

Exercises – Lecture 10

BIO-212

Question 1

The two accessible conformations of a protein differ by 2 kJ/mol. What percentage of proteins will be in the higher energy state at 270 K?

Question 2

The Boltzmann distribution describes the most probable distribution of particles in different energy states for a given system. Thinking about each particle as being a protein and remembering that each different possible conformation of a protein has a different energy, use the Boltzmann distribution to explain why at extremely high temperatures proteins are unfolded.

Question 3

A protein can transition between two conformations which differ by 5 kJ/mol. Which of the following statements is false?

- a. 15 % of the protein is in the higher energy state at 350 K
- b. 10 % of the protein is in the higher energy state at 270 K
- c. The protein can change conformation at room temperature
- d. 90 % of the protein is in the lower energy state at 300 K

Question 4

A particular sidechain has a dihedral angle for which the energy is governed by the following equation:

$$U_{\text{dihedral}} = 2 \times \cos(3 \times \text{angle}) \text{ kJ/mol}$$

- A. What is the torsional energy of the sidechain when the angle is 60 °?

- B. And when the angle is 120° ?
- C. What is the relative population of sidechains with an angle of 60° vs 120° at 300 K?
- D. Would it be possible to visit a state with a dihedral angle of 180° at 300 K, given that the initial dihedral angle is 60° ? Explain your answer considering possible energy barriers.

Question 5

The energy associated a specific torsional angle of a given molecule can be described by the following potential: $U(\vartheta) = U_0 (1 + \cos 4 \vartheta)$ with $U_0 = 6$ kJ/mol. Which of the following statements is false?

- The maximum energy value associated with the interaction is 12 kJ/mol
- The torsional angle has 4 possible minima
- At the minima the energy is zero
- The minimal amount of energy required to jump between two minima is 6 kJ/mol

Question 6

A system at 275 K in state A has an enthalpy of -25 kJ and an entropy of $2 \text{ J}\cdot\text{K}^{-1}$. In state B, it has an enthalpy of -20 kJ and an entropy of $10 \text{ J}\cdot\text{K}^{-1}$. Will state A convert spontaneously to state B?

	State A	State B
H	-25 kJ	-20 kJ
S	$2 \text{ J}\cdot\text{K}^{-1}$	$10 \text{ J}\cdot\text{K}^{-1}$

Question 7

Assume that entropy and enthalpy changes are independent of temperature. A system in state A has an enthalpy of -22 kJ and an entropy of $7 \text{ J}\cdot\text{K}^{-1}$. In state B, it has an enthalpy of -12 kJ and an entropy of $15 \text{ J}\cdot\text{K}^{-1}$. At what temperatures will state B be favored?

	State A	State B
H	-22 kJ	-12 kJ
S	7 J•K ⁻¹	15 J•K ⁻¹

Question 8

The potential energy between two atoms is described by a **Lennard-Jones potential**:

$$U_{VdW} = \sum_{i>j}^N \epsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^6 \right]$$

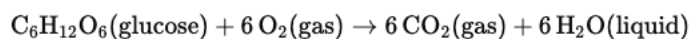
Given:

- $\epsilon = 2 \text{ kJ/mol}$,
- $r_0 = 0.4 \text{ nm}$

- Calculate the potential energy $U(r)$ at $r = 0.45 \text{ nm}$.
- At what distance r is the potential energy at its minimum?
- Choose the correct interpretation of the potential:
 - The term $\left(\frac{r_0}{r}\right)^{12}$ describes the attractive force.
 - The term $\left(\frac{r_0}{r}\right)^6$ describes the repulsive force.
 - The potential $U(r)$ accounts for both attractive and repulsive interactions.
 - The distance $r = r_0$ corresponds to the strongest attractive force.

Question 9

During cellular respiration, a glucose molecule is gradually broken down into carbon dioxide and water. Below you have a reaction:



Using a table from the lecture:

Compound	ΔG° (kJ·mol ⁻¹)
acetate ⁻	-369.2
CO ₂ (gas)	-394.4
CO ₂ (aqueous solution)	-386.2
carbonate ion	-587.1
ethanol	-181.5
fructose	-915.4
fructose-6-phosphate ²⁻	-1758.3
α -D-glucose	-917.2
glucose-6-phosphate ²⁻	-1760.2
H ⁺ (aqueous solution)	0.0
H ₂ (gas)	0.0
H ₂ O (liquid)	-237.2
isocitrate ³⁻	-1160.0
lactate ⁻	-516.6
OH ⁻	-157.3
pyruvate ⁻	-474.5
succinate ²⁻	-690.2

a) Calculate the standard Gibbs free energy change (ΔG) for the reaction

b) Interpret the result: Is the reaction thermodynamically favorable under standard conditions?

Question 10:

In the lecture you had 2 pathways (1) and (2) on the picture below.

Check what would be the Gibbs energy for both. Use the table from question 10. What you can say?

