Seoul National University

457.620.001

Water Contaminants

FINAL EXAMINATION

TIME ALLOWED: 90 MINUTES

May 30, 2019

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1. Students may use one double-sided, A4 notes prepared in their own handwriting. Mechanical or electronic reproduction of any notes are not allowed.

2. Students should bring their own calculator which is not pre-programmed with formulae from the class.

3. Be aware that the cheated student will get 80% of the lowest score in class! There is no tolerance at all.

4. Make sure your answers include units if appropriate. Watch your units! Prepare your answers in a logical, easy-to-follow format.

5. If needed, use the following constants:

   Ideal gas constant, $R = 8.21 \times 10^{-2}\ L-atm/mol-K = 8.31 \times 10^{-3}\ kJ/mol-K$

   Faraday constant, $F = 96500\ Coulomb/mol = 96.5\ kJ/mol-V$

   Water dissociation constant, $K_w = [H^+][OH^-] = 10^{-14}$

6. **Assume 25 °C, 1 atm and activity = molarity in an aqueous solution unless specified in the question.**

1. Mark T or F for the following statements. (2 points each)

1) All of the carbon atoms in ethylbenzene are in the same plane.

2) The COD/TOC ratio of ethylene (C_2H_4) is higher than that of acetylene (C_2H_2).

3) The pK_a value of 2,4-dichlorophenol is higher than that of phenol.

4) Persistent organic pollutants (POPs) always show conservative properties in water.

5) Exothermic reactions always occur spontaneously.

6) The rate of an S_N1-type nucleophile substitution reaction does not depend on the property of a leaving group.

7) Under the same light radiation condition above the water surface, phenanthrene in clear water exhibits shorter direct photolysis half-life than phenanthrene in turbid water.

8) The performance reference compound (PRC) method employed for non-equilibrium passive sampling for hydrophobic organic contaminants (HOCs) in sediment pore-water assumes isotropic exchange kinetics at the passive sampler-sediment interface.

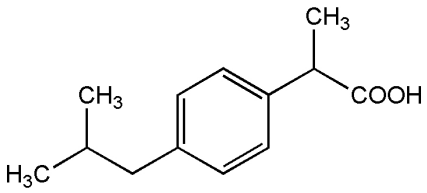
9) The higher the wind speed above the water surface, the greater the total resistance (R_{tot}) of interphase mass transfer between air and water.

10) For a given value of longitudinal dispersivity, the Peclet number generally increases with increasing length of a system.

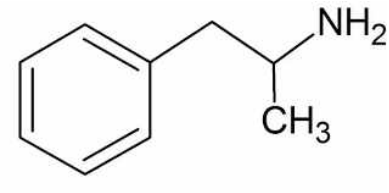
2. Answer the following questions.

1) A chemical that has at least one pair of enantiomers (optical isomers) is called to be “chiral”. For each of chemicals listed below, determine if it is chiral and if so, provide the total number of enantiomers. (7 points)

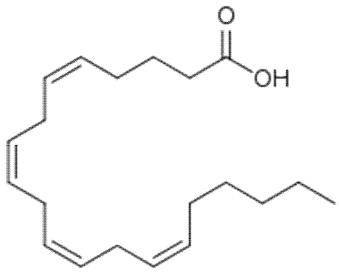
i) ibuprofen



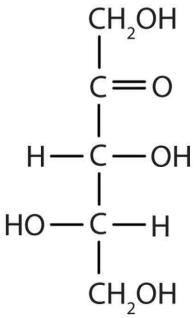
ii) amphetamine



iii) arachidonic acid



iv) ketopentose



2) Among ethane (C_2H_6), ethanol (C_2H_5OH), and hexachloroethane (C_2Cl_6), which one will be the most soluble in water and which one the least? Describe the reason for your decision. (6 points)

3) Describe the potential impact of the presence of natural organic matter (NOM) in water and wastewater treatment. (5 points)

4) Soil organic matter (SOM) can be divided into i) those exhibiting a rubbery (i.e., soft) structure which allows organic contaminants to easily penetrate below the surface and ii) those exhibiting a glassy (i.e., hard) structure which does not allow the penetration. The glassy-type is known to show high affinity to organic contaminants. For the Freundlich isotherm of an organic contaminant described by $C_s = K_F \cdot C_{aq}^{1/n}$, predict what the n value is likely to be, n<1, n close to 1, or n>1 for each type of soil organic matter (i.e., rubbery and glassy). Briefly describe your rationale. (7 points)

3. Carbon tetrachloride (CCl_4) may react with hydrogen gas (H_2) to be reduced into chloroform ($CHCl_3$). Using the following half reactions, calculate the minimum hydrogen partial pressure required for the reaction to be thermodynamically favorable until the chloroform to carbon tetrachloride molar concentration ratio (i.e., $[CHCl_3]/[CCl_4]$) reaches 10^6. Use T = 25 °C, pH = 7.0, and $[Cl^-] = 10^{-3}$ M.

$CCl_4 + H^+ + 2e^- = CHCl_3 + Cl^-, \quad E_H^0 = 0.79\ V$

$2H^+ + 2e^- = H_2(g), \quad E_H^0 = 0.00\ V$

(15 points)

4. Using the following rate constants for ethyl acetate ($CH_3COOC_2H_5$), determine the value of I_{AB} (i.e., the pH at which the rates for acid- and base-catalyzed hydrolysis reactions are the same). What is the hydrolysis half-life at pH = I_{AB}?

k_A	k_N	k_B
$1.1\times10^{-4}\ M^{-1}s^{-1}$	$1.5\times10^{-10}\ s^{-1}$	$1.1\times10^{-1}\ M^{-1}s^{-1}$

k_A = 2nd order acid-catalyzed hydrolysis rate constant
k_N = pseudo 1st order neutral hydrolysis rate constant
k_B = 2nd order base-catalyzed hydrolysis rate constant

(15 points)

5. During his Ph.D. study, Prof. Choi used polyethylene (PE) passive samplers to determine the sediment-water partitioning coefficient, K_p, of 2-methyl naphthalene. In a 40-mL amber vial, he added **10 g sediment (in dry weight), 30 cm^3 water, and 20 mg PE passive sampler, leaving 5 cm^3 as head space (i.e., air).** The initial concentration of 2-methyl naphthalene in the sediment was 10 nmol/g sediment dry weight, and no 2-methyl naphthalene was present in any other phases at the beginning. After 1 month of continuous mixing, which was sufficient to establish equilibrium partitioning for 2-methyl naphthalene, he sampled the PE passive sampler. The 2-methyl naphthalene

concentration in the PE passive sampler was measured to be 7.5 nmol/g PE. Using T = 25 °C and the values listed in the table, answer the following.

Parameter	H_{pc} (cm^3-atm/mol)	K_{PE} (cm^3 water/g PE)
Value	520	2.2×10^3

K_{PE}: PE-water partitioning coefficient

1) Determine the fugacity of the system. (6 points)

2) Prove that the 2-methyl naphthalene loss from the sediment to water, PE, and head space is all negligible. (10 points)

3) Calculate the sediment-water partitioning coefficient, K_p, of 2-methyl naphthalene in cm^3 water/g sediment dry weight. (4 points)

6. You bought a bottle of "super oxygen water" from a market, which is highly supersaturated with oxygen (dissolved oxygen concentration = 60 mg/L). You poured 200 cm^3 of the drink to a cup in a cylindrical shape with an inner diameter of 8 cm and left it for 3 hours. What will be the dissolved oxygen concentration of the drink then? Use an overall mass transfer coefficient (K_L) of 1.00×10^{-2} m/h and the saturated dissolved oxygen concentration of 8.3 mg/L.

(15 points)