UNIVERSITY OF CALIFORNIA, BERKELEY
CHEM C130/MCB C100A
MIDTERM EXAMINATION #2
October 22, 2014

INSTRUCTORS: John Kuriyan and David Savage

THE TIME LIMIT FOR THIS EXAMINATION: 1 HOUR 50 MINUTES

SIGNATURE:

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Please **SIGN** your name on the line above in **INDELIBLE INK**.

YOUR NAME:

____

PLEASE PRINT your name (**IN INDELIBLE INK**) on the line above (& on the top right hand corner of every page).

PLEASE CIRCLE the name of your GSI:

Pradeep Bandaru   Caroline Cypranowska

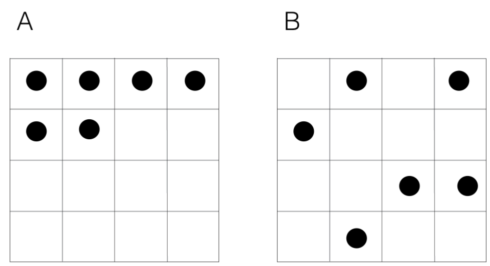
Julian Hassinger   Madeleine Jensen

Laura Nocka

PLEASE WRITE all of your answers **AS LEGIBLY AS POSSIBLE**.
Note that any exam submitted for a regrade should be written in indelible ink.
SCORING. The exam consists of 5 questions totaling 100 pts as broken down in this table:

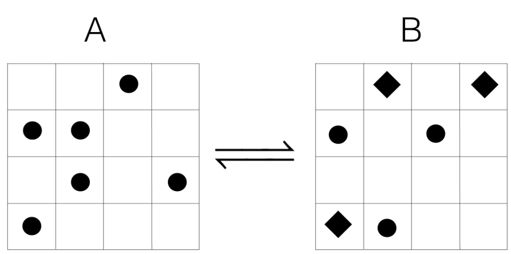
Question	Part A	Part B	Part C	Part D	Your Total	Max Score
1.	6	14	---------------	---------------		20
2.	10	10	---------------	—————		20
3.	9	11	---------------	---------------		20
4.	14	6	---------------	---------------		20
5	----------	-------------	---------------	---------------		20
				TOTAL		100

Q1 (20 points) Q1A (6 points)
(i) (2 points) Shown below are two microstates (instantaneous configurations) of a system of non-interacting particles.



Which microstate is more probable? Briefly explain your answer.

(ii) (4 points) A system of non-interacting particles can interconvert between two states, shown below. The transition involves a conformational change in some of the molecules, with the two conformations indicated by circles and diamonds, respectively. The two conformations have the same energy.



Will State A convert spontaneously to State B? Justify your answer by calculating the relative probability of State B versus State A.

Q1B (14 points) A piston contains 3 moles of an ideal gas. The gas expands isothermally and in a near-equilibrium (reversible) process at 200K. The volume increases from 1 liter to 3 liters during the expansion.

(i) (2 points) What is the change in energy of the gas?

(ii) (3 points) What is the change in entropy of the gas? What are the units of the entropy change?

(iii) (3 points) What is the final value of the enthalpy of the gas? Express your answer in Joules.

Q1B (iv) (3 points) How much heat is transferred to the system during this process, in units of J?

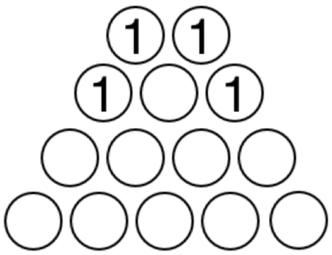
(v) (2 points) Would the energy change be the same if the gas were carbon dioxide? Briefly explain your answer.

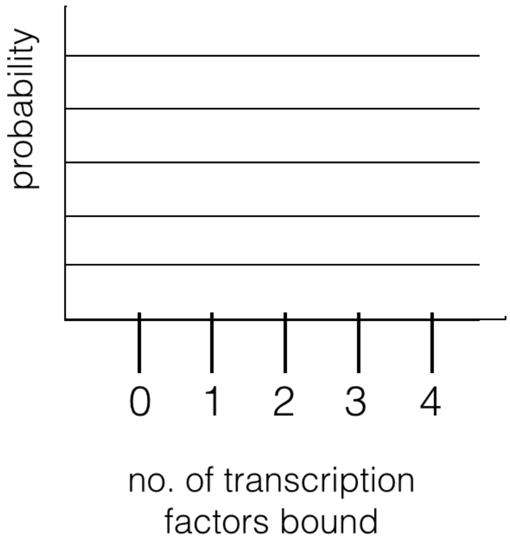
Q2. (20 points)
Q2(A) (10 points)
(i) (2 points) Fill in the blank entries in Pascal's Triangle, shown on the next page.

(ii) (6 points) A segment of DNA that controls gene transcription, known as an operator, contains 4 bindings sites for a transcription factor protein. Under particular conditions in the cell the probability of a transcription factor being bound to a binding site is 0.6.

In the diagram shown on the next page, draw a histogram showing the probability of 0, 1, 2, 3 and 4 transcription factors being bound to the operator. Write down the numerical value for each probability that you calculate above the corresponding bar in the histogram.

Show the formula you use to calculate the probabilities, and show your calculations. Specify which row of Pascal's triangle enters into your calculation.





(iii) (2 points) Transcription is initiated from the operator whenever two or more transcription factors are bound. What is the probability of transcription being initiated? Show all the steps of how you work out the answer.

Q2B (10 points)
(i) 2 points. A system consists of several energy levels and $15X10^{10}$ molecules and is at equilibrium at 300K. The entropy associated with the energy is 1.0 $J.K^{-1}$. What would be the entropy of a system with the same energy levels, at equilibrium at 300K, if the number of molecules was increased to $30X10^{10}$?

(ii) (4 points) A system is coupled to a heat bath. Consider the potential energy distribution shown below.

$U=10\ kJ.mol^{-1}$, $n_1=18.3X10^{20}$

$U= 0\ kJ.mol^{-1}$, $n_0=1000X10^{20}$

Calculate the **entropy per mole** of the system. Show all the steps of how you work out the answer. Report your answer in units of $J.mol^{-1}.K^{-1}$.

(more blank space on next page)

Q2B(iii) (2 points) Does this correspond to an equilibrium distribution at 300K? Explain your answer.

(iv) (2 points) What is the value of the partition function of the system? Explain the relationship between the value of the partition function and the heat capacity of the system, discussing whether high partition functions correspond to low or high heat capacity.

Q3.

(A) (9 points) The interaction between two atoms separated by a distance r is given by the following equation:

(1) $F = -k(r - r_0)$ r_0 is the equilibrium bond length, which is 2.7 Å.

(2) The magnitude of the force is 15.0 kJ.mol^{-1}.Å^{-1} when r = 5.0 Å.

(i) (3 points) What is the value of the force constant, k? Specify the units.

(ii) (3 points) Write down the equation for energy as a function of distance, $U(r)$, corresponding to the force equation given above:

(iii) (3 points) What is the magnitude of the work done in moving the atoms from a separation of 4 Å to 10 Å?

Q3B (11 points)

(i) (4 points) An aspartate sidechain and a protonated histidine sidechain form an ion pair such that the charged atoms are 4.0 Å apart. The electrostatic interaction energy between the sidechains is -174 $kJ.mol^{-1}$. Based on this information, is the ion pair exposed on the surface of the protein, or is it buried in the hydrophobic core? Justify your answer.

(ii) (4 points) A protein with a net positive charge binds to a small substrate molecule with a net positive charge. A scientist measures the rate of binding of the small molecule to the protein and observes that the binding occurs *faster* than the rate predicted from diffusion of the molecule in water. Explain briefly what properties of the protein underlie the faster than diffusion rate of binding.

(iii) (3 points) The Morse potential and Hooke's Law are both equations that are used to describe the energy of a covalent bond. A scientist wishes to calculate the covalent bond energy for a protein molecule in which one carbon-carbon covalent bond has been stretched to 2.5 Å. Would he get an accurate answer by using the Hooke's law equation? Explain the reasoning behind your answer.

Q4. On a recent expedition to Saturn's moon Titan, astronauts have isolated a novel kind of bacterium named *Titanus tmol*. Confident that exploring this organism's physiology may one day land you a high-profile research position, you make a number of careful measurements to understand out how this organism is able to make a living in extreme conditions. Interpret and answer the following questions.

(A) (14 points) You realize that all metabolism in *Titanus* revolves around the reaction:
A + 3B $\rightleftharpoons$ **Z**, where molecule Z is an energy storage compound unlike anything seen on Earth but conceptually similar to ATP in that it drives much of the rest of metabolism.

(i) (5 points) *Titanus* is found to grow near thermal vents that produce a constant temperature of 400K. Use the enthalpy and entropy of formation values (assume they're constant with temperature) in the table below to calculate the value of ΔG° for the production of Z at 400K.

	A	**B**	**Z**
$\Delta_f H°$ (kJ/mol)	-94	-2	-150
$\Delta_f S°$ (J/(K mol))	20	50	0

(ii) (2 points) What does this value indicate for the spontaneity of the reaction?

(iii) (2 points) Is this free energy calculation valid for constant volume or constant pressure?

Q4A (iv) (3 points) More careful study of *Titanus*'s natural environment reveals that there are huge temperature swings: the temperature drops to 235K when the thermal vents are not active. Suppose that the metabolic strategy of *Titanus* exploits these natural temperature oscillations. Recalculate $\Delta G°$ at 235K and describe what the metabolism of *Titanus* appears to be doing. Make sure to include a discussion of spontaneity.

(v) (2 points). While writing a paper describing these results, you'd like to compare this result with what occurs in normal bacteria isolated on Earth. ATP synthesis in cells should be highly unfavorable and yet it does occur. Briefly state how cells accomplish this.

Q4 (B) (6 points).

(i) (4 points) Cell biologists investigating chemotaxis in *Titanus* identify a molecular motor that is able to use the consumption of molecule Z (i.e. the reverse reaction to that described above). The motor take 10 nm steps and is able to move cargo against a resistive force of 3.3 pN *in vivo*. Assuming perfect mechanochemical coupling (all free energy is converted to work), what is the free energy for the consumption of Z *in vivo?*

(ii) (2 points). This value is somewhat different than what was calculated for the consumption of Z in Q4A. Justify this difference based upon Le Chatelier's principle.

Q5. (20 points) Multiple choice and True/False questions. Circle the correct option (or circle either TRUE or FALSE). +2 points for each correct answer, -1 point for each wrong answer. To get the maximum score you do not need to answer all the questions, so be careful not to answer questions incorrectly. Unanswered questions do not change the score. Minimum points: 0.

(i) The heat transferred for a process occurring under constant pressure conditions is equal to the enthalpy change (TRUE / FALSE)

(ii) For a process occurring under reversible conditions the heat transferred is a state function (TRUE / FALSE)

(iii) A piston contains protein molecules dissolved in water. During an isothermal and reversible expansion of the system the total energy of the system must stay constant. (TRUE/FALSE)

(iv) The entropy of a system can decrease spontaneously if it is coupled to an energy source. (TRUE/FALSE)

(v) The magnitude of the work done in a reversible process is always _______ the magnitude of the work done in an irreversible process. Circle the best answer.
- less than
- greater than
- equal to

(vi) The force required to break a non-covalent interaction in a protein is in the range of:

(a) 10 – 100 piconewtons
(b) 10 – 100 nanonewtons
(c) 10 – 100 micronewtons
(d) 10 – 100 millinewtons

(vii) A valid unit for force is calories per Å. (TRUE/ FALSE)

(viii) Water reduces the effective strengths of hydrogen bonds in proteins. Choose the best explanation:

(a) Water weakens electrostatic interactions
(b) Water competes with polar groups for hydrogen bonds
(c) Both (a) and (b)
(d) The statement is false. Water has no effect on hydrogen bonds.

(ix) There is no specific energy function describing the hydrophobic interaction because it is the net result of many electrostatic interactions and entropic effects. (TRUE / FALSE)

(x) Entropy is an additive function because the multiplicities of independent events are multiplied (TRUE/ FALSE)

(xi) The total entropy of a system is equal to the product of the positional entropy and the entropy of energy distributions when the energy of the molecules does not depend on their relative positions.TRUE / FALSE

(xii) The change in free energy around a thermodynamic cycle _________: (circle the best choice)

(a) depends on whether reactants and products are in their standard states
(b) is zero
(c) is greater than zero
(c) is less than zero