

Time: 90 MINUTES.

ANSWER ALL QUESTIONS.

FULL MARKS: 30

Useful Information:

- Boltzmann constant,  $k_B = 1.3806 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$
- Gas constant,  $R = 8.3144 \text{ J mol}^{-1} \text{ K}^{-1}$
- Planck's constant,  $h = 6.6261 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$

**Q1.** Clearly write your selection(s) for each question below. (2 x 3 = 6 marks; wrong selection: -0.5)

- i) Assume room temperature to be 27 °C. Select the closest equivalent of **1  $k_B T$**  from the choices below.
- 4.1 nanoNewton-metre
  - 4.1 picoNewton-nanometre
  - $4.1 \times 10^{-9}$  Newton-metre
  - 41.4 picoNewton-metre
  - 4.1 picoNewton-picometre
- ii) A bio-molecular complex has four domains that independently adopt W1, W2, W3 and W4 microscopic states.
- The overall complex has  $[W1 + W2 + W3 + W4]$  microscopic states
  - The overall entropy is proportional to  $[\ln(W1 + W2 + W3 + W4)]$
  - The overall entropy is proportional to  $[W1 \times W2 \times W3 \times W4]$
  - The overall entropy is proportional to  $[\ln(W1) + \ln(W2) + \ln(W3) + \ln(W4)]$
  - None of the above is correct.
- iii) A trainee assumes that the shape of organisms can be approximated as spheres, and that the metabolism rate scales as their volume. He then collects a large (surface to volume) data set and metabolism rates. If his hypothesis is correct, which should hold true?
- The (surface to volume) ratio of the organisms will have (linear  $r$ ) dependence
  - The (surface to volume) ratio of the organisms will have ( $r^{-2}$ ) dependence
  - The metabolism rates will scale as (surface to volume) ratio
  - The metabolism rates will scale independently of (surface to volume) ratio
  - The metabolism rates will scale as the cubical inverse of (surface to volume) ratio

**Q2.** (2 + 3 + 3 = 8 marks)

A researcher decides to approximate the entropy ( $S$ ) protein solutions at equilibrium with the ideal gas entropy. Thereby, for 'N' protein molecules, each of mass 'm' in system volume 'V', she uses a constant 'B' and writes,

$$S = k_B \ln \left[ (V (2mE)^{3/2})^N \right] + B$$

- What are the assumptions about the quantity 'E', if any? How does 'E' depend on the temperature?
- A protein solution is found to undergo volume expansion at constant temperature, from an initial volume 'V' to a final volume '1.5 V'. Derive an expression for the *entropy change* estimate within the system. Thereby, comment on the spontaneity of the expansion.
- The expansion occurred for the solution with 1 mole of protein of molecular weight 1500 g/mol. Find the entropy change in *SI units*.

**Q3.**

(2 + 4 + 2 = 8 marks)

Consider a small peptide molecule in solution with ' $M$ ' number of possible energy states, with the  $j^{\text{th}}$  state having the probability,  $P_j$ .

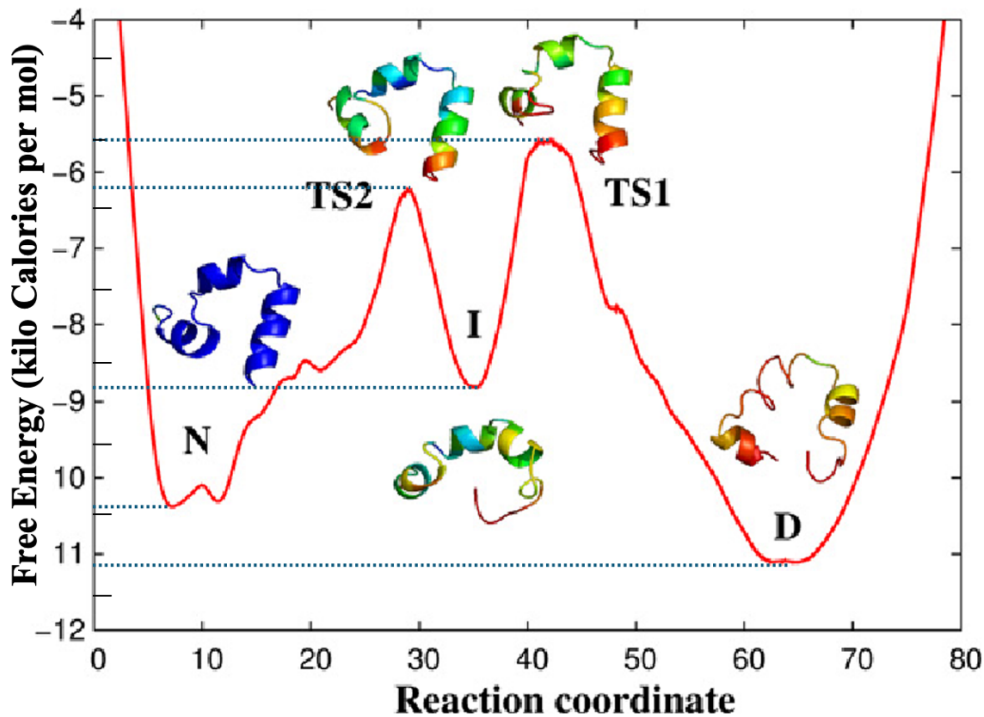
- Write down the level of disorder (say  $I$ ) in the system using Shannon's formula. Include additional constants if required.
- Assume  $M = 4$ . Use Shannon's formula to show that the level of disorder is maximum when all  $P_j$  are equal. When is the level of disorder a minimum?
- Now assume that the  $j^{\text{th}}$  state is associated with energy  $E_j$ . Write down the probability of occupation of the state, using proportionality constant(s) of your choice. Simplify Shannon's formula with this information.

**Q4.** Refer to a protein's Free Energy Landscape below.

Free energies of the *observable configurations*, Native ( $N$ ), Intermediate ( $I$ ) and Disordered ( $D$ ), are provided along with those for the two *transitory configurations* (TS2 and TS1).

Assume equilibrium at physiological temperature.

Free Energies should be rounded up to the nearest 0.5 value.



(4 + 4 = 8 marks)

- Designate the most probable configuration as ' $MP$ '; give reasons. Find the population ratio of  $MP$  with the other two observable configurations. Show all steps clearly.
- Configuration  $I$  can go to either  $N$  or  $D$ . Find the ratio of the rates of the two possible transitions. Show all steps clearly.