

**Seoul National University**

**457.620.001**

**Water Contaminants**

***FINAL EXAMINATION***

**TIME ALLOWED: 75 MINUTES**

**June 04, 2020**

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1. Students may use two 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.

1. Mark O or X for the following statements.

(+2 points for correct answers; -2 points for incorrect answers)

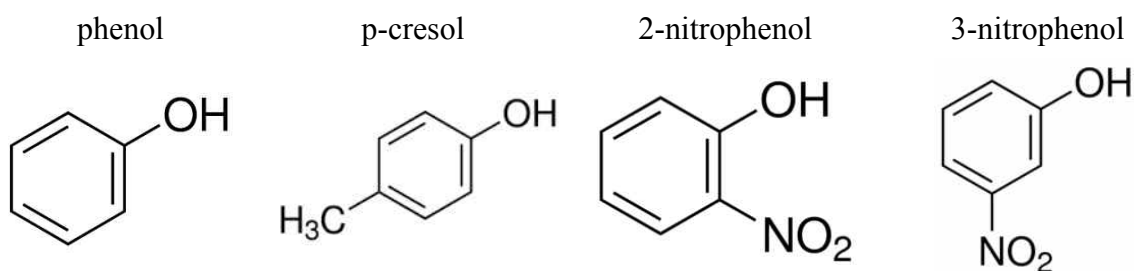
- 1)  $\text{Ca}^{2+}$  ion in a water sample with an ionic strength of  $10^{-2}$  has a smaller activity coefficient value than that of  $\text{Na}^{+}$  ion in the same water sample.
- 2) The COD/TOC ratio of acetic acid ( $\text{CH}_3\text{COOH}$ ) is smaller than the COD/TOC ratio of ethanol ( $\text{C}_2\text{H}_5\text{OH}$ ).
- 3) Toluene ( $\text{C}_6\text{H}_5\text{CH}_3$ ) is a planar molecule.
- 4) 1,3-butadiene ( $\text{C}_4\text{H}_6$ ) has a conjugated double bond.
- 5) Persistent organic pollutants are often used as conservative tracers.
- 6) Reductive dechlorination of trichloroethene occurs at an appreciable rate (half life in the order of months) abiotically in the dark in the absence of catalysts.
- 7) Transformation of a molecule structure always occur if the molecule absorbs a photon with sufficient energy to induce the transformation.
- 8) The resistance at the gas phase boundary layer dominates the overall resistance of mass transfer at the air-water interface for highly volatile compounds.
- 9) The greater the Peclet number, the more dominant the dispersion over advection.
- 10) For rivers, the overall dispersion coefficient in the longitudinal direction is typically much smaller than the overall dispersion coefficient in the vertical direction.

2. For a compound represented by a molecular formula of  $\text{C}_3\text{H}_4\text{Br}_2$ , answer the followings.

- 1) Provide all possible structures (i.e., constitutions) and indicate the systematic names for each. (8 points)

2) Does any of the structural isomers have a pair of stereoisomers? If yes, provide the geometry of the stereoisomeric compounds. (6 points)

3. Compare the  $pK_a$  values of the compounds given below. Explain your rationale. (9 points)



4. Compound A is being chemically reacted to generate a final product C. As shown in the following, the reaction occurs in two steps that are in series. Both steps are irreversible and are expressed as a first-order reaction with rate constants  $k_1$  and  $k_2$ .



The initial concentrations for the compounds are as follows:

$$[A]_0 = 5 \text{ mM} \qquad [B]_0 = 3 \text{ mM} \qquad [C]_0 = 2 \text{ mM}$$

Calculate the concentration of B after 2 days. (10 points)

5. Determine the pH at which the hydrolysis rate of  $\text{CH}_3\text{Br}$  with  $\text{H}_2\text{O}$  as a reactant and the hydrolysis rate of  $\text{CH}_3\text{Br}$  with  $\text{OH}^-$  as a reactant are identical, in other words, the  $I_{\text{NB}}$  value for the hydrolysis of  $\text{CH}_3\text{Br}$ . Assume molarity = activity, temperature =  $25^\circ\text{C}$ , and use  $n_{\text{OH}^-, \text{CH}_3\text{Br}} = 4.2$ . (10 points)

6. Plumlee & Reinhard (2007) reported the overall specific light absorption rate of 0.12~0.24 einstein/mole-hr for n-dimethylnitrosamine (NDMA) in a natural river with 1 m mixed water depth under midday solar irradiance condition of Southern California, USA. They also reported a reaction quantum yield value of 0.41 for NDMA.

The second-order rate constant for reaction between hydroxy radical ( $\cdot\text{OH}$ ) and NDMA is reported as  $4.0 \times 10^8$  L/mole-s in the literature. In addition, Brezonik & Fulkerson-Brekken (1998) reported an annual average steady-state  $\cdot\text{OH}$  concentration of  $2.1 \times 10^{-18}$  M in a Southern California river.

Decide whether direct or indirect photolysis is dominant for photochemical transformation of NDMA in Southern California rivers. Conduct quantitative analysis to answer. Assume  $\cdot\text{OH}$  is the only relevant photochemically-produced reactive intermediate (PPRI) for indirect photolysis of NDMA.

(10 points)

7. The pesticide DDT (MW = 354.5) has the following properties:

Vapor pressure =  $10^{-9.87}$  atm (25°C)

Aqueous solubility =  $10^{-7.85}$  mole/L (25°C)

Octanol-water partitioning coefficient,  $K_{ow} = 10^{6.36}$

1) Calculate the Henry's constant at 25 °C expressed as a dimensionless concentration ratio,  $H_{cc}$ . (5 points)

2) In a 40-mL vial, you added 5 g soil and 20 mL water, spiked some DDT, and agitated the contents until equilibrium was established. The air volume in the vial was 17 mL. Determine how mass of the spiked DDT is distributed at each phase (i.e., mass fraction in air, water, and soil relative to the total mass spiked). The soil-water distribution coefficient,  $K_d$ , is estimated to be  $1.5 \times 10^5$  L/kg.

(14 points)

3) Qualitatively predict the fate of DDT applied to agricultural area. Neglect the transformation reactions of DDT. (8 points)