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Sample Question Solutions for the Chemistry of Coffee Topic Test

1. During the 2013 Barista Championship, one of the contestants used a distillation apparatus to deliver a “distilled coffee” product as his specialty drink. In chemistry, distillation is traditionally used to separate compounds by boiling point.

a. This Barista first brewed coffee normally and then collected the first distillate as his flavorful product for the judges. If caffeine has a boiling point of 178°C, would the drink served to the judges contain any caffeine? What color would the drink be?

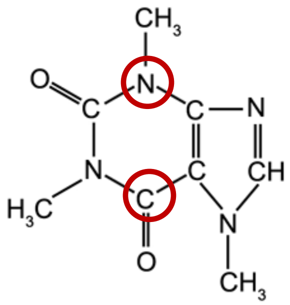
No- since coffee is brewed in water, with a bp of 100°C, the product would not contain any caffeine.

The product would be colorless.

b. If the barista had first added sugar to the coffee before putting it through the distillation apparatus, would the judges have to wait a shorter or longer time to get their first taste of his drink?

Longer time: boiling point of a liquid is elevated with the addition of a solute

c. Looking at the caffeine molecule, which type of intermolecular interactions contribute most to its high boiling point? Please circle 2 parts of the molecule where these interactions would occur and explain your choice (in 1 sentence).



In aqueous solution (around pH of 7), caffeine molecule is protonated (+ charge on nitrogen atoms) and therefore can interact with water via Hydrogen bonding and internally via dipole-dipole interactions and dipole-induced dipole interactions between positively charged N atoms and carbonyl O.

Any of the nitrogen atoms and oxygen atoms may be circled for full credit since these atoms are the predominant players in intermolecular interactions for a caffeine molecule.

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2. Caffeine metabolism follows first-order kinetics. Studies have shown that the half-life of caffeine in the body of a healthy adult is 6 hours, and that an average person can only fall asleep when the average amount of caffeine drops below 2.5 milligrams per kilogram of body mass.

a. A 12 oz. cup of "Death Wish Coffee" contains 650 mg of caffeine. If Over-caffeinated Oscar consumes one 12 oz. cup of this coffee at 8:00 A.M., how many grams of caffeine will remain in his system at 5:30 P.M.?

Hint: For first-order kinetics, if $[A_t]$ is the amount of substance at a time t, and $[A_0]$ is the initial amount of substance, then the following equation applies

$$\ln[A_t] = \ln[A_0] - kt \text{ , where k is a constant}$$

$$\ln\left[\frac{A_t}{A_0}\right] = -kt \Rightarrow \frac{A_t}{A_0} = e^{-kt} \Rightarrow A_t = A_0 e^{-kt}$$

$$\frac{A_t}{A_0} = \frac{1}{2} = e^{(-k)(6\text{ hr})} \Longrightarrow k = 0.1155\text{ hr}^{-1}$$

$$\text{8:00 A.M. to 3:30 P.M. is 7.5 hours, so } A_t = (650\text{ mg})e^{(-0.1155\text{ hr}^{-1})(7.5\text{ hr})}$$

$$A_t = 273.34\text{ mg}$$

273.34 milligrams of caffeine remain in Oscar's system at 3:30 P.M.

b. How long after drinking the cup of Death Wish Coffee will Oscar finally be able to fall asleep? Oscar has a mass of 85 kg; assume the caffeine is evenly distributed in his body.

$85\text{ kg body mass}\left(\frac{2.5\text{ mg caffeine}}{1\text{ kg body mass}}\right) = 212.5\text{ mg caffeine.}$ Below this threshold, Oscar will be able to fall asleep.

$$\frac{A_t}{A_0} = \frac{212.5\text{ mg}}{650\text{ mg}} = 0.3269 = e^{(-0.1155\text{ hr}^{-1})(t)}$$

$$t = \frac{\ln(0.3269)}{-0.1155\text{ hr}^{-1}} = \mathbf{9.68\ hours}$$

(This question continues on the next page.)

c. 2 grams of caffeine is considered a dangerous dose. If an average person were to consume one cup of Death Wish coffee every hour, with the first cup being consumed at $t = 0$ hours, how long will it take for the level of caffeine in the body to first exceed 2 grams? Afterwards, will the total amount of caffeine ever drop below 2 grams again?

$$\text{From part (a)}, A_t = A_0 e^{-kt}$$

$$\text{At } t = 0 \text{ hours, 650 mg caffeine are consumed. } A_t = 650 \text{ mg.}$$

$$\text{Just before 1 hour has elapsed, } A_{0.9999} \approx (650 \text{ mg}) e^{(-0.1155 \text{ hr}^{-1})(1 \text{ hr})} = 579 \text{ mg.}$$

$$\text{At } t = 1 \text{ hour, another 650 mg are consumed. } A_1 = 579 + 650 = 1229 \text{ mg.}$$

$$\text{Using same method as above, just before } t = 2 \text{ hr, } A_{1.9999} \approx 1094 \text{ mg.}$$

$$A_2 = 1745 \text{ mg, just before } t = 3 \text{ hr, } A_{2.9999} \approx 1555 \text{ mg.}$$

$$A_3 = 2205 \text{ mg, which is greater than 2 grams.}$$

It will take 3 hours for the level of caffeine to reach 2 grams.

$$\text{Just before } t = 4 \text{ hr, } A_{3.9999} \approx 1964 \text{ mg.}$$

The level of caffeine will drop below 2 grams again at some point between t= 3 hr and t=4 hr.

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3. It has been said that there is a time and a place for decaffeinated coffee-- never and in the trash.

a. One method of decaffeinating coffee beans is called the Swiss Water Process. It involves soaking a batch of fresh coffee beans in very hot water to extract all the caffeine, oils, and flavorful molecules. The caffeine is selectively removed, and this mixture is heated with a fresh batch of coffee beans. Use solubility principles to explain why this will result in decaffeination of the second batch of beans without a huge loss of oils and flavor molecules.

This process works because there is some equilibrium between the amounts of caffeine and oils/flavors present in the beans and in the solution. In the second round of heating, there is a lot of caffeine in the beans but none in the water, so the caffeine will be extracted and dissolve in the water until this equilibrium is reached. However, the water already contains a significant amount of oils/flavor molecules so the solution is nearly saturated with respect to these molecules, and there will not be a huge loss of oils/flavors.

b. It would be unacceptable to just throw all of that caffeine away, so let's further investigate how we might be able to isolate/purify the caffeine into a useful form. The first step to separating the caffeine from the rest of the solution is to convert it from its protonated form to its neutral form. Should we use an acid or a base to accomplish this?

The Bronsted-Lowry definition of acids and bases tells us that acids are proton donors and bases are proton acceptors, therefore we should add a base.

c. Now, we want to choose a solvent that will selectively dissolve the caffeine and allow us to separate it from the aqueous solution by forming 2 distinct layers. Choose between: H_2O (water), CH_3CH_2OH (ethanol), and CH_2Cl_2 (dichloromethane) and justify your answer.

Even without any knowledge of organic chemistry, students should be able to solve this problem based on knowledge of intermolecular forces. H_2O can be eliminated because we've already established that water will dissolve all of the components of the solution. CH_3CH_2OH could potentially be useful in dissolving caffeine since it's a polar molecule, however ethanol is miscible with water and we would not be able to separate the two solutions. That leaves CH_2Cl_2 which is a polar solvent that is not miscible with water and is therefore perfect for dissolving caffeine.

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d. Once we separate the two solvents from one another, we still need to figure out a way to remove the solvent and obtain our caffeine crystals. One method to do this is through distillation. Suppose, however, that you want to speed up the process or avoid exposing the caffeine to heat. How could you accomplish this? Hint: think about the definition of boiling or how we can manipulate the boiling point of a substance.

The boiling point of a substance is defined as the temperature at which its vapor pressure becomes equal to the external pressure. Therefore, in order to lower the boiling point of a substance we can either find a way to change the vapor pressure of the substance or the external pressure. The best option is to change the external pressure, which we can accomplish by putting the solution under vacuum. This lowers the external pressure and therefore the boiling point.

e. In part c we mentioned that CH_2Cl_2 might be useful in the decaffeination process. Say that Jim has a supply of methane and chlorine gas, and he wants to synthesize dichloromethane. Write a balanced overall reaction for this synthesis. Hint: Jim will need a good way to deal with formation of a strong acid.

$CH_4+2Cl_2 \rightarrow CH_2Cl_2+2HCl$

f. Ethyl acetate, CH3CO2C2H5, is another compound commonly used in decaffeination. If 30 grams of ethyl acetate are combusted in excess oxygen and the reaction goes to completion, how many liters of gas are present when the product mixture is at 120 ºC and 1 atm? Assume ideal behavior.

First write the balanced equation for the combustion of ethyl acetate:

$$CH_3CO_2C_2H_5+5O_2 \rightarrow 4CO_2+4H_2O$$

Then calculate how many moles of products will be formed:

$$30\text{ g } CH_3CO_2C_2H_5 \text{ x } (1\text{ mol } CH_3CO_2C_2H_5/88.11\text{g}) = 0.34\text{ mol } CH_3CO_2C_2H_5$$

$$0.34\text{ mol } CH_3CO_2C_2H_5 \text{ x } (4\text{ mol } CO_2/1\text{ mol } CH_3CO_2C_2H_5) = 1.36\text{ mol } CO_2 \text{ produced}$$

$$0.34\text{ mol } CH_3CO_2C_2H_5 \text{ x } (4\text{ mol } H_2O\ /1\text{ mol } CH_3CO_2C_2H_5) = 1.36\text{ mol } H_2O \text{ produced}$$

At 120 C, both products will be in the gas phase, so we have 2.72 mol of gas.

Then use the ideal gas law to calculate volume:

$$PV=nRT$$

$$(1\text{ atm})V=(2.72\text{ mol})(0.08206\text{ L*atm/mol*K})(393\text{ K})$$

V=87.7 L of gas