

Exam 1 – Spring 2019
BCH 341 - Physical Chemistry with a Biological Focus
Professor Jeff Yarger & Vladimiro Mujica

January 23-24, 2019

DUE Thursday, Jan 24, 2019 by 11:59 PM (UTC-7). Turn in completed exam as a single PDF document into the assignment link on ASU Canvas. Please make sure the completed exam is organized, self-contained and legible.

Initials: _____ Email: _____

To aid in the anonymous peer review process, you do NOT need to include your full name, just your first and last initials, and an email address for contact purposes. The exam consists of 8 numerical problems. The first 4 problems are worth 10 pts each and the last 4 problems are worth 15 pts each. Hence, the exam is worth a total of 100 points. You are required to explicitly show all equations, numerical calculations and associated units. 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.

1. The composition of planetary atmospheres is determined in part by the speeds of the molecules of the constituent gases because the faster moving molecules can reach escape velocity and leave the planet (often called Jeans escape, named after British astronomer Sir James Jeans). The major constituents of earth's atmosphere (air) are nitrogen, oxygen, argon, carbon dioxide, dihydrogen monoxide, neon, helium, methane, krypton and hydrogen gases. In general, the earth is too large to lose a significant proportion of its atmosphere through Jeans escape. (A) Of the major constituent gases in the earth's atmosphere, which are most susceptible to Jeans escape? (B) The exosphere is the high-altitude region where atmospheric density is sparse and Jeans escape occurs. For the atmospheric gases susceptible to Jeans escape (part-A), estimate the fraction of molecules traveling at a speed above the earth's escape velocity.

2. (A) The helix to coil transition of an alanine peptide in water has been observed using numerous experimental techniques, which includes standard calorimetry. The two conformations of neighboring peptide groups in a polypeptide are shown to differ in energy by 1.3 kcal/mol. At body temperature what is the expected ratio of populations of the two conformations? (B) How do you expect the population of these two conformations to change over that standard temperature range of water (0°C to 100°C)? The 1.3 kcal/mol per residue was determined from the following journal article: Scholtz, J., et. al., *Proc. Natl. Acad. Sci. USA*, 88, 2854-2858 (1991). There are numerous other journal articles on the helix to coil transition in alanine peptides. It sometimes helps to look up other journal articles to get several perspectives and determine the variation in the experimentally determined energy. [Put a box around your numerical answer in part-A. For part-B, the recommended way to illustrate the answer is through a plot of population versus temperature.]

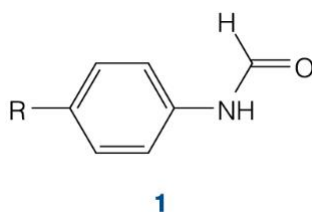
3. (A) Plot the Coulomb potential due to the nuclei at a point in a Li^+F^- ion pair located on a line half-way between the nuclei as the point approaches from infinity and ends at the mid-point between the nuclei. (B) Formation of LiF from the elements releases one of the highest energy per mass of reactants. What is the energy per mass of reactants for LiF and briefly discuss (from a chemical and/or molecular point of view) why it has one of the highest energies per mass of reactants. Also, provide the name and chemical formula of a compound that has a higher energy per mass of reactants.

4. Each student has been assigned a common gas or volatile liquid compound. (A) Do you expect the compound you have been assigned to behave like an ideal gas at standard temperature and pressure? This can be quantified by comparing the molar volume (density) of the compound using the Van der Waals equation of state to that of the ideal gas equation of state. (B) For the compound you have been assigned, under what temperature and/or pressure conditions do you start to get significant deviations from ideality? This can be quantified by comparing the Van der Waals equation of state to that of the ideal gas equation of state at various temperatures and/or pressures and determining where the two equations of state start to vary significantly (e.g., there is a $> 10\%$ deviation between the two equations of state).

5. Use the equipartition theorem to calculate the contribution of molecular motion to the total energy of a sample of 1 mole of (i) argon, (ii) nitrogen, (iii) carbon dioxide, (iv) water vapor and (v) methane at room temperature and pressure. (B) Compare the values calculated using the equipartition theorem to those from ab initio electronic structure computational calculates (from a program like molcalc.org).

6. (A) A sample of the sugar D-ribose of mass 1.525 g was placed in a constant volume calorimeter and then ignited in the presence of excess oxygen. The temperature rose by 1.91°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-ribose. (B) Calculate the enthalpy of formation of D-ribose 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). (C) Briefly compare the results from the calorimetric method used in part-A to the method used in part-B.

7. The following is an example of a structure-activity relation (SAR), in which it is possible to correlate the effect of a structural change in a compound with its biological function. The use of SARs can improve the design of drugs for the treatment of disease because it facilitates the prediction of the biological activity of a compound before it is synthesized. The binding of non-polar groups of amino acid to hydrophobic sites in the interior of proteins is governed largely by hydrophobic interactions. (A) Consider a family of hydrocarbons R-H. The hydrophobicity constants, π , for R = CH_3 , CH_2CH_3 , $(\text{CH}_2)_2\text{CH}_3$, $(\text{CH}_2)_3\text{CH}_3$, and $(\text{CH}_2)_4\text{CH}_3$, are, respectively, 0.5, 1.0, 1.5, 2.0 and 2.5. Use these data to predict the π value of $(\text{CH}_2)_7\text{CH}_3$. (B) The equilibrium constant K_1 for the dissociation of inhibitors (1) from the enzyme chymotrypsin (Atlas P3) were measured from different substituents R:



R	CH₃CO	CN	NO₂	CH₃	Cl	(CH₂)₂CH₃
π	-0.20	-0.025	0.33	0.50	0.90	1.5
K_1	2.34×10^{-2}	1.26×10^{-2}	3.72×10^{-3}	1.78×10^{-3}	3.98×10^{-4}	5.01×10^{-5}

Plot K_1 against π and determine the best fit to the data that allows for extrapolation. Hint: If the direct plot of K_1 against π is not linear, it is typically possible to find a functional form of K_1 and π that produces a

linear plot and then use a standard linear fitting algorithm for the best fit to the data. (C) Predict the value of K_1 for $R = H$ and $R = (CH_2)_7CH_3$.

8. Find and read a recent 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. (B) Summarize the significance of the paper in one paragraph. (C) List the thermodynamic parameters determined and what methods were used to measure or compute the thermodynamics presented in the paper. 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.