2022 WUCT: Chemistry of Medicine

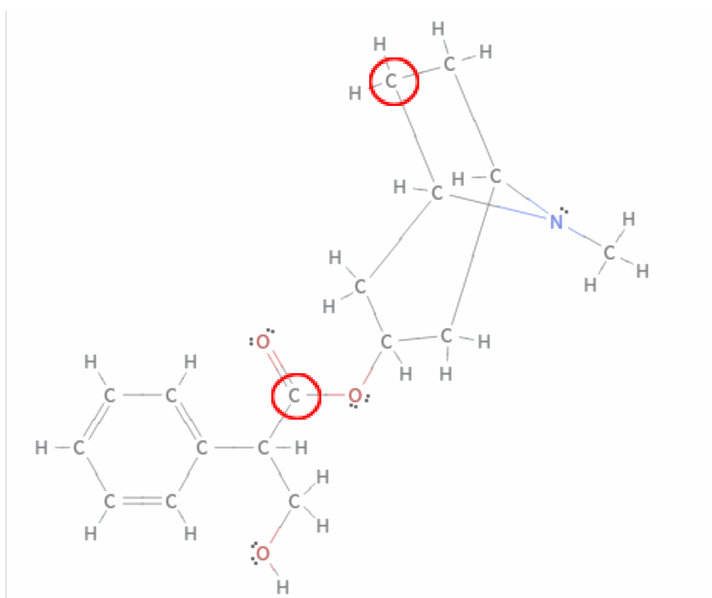
This exam consists of 7 questions and is worth 100 points. You will work together with a partner to answer the questions. You will have 1 hour to take the exam, followed by 10 minutes of upload time during which you cannot make changes to your exam. The only allowed resources for this exam are a calculator and the provided equation sheet. You may NOT use any other notes, books, or websites (other than Gradescope and HopIn). You must show your work and box your final answer to receive credit for a problem. NOTE: If you get the answer to an early part of a question incorrect but later use that answer for a subsequent part of the question, you can still earn full credit for those subsequent parts. Please write your answer in the designated space on the answer sheet. If you need additional space for a problem, you may use scratch paper, but make sure to clearly indicate in the problem's designated space where the rest of your work can be found. Dark pencil or pen is preferred so that your writing clearly shows on your submitted document in Gradescope.

Problem #1: ***(13 points)***

Atropine is commonly used as a medication to treat the symptoms of bradycardia, an abnormally low heart rate. The molecular formula of atropine is $C_{17}H_{23}NO_3$.

a) What is the molecular mass of $C_{17}H_{23}NO_3$? ***(2 points)***

b) Shown below is the lewis structure of atropine. Write the correct hybridizations of the circled carbons. Also write how many hydroxyl groups are present in the molecule. ***(3 points)***

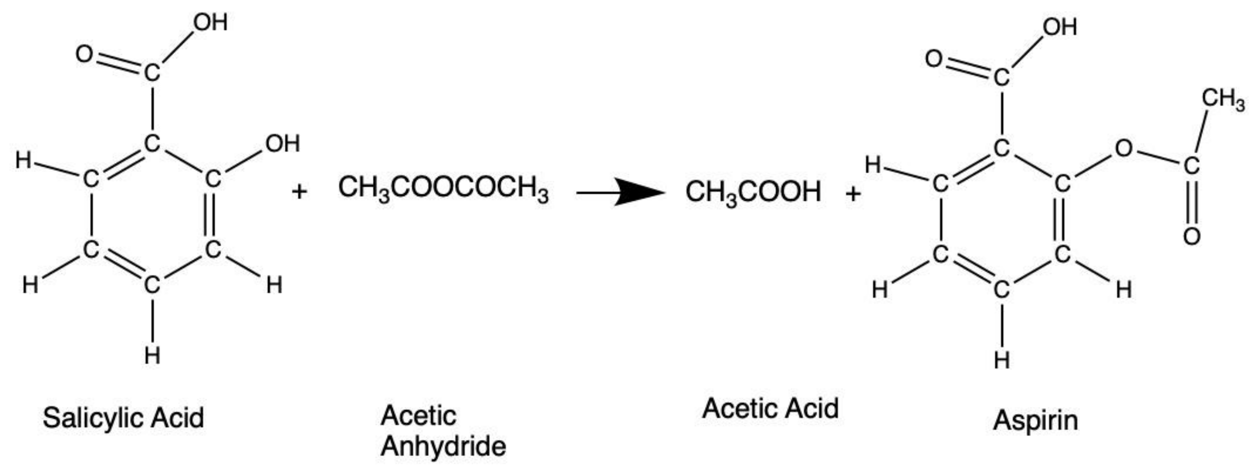


c) Assume a researcher is conducting an experiment with the compound and has a step in the procedure that calls for the addition of 1.50 mL of a 3.0% by mass $C_{17}H_{23}NO_3$ solution. How many moles of $C_{17}H_{23}NO_3$ are added in this step? Since the concentration of $C_{17}H_{23}NO_3$ is quite low, you can assume that the density of the $C_{17}H_{23}NO_3$ solution is the same as water, 1.0 g/mL. Show your work below and round your answer to two decimal places. ***(4 points)***

d) In a second portion of the experiment, the researcher is working with the elements xenon and chlorine. Together, they form a neutral compound, $XeCl_n$, where n is a whole number integer. The mass of 7.0544×10^{20} molecules of $XeCl_n$ is 0.3199 g. Determine the whole number integer value of n. ***(4 points)***

Problem #2: ***(15 points)***

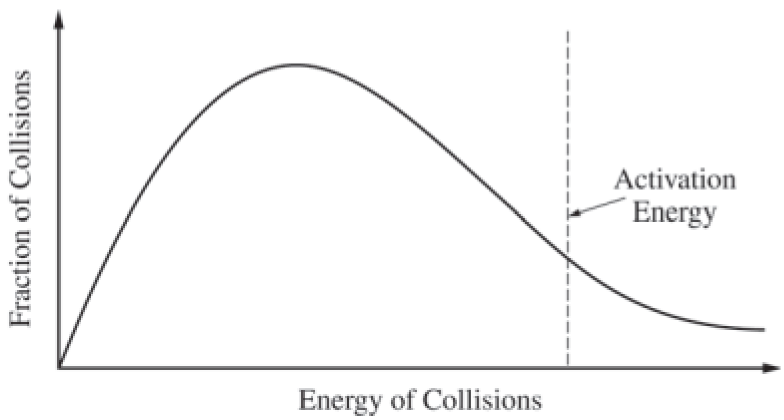
Aspirin is a common drug for relieving minor aches, pains, and fevers. The production of aspirin from raw materials can be divided into four separate reactions, the last of which is shown below:



a) Draw the missing Lewis structures for acetic anhydride and acetic acid. ***(4 points)***

b) What is the hybridization of each of the two carbon atoms in acetic acid? ***(2 points)***

c) The graph below shows a distribution for the collision energies of reactant molecules at room temperature. Heat is commonly applied to the starting materials to facilitate solvation and speed up the reaction. Draw a second curve on the graph that shows the distribution for the collision energies of reactant molecules when they are heated to a higher temperature. ***(2 points)***



d) Given the following standard enthalpies of formation, predict which species, salicylic acid or aspirin, will increase in concentration following the temperature change described in part (c). Justify your answer. ***(3 points)***

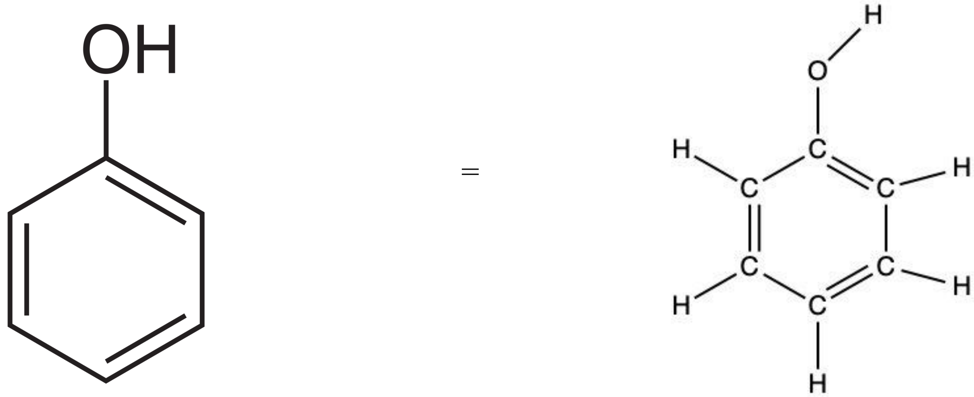
Compound	**ΔH°f (kJ/mol)**
Salicylic acid	-585
Acetic anhydride	-625
Acetic acid	-484
Aspirin	-140

e) Predict which side of the reaction is favored at *equilibrium*. Include a discussion of the standard entropy of the reaction based on the number of reactants consumed and products formed. ***(2 points)***

f) In a different reaction, acetic anhydride can combine with H_2O to form acetic acid. This reaction favors the formation of products. Explain how the equilibrium constant, K, of this reaction compares to that of the original reaction. ***(2 points)***

<u>Problem #3</u>: *(12 points)*

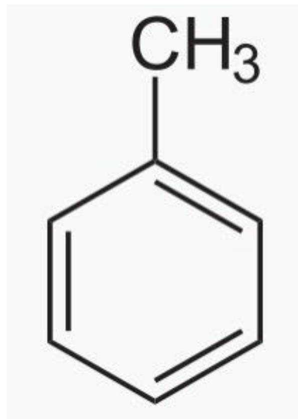
Over 60% of FDA approved small molecule drugs contain at least one aromatic ring motif. Below is an example, phenol (molecular formula: C_6H_6O). Phenol is used to relieve pain and irritation caused by sore throat, sore mouth, or canker sores. One of the reasons behind this application is the stability the ring provides, allowing the drug to bind better to biological molecules.



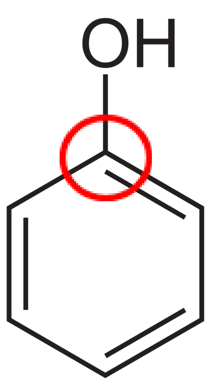
a) Explain the stability in terms of the bonding pattern of the ring. Note: There is a carbon atom everywhere there is a vertex. When the carbon atom has less than 4 bonds, it is assumed that the carbon atom is bonded to as many hydrogen atoms as needed to bring it to a total of 4 bonds. ***(3 points)***

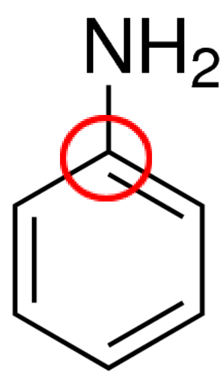
b) Another important characteristic of phenol is that it can participate in hydrogen bonding. Draw at least three molecules of phenol with this intermolecular interaction, with relevant partial positive and negative charges. ***(4 points)***

c) Structurally, a compound known as toluene looks very similar (see picture below). However, toluene has a different boiling point than phenol. Please identify which compound has the higher boiling point and explain. ***(3 points)***



d) Please identify the geometries about the circled atom in both phenol and aniline. ***(2 points)***





Problem #4: ***(13 points)***

Sulfuric acid, H_2SO_4, is a strong acid that is a common component in many chemotherapy drugs due to its ability to break down cancerous cell DNA. A researcher is working with sulfuric acid in a lab, configuring a set of experiments in an attempt to determine its quantity and concentration limits for an emerging chemotherapy drug. At 25˚C, the pH of a 25.0 mL sample of 0.15 *M* H_2SO_4 is 1.07. It reacts with water as shown in the equation below:

$$H_2SO_{4(aq)} + H_2O_{(l)} \rightarrow H_3O^+_{(aq)} + HSO_4^-{}_{(aq)}$$

a) Identify a Brønsted-Lowry conjugate acid-base pair in the reaction. Label which is the acid and which is the base. ***(2 points)***

b) Determine the K_a for sulfuric acid at 25˚C. Round your answer to three decimal places. ***(4 points)***

c) Read the statement below and determine if it is true or false. Justify your reasoning in 2-3 sentences. ***(2 points)***

If the pH of an acetic acid solution is the same as the pH of a sulfuric acid solution, then the molar concentration of the sulfuric acid solution must be less than the molar concentration of the acetic acid solution.

d) Assume a researcher wants to conduct a test to see if acetic acid is a valid substitute for sulfuric acid in the chemotherapy drug. In the process, he finds that creating a buffer and calculating its pH will reveal the effectiveness of the substitution. The researcher creates a buffer solution by dissolving 8.0 grams of sodium acetate in 160.0 mL of 1.2 M acetic acid. Assuming the researcher neglects any changes in volume from the sodium acetate, calculate the pH of the acetic acid/sodium acetate buffer solution. The K_a for acetic acid is 1.8×10^{-5}. Round to two decimal places. ***(5 points)***

Problem #5: ***(16 points)***

Imagine that it has been found that Atorvastatin, a commonly prescribed drug that is used to lower patients' cholesterol, actually has two differing existing chemical compositions each with their respective properties. Medical professionals deliberate about the effectiveness of the two drugs, known as Atorvastatin A and Atorvastatin B, and carry out research to analyze the effectiveness of each composition. Assume Atorvastatin A has a half life of 8 hours and Atorvastatin B has a half life of 6 hours.

a) Assuming that 1 g samples of both drugs are collected for experimentation, find the rate constant k of each. Round to the nearest thousandth. ***(5 points)***

b) Using the k rate constants calculated in part (a), how much of Atorvastatin A and Atorvastatin B will remain after one and a half days? Round to the nearest thousandth. ***(5 points)***

c) Doctors want to ensure that the Atorvastatin is out of the bloodstream as quickly as possible. As a result, they want to find which version of the drug takes the least amount of time to be cleared (1% remaining). In a written statement, identify which drug this is by finding the time it takes for each drug to be 99% cleared from the bloodstream. Round your answer to the nearest thousandth. ***(6 points)***

Problem #6: ***(15 points)***

Hearing aids are most commonly powered by silver oxide batteries. A silver-oxide battery uses silver (I) oxide as the cathode, zinc as the anode, plus an alkaline electrolyte, usually sodium hydroxide (NaOH) or potassium hydroxide (KOH).

a) Write the balanced half cell reactions that occur at each electrode. ***(2 points)***

b) Using the information provided in the Table of Standard Reduction Potentials, determine whether this cell is a Galvanic cell. Please give evidence for your answer. ***(3 points)***

c) In which direction do electrons flow? ***(2 points)***

d) For nonstandard conditions (specifically, nonstandard molar concentrations), a version of the Nernst equation can be used to find $\Delta\varepsilon$.

$\Delta\varepsilon = \Delta\varepsilon° - \frac{0.0257}{n}(\ln Q)$, where n is the number of moles of e- per mole of reaction

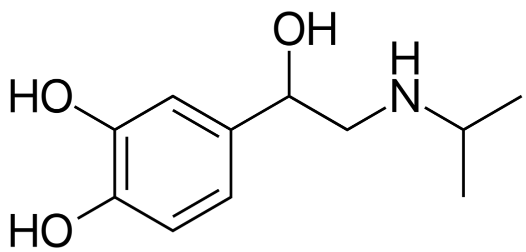
After the cell runs spontaneously for a certain period of time, the concentration of silver ions has decreased to 0.5 M, while the concentration of zinc ions has increased to 1.25 M. Assume the volume stays constant.

What is the cell potential at this point? It may be helpful to write out the overall electrochemical reaction. ***(4 points)***

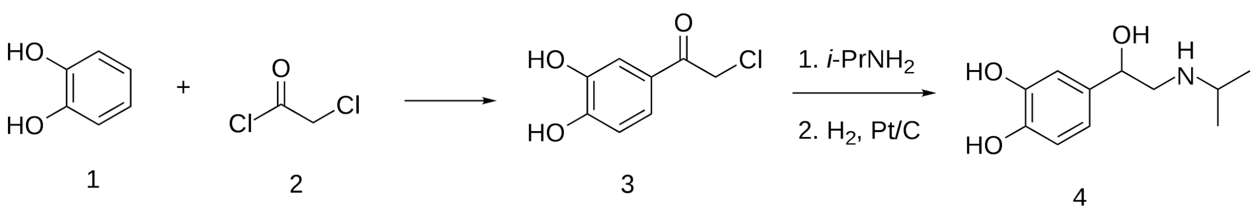
e) Calculate the solubility product constant, Ksp, of AgBr in pure water at 25°C. ***(4 points)***

Problem #7: ***(16 points)***

Isoprenaline, also known as isoproterenol, is an organic compound that can imitate the effects of the sympathetic nervous system. Isoprenaline is often used for treatment of various heart diseases, including bradycardia and heart block. It is also sometimes used to treat asthma. The molecular structure of isoprenaline is shown below.



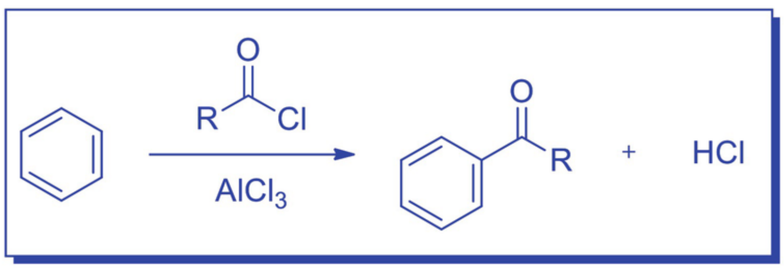
Isoprenaline is often made using a friedel-crafts acylation reaction, as shown below, between 1,2-dihydoxylbenzene (molecule #1) and chloroacetyl chloride (molecule #2) in the presence of an $AlCl_3$ catalyst. During the reaction, it forms an intermediate compound, 2-chloro-3′,4′-dihydroxyacetophenone (molecule #3), before becoming the final product, isoprenaline (molecule #4).

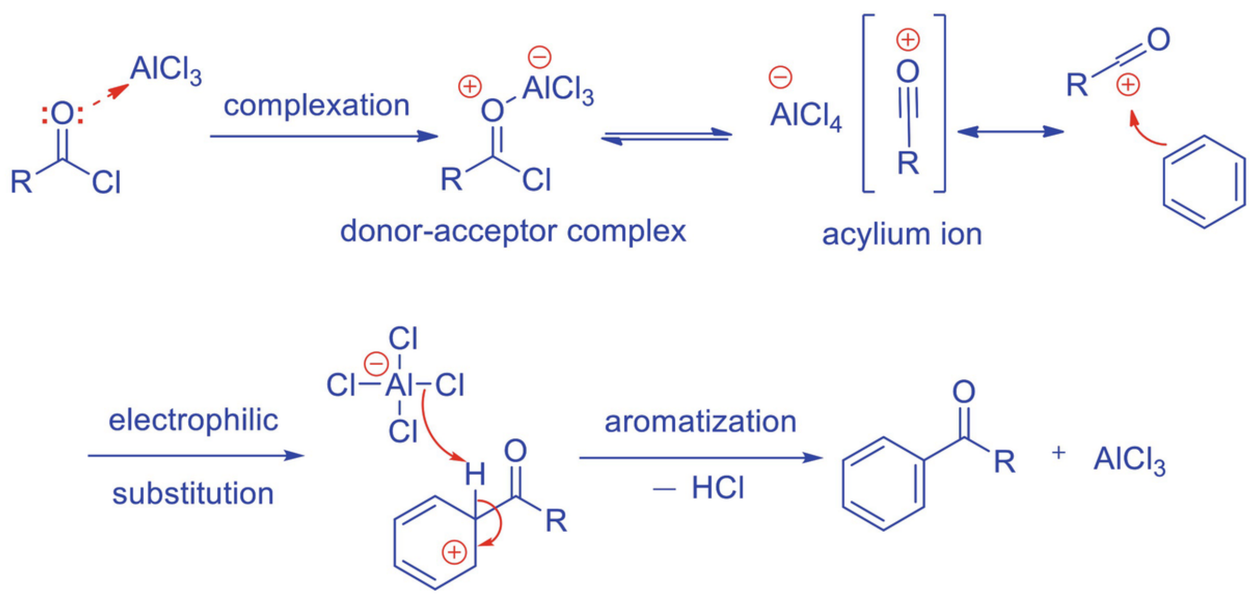


a) Write out the molecular formula for 1,2-dihydoxylbenzene (molecule #1) ***(2 points)***

b) What is the empirical formula for 1,2-dihydoxylbenzene (molecule #1)? ***(2 points)***

c) A friedel-crafts acylation reaction between 1,2-dihydoxylbenzene (molecule #1) and chloroacetyl chloride (molecule #2) in the presence of an $AlCl_3$ catalyst results in the formation of 2-chloro-3′,4′-dihydroxyacetophenone (molecule #3). The chemical mechanism behind a friedel-craft's acylation reaction between benzene and ROCl in the presence of $AlCl_3$ catalyst is shown below. In the space below, show the entire mechanism of the reaction between 1,2-dihydoxylbenzene (molecule #1) and chloroacetyl chloride (molecule #2) in the presence of an $AlCl_3$ catalyst forming the intermediate compound, 2-chloro-3′,4′-dihydroxyacetophenone (molecule #3). ***(12 points)***





(space for answer for part c)