Study guide for the first midterm

Chemistry 342, Spring 2016
Friday, Feb. 19, in class
Physical Chemistry of Biochemical Systems

1 Key concepts and equations

For the following, you should understand the concepts, know (have memorized) the key equations, understand what all the symbols mean, and be able to explain the equations in words and to appreciate their context. Please pay close attention to the *Summary* and the *Mathematics Needed* sections at the end of the chapters. Please bring a calculator to the exam. Be sure to *show your work* for each problem.

Some constants: $N_A = 6.022 \times 10^{23}$ mol^{-1}; R=8.314 J $K^{-1}mol^{-1}$; h (Planck's constant) = 6.63 $\times 10^{-34}$ J s; $4\pi\varepsilon_0$= 1.11 $\times$ $10^{-10}C^2$/(Jm); 1 Å = 10^{-10}m; e (charge of the electron) = 1.602 $\times$ 10^{-19} C

1.1 Chapter 10: Enzyme kinetics

- Michaelis-Menten kinetics: initial rate $v_0 = V_{max}[S]/(K_M + [S])$, where $V_{max} = k_2[E]_0$
- Form of a Lineweaver-Burke plot

1.2 Chapter 11: Basics of quantum mechanics

- Bohr frequency relationship: $\Delta E = h\nu$
- de Broglie relation: $\lambda = h/p$
- Schrodinger equation: $-(\hbar^2/2m)(d^2\psi/dx^2) + U(x)\psi = E\psi$
- Harmonic oscillator: $E_n = (n + \frac{1}{2})h\nu$, where $\nu = \frac{1}{2\pi}\left(\frac{k}{\mu}\right)^{1/2}$
- Coulomb's law: $(q_1q_2)/(4\pi\varepsilon_0 r)$

2 Sample exam questions

1. Explain (define in words) each of the symbols in the above expressions; explain their limitations (what they assume)
2. The Michaelis-Menten mechanism is broadly applicable to many enzyme reactions, where "E" (enzyme) catalyzes the conversion of "S" (substrate) to "P" (product).

   (a) Write down this mechanism, showing rate constants for the elementary steps.

(b) Write an expression for the Michaelis constant, K_M, in terms of the elementary rate constants identified in part *(a)*.

(c) Experiments often measure v, the rate of production of products, as a function of substrate concentration, at a fixed concentration of total enzyme. Draw a qualitative plot of rate *vs.* substrate concentration for reactions following this mechanism.

3. Red light has a wavelength of 700 nm. What is its frequency? How much energy does it have in wavenumbers (cm^{-1})? What is the energy (in cm^{-1}) of light with a wavelength half that of red light?

4. Infrared spectroscopy involves excitations of vibrational motion of chemical bonds. For a typical C–H bond, an approximate potential energy is that of the harmonic oscillator:

$$V(x) = \frac{1}{2}k(x - x_0)^2$$

Here k is a force constant, x is the C–H bond length, and x_0 is the ideal bond length.

(a) Given that the atomic mass of carbon is 12.0 atomic mass units (amu), and that of hydrogen is 1.0 amu, what is the reduced mass μ of the C–H bond? Express your answer in both amu and kg.

(b) The fundamental vibrational frequency of the harmonic oscillator is $\nu = (1/2\pi)(k/\mu)^{1/2}$. Given a force constant of 2500 kJ mol^{-1} Å^{-2}, compute the frequency (expressed as wavenumbers) for a C–H bond. (*Hints*: 1 J = 1 kg m^2 s^{-2}; 1 amu = 1 g mol^{-1}.)

5. What is the potential energy between two electrons that are 1 Å apart? Express your answer in J/mol.

6. Consider the LiH molecule, where the two nuclei can be considered as fixed points. Let “A” and “B” represent the two nuclei, so that R_{AB} is the distance between them. Let r_{1A} and r_{1B} be the distances of electron “1” from the nuclei, (with similar expressions for the other electrons); and r_{12} be the distance between electrons “1” and “2”, (again, with similar expresions for the other electrons). Write the Schrodinger equation for the motion of the electrons in this system; identify the parts of the equation that refer to the kinetic, potential and total energies of the system. [The potential energy part should be expressed in terms of the electron charge e, the distances described above, and any needed universal constants.]