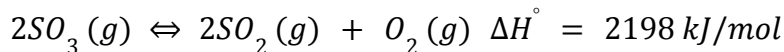


2023 WUCT: Team Exam **ANSWER KEY**

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.

Problem #1: (12 points)

Consider the following reaction:



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 : _____ decrease

SO_2 : _____ increase

O_2 : _____ increase

+ 1 point for having all 3 answers correct

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

SO_3 : _____ decrease

SO_2 : _____ increase

O_2 : _____ increase

+ 1 point for having all 3 answers correct

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

SO_3 : _____ increase

SO_2 : _____ decrease

O_2 : _____ N/A

+ 1 point for having all 3 answers correct

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

SO_3 : _____ same

SO_2 : _____ same

O_2 : _____ same

+ 1 point for having all 3 answers correct

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. $PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g)$

_____ right

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

_____ left

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

_____ right

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

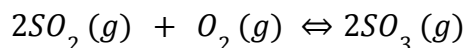
_____ no shift

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

_____ left

+ 0.5 points for each correct answer (total of 2.5 points)

Consider the reverse of the first reaction:



The equilibrium constant, K , for the reaction as written is 9.64×10^{-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 points)

	$2SO_2(g)$	+	$O_2(g)$	\rightleftharpoons	$2SO_3(g)$
I	0.4 atm		0 atm		1.2 atm
C	+1.2		+0.6		-1.2
I'	1.6 atm		0.6 atm		0 atm
C'	-2x		-x		+2x
E'	1.6 - 2x		0.6 - x		2x

$$K = \frac{(P_{SO_3})^2}{(P_{SO_2})^2 (P_{O_2})}$$

$$K = \frac{(2x)^2}{(1.6-2x)^2(0.6-x)} = 9.64 \times 10^{-5}$$

Because K is very small, we can assume that $x \ll 1.6$ and $x \ll 0.6$. Therefore, we can do Method of Successive Approximations.

$$\frac{(2x)^2}{(1.6)^2(0.6)} = 9.64 \times 10^{-5}$$

$$x_1 = 0.0060842$$

$$x_2 = 0.0060072$$

$$x_3 = 0.0060082$$

$$x_4 = 0.0060082$$

Finally: $x = 0.0060082 \text{ atm}$

Equilibrium partial pressure of the $SO_2(g)$:

$$1.6 - 2x = 1.6 - 2(0.0060082) = 1.58798359 \text{ atm} = 1.5880 \text{ atm}$$

+1.5 points for using ICE tables

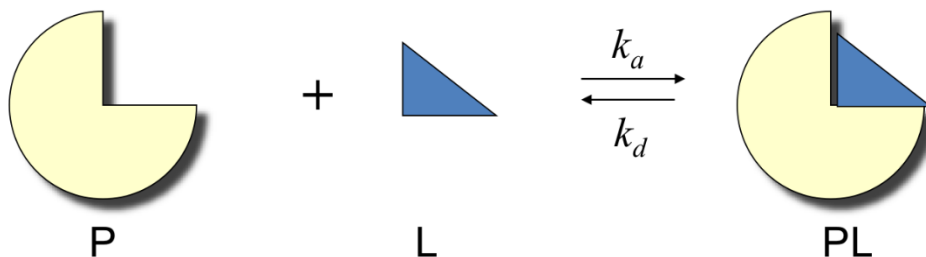
+1 point for setting up correct K equation

+1 point for correctly solving for $x = 0.006$

+2 points for correct final answer with 4 decimal places

Problem #2: (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)

$$K_a = \frac{[PL]}{[P][L]}$$

+2 points for correct answer

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

$$K_a = 1/K_d$$

+2 points for correct answer

- 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)

Myoglobin has a higher affinity for oxygen. Since it has a lower K_d , that signifies that there is a lower concentration of unbound protein and ligand and a higher concentration of bound protein at equilibrium.

+1 point for correct answer

+2 points for correct explanation

- 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)

K_a decreases

K_d increases

[P] is stabilized and therefore will be present in a greater concentration at equilibrium, in the numerator of K_d , in the denominator of K_a

+1 point for correct K_a

+1 point for correct K_d

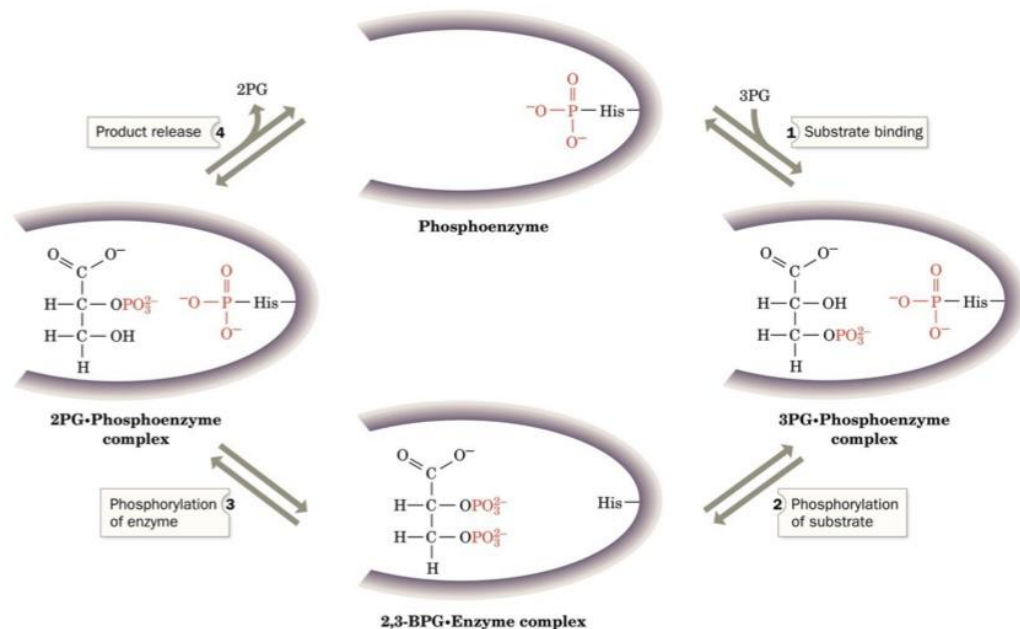
+1 point for correct answer

- 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)

BPG increases K_d , lowers the oxygen affinity of hemoglobin, more oxygen released

+2 points for correct answer

- 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)



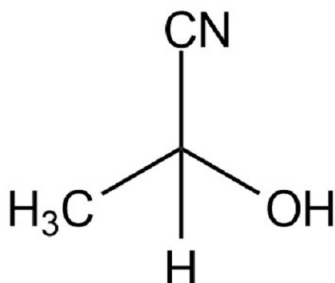
The enzyme would remain dephosphorylated, inactive and would not be able to react again.

+1 point for correct answer

+1 point for mentioning phosphate group

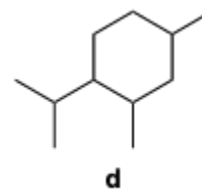
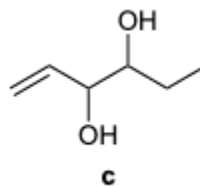
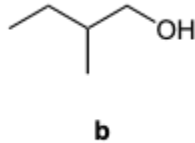
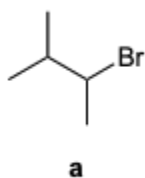
Problem #3: (12 points)

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.

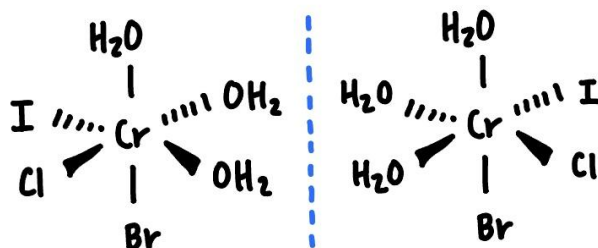
- a. Assess whether the following molecules are chiral or achiral. (4 points)



All are chiral

+1 point for each answer (total of 4 points)

- b. The coordination compound $[\text{Cr}(\text{H}_2\text{O})_3\text{ClBrI}]^-$ 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)



+2 points for each correct structure (total of 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 $[\text{Cr}(\text{H}_2\text{O})_3\text{ClBrI}]$ be separated by fractional distillation? Explain. (2 points)

No, they'll have the same melting and boiling points.

+1 point for saying no

+1 point for correct explanation

- 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)

Yes, they'll have different melting and boiling points so they will evaporate at different times.

+1 point for saying yes

+1 point for correct explanation

Problem #4: (15 points)

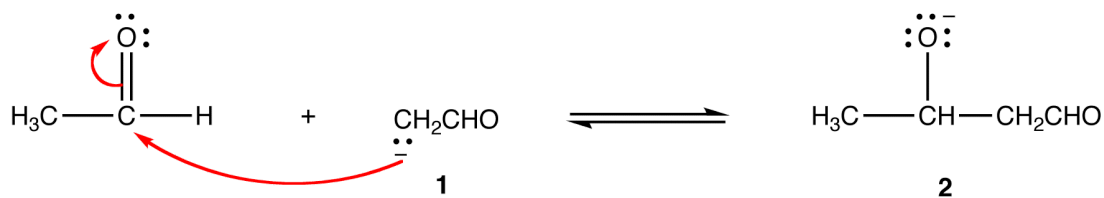
An aldol condensation is a condensation reaction in which an enol or an enolate ion reacts with a carbonyl compound to form a β -hydroxyaldehyde or β -hydroxy ketone, followed by a dehydration reaction to form a conjugated enone.

Step by step explanation of an aldol condensation:

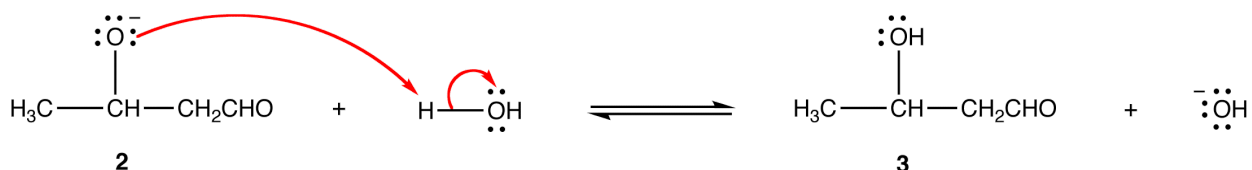
Step 1: The hydroxide ion deprotonates the aldehyde reversibly.



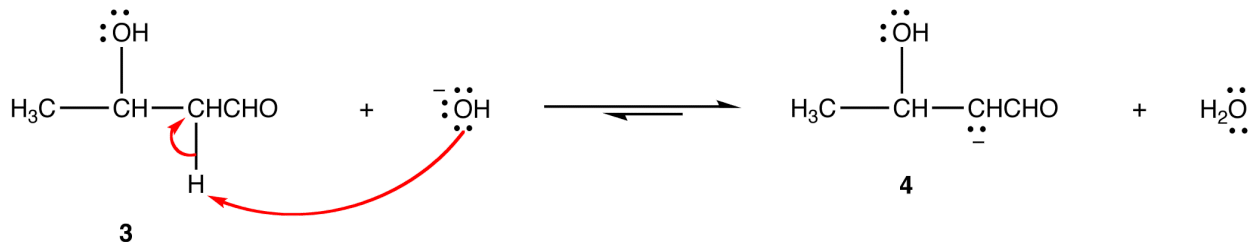
Step 2: Enolate ion 1 adds to the unreacted aldehyde.



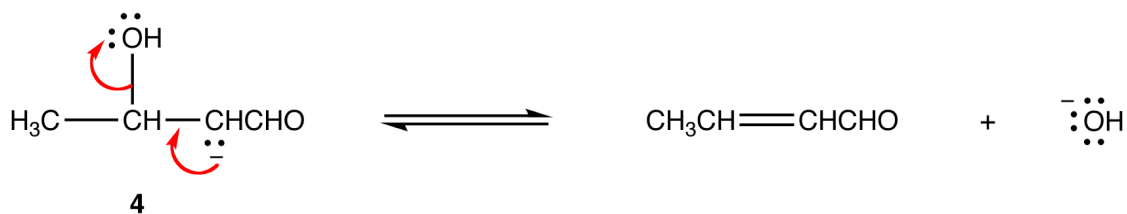
Step 3: Alkoxide ion 2 is protonated by water.



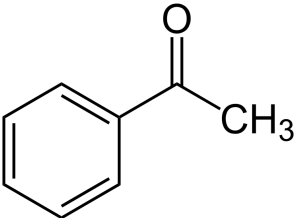
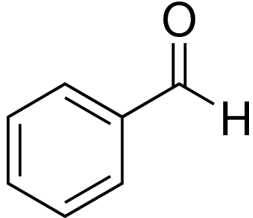
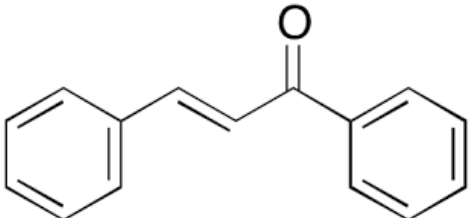
Step 4: Aldol 3 is an enolizable aldehyde. A small amount of it is converted to the corresponding enolate ion (4) by the hydroxide ion.



Step 5: Enolate ion 4 loses a hydroxide ion.



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-ene-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)

17 sigma, 4 pi bonds

+1 point for correct number of sigma bonds

+1 point for correct number of pi bonds

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

Acetophenone has a ketone group (C=O) that is polar but also has a large benzene ring, which is nonpolar.

+2 points for correct explanation

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

sp²

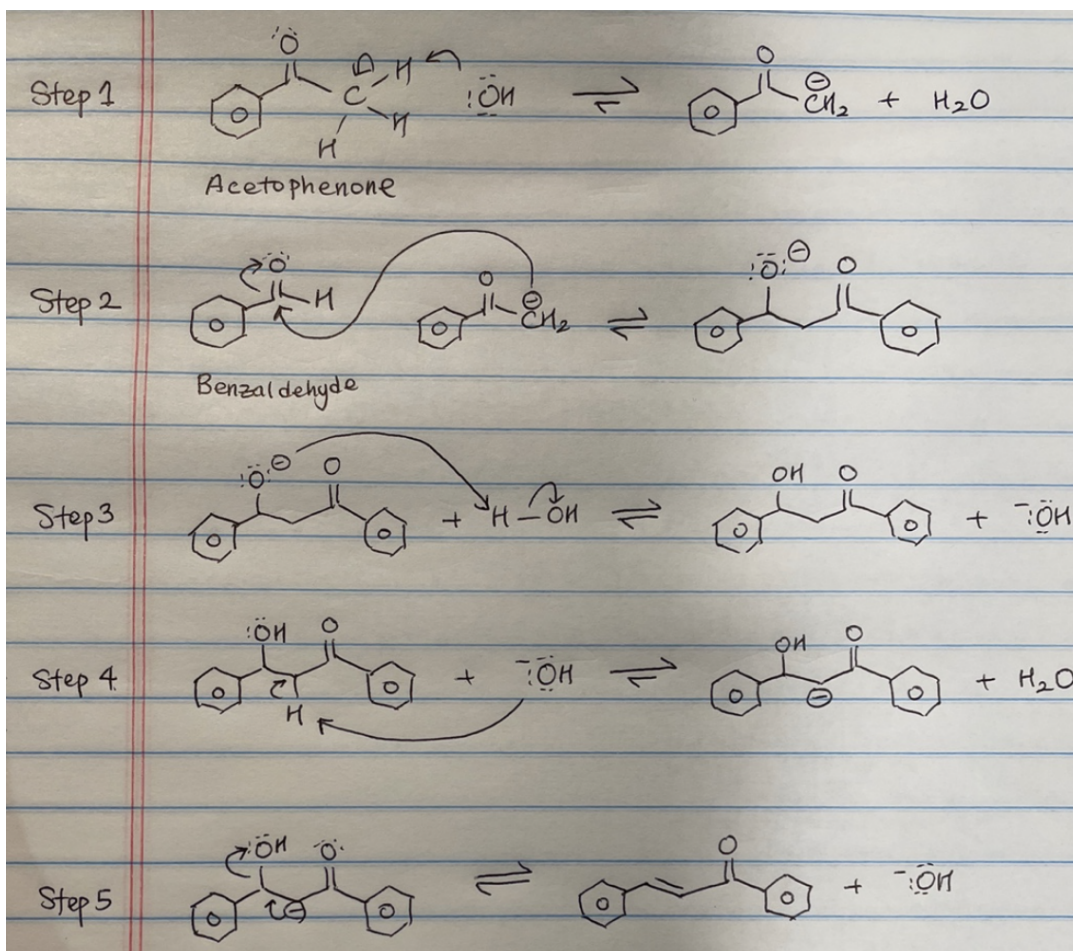
+2 points for correct answer

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



+2 points for correct answer

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)



+1 point for using Acetophenone as the nucleophile and Benzaldehyde as the electrophile

+2 points for correct step 1

+1 point for correct step 2

+1 point for correct step 3

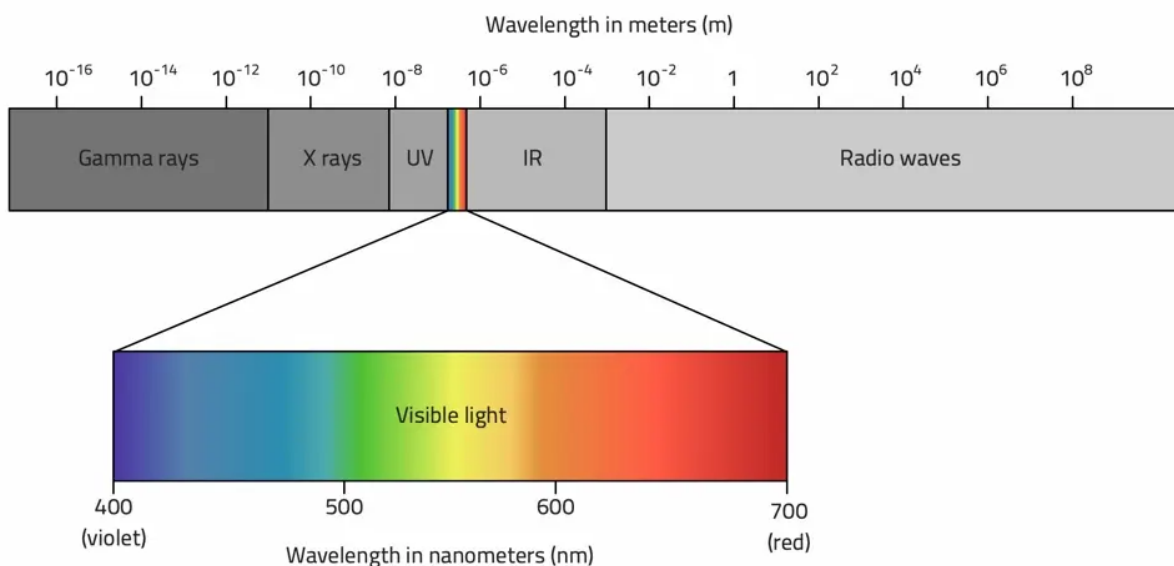
+1 point for correct step 4

+1 point for correct step 5

Problem #5: (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 leads to excitations of electrons.

- Microwaves are not shown on the spectrum above. Where would microwaves fall on the spectrum? **(1 point)**
Between IR and radio waves
+1 point for correct answer
- 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.
 - 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 $2.67 \mu\text{m}$. Which molecule absorbs infrared light of more energy and by how much? (4 points)

Methanol absorbs a photon of infrared light with more energy. The photon for methanol is $8.840 \times 10^{-21} \text{ J}$ higher in energy than the photon for water.

$$2.67 \mu\text{m} \times \frac{1 \times 10^{-6} \text{ m}}{1 \mu\text{m}} = 2.67 \times 10^{-6} \text{ m}$$

$$3.03 \mu\text{m} \times \frac{1 \times 10^{-6} \text{ m}}{1 \mu\text{m}} = 3.03 \times 10^{-6} \text{ m}$$

$$E = \frac{hc}{\lambda}$$

$$E(\text{methanol}) = \frac{(6.626 \times 10^{-34} \text{ Js})(2.998 \times 10^8 \text{ m/s})}{(2.67 \times 10^{-6} \text{ m})} = 7.43998052 \times 10^{-20} \text{ J}$$

$$E(\text{water}) = \frac{(6.626 \times 10^{-34} \text{ Js})(2.998 \times 10^8 \text{ m/s})}{(3.03 \times 10^{-6} \text{ m})} = 6.55602244 \times 10^{-20} \text{ J}$$

$$E(\text{methanol}) - E(\text{water}) = 7.43998052 \times 10^{-20} \text{ J} -$$

$$6.55602244 \times 10^{-20} \text{ J}$$

$$= 8.8395808 \times 10^{-21} \text{ J}$$

$$= 8.840 \times 10^{-21} \text{ J}$$

+1 point for using $E = hc/\lambda$ equation

+1 point for correct answer: stating that methanol absorbs more energy

+2 points for correct calculations: stating that there is a difference of $8.840 \times 10^{-21} \text{ J}$

- 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:

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

Calculate the wavenumber of the following photons.

- 1) A photon with a wavelength of $4,395 \text{ nm}$. (2 points)

$$4395 \text{ nm} \times \frac{1 \times 10^{-9} \text{ m}}{1 \text{ nm}} \times \frac{100 \text{ cm}}{1 \text{ m}} = 4.395 \times 10^{-4} \text{ cm}$$

$$w = \frac{1}{\lambda} = \frac{1}{(4.395 \times 10^{-4} \text{ cm})}$$

$$= 2275.31 \text{ cm}^{-1}$$

+2 points for correct answer

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

$$c = \lambda\nu \rightarrow \lambda = \frac{c}{\nu}$$

$$w = \frac{1}{\lambda} = \frac{\nu}{c} = \frac{(4.95 \times 10^{13} \frac{1}{s})}{(2.998 \times 10^8 \frac{m}{s})} = 165110.0734 \frac{1}{m} \times \frac{1 m}{100 cm}$$

$$= 1651.10 \text{ cm}^{-1}$$

+2 points for correct answer

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

$$0.434 \text{ eV} \times \frac{1.6021773 \times 10^{-19} \text{ J}}{1 \text{ eV}} = 6.95344948 \times 10^{-20} \text{ J}$$

$$E = h\nu \rightarrow \nu = \frac{E}{h}$$

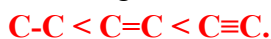
$$c = \lambda\nu \rightarrow \lambda = \frac{c}{\nu} = \frac{c}{\frac{E}{h}} = \frac{hc}{E}$$

$$w = \frac{1}{\lambda} = \frac{E}{hc} = \frac{(6.95344948 \times 10^{-20} \text{ J})}{(6.626 \times 10^{-34} \text{ Js})(2.998 \times 10^8 \text{ m/s})} = 350039.6523 \frac{1}{m} \times \frac{1 m}{100 cm}$$

$$= 3500.40 \text{ cm}^{-1}$$

+2 points for correct answer

- 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)



Single bonds are weaker than double bonds, which are weaker than triple bonds. Weaker bonds require less energy to increase the vibrational frequency, and since energy is directly related to wavenumber, weaker bonds will experience an increase in vibrational frequency at a lower wavenumber of infrared light. Thus, single bonds require the lowest wavenumber, followed by double bonds, followed by triple bonds.

+1 point for correct ranking


+2 points for correct explanation

- 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.

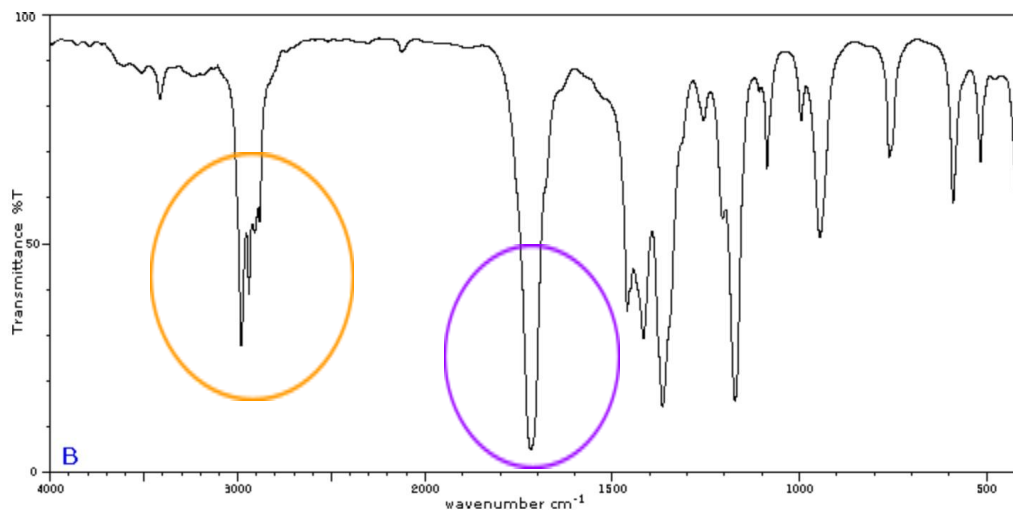


Different functional groups absorb infrared light of different energies, which again leads to a higher energy vibration of the functional group bonds. Using what we know about which functional group absorbs light around which regions allows chemists to identify and visualize the structure of a molecule.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

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

- i) 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 $600\text{-}1500\text{ cm}^{-1}$. 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: **C-H bonds**

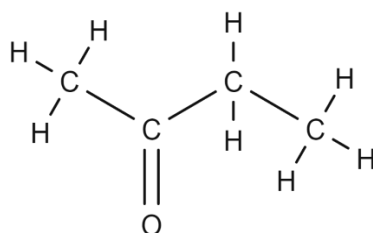
Purple circle: **C=O bonds**

+1 point for correct answer for orange circle

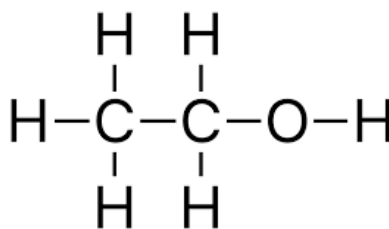
+1 point for correct answer for purple circle

- ii) 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.

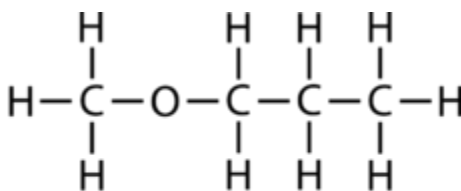
a) 2-butanone (**3 points**)



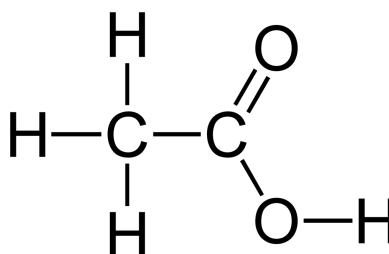
b) Ethanol



c) Methyl propyl ether



d) Acetic acid

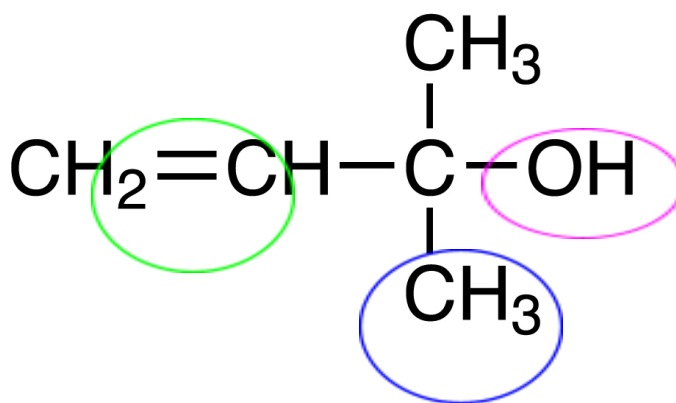


A, because the spectrum shows the carbonyl (C=O) group, as well as the C-H bonds. There are no broad peaks in the 3000s cm^{-1} that would indicate an acid or alcohol OH group. In addition, C (methyl propyl ether) would not give the carbonyl peak that does show up at the spectrum.

+1 point for correct answer

+2 points for correct explanation

- iii) 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: _____

Green circle: **1680-1600 cm^{-1} ; medium intensity**

Blue circle: **3300-2700 cm^{-1} ; medium intensity**

Purple circle: **3650-3200 cm^{-1} ; strong, broad intensity**

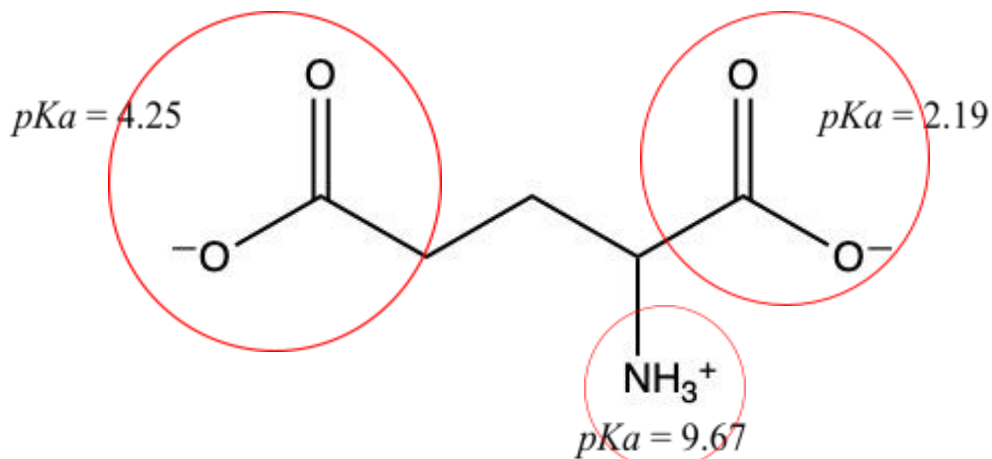
+1 point for correct wavenumbers and intensity for the green circle

+1 point for correct wavenumbers and intensity for the blue circle

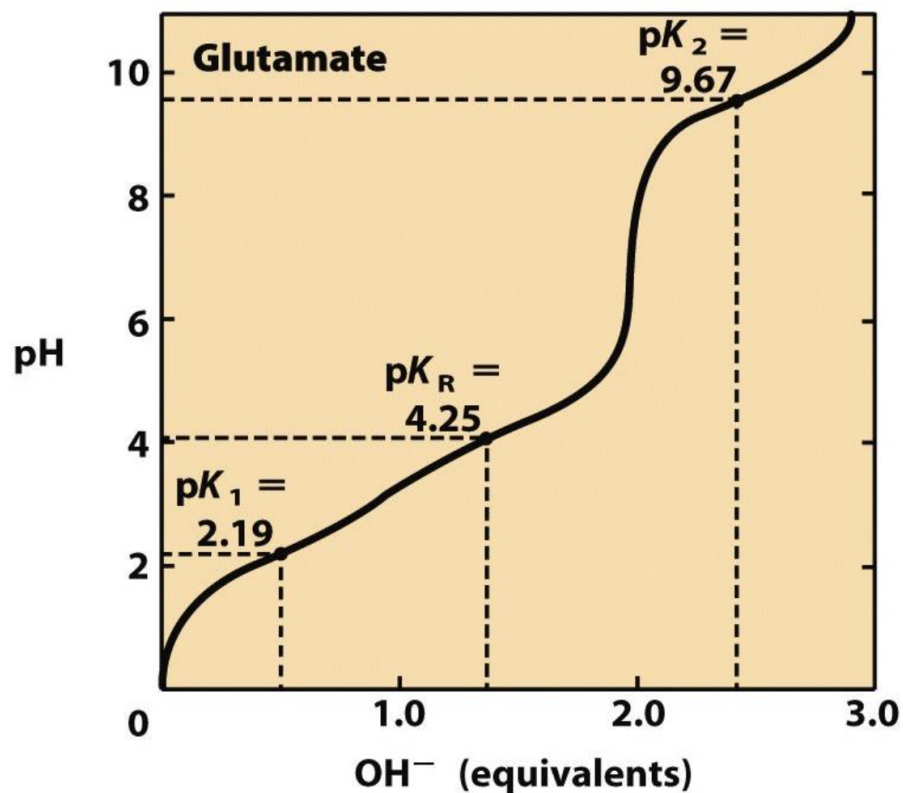
+1 point for correct wavenumbers and intensity for the purple circle

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:

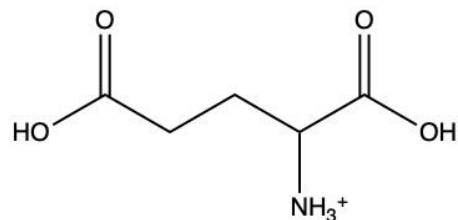


- Circle the groups of glutamate that can be ionized on the structure above. (3 points)
+ 1 point for each correctly circled group (total 3 points)
- The image below shows a titration curve for the amino acid glutamate with a strong base.

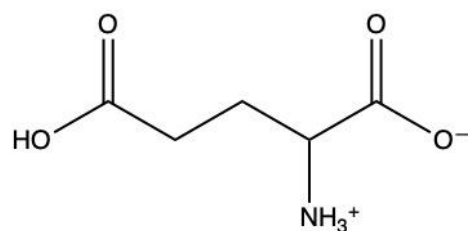


Using the titration curve and the given pKa values of each functional group, draw the structure of the dominant form of glutamate in each of the following ranges of pH. (4 points)

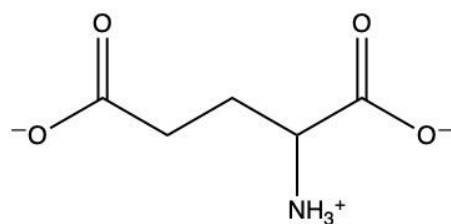
0 - 2.19:



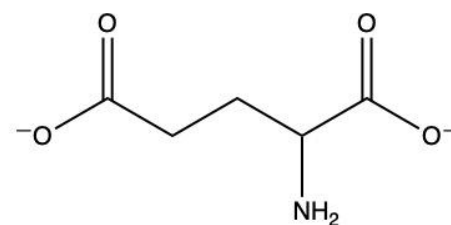
2.19 - 4.25:



4.25 - 9.67:



9.67 - 12:



+1 point for each correct structure

- 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)

Glutamate would be a good buffer at the pHs of 2.19, 4.25, and 9.67. This is because a buffer is able to resist pH change because the two components (conjugate acid and conjugate base) are both present in appreciable amounts at equilibrium. At those pHs, glutamate has an equal amount of conjugate acid and a conjugate base present to neutralize small amounts of H⁺ and OH⁻.

+1 for correct pHs of the buffers

+2 for the correct explanation

- 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)

At around 3.22 [$= \frac{2.19 + 4.25}{2}$], the pH of the solution is only strong enough to protonate the side chain carboxylic group and the amine but not strong enough to protonate the carboxylic group attached to the α -carbon. Since the amine group gains a positive charge and one of the carboxylic groups loses its negative charge, the overall charge of glutamate is zero.

+1 for correct pH of isoelectric point

+2 for the correct explanation

Problem #7: (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 ($6.626 \times 10^{-34} \text{ m}^2 \text{ kg/s}$), 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)

$$\lambda = \frac{6.626 * 10^{-34} \text{ m}^2 \text{ kg/s}}{9.11 * 10^{-31} \text{ kg} * 0.02 * 3 * 10^8 \text{ m/s}} = 1.212 * 10^{-10} \text{ m}$$

+2 points for correct answer

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

$$v = \frac{h}{m\lambda} = \frac{6.626 * 10^{-34} \text{ m}^2 \text{ kg/s}}{16,000 \text{ kg} * 2.96 * 10^{-39} \text{ m}} = 13.99 \text{ m/s}$$

+2 points for correct answer

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:

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

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 45m/s is 1% of its momentum. What is the uncertainty in position? The mass of the baseball is 0.15kg. (2 points)

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

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

$$\Delta x \geq \frac{6.626 * 10^{-34} \text{ m}^2 \text{ kg/s}}{4\pi * 0.01 * (0.15 \text{ kg} * 45 \text{ m/s})} = 7.811 * 10^{-34} \text{ m}$$

+2 point for correct answer

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 O₂ 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:

$$x = \int \Psi^* x \Psi dx$$

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 inverts 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)**

$$x = \int_0^L \sqrt{\frac{2}{L}} * \sin(\frac{n\pi x}{L}) x \sqrt{\frac{2}{L}} * \sin(\frac{n\pi x}{L}) dx$$

*** In the problem, $\Psi = \Psi^*$ because there are no complex numbers in Ψ

+2 points for correct set up

- 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)**

$$x = \int_0^L \sqrt{\frac{2}{L}} * \sin(\frac{n\pi x}{L}) x \sqrt{\frac{2}{L}} * \sin(\frac{n\pi x}{L}) dx = \frac{2}{L} * \int_0^L x \sin^2(\frac{n\pi x}{L}) = \frac{2}{L} * \frac{L^2}{4} = \frac{L}{2}$$

+2 points for correct answer

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

(2 points)

The length of the box is L and the expectation value is $\frac{L}{2}$, which tells us that you are most likely to find the particle in the middle of the box.

+2 points for stating “middle of the box”