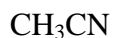


## CHEM106 Midterm Exam

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:



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 [ $\text{CH}_3\text{COCH}_3$ ] molecules. Clearly and fully support your reasoning.
3. Draw the mechanism for the reaction of a hydrogen phosphate ion [ $\text{H}_2\text{PO}_4^-$ ] with a choline ion [ $\text{HOCH}_2\text{CH}_2\text{N}(\text{CH}_3)_3^+$ ]. 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:
- Define explicitly what P is using both a formula and an explanation.
  - 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.
  - 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).
- 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.
  - 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.
- Calculate  $V_{max}$  and  $K_M$  for this reaction. Show all equations, substitutions and units.
  - 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  $\mu\text{M}$  and 0.96  $\mu\text{M}$  for COX-1 and COX-2 respectively. Inhibitor B has IC-50 values of 6.70  $\mu\text{M}$  and 0.87  $\mu\text{M}$  for COX-1 and COX-2 respectively.
- 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.
  - 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:
- Alanine
  - Cysteine
  - Threonine
  - Phenylalanine
  - Valine
  - Lysine