Exam 1 – Fall 2019

BCH 341 - Physical Chemistry with a Biological Focus

Professor Jeff Yarger

September 8-10, 2019

DUE Tuesday September 10, 2019 by 11:59 PM (UTC-7). Turn in completed exam as a typeset (no handwriting allowed) single PDF document into the assignment link on ASU Canvas. Please make sure the completed exam is organized, self-contained and all text, equations, figures and images are typeset, clear and legible.

REQUIRED Identification:

ASU ID #:____

(10-digit number (typically starting with 12xxxxxxxx or 10xxxxxxxx))

OPTIONAL Identification:

Initials: _______ Email: _____________________________________

Exam General Instructions

To aid in the anonymous peer review process, you do NOT need to include your full name, just your ASU student ID. There is the option of including your first, middle and last initials, and an email address for contact purposes (which is really helpful).

There are 5 multi-component questions on examination 1 (exam 1). Pick 4 of these problems to work on this examination. Each of the multi-component numbered problems is worth 25 points and you are required to pick 4 of them. Hence, the exam is worth a total of 100 points. If you don't include a number in the space below and provide answers for all 5 questions on the exam, then the first 4 will be graded. You are required to explicitly show all equations, numerical calculations and associated units. All points are associated with explicitly showing all your work and no points are awarded for just determining the correct numerical answer. All assumptions need to be clearly and concisely stated. If thermodynamic parameters are used, the citation, reference or link to where this thermodynamics data came from must be stated. The completed exam should be typeset (no handwriting of equations or numerical values and associated units).

Please write down the problem number you want **omitted (not graded)**: _____ (1, 2, 3, 4 or 5)

Peer-Review (Peer-Grading) Information

This is a new feature and a trial in ASU Canvas as an additional option for an 'assignment' (exam 1 in Canvas). Details about the peer review process will be provided immediately after the due date for this exam. A rubric will be provided to aid in the peer review (grading) process.

1. (A) Provide brief molecular interpretations of (i) heat, (ii) temperature and (iii) heat capacity (please limit your answers to 1-2 paragraphs and include associated citations, 10 pts).

(B) Pick a molecular system that you feel best allows you to illustrate the molecular interpretation of heat, temperature and heat capacity. The most common example molecular systems used by textbooks include the kinetic model of gases (pick your favorite common gas molecule, H_2, He, N_2, CO_2, etc) and/or one or more of the various phases of H_2O (ice, water, vapor). Given that this course has a biological focus, you are encouraged to pick an example with biological relevance, i.e., your favorite biological molecule (peptide, protein, nucleic acid, lipid molecule, etc). Points are awarded for creative, insightful and unique molecular examples with clear visual illustrations (plots or graphs are typically very useful as visual illustrations, provide links or citations to any existing material used in your illustrations/examples, 15 pts).

2. (A) Calculate the change in enthalpy (ΔH) for 1.0 mol of carbon dioxide (CO_2) initially at a volume of 5.00 L and a temperature of 298 K to a final volume of 10.00 L and a temperature of 373 K. Explicitly state all assumptions along with a justification for any and all assumptions made. Express your answer in units of kilojoules per mole (kJ/mol) (15 pts).

(B) The enthalpy is a common form of energy used in biochemical thermodynamics and is a state function, meaning the change in enthalpy (ΔH) for the process above should be independent of the path. Explicitly illustrate this point by calculating the change in enthalpy for the expansion process above along a different path than you did in part (A) of this problem (5 pts).

(C) This problem is inspired from a Module 1 quiz question and further YellowDig discussion. The numerical value that was correct on the quiz is NOT the answer to part (A) of this problem. Why? The change of system from helium to carbon dioxide plays a critical role (another example of understanding thermodynamics from a molecular perspective). Calculate the change in enthalpy for the exact initial and final conditions stated in part (A) but the helium instead of carbon dioxide as the molecular system. Explain or illustrate how this change in molecular system changes the calculated change in enthalpy (ΔH) for this process. (5 pts)

3. (A) Predict whether the change in entropy (ΔS) is positive, negative or near zero for the following processes at 298K (4 pts). Provide a molecular level explanation or justification for your prediction (8 pts). (B) Now calculate the change in entropy (ΔS) for the following processes at 298K (8 pts). Write a brief explanation on how your predicted vs. calculated results compare (5 pts).

i. H_2O (*s*) → H_2O (*l*), melting of ice.
ii. Formation reaction for steam (water vapor, H_2O (*g*)).
iii. C_3H_8 (*l*) → C_3H_8 (*aq*), Liquid propane going to aqueous propane.
iv. The hydrolysis of the dipeptide glycylglycine.

4. (A) A sample of the monosaccharide (sugar) D-threose of mass 1.15 g was placed in a constant volume calorimeter and then ignited in the presence of excess oxygen. The temperature rose by 1.48°C. In a separate experiment in the same calorimeter, the combustion of 0.917 g of benzoic acid, for which the internal energy of combustion is -3226 kJ/mol, gave a temperature rise of 1.94°C. Calculate the enthalpy of formation of D-threose (10 pts). (B) Calculate the enthalpy of formation of D-threose and benzoic acid using either an arithmetic method (e.g., bond dissociation energies) or a computational method (e.g, *ab initio* electronic structure computational program like molcalc.org) (10 pts). (C) Compare the results from the calorimetric method used in part-A to the method used in part-B and provide a brief molecular level explanation for any potential differences (5 pts).

5. Find and read a recent and original paper in the scientific literature that sounds interesting to you and which common thermodynamic parameters (i.e., ΔH, ΔS, ΔG, or C_p …) have been measured or computed. (A) Record the reference (citation) to this scientific paper (5 pts). (B) Summarize the significance of the paper in one paragraph (5 pts). (C) List the thermodynamic parameters determined and what methods were used to measure or compute the thermodynamics presented in the paper (15 pts).

Please try to choose a public open-access journal article and provide a link to the web or pdf version of the manuscript. If you choose a copyrighted article that is not publicly accessible, please provide a method of linking to this article. It is recommended that you make a web-accessible (publicly available) shared link to a pdf electronic version of the paper. This can be done from any of the commonly used cloud-storage services, i.e., Dropbox, Google Drive, Amazon Drive, Box, etc.

Extra Credit: After your exam is turned in, it will be put into an anonymous peer review system and students will have 1-2 days to peer review (peer grade) three randomly assigned exams. Students who provide insightful comments and accurate evaluation (correct number of points) will receive 15 extra credit points (5pts/exam). These points will only be given to students that provide detailed corrections, scores and comments on each of the 3 assigned exams and for each problem within the submitted exam. These comments and recommended scoring (points) for each problem can be done directly as comments in the Canvas LMS. However, it is recommended that the peer reviewer be provided as a separate single PDF annotated document with the associated corrections, comments, scores/points, etc (i.e., a graded annotated PDF document) added to the students originally submitted document.