

NAME/TEAM: \_\_\_\_\_

## Fourier Transform Infrared Spectroscopy Postlab

*Last modified: June 17, 2014*

1) Summarize your results in the following table:

v/v % MTBE in gasoline	
v/v % ethanol in vodka	
v/v % ethanol in mouthwash	

2) Based on your results, what is the proof of your vodka and the v/v% ethanol in mouthwash?

3) What was your percent relative error (% RE) for the vodka proof and mouthwash v/v%:  
(see the container bottles for the manufacturer's values)

$$\% \text{ RE} = \frac{|\text{lit. value} - \text{your value}|}{\text{lit. value}} \times 100$$

4) Convert your v/v % MTBE in gasoline to units of mass % (w/w %) of oxygen in gasoline. Density of MTBE = 0.74 g/mL, Density of gasoline = 0.66 g/mL, Molar Mass of MTBE = 88.15 g/mol. You may need your TA to review dimensional analysis & conversion factors for this one!

NAME/TEAM: \_\_\_\_\_

- 5) What was your % RE for your measured mass % of oxygen in gasoline vs. the 1990 Clean Air Act Amendment minimum value of 2 % oxygen by mass?
- 6) Estimate the total mass of gasoline consumed each year in the U.S. (density of gasoline is 0.66 g/mL). If ethanol was used as the oxygen additive, approximately what volume of ethanol (in gallons) would be required each year, based on your answer to #4. (density of ethanol = 0.789 g mL<sup>-1</sup>; 1 gal = 3.7854 L). How many Olympic sized swimming pools would this fill (1 pool = 660,000 gal)?
- 7) If MTBE was phased out completely in the U.S. and replaced with ethanol as the oxygen additive to gasoline, discuss the economic and political ramifications of this change. (Approximate ethanol production in the U.S. is 14 billion gallons per year)

NAME/TEAM: \_\_\_\_\_

## GC/MS of Gasoline Postlab

*Last modified: June 17, 2014*

1. List the elution times from your gas chromatogram for benzene, toluene, and o-xylene. Can you find the qualitative relationship between these elution times and the structural attributes of the compounds?

Compound	Elution Time
Ethanol	
Benzene	
Toluene	
o-xylene	

2. You identified the molecules at specific retention times by their mass spectra. Fill the following table based on your observations. Explain why the mass corresponding to the highest peak in the observed mass spectrum is not the same as the molecular weight.

Compound	Molar Mass (g/mol)	1 <sup>st</sup> highest peak in mass spectrum	2 <sup>nd</sup> highest peak in mass spectrum	3 <sup>rd</sup> highest peak in mass spectrum
Ethanol				
Benzene				
Toluene				
o-xylene				

NAME/TEAM: \_\_\_\_\_

3. List your (v/v) % values in the following table:

Compound	Volume concentration (%)	(w/w) %
Ethanol		
Benzene		_____

Convert your v/v % ethanol in gasoline to units of mass % (w/w %) of oxygen in gasoline. (Density of ethanol = 0.789 g/mL, Density of gasoline = 0.66 g/mL). Use dimensional analysis properly for this one! List your answer in the Table above.

4. The 1990 Clean Air Act Amendment required a minimum value of 2.0 % oxygen by mass in gasoline. Compare this to the value you measured in step 4 using % relative error.
5. The 1990 average v/v % of benzene in gas is approximately 0.95%. Compare this to the value you measured using % relative error.
- $$\%RE = \frac{|\text{true value} - \text{your value}|}{\text{true value}} \times 100$$

NAME/TEAM: \_\_\_\_\_

## **HPLC of PAH Postlab**

*Last modified: June 17, 2014*

- 1) Summarize your results in the following Table:

ng benz[a]anthracene in one cigarette via UV absorption	

- 2) (a) Based on your results, determine how many milligrams of benz[a]anthracene a smoker would ingest over 40 years if they smoked 10 cigarettes a day.

(b) If the smoker weighed 185 pounds, what would be the amount ingested in mg benz[a]anthracene per kilogram body weight? How does this compare to the LD<sub>50</sub> value in the literature?

**NAME/TEAM:** \_\_\_\_\_

4) In your opinion, should smoking be banned on school and college campuses? Why or why not? Try to come up with both cons and pros for the ban.

5) List 5 chemicals in cigarettes and a major health concern of each:

NAME/TEAM: \_\_\_\_\_

## **LIBS Postlab**

*Last modified: June 17, 2014*

1. Observations for the spectra of different radiation sources:

<b>Source</b>	<b>Visual Appearance</b>	<b>Wavelengths</b> of 3-4 largest peaks in the emission spectrum (nm) – in the order of decreasing intensity

NAME/TEAM: \_\_\_\_\_

<b>Source</b>	<b>Visual Appearance</b>	<b>Wavelengths</b> of 3-4 largest peaks in the emission spectrum (nm) – in the order of decreasing intensity

2. Summarize your observations for the emission spectra and plasma of the metal samples in the following table :

Sample Number	Visual appearance	Observed emission color from this sample	Wavelengths of 3-4 largest peaks in the emission spectrum (nm) – in the order of decreasing intensity	Your guess for what this material is
1				
2				
3				
4				
5				

NAME/TEAM: \_\_\_\_\_

6				
7				
8				



NAME/TEAM: \_\_\_\_\_

6. Discuss what you learned from the spectra of different light sources
  - a. What are the qualitative differences between the spectra of the laser sources, spectra of plasma-driven lamps, spectra of LED lamps, and spectra of incandescent lamps?
  - b. What lines do you observe in the Hg lamp spectrum? Do they agree with the literature values (refer to the Hg-lamp paper on the course website)? Does your spectrometer measure wavelength accurately?
  - c. Are the spectra from the fluorescence room lights, white LED, or white monitor screen truly “white”?
  - d. Why do you think a TV remote is manufactured to emit in the region you measured?

NAME/TEAM: \_\_\_\_\_

7. One of the emission lines from a hydrogen lamp is due to an electron relaxing from the  $n = 5$  to  $n = 2$  energy levels. Calculate the wavelength and color of the photons emitted using Bohr theory for a 1 electron species ( $E_n = -R_H/n^2$ ) and Planck's Equation:  $E_{\text{photon}} = hc/\lambda$ . Note that  $\Delta E = E_{\text{final}} - E_{\text{initial}}$  and that for emission,  $E_{\text{photon}} = |\Delta E|$ .  $R_H = 2.179 \times 10^{-18}$  J. This problem is a great review for quantum theory in General Chemistry. (Bohr Theory does NOT work for the Hg lamp emission lines since Hg has 80 electrons). ( $h = 6.626 \times 10^{-34}$  J s;  $c = 3.00 \times 10^8$  m s<sup>-1</sup>).

NAME/TEAM: \_\_\_\_\_

## Catalytic Converter Postlab

- 1) Please summarize the results of your NO<sub>x</sub> sampling experiments in the following table

Car #1 make: \_\_\_\_\_ Car model: \_\_\_\_\_ Year: \_\_\_\_\_

Car #2 make: \_\_\_\_\_ Car model: \_\_\_\_\_ Year: \_\_\_\_\_

### NO<sub>x</sub> mixing ratio in car exhaust (in ppmv)

	Car #1	Car #2
<b>Cold start exhaust:</b>		
<b>Warm exhaust:</b>		

- 2) What is the apparent efficiency of the catalytic converter in removing NO<sub>x</sub> from the engine exhaust? One way to answer this is to calculate the percent reduction of NO<sub>x</sub> in the exhaust stream between samples collected before and after the catalytic converter has warmed up.

- 3) Provide an estimate of the amount of NO<sub>x</sub> (in grams) emitted by your car as you drove to UCI to attend the workshop. To do this, assume that the exhaust flows out of the tailpipe at a rate of 50 liters per second at all times regardless of the car's speed. If 4 million people commute to work in Los Angeles County daily and each person spends one hour per day driving to and from work, how much NO<sub>x</sub> would be emitted by these cars in one day? (Assume the temperature is 25 °C). Passenger cars are not the only emitters of NO<sub>x</sub>. Can you name other sources of NO<sub>x</sub> to the atmosphere and identify most important emitters?

**NAME/TEAM:** \_\_\_\_\_

4) Do catalytic converters last for the lifetime of the car? If not, why (since catalysts are not used up in the course of catalyzing a chemical reaction).

5) Have you ever had to replace a catalytic converter? How much did this cost? Why do you think it was so expensive to replace (disregarding labor!)

NAME/TEAM: \_\_\_\_\_

*Summer Teaching Program in Environmental Chemistry  
Computational Chemistry Laboratory Worksheet*

**Using Spartan to Investigate the Molecular Properties of  
Atmospherically Relevant Greenhouse Gases**

*Last modified: June 17, 2014*

**1. Geometry optimization**

(a) Perform the optimization of the geometry of each molecule as described in the lab manual and enter the calculated values of the geometric parameters in the table below.

molecule	parameter	values	
		calculated	experimental (CRC)
CO <sub>2</sub>	CO bond (Å)		
	OCO angle (°)		
H <sub>2</sub> O	OH bond (Å)		
	HOH angle (°)		
N <sub>2</sub> O	NN bond (Å)		
	NO bond (Å)		
	NNO angle (°)		
O <sub>3</sub>	OO bond (Å)		
	OOO angle (°)		

(b) Look up experimental values of the geometric parameters in the online CRC Handbook ([www.hbcponline.com](http://www.hbcponline.com)) and add them to the table.

(c) Briefly discuss the level of agreement between your calculated geometric parameters and the corresponding experimental values.

NAME/TEAM: \_\_\_\_\_

## 2. Vibrational analysis

(a) Perform the computation of the vibrational frequencies of each molecule as described in the lab manual and enter the values in the following table:

molecule	mode	frequencies ( $\text{cm}^{-1}$ )		IR active?	experimental wavelength ( $\mu\text{m}$ )	overlap with BB spectrum?
		calculated	experimental (NIST)			
$\text{CO}_2$	sym. str.					
	asym. str.					
	bend					
$\text{H}_2\text{O}$	sym. str.					
	asym. str.					
	bend					
$\text{N}_2\text{O}$	NN str.					
	NO str.					
	bend					
$\text{O}_3$	sym str.					
	asym. str.					
	bend					

(b) Look up experimental values of the vibrational frequencies in the NIST database (<http://webbook.nist.gov/chemistry/form-ser.html>) and add them to the table.

(c) Briefly discuss the level of agreement between your calculated vibrational frequencies and the corresponding experimental values.

NAME/TEAM: \_\_\_\_\_

### 3. Charge distribution

Examine the electrostatic potential surface of each molecule to get an idea of how the charge is distributed. In the space below, sketch the molecules and label each atom with partial charges (i.e.,  $\delta^+$  or  $\delta^-$ ). Draw arrows indicating the direction of the bond dipoles. Indicate whether or not the molecule has a net dipole moment.

(a) CO<sub>2</sub>

(b) H<sub>2</sub>O

(c) NO<sub>2</sub>

(d) O<sub>3</sub>

### 4. Infrared activity

Animate each of the vibrational modes of your molecule. In the space below, make a sketch of each vibrational mode, using double-headed arrows the relative motion of the atoms for each mode. Indicate which modes are IR active (i.e., change the dipole moment of the molecule) in the vibrational analysis table on p. 2.

(a) CO<sub>2</sub>

(b) H<sub>2</sub>O

(c) N<sub>2</sub>O

NAME/TEAM: \_\_\_\_\_

(d) O<sub>3</sub>

### 5. Overlap of IR active modes with Earth's blackbody radiation spectrum

(a) For each IR active mode of each molecule, convert the experimental vibrational frequency in  $\text{cm}^{-1}$  to wavelengths in  $\mu\text{m}$ , and enter the result in the vibrational analysis table on p. 2.

(b) Compare the wavelengths of the IR active modes with Earth's theoretical blackbody radiation spectrum (found on the last page of the COMPUTATIONAL CHEMISTRY LAB MANUAL). Indicate in the vibrational analysis table on p. 2 which modes absorb radiation at wavelengths that overlap with the theoretical blackbody (BB) spectrum. Do you see evidence of absorption from the modes you identified in the experimentally measured spectrum of radiation leaving the upper atmosphere?