CHEM106 Midterm Exam
You must show all equations and all work to receive any credit

1. Draw the complete Lewis structures (include all nonzero formal charges and total charges) for:

   CH_3CN $BrCl_5$ CH_3COCH_3

2. Compare the magnitude of attractive London dispersion forces present between two water molecules with the magnitude of London dispersion forces present between two dimethyl ether [CH_3COCH_3] molecules. Clearly and fully support your reasoning.

3. Draw the mechanism for the reaction of a hydrogen phosphate ion [$H_2PO_4^-$] with a choline ion [$HOCH_2CH_2N(CH_3)_3^+$]. You must draw complete Lewis structures—to include all atoms, all bonds, all lone electron pairs and all full (not partial) charges--for both reactants and expected products. You must clearly show the mechanism for the reaction.

4. Chemical bond energies are typically in the range of 200-400 kJ/mole. For a bond energy of 300 kJ/mole, calculate the fraction of molecules at a temperature of 10,000 K that is expected to have a kinetic energy in excess of this bond energy.

5. Log P values are widely used in the pharmaceutical industry for drug discovery applications; in the environmental health industry to predict toxic substance accumulation in organisms, and in the agricultural industry to research improved insecticides, herbicides, and fertilizers. Not surprisingly, log P values are very closely related to biological activity. Answer each of these related questions:
    a. Define explicitly what P is using both a formula and an explanation.

    b. Rank—low to high--the P values for these substances: propanol [C_3H_7OH], water, octane [C_8H_{18}], methanol [CH_3OH], and 1-octanol [$C_8H_{17}OH$]. Provide clear reasons for your answer.

    c. A commercially available crosslinker chemical product, DSS, was found to have a log P value of -0.046. 100.0 mmoles of DSS are added to a solution containing 50.0 mL of water and 500.0 mL of 1-octanol. Calculate the number of mmoles of DSS that partitions into the 1-octanol phase.

6. The amino acid glutamic acid has pKa's of 2.10, 9.47, and 4.07 (side group).
    a. Draw the complete Lewis structures of the two most abundant forms of glutamic acid that would be present at a stomach pH of 1.50. Clearly show which is the more concentrated.

    b. For a pH of 1.50, calculate the ratio of the two most concentrated forms of glutamic acid.

7. A Lineweaver-Burk enzyme plot gave a slope of 0.0347 min and a y-intercept of 0.7645 min/mM.
    a. Calculate V_{max} and K_M for this reaction. Show all equations, substitutions and units.

    b. Assuming an enzyme concentration of 5 micromolar, calculate the enzyme's turnover number and discuss what turnover number explicitly refers to.

8. Approximately 1% of the world's population develops rheumatoid arthritis (RA). NSAIDs are often given to patients affected by RA; substances A and B are two different COX inhibitors widely used to treat RA. Inhibitor A has IC-50 values of 0.08 μM and 0.96 μM for COX-1 and COX-2 respectively. Inhibitor B has IC-50 values of 6.70 μM and 0.87 μM for COX-1 and COX-2 respectively.

    a. Draw two separate dose-response curves (one for inhibitor A, one for inhibitor B) that show how these substances affect COX-1 and COX-2 enzyme activity.

    b. If one of your family members develops rheumatoid arthritis and needed to use an NSAID daily for long-term treatment of pain and inflammation, which of these two COX inhibitors would you recommend that they take; more importantly, why (be very specific).

9. Draw the molecular structure for each of the following amino acids in the form that is most abundant at a physiological pH of 7.4. Except for aromatic rings, show all atoms, bonds, lone pairs, and full charges (not partial charges) for these compounds:

    a. Alanine

    b. Cysteine

    c. Threonine

    d. Phenylalanine

    e. Valine

    f. Lysine