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CS/M.TECH/MBIN/SEM-2/MBIN-201/2013

2013

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 Question No. **1** and any *six* from the rest taking at least *one* from each Group.

1. Answer any *ten* questions for the following : $10 \times 1 = 10$

   i) What do you mean by an ideal gas ?

   ii) What is an adiabatic process ?

   iii) Define Gibb's free energy.

   iv) Why are the peptide bonds rigid ?

   v) Does the entropy increase or decrease when a random coil protein folds ?

vi) Which pulse will give higher intensity in NMR signal ?

a) 45°   b) 180°.

Fill in the blanks :

vii) Concentration of sample required for CD analysis is .... than required for NMR.

viii) S/N ratio of a spectrum will be enhanced by a factor of .... if you repeat the experiment by 100 times.

ix) Name the programme that helps you to get the structure to deposit in PDB from NMR spectral data.

x) Write the equation showing the relation between $^3J_{N\alpha}$ and dihedral angle Φ.

Choose the correct alternatives :

xi) The highest point group in a crystal is exploited in a crystal structure solution to

a) reduce the volume of the cell

b) reduce the volume of the asymmetric unit

c) reduce the length of the basis vectors *a, b, c*

d) reduce the density of the crystal.

xii) Addition of an independent centre of inversion to point group 2 results in

a) 222 b) $2/m$

c) m d) 4.

xiii) X-ray scattering in a crystal is primarily due to

a) electrons b) protons

c) neutrons d) nucleus.

xiv) Fourier transform of the electron density function gives the

a) electronic wave function

b) reciprocal lattice

c) structure factor

d) interplanar spacing.

GROUP – A

2. a) For an isothermal reversible expansion of 1 mole of an ideal gas from volume V_1 to V_2 show that the change in entropy $\Delta S = R\ ln(V_2 / V_1)$, where R is the gas constant.

b) In the cylinder of a certain engine, 0·8 mole of an ideal diatomic gas expands rapidly and adiabatically against a weightless piston. In the process of expansion, the temperature drops from 1250 K to 750 K. How much work does the gas do ? (Given R = 8·3 J/mole/K).

5 + 5

3. A three-level molecular system has a ground state and two equally spaced excited states, each separated by an energy gap of 1·2 kcal/mole. If the first excited state is 3-fold degenerate, and the second excited state is 5-fold degenerate, calculate —

a) the partition function of the system

b) the percentage of molecules in the ground state at 300 K. (Given R = 2 cal/mole/K). 5 + 5

4. a) How much energy is required to rotate a single bond by $40°$ about its minimum energy position $(\theta = 0)$, if the torsion potential energy is $V(\theta) = V_0(1 - \cos 3\theta)/2$ and the maximum energy barrier for the rotation $V_0 = 2 \cdot 0$ kcal/mole ?

b) Assuming that there are 3 equally probable isomers for each of the torsion angles ϕ and ψ in a 'random coil' protein molecule, estimate the amount of nucleation energy required to initiate an α-helix at 300 K. 5 + 5

GROUP – B

5. a) ^{13}C NMR is less sensitive in comparison to ^{1}H NMR. Justify the comment with proper reason. How can you increase the sensitivity of ^{13}C NMR experiment ?

b) Which relaxation process in NMR spectroscopy helps to obtain excess ground state population ? How is the initial delay related to this relaxation process ?

c) ^{1}H NMR spectrum of a peptide have sequence of Gly-Gly-Ala-Gly is taken in water initially and then in D_2O. What changes do you expect in 1D spectrum of Ala during such solvent shift considering that the spectrum for individual residue is well dispersed and resolved ? If Ala is mutated by Asp, how do you authenticate the mutation using 2D TOCSY ^1H NMR spectrum ?

3 + 2 + 5

6. a) What is Cotton effect ? How do you obtain positive cotton effect ?

   b) A short helical peptide is treated with varying concentration of GnCl to study the unfolding process. Using CD, IR and ^1H, ^{13}C NMR (1D and 2D) spectroscopy how do you justify this 'helix-coil transition' ? 2 + 8

7. a) How do you distinguish between an intramolecular H-bonded N-H and an intermolecular hydrogen bonded N-H using FTIR stretching mode ?

   b) A conjugated ene-one system in CCl_4 shows λ_{max} at 230 nm and 275 nm (with reduced intensity). Draw the expected UV spectral pattern of that sample if the solvent is changed to H_2O.

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c) What characteristic changes do you expect in UV spectrum for Tyr if you take the spectrum in pH10 instead of pH1 ?

d) Why is the spectral width of UV spectrum broad while that of NMR in sharp ? 3 + 3 + 2 + 2

GROUP – C

8. Protein X crystallizes in the space group P4 with cell parameters :

$a = b = 145{\cdot}2$, $c = 75{\cdot}8$ Å, $\alpha = \beta = \gamma = 90°$.

the equivalent positions for P4 are $(x, y, z), (-x, -y, z)$, $(-y, x, z), (y, -x, z)$.

i) Calculate the volume of the asymmetric unit.

ii) X contains an iron atom with fractional coordinates : (0·2036, 0·1567, 0·7312). Write down all the equivalent positions for this atom.

iii) What do you understand by the term 'special position' ?

iv) Protein X is a tetramer consisting of 4 identical subunits. If there are 8 subunits in the asymmetric unit, how many protein molecules are there in the cell ?

v) Is the point group $4/m$ centric ? 5 × 2

9. a) Prove $|G_{hkl}| = 1/d_{hkl}$.

b) Write a short notes on the Phase Problem in crystallography.

c) A cubic crystal has cell parameters $a = b = c = 60Å$. Calculate the Bragg angle of scattering for the Bragg planes (1, 1, 1). 3 + 3 + 4

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