Name ______________________________ Team ID # ________________________

Team Name ______________________________________

2023 WUCT: TEAM EXAM

April 1st, 2023
2:15 – 3:15 p.m.

Please fill in the numbers of your 6-digit team ID:

Team ID					
⑨	⑨	⑨	⑨	⑨	⑨
⑧	⑧	⑧	⑧	⑧	⑧
⑦	⑦	⑦	⑦	⑦	⑦
⑥	⑥	⑥	⑥	⑥	⑥
⑤	⑤	⑤	⑤	⑤	⑤
④	④	④	④	④	④
③	③	③	③	③	③
②	②	②	②	②	②
①	①	①	①	①	①
⓪	⓪	⓪	⓪	⓪	⓪

1 HOUR will be allowed for the exam. The examination contains **7** questions on **23** numbered pages, including the last **SCRATCH PAGE**.

TURN IN THE ENTIRE EXAM (INCLUDING THE SCRATCH PAGE) WHEN YOU ARE FINISHED!

Exam Points Breakdown:

1. (12 pts)
2. (14 pts)
3. (12 pts)
4. (15 pts)
5. (22 pts)
6. (13 pts)
7. (12 pts)
Total Points: (100 pts)

2023 WUCT: Team Exam

This exam consists of 7 questions and is worth 100 points. You will complete this exam as a team. You will have 1 hour to take the exam. The only allowed resources for this exam are a calculator and the provided equation sheet. You may NOT use any other notes or books. 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 the blank scratch page at the end of the exam. Make sure to clearly indicate in the problem's designated space where the rest of your work can be found. Any work anywhere other than the exam or the scratch page will not be graded. Dark pencil or pen is preferred.

<u>Problem #1</u>: ***(12 points)***

Consider the following reaction:

$$2SO_3\,(g) \Leftrightarrow 2SO_2\,(g) + O_2\,(g) \qquad \Delta H^\circ = 2198\,kJ/mol$$

How will the concentrations of SO_3, SO_2, and O_2 be affected by each of the following changes? Fill in the blanks with the words **increase, decrease, same, or N/A**.

1. The temperature is increased ***(1 point)***

   SO_3: ______________________________

   SO_2: ______________________________

   O_2: ______________________________

2. The pressure is decreased through an appropriate change in volume ***(1 point)***

   SO_3: ______________________________

   SO_2: ______________________________

   O_2: ______________________________

3. The concentration of O_2 is increased ***(1 point)***

   SO_3: ____

   SO_2: ____

   O_2: ____

4. A catalyst is added ***(1 point)***

   SO_3: ____

   SO_2: ____

   O_2: ____

State the direction each reaction will shift in when the volume of the container is decreased. Fill in the blanks with the words **left, right, or no shift**. ***(2.5 points)***

1. $PCl_3(g) + Cl_2(g) \leftrightarrows PCl_5(g)$

   ____

2. $2NBr_3(g) \leftrightarrows N_2(g) + 3Br_2(g)$

   ____

3. $CO(g) + Cl_2(g) \leftrightarrows COCl_2(g)$

   ____

4. $H_2(g) + B_2(g) \leftrightarrows 2HBr(g)$

   ____

5. $MgCO_3(s) \leftrightarrows MgO(s) + CO_2(g)$

   ____

Consider the reverse of the first reaction:

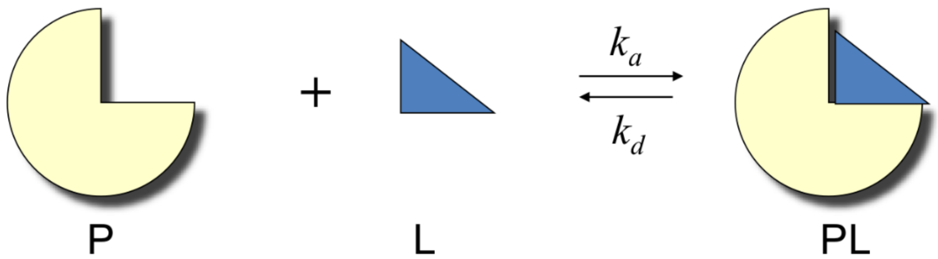
$$2\,SO_2\,(g)\ +\ O_2\,(g)\ \Leftrightarrow 2\,SO_3\,(g)$$

The equilibrium constant, K, for the reaction as written is $9.64\ \times\ 10^{-5}$ at 400K. If a sealed 1.0L reaction vessel contains 0.4 atm of $SO_2\,(g)$ and 1.2 atm of $SO_3\,(g)$ (no $O_2\,(g)$ initially), then what is the equilibrium partial pressure of the $SO_2\,(g)$ **expressed to 4 decimal places**?

(5.5 point)

<u>Problem #2</u>: ***(14 points)***

Hemoglobin is an enzyme-like protein that transports oxygen in red blood cells. In this case, oxygen is the ligand, or a molecule that binds to another larger molecule. Myoglobin is a protein that facilitates oxygen storage in the muscle. The process in which a ligand (L) binds reversibly to a site in a protein (P) can be described as follows:



k_a is the association rate constant; k_d is the dissociation rate constant. The equilibrium composition is characterized by the equilibrium association constant K_a or the equilibrium dissociation constant, K_d.

a. Represent K_a in terms of the concentrations of unbound protein, bound protein, and ligand. ***(2 points)***

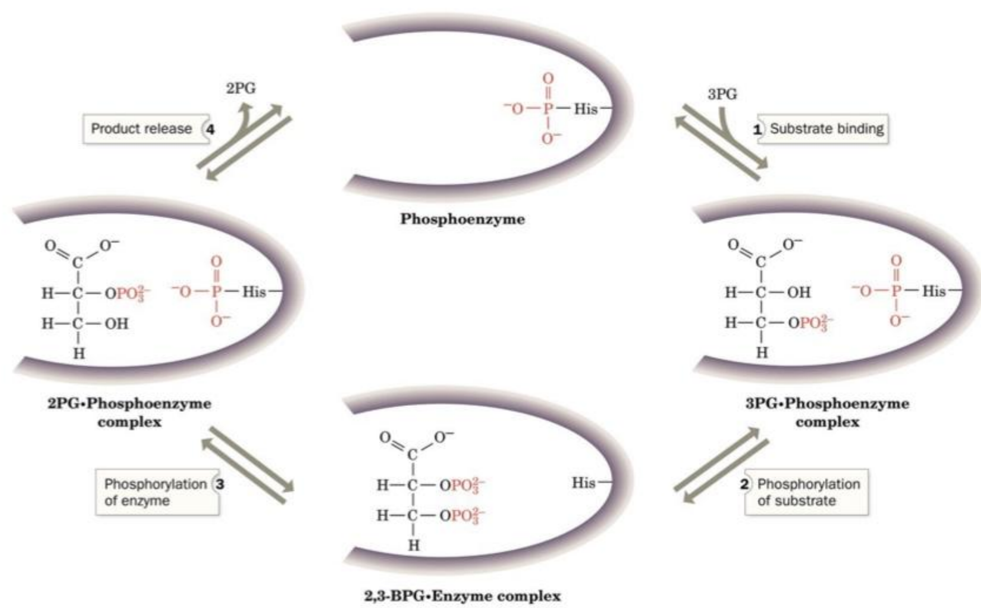
b. What is the relationship between K_a and K_d? ***(2 points)***

c. Given that the K_d of hemoglobin is 26, and that of myoglobin is 3, which protein has a higher affinity for oxygen? Explain. ***(3 points)***

d. 2,3-BPG is an allosteric inhibitor that stabilizes the unbound, free protein version of hemoglobin. This means that it binds to hemoglobin at a site different from that which oxygen binds. Predict how the K_a and K_d of hemoglobin would be affected by an increase in 2,3-BPG content. ***(3 points)***

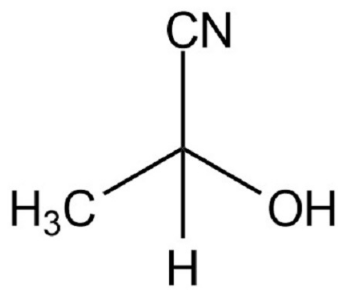
e. Why might 2,3-BPG content be higher specifically in red blood cells? Red blood cells compose the blood that flows in the human circulatory system and helps deliver oxygen to the body's tissues. (Hint: relate your answer to oxygen affinity and the function of red blood cells). ***(2 points)***

f. 2,3-BPG is also an important intermediate in a metabolic process known as glycolysis, which extracts energy from glucose sugar. Given the following mechanism, or steps of the reaction, predict what would happen to the phosphoenzyme if 2,3-BPG diffuses out of the cell. Make sure you identify the functional group that is moved in this reaction. ***(2 points)***



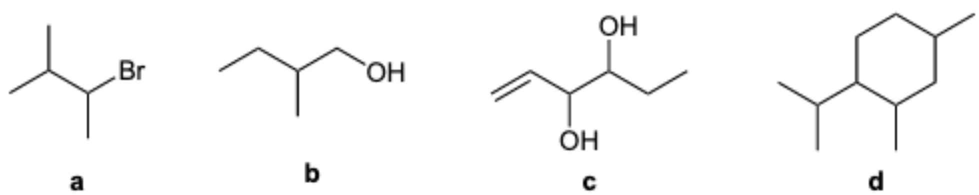
<u>Problem #3</u>: *(12 points)*

A molecule is defined as chiral if it has a non-superimposable mirror image. A molecule is defined as achiral if it has a mirror image that can be translated or rotated so that it is identical to the original molecule. For example, this molecule:



is chiral, while methane (CH_4) is achiral.

a. Assess whether the following molecules are chiral or achiral. ***(4 points)***



b. The coordination compound $[Cr(H_2O)_3ClBrI]^-$ has octahedral geometry. There are 5 total isomers, 2 of which are chiral and 3 of which are achiral. Draw the VSEPR geometry for the 2 chiral isomers. ***(4 points)***

c. A pair of non-superimposable mirror images are also known as a pair of enantiomers. Enantiomers have the same chemical and physical properties unless they are interacting with something else that is chiral. Given this information, can the two chiral isomers of $[Cr(H_2O)_3ClBrI]^-$ be separated by fractional distillation? Explain. ***(2 points)***

d. Diastereomers, on the other hand, are defined as non-mirror image, non-identical stereoisomers. They have a different spatial arrangement of their atoms. This gives them different chemical and physical properties. Given this information, can diastereomers be separated by fractional distillation? Explain. ***(2 points)***

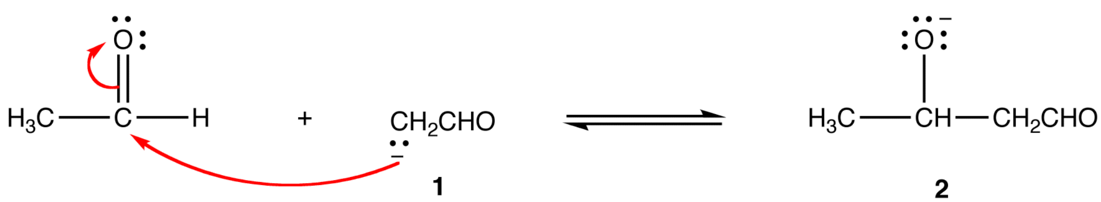
<u>Problem #4</u>: *(15 points)*

An aldol condensation is a condensation reaction in which an enol or an enolate ion reacts with a carbonyl compound to form a B-hydroxyaldehyde or B-hydroxy ketone, followed by a dehydration reaction to form a conjugated enone.

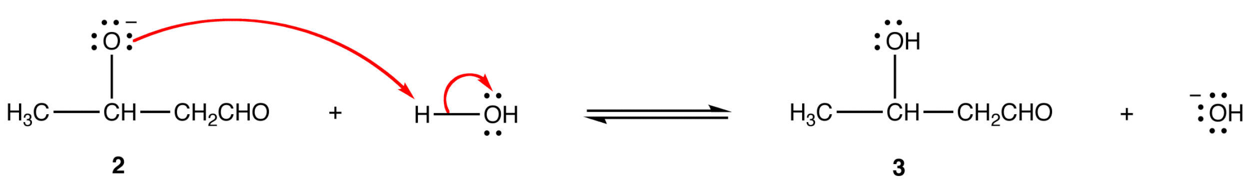
Step by step explanation of an aldol condensation:

Step 1: The hydroxide ion deprotonates the aldehyde reversibly.

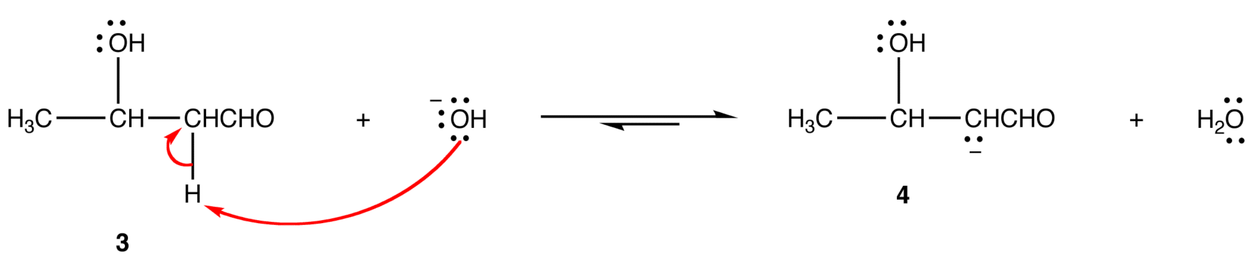
Step 2: Enolate ion 1 adds to the unreacted aldehyde.



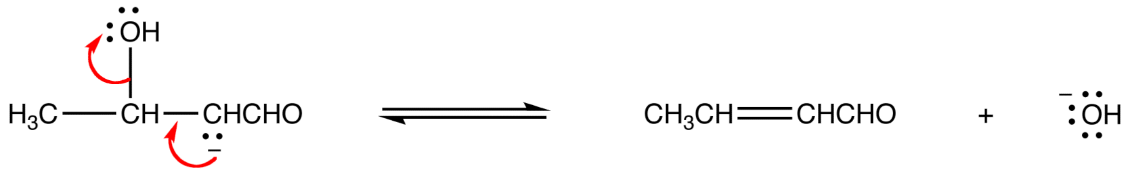
Step 3: Alkoxide ion 2 is protonated by water.



Step 4: Aldol 3 is an enolizable aldehyde. A small amount of it is converted to the corresponding enolate ion (4) by the hydroxide ion.



Step 5: Enolate ion 4 loses a hydroxide ion.



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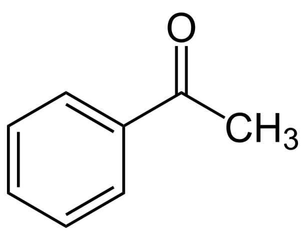
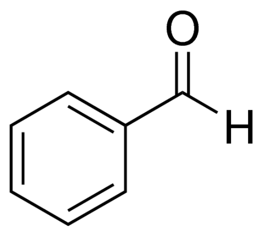
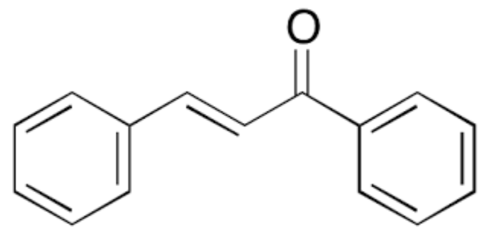
An aldol condensation reaction forms between an acetophenone and benzaldehyde to form 1,3-Diphenylprop-2-ene-1-one. The structure of the 3 molecules are shown below.

Acetophenone	**Benzaldehyde**	**1,3-Diphenylprop-2-en-1-one**
		

In organic chemistry, structures can be simplified into line drawings as shown above. This allows you to omit writing out carbons and represent them as vertices when two lines intersect.

a. How many sigma bonds and pi bonds are in acetophenone? ***(2 points)***

b. Why does acetophenone show partial polar and partial nonpolar properties? ***(2 points)***

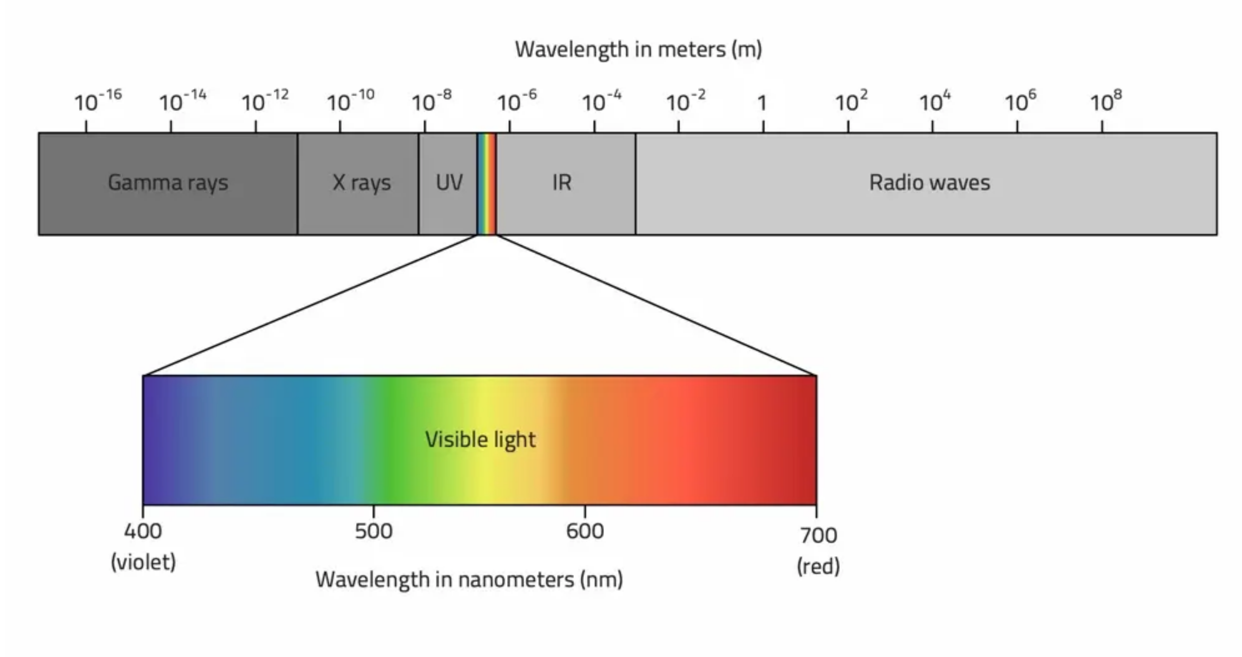
c. What is the hybridization of the carbon that is attached to the oxygen in benzaldehyde? ***(2 points)***

d. Write out the empirical formula of 1,3-Diphenylprop-2-en-1-one. ***(2 points)***

e. Write out the full mechanism of this reaction between an acetophenone and benzaldehyde using the 5 steps that are described above given that there are plenty of hydroxide ions and water present in solution. (*Hint*: in step 1, the hydroxide ion deprotonates acetophenone) ***(7 points)***

<u>Problem #5</u>: *(22 points)*

Light waves are electromagnetic waves, which consist of oscillating electric and magnetic fields that are perpendicular to each other and to the direction of the light's propagation. Electromagnetic waves can be characterized by the electromagnetic spectrum, where they are arranged on the basis of their wavelength, frequency, and energy. The electromagnetic spectrum is shown below.



Light in different regions of the electromagnetic spectrum excites different motions in molecules. For instance, microwaves excite molecular rotations, infrared waves excite vibrations of chemical bonds, and visible and ultraviolet light lead to excitations of electrons.

a. Microwaves are not shown on the spectrum above. Where would microwaves fall on the spectrum? ***(1 point)***

b. When an atom or molecule absorbs a photon of the right energy, this leads to an excitation from a lower energy state to a higher energy state. Depending on the energy of light, this transition could be between vibrational states, rotational states, or electron energy levels. The following questions will focus on different vibrations induced by the absorption of infrared waves.

i) A photon of infrared light having a wavelength of 3.03 μm is absorbed by a water molecule. A molecule of methanol, CH_3OH, absorbs an infrared photon with a wavelength of 2.67 μm. Which molecule absorbs infrared light of more energy and by how much? ***(4 points)***

ii) When you shine infrared light on a sample of a certain molecule, the molecule will absorb photons of certain energies and let others pass through. This information is shown on a spectrum called an Infrared Spectrum, with the units of light often being given in wavenumbers (cm^{-1}). The wavenumber (w) is calculated via the following equation:

$$w = \frac{1}{(wavelength)}$$

Calculate the wavenumber of the following photons.

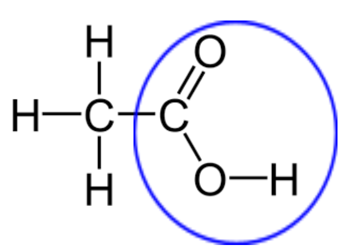
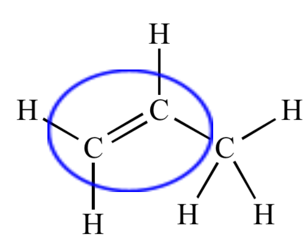
1) A photon with a wavelength of 4,395 nm. ***(2 points)***

2) A photon with a frequency of 4.95×10^{13} Hz. ***(2 points)***

3) A photon with an energy of 0.434 eV. ***(2 points)***

c. As mentioned before, infrared waves cause molecules to go from one frequency of vibration to a higher frequency of vibration. Picture a spring that is contracting and expanding slowly. If you put more energy into it, that spring will contract and expand at a faster rate. That is essentially how we can imagine chemical bonds reacting to an increase in energy given by the absorption of infrared light. Rank the following bonds (C-C, C=C, C≡C) from lowest to highest wavenumber of infrared light needed to excite them from the lowest vibrational frequency to the next highest vibrational frequency. Explain your reasoning in 2-3 sentences. ***(3 points)***

d. A functional group is a group of atoms in a molecule that is very important in determining its chemistry. Some examples include a carboxylic acid group (-COOH) and a carbon-carbon double bond (-C=C). These are shown from left to right below, with the respective functional group in the blue circle.

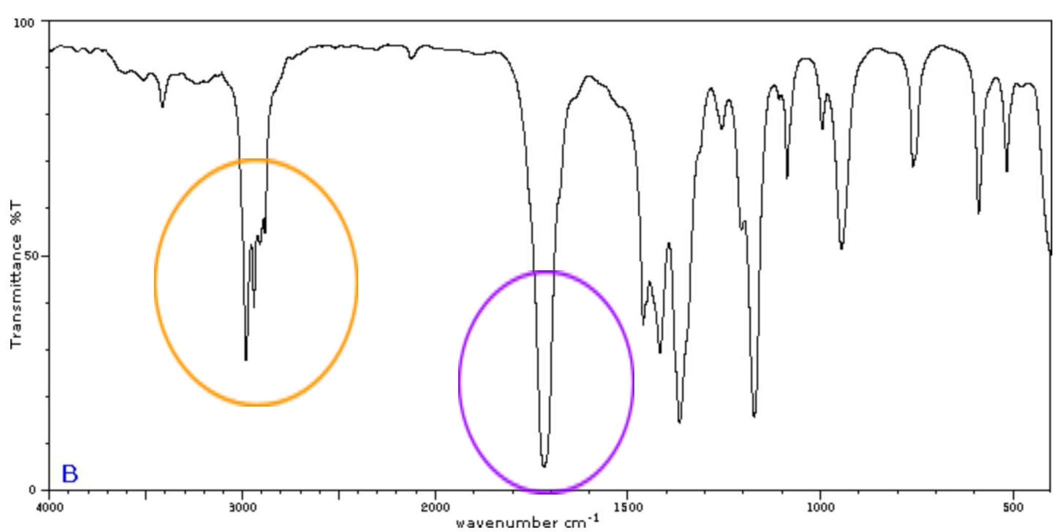
Different functional groups absorb infrared light of different energies, which again leads to a higher energy vibration of the functional group bonds. Using what we know about which functional group absorbs light around which regions allows chemists to identify and visualize the structure of a molecule. The following chart shows the connection between functional groups and wavenumber of the photon absorbed.

Table 13.4 Important IR Stretching Frequencies

Type of bond	Wavenumber (cm^{-1})	Intensity
C≡N	2260–2220	medium
C≡C	2260–2100	medium to weak
C=C	1680–1600	medium
C=N	1650–1550	medium
	~1600 and ~1500–1430	strong to weak
C=O	1780–1650	strong
C—O	1250–1050	strong
C—N	1230–1020	medium
O—H (alcohol)	3650–3200	strong, broad
O—H (carboxylic acid)	3300–2500	strong, very broad
N—H	3500–3300	medium, broad
C—H	3300–2700	medium

The infrared spectrum maps which wavenumbers of infrared light are absorbed by a certain molecule. The peaks give an idea of which functional groups are present.

iii) On the infrared spectrum shown below, identify which circled peak corresponds to which functional group. HINT: Pay attention to the size of the peaks (none of these would be considered broad peaks). Ignore the peaks located at between 600-1500 cm^{-1}. This region is known as the "fingerprint region," and usually consists of a complicated set of peaks unique to the compound being studied. ***(2 points)***

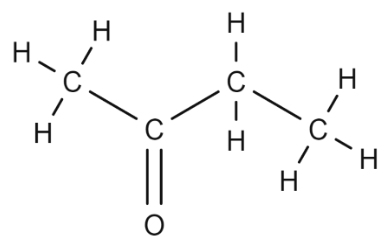


Orange circle: ___________________________________

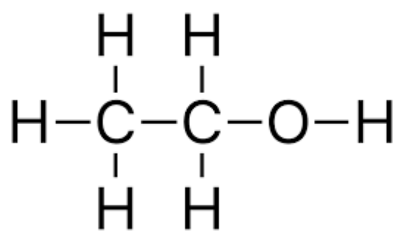
Purple circle: ____________________________________

iv) Which of the following molecules could this spectrum correspond to? There may be more than one correct answer. Justify your reasoning in 1-2 sentences. ***(3 points)***

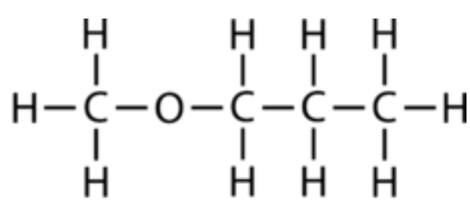
a) 2-butanone



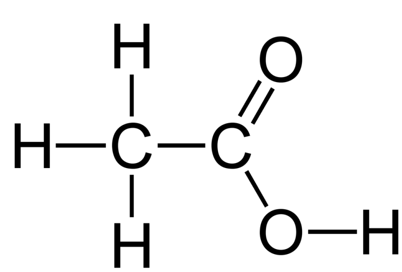
b) Ethanol



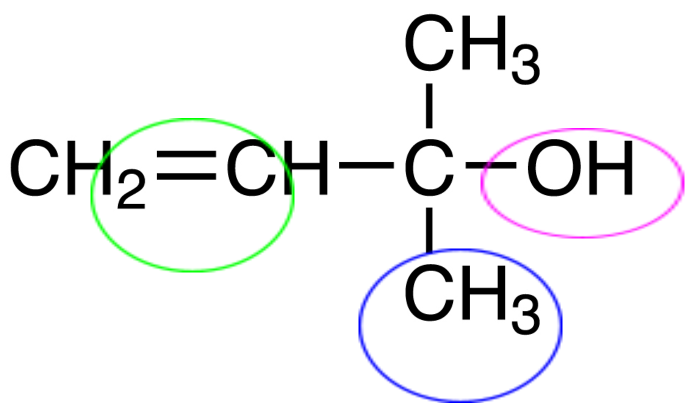
c) Methyl propyl ether



d) Acetic acid



v) Given the following molecule, predict where the peaks would be on the molecule's infrared spectrum (in wavenumbers), as well as what their intensity would be. ***(3 points)***



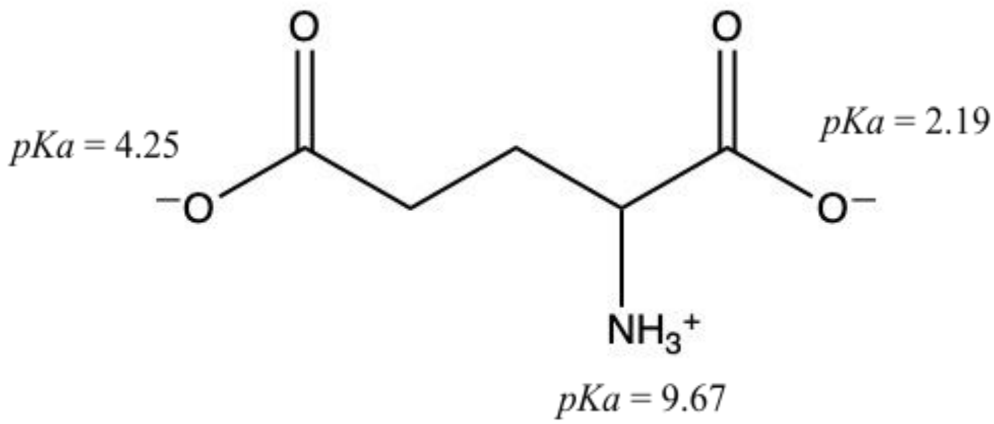
Green circle: ____

Blue circle: ____

Purple circle: ____

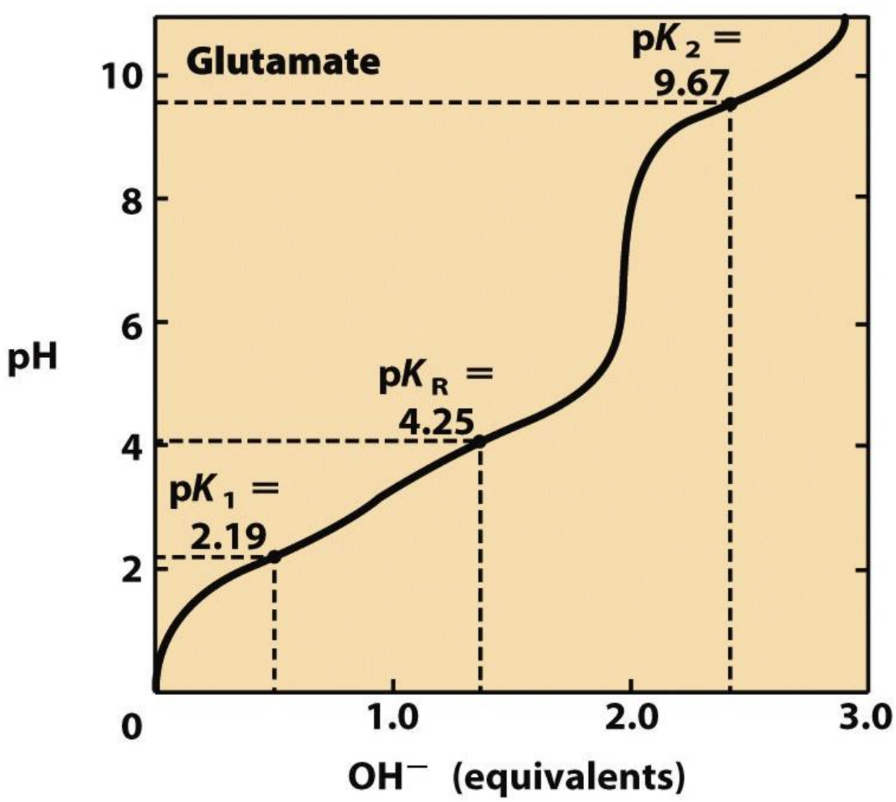
Problem #6: ***(13 points)***

Glutamate is one of 20 natural amino acids found in all living things. One of the features of glutamate (and amino acids in general) is that multiple groups can be ionized. In other words, amino acids can acquire a negative or positive charge by gaining or losing electrons. The structure of glutamate at pH of 7 is shown below:



a. Circle the groups of glutamate that can be ionized on the structure above. ***(3 points)***

b. The image below shows a titration curve for the amino acid glutamate with a strong base.



Using the titration curve and the given pKa values of each functional group, draw the structure of the dominant form of glutamate in each of the following ranges of pH. ***(4 points)***

0 - 2.19:

2.19 - 4.25:

4.25 - 9.67:

9.67 - 12:

c. A buffer is a solution that can resist pH change upon the addition of acidic or basic components. At what pH or pHs would glutamate be a good buffer? Explain why glutamate can be a good buffer and how a buffer works. ***(3 points)***

d. The isoelectric point (pI) is the pH at which a molecule as a whole has a net charge of zero. What is the approximate pI of glutamate? Explain your reasoning. ***(3 points)***

<u>Problem #7</u>: *(12 points)*

All particles exhibit wave-like properties. In 1924, French scientist Louis de Broglie derived an equation that described the wave nature of a particle. This equation can be written in the form below:

$$\lambda=h/mv$$

with λ being the wavelength, h being Planck's constant (6.626 x 10^{-34} m^2 kg/s), m being mass and v being velocity.

a. Calculate the de Broglie wavelength for an electron moving at 2% speed of light in a vacuum. ***(2 points)***

b. A 16,000 kg bus emits a de Broglie wavelength of 2.96 x 10^{-39} m. At what speed is the bus moving at? ***(2 points)***

In 1927, scientist Werner Heisenberg came up with the idea of the uncertainty principle. This principle states that we cannot precisely know the position and momentum of a particle at the same time. The uncertainty principle can be modeled by the equation below:

$$\mathbf{\Delta x \Delta p} \geq \frac{h}{4\pi}$$

In the equation, Δx represents the uncertainty in position of the particle and Δp represents the uncertainty in momentum of the particle.

c. The uncertainty of momentum of a baseball thrown during a game at 45 m/s is 1% of its momentum. What is the uncertainty in position? The mass of the baseball is 0.15 kg. ***(2 points)***

In quantum mechanics, a *particle in a box model* describes a system in which a particle is free to move around in a small space that is surrounded by impenetrable barriers. For instance, a single O_2 molecule that is freely floating around in a 1D box with a length of 1m can be described by a *particle in a box model*. The expectation value describes the most probabilistic location at which you are most likely to find the particle in a box. This value can be described by the equation below:

$$\text{x} = \int \Psi^* \, x \, \Psi \, dx$$

In the equation, Ψ represents the wavefunction that describes the particle in a box system. Ψ^* is the complex conjugate of Ψ. A complex conjugate simply inverses complex numbers. For instance, the complex conjugate of 2i is -2i. If an equation does not have any complex numbers, Ψ^* will be equal to Ψ. The bounds of the integral will start from the left side of the particle in a box to the right side of the box.

d. Given that the particle in the box system is from 0 to L, and the $\Psi = \sqrt{\frac{2}{L}} * \, sin(\frac{n\pi x}{L})$, set up the equation for solving the expectation value of position. ***(2 points)***

e. Given that the integral of $\int_0^L x \, sin^2(\frac{n\pi x}{L}) = \frac{L^2}{4}$, solve for the expectation value of position for particles in a box. ***(2 points)***

f. What does the answer in part (e) represent? Where are you most likely to find a particle? ***(2 points)***

Scratch Page