Chem 101, Fall 2017 Discussion # 4 **Chapter** 3

Things you should know when you leave Discussion today:

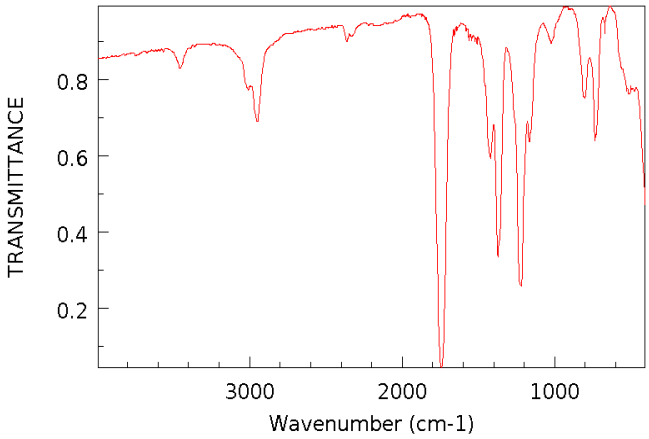
IR and MS

KEY

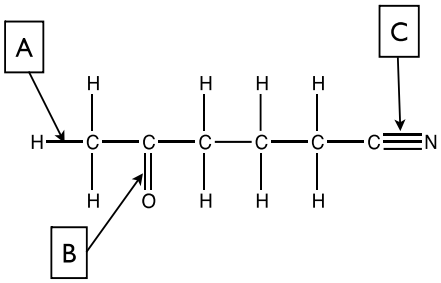
1. IR theory questions:
   a. In the IR spectrum the detector records light that :
   Interacts with the sample. Does not interact with the sample.

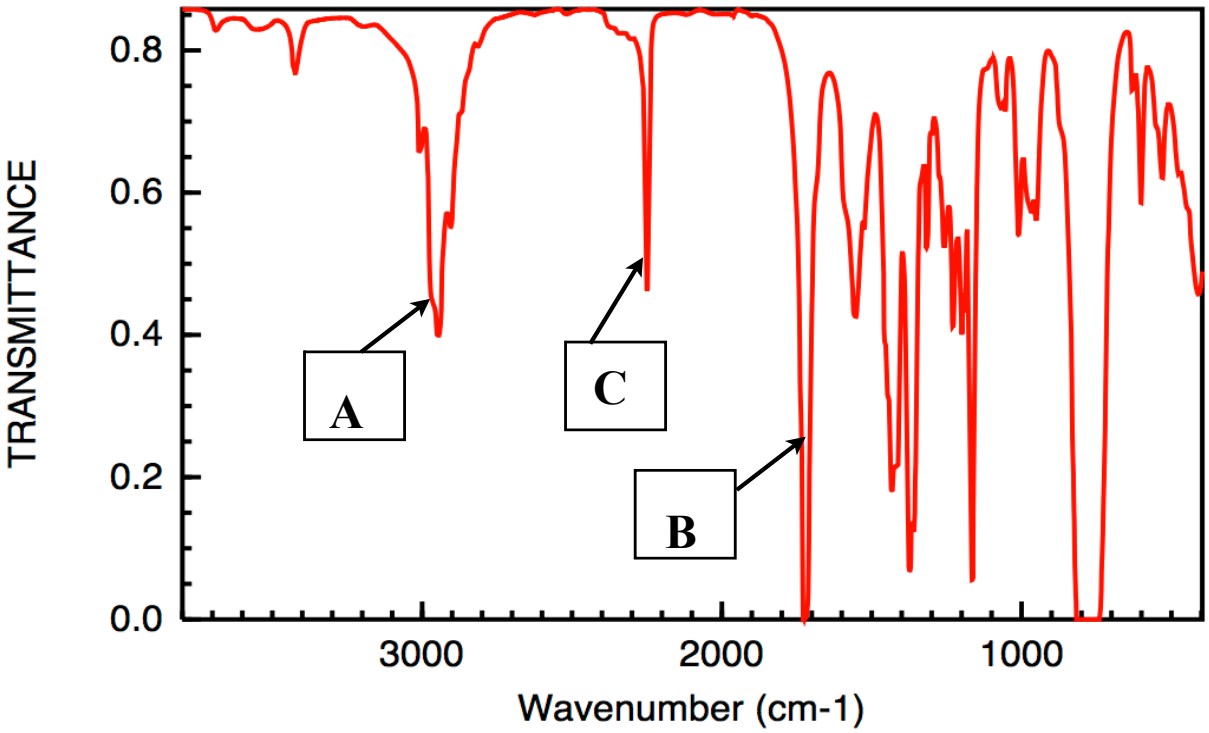
   b. From the IR spectrum, at what wavenumber is the most light absorbed by the sample?
   1800

   c. How do you know that light is absorbed and not emitted?



2. Keeping in mind that $\upsilon \sim \sqrt{\frac{k}{m}}$ where k represents the strength of the bond and m represent mass. Match the labeled bonds to the corresponding band in the infrared spectrum.





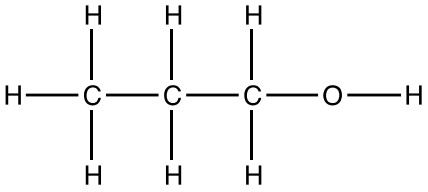
a. Calculate, to one significant figure, the frequency, in Hz, of light resonant at location **A**.

$$\nu = c * \tilde{\upsilon} = \frac{2.99 \cdot 10^{8} m}{s} \cdot \frac{3000}{cm} \cdot \frac{10^{2} cm}{1m} = 9 \cdot 10^{13} \frac{1}{s}$$

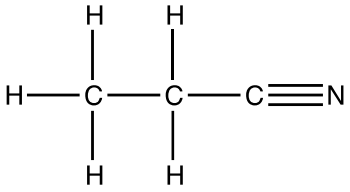
$$\lambda = 1/\tilde{\upsilon} = \frac{1}{3000 \frac{1}{cm}} \cdot \frac{1m}{100cm} \cdot \frac{10^{9} nm}{1m} = 3333.3nm = 3 \cdot 10^{3} nm$$

3. Match the structures of the following molecules with their corresponding infrared spectra. Circle the feature in the spectrum you used to make the assignment of the structure.

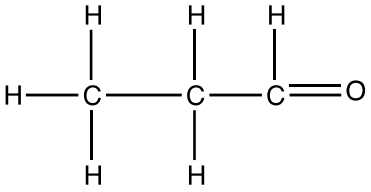
A) **Propanol**



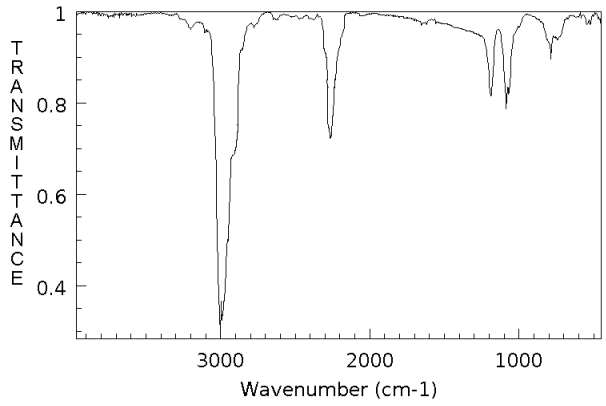
B) **Propionitrile**



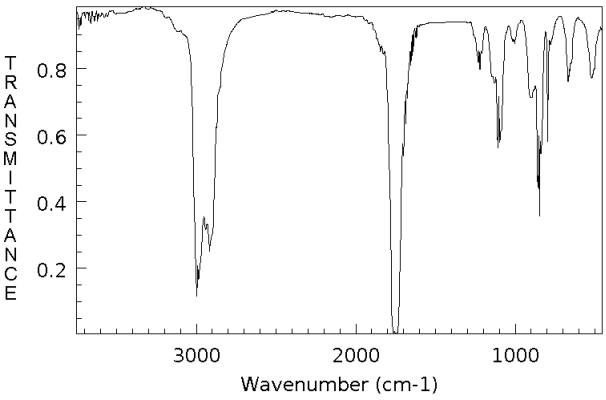
C) **1-Propanal**



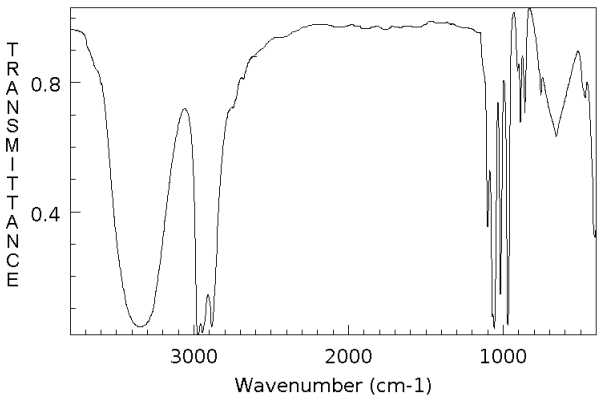
B



C



A



4. Arrange the following in order of increasing energy?
    a. Blue light
    b. Red light
    c. UV light
    d. An C-H stretch from problem 3
    e. An O-H stretch from problem 3

    D(IR at 3000cm^{-1}) <E(IR at 3500)<B(red) < A(blue) <C(UV)

5. Circle T or F according to whether each of the following statements about atmospheric warming is true of false.

    T / **F** A major source of warming is the absorption of sunlight by greenhouse gases.

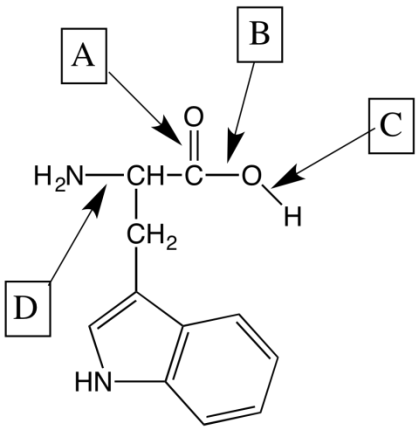
    T / **F** A major source of warming is IR light in the 3500 cm^{-1} region.

    T / **F** The primary source of warming is absorption of IR light by the major atmospheric gases O_2 and N_2.

    T / F The primary source of warming is absorption of IR light given off by Earth.

    T / F Water vapor is a major contributor to atmospheric warming.

6. Tryptophan (depicted below) is an amino acid that, although it is not synthesized in humans, is an essential amino acid and is required for the production of serotonin. Consider the four bonds (indicated by arrows labeled A, B, C, and D) selected in the figure when answering the following questions.



    a. Arrange the bonds A, B, and C, in order of increasing fundamental IR stretching frequency.

        B<A<C

    b. Laser light has a single frequency. A laser is used to excite the bond B stretch. If the same laser is used, how much light will be absorbed by bond D? (Circle only one of the choices below)

Less light	The same amount of light	More light	**No light will be absorbed**

7. "Visible light" refers to the part of the electromagnetic spectrum that a typical human eye will respond to: 390 to 780 nm. What is the highest frequency (in Hz) light that the typical human eye can detect? What will be the corresponding wavenumber (in cm^{-1}) (Answer:7.7·10^{14}, 2.6·10^{4})

    Highest frequency means lowest wavelength

    frequency: $\nu = c/\lambda = \frac{2.99\cdot10^{8}\,m}{s}\cdot\frac{1}{390nm}\cdot\frac{10^{9}\,nm}{1m} = 7.7\cdot10^{14}\,\frac{1}{s}$

    wavenumber: $\bar{\upsilon} = 1/\lambda = \frac{1}{390nm}\cdot\frac{10^{9}\,nm}{1m}\,\frac{1m}{100cm} = 2.6\cdot10^{4}\,\frac{1}{cm}$

8. Spectroscopists use isotopes to help identify molecules. Frequently, hydrogen atoms (^1H) are replaced by deuterium atoms (^2H). The ^1H–O stretch absorbs infrared light of 3600 cm^{-1}. Assuming that the strength of the bond remains the same, circle the appropriate relationship in the parentheses for the statements below.

   a. The frequency of the light absorbed by the ^1H-O stretch is (***greater than*** / *less than* / *equal to*) the frequency of the light absorbed by the ^2H-O stretch.

   b. The wavelength of the light absorbed by the ^1H-O stretch is (*greater than* / ***less than*** / *equal to*) the wavelength of light absorbed by the ^2H-O stretch.

9. Use dimensional analysis to answer the following question. In recent years the concentration of carbon dioxide, CO_2, in the atmosphere has increased from 309 to 397 ppm (parts per million). For CO_2, 1 ppm is equal to 2 mg of CO_2 per cubic centimeter, cm^3. Express the *change* in concentration of carbon dioxide in the air as molecules of CO_2 per cm^3.(Answer: $24*10^{20}$)
   397-309=88ppm

$$\frac{88\,ppm}{1cm^3}\cdot\frac{2mgCO_2}{1ppm}\cdot\frac{1g}{10^3mg}\cdot\frac{1molCO_2}{44gCO_2}\cdot\frac{N_A ofCO_2}{1molCO_2}=24\cdot10^{20}\frac{CO_2}{cm^3}$$

10. Atmospheric levels of **CO_2** increased by 40 ppm (40/364 x 100% = 10.9% CO_2 1997: 364 ppm → 2016: 404 ppm). Consider that 40 ppm is equivalent to 40 µmol **of CO_2 per 1** mol air. If atmosphere is 5.2 x 10^{18} kg and air is composed of 80% N_2 and 20% O_2 how many kg of CO_2 were added to atmosphere since 1997? (Hint: first find the molar mass of atmosphere) (Answer: $3*10^{14}$)

    Air= 0.8*28+0.2*32=28.8g/mol

$$\frac{40\mu molCO_2}{1molair}\cdot\frac{1molAir}{29gair}\cdot\frac{10^3gAir}{1kgAir}\cdot\frac{5.2\cdot10^{18}kgAir}{1}\frac{44gCO_2}{1molCO_2}\frac{1molCO_2}{10^6\mu molCO_2}=3\cdot10^{14}kgCO_2$$

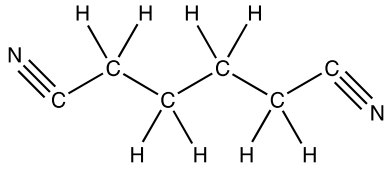
11. A newspaper article about the danger of global warming from the accumulation of greenhouse gases such as carbon dioxide states that "reducing driving your car by **40** miles a week would prevent release of over **2000** pounds of CO_2 per year into the atmosphere." To decide if this is a reasonable statement, calculate the reduction in the number of pounds of CO_2 a car would release in a year if its use was decreased by **40.0** miles per week. In your calculations, assume that gasoline is **isooctane** (C_8H_{18}) and that it is burned completely to CO_2 and H_2O in the engine of your car. Also assume that the car averages **21.8** miles per gallon and that the density of **isooctane** is **0.692** g cm^{-3}.

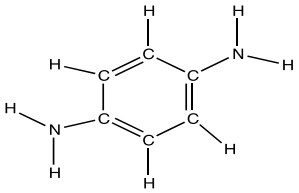
$$C_8H_{18} + 25/2\ O_2 \rightarrow 8CO_2 + 9H_2O$$

$$\frac{40miles}{1week}\frac{52weeks}{1year}\frac{1gal}{21.8miles}\frac{3.75L}{1galon}\frac{10^3mL}{1L}\frac{1cm^3}{1mL}\frac{0.693gC_8H_{18}}{1cm^3}\frac{1molC_8H_{18}}{114gC_8H_{18}}\frac{8molCO_2}{1molC_8H_{18}}\frac{44gCO_2}{1molCO_2}\frac{1lb}{453g}=1700lb$$

FALSE

12. Below is the structure of two molecules, hexanediamine (left) and 1,4 benzediamine (right) each of which have the formula $C_6H_8N_2$. Would you use IR or mass spectrometry to identify these species? Justify your response. Check your answers by using the IR (choose the gas phase spectrum) and mass spectrum of the two compounds provided by
NIST: Hexanediamine: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111693&Units=SI
1,4 benzediamine: http://webbook.nist.gov/cgi/cbook.cgi?ID=C106503&Units=SI





13. Consider two waves of light, light wave "A" with wavelength of 800 nm and light wave "B" with wavelength 1600 nm. Circle all the appropriate relationships in the parentheses for the five statements below. (Keep in mind that $\upsilon \sim \sqrt{\frac{k}{m}}$ where *k* represents the strength of the bond and *m* represent mass.)

a. The speed of light wave "A" is (*greater than / less than /* ***equal to***) the speed of light wave "B".

b. The wavenumber of light wave "A" is **(** ***greater than*** */ less than / equal to*) the wavenumber of light wave "B".

c. The frequency of light wave "A" is (***greater than*** */ less than / equal to*) the frequency of light wave "B".

d. Assuming the same atom masses, light wave "A" will match the frequency of bonds that are (***stronger than*** */ weaker than / the same strength as*) the bonds that match the frequency of light wave "B".

e. Assuming the same bond strength, light wave "A" will match the frequency of bonds that contain atoms that are (*heavier /* ***lighter***) than the bonds that match the frequency of light wave "B".