmetric unit how many protein molecules are there in the cell ?



- d) If there is only one subunit of the protein in the asymmetric unit, then is the protein molecule located at a special position ? What can you infer regarding the symmetry of its quaternary structure ?
- e) Addition of a centre of inversion ($-x, -y, -z$) converts point group 222 to $2/m 2/m 2/m$. What are equivalent positions of $2/m 2/m 2/m$?
9. a) Consider a cubic crystal with cell parameters $a = b = c = 25.67 \text{ \AA}$, $\alpha = \beta = \gamma = 90^\circ$. Given $\lambda = 1.5418 \text{ \AA}$. Calculate the Bragg angle of scattering for the planes with Miller indices (222).
- b) What do you understand by the term 'resolution' of a crystal structure ? Why is it important in building a database of protein crystal structure ?
- c) Given all the structure factors $F_{hkl} \left(|F_{hkl}| e^{i\phi_{hkl}} \right)$. Write down the steps to solve the crystal structure and obtain the coordinates of the atoms in the cell.

5 × 2

5 + 2 + 3

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