Title Page
Title (1 pts)
Incapacitating Gas
Nick Pekor – ntp11@pitt.edu

Two Hypotheses (4 pts)

      The speed of sound calculated through the system is correlative to the pressure of the system. This is hypothesized because of the physical definition of sound. Sound is produced by a waveform function of differing pressure over time. If the pressure is lower, that means that there are less gas particles present in the system, and there are weaker overall intermolecular forces interacting in the system, so much less energy is needed to excite the particles when the sound wave is introduced.

      It is believed that the heat capacity values of the gases will be inversely proportional to the molar mass of the gas molecules, meaning that a higher heat capacity would imply a lower molar mass. This is because of the energy needed to move the gas molecules. A heavier gas would need more energy to move and disrupt the pressure equilibrium of the system.

Abstract (5 pts)

      Sound is not necessarily caused by its own physical wave, but rather a theoretical wave that causes molecules in the air to vibrate at certain frequencies. The frequencies that the gas particles vibrate at determine the pitch of the sound that is heard. Since audible sound is caused by the vibration of molecules, in a vacuum, sound does not technically exist, as there are no molecules present to vibrate. The vibration of molecules gives insight into the energetic and thermodynamic properties that the gases have. For this experiment, multiple gases are pumped into a tube under vacuum, and a sound wave is passed through the system. The speed of the sound in the system can be found through this and eventually allow for the heat capacities of the multiple gases to be determined.

Results (35 pts)

      Before the experimental procedure is pursued, it is important to record some control values, as these will be needed for future calculations to determine the specific heats. Later on in the experiment, when a second run is done, the Kundt's Tube Length will be changed to confirm the guesses for the identity of the gases used in the experiment.

Table 1 – Significant values needed for calculation for the initial run	
Kundt's Tube Length (m)	Temperature (K)
0.9300	296.2

      After the respective gases were pumped into the Kundt's tube, the sound wave was pumped through the gas at a set length. The oscilloscope reading would show the harmonic overtone frequencies. These frequencies were plotted, as they are necessary to determine the heat capacities of the gases. The values are used in calibration curves, for each of the unknown gases.
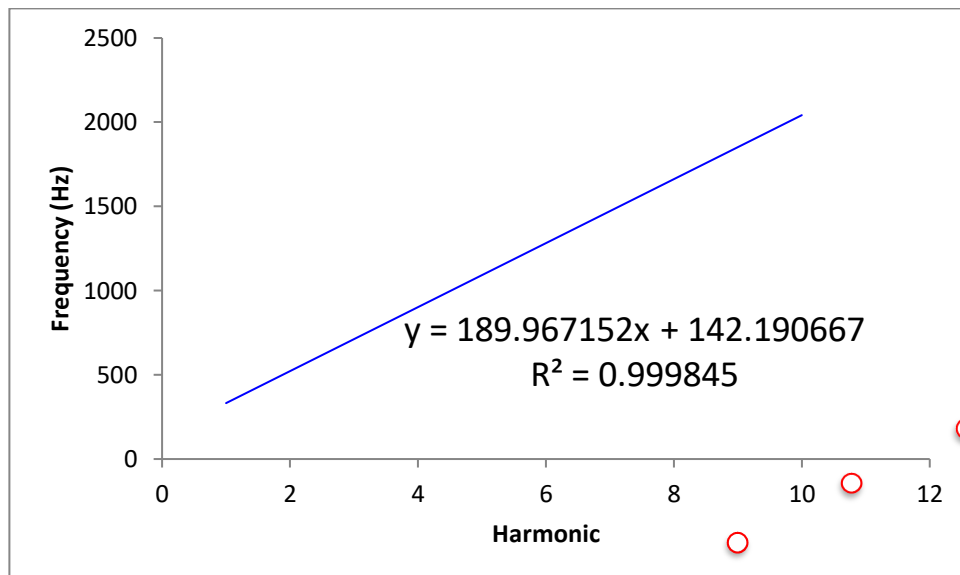
Figure 1 – Calibration curve of the initial run of the 1 gas. The axes are plotted harmonic vs frequency.

The value of the slope is gathered to continue the calculation process. Likewise, the standard uncertainty of the slope is calculated through excel by the LINEST function. The value of the slope, as detailed in the lab instructions, is equivalent to (c/2L), where L is the length of the Kundt's tube, and c is the speed of the sound wave. Through all of this, the individual speeds of the sound waves through the individual gases can be determined.

Sample	Slope (Hz/n)	Speed of Sound (m/s) [1] {1}
Table 2 – Values of the slopes of the calibration curves, and the calculated speed of sound values for the initial run of each gas.		
Gas 1	190.0 ± 0.8	353.3 ± 2
Gas 2	143.8 ± 0.9	267.5 ± 2
Gas 3	536.0 ± 7	996.9 ± 10
Gas 4	87.8 ± 0.4	163.3 ± 1

Through the speed of sound calculations, the heat capacity fraction of the individual gases can also be found. By using these heat capacity fraction values, and comparing it to the ideal value, 1.666, a guess for the identities of the gases. The identities can be determined by knowing the theoretical heat capacities of the gases and comparing their fractions, but in this case standard trial and error by plugging in the molar mass of the gases for each run will work. The closer the resulting value is to the 1.666 value determines the identity of the gases.

Sample	γ [2] {2}	Gas Identity
Table 3 – Values of the slopes of the calibration curves, and the calculated speed of sound values for the initial run of each gas.		
Gas 1	1.420 ± 0.01	N_2
Gas 2	1.279 ± 0.02	CO_2
Gas 3	1.616 ± 0.04	He
Gas 4	1.105 ± 0.009	CF_3CH_2F

As of right now, the identity of the gases is just an initial guess. Later on in the procedure, a second run will be done with a different Kundt's tube length to confirm the guess.

Now that the heat capacity fraction of the gases was found, the heat capacity values for each gas can be determined. To consider the accuracy of the heat capacity values, the theoretical heat capacity values must be calculated. The error between the two readings can show the error that the experimental run has on the values.

The theoretical values of the heat capacities are found through a number of calculations and definitions of heat capacity depending on the shape of the molecule. The definitions, and calculation values are shown below, as well as the experimental and theoretical heat capacities.

The theoretical C_v values of the gases are found by adding up all of the components of the energy the gas molecules have, $C_{v\ trans}$, $C_{v\ rot}$, and $C_{v\ vib}$, which account for the translational, rotational, and vibrational heat capacities respectively. The determination of $C_{v\ trans}$ and $C_{v\ rot}$ is fairly simple, as the values can be determined by just examining the shape of the gas molecule. $C_{v\ vib}$, however, needs to be found by much more intricate calculations. For this experiment, Scigress is used to model the gas molecules, and use built-in analysis options to examine the IR absorption peaks, ignoring degenerate values. The wavenumbers of the peaks are then plugged into an involved equation to determine the total $C_{v\ vib}$ interaction that the molecule has.

Table 4 – Theoretical component C_v values, and the calculated theoretical C_v and C_p values for the initial run.

Sample	$C_{v\ trans}$ (J/molK)	$C_{v\ rot}$ (J/molK)	$C_{v\ vib}$ (J/molK) [4, 5]	C_v theo (J/molK) [6]	C_p theo (J/molK) [7]
Gas 1 (N_2)	1.5R	R	1.022×10^{-3}	20.79	29.10
Gas 2 (CO_2)	1.5R	R	0.6285	21.41	29.73
Gas 3 (He)	1.5R	0	0	12.47	20.79
Gas 4 (CF_3CH_2F)	1.5R	1.5R	6.124	31.07	39.38

Table 5 – Experimental and Theoretical C_p and C_v values, as well as their respective error for the initial run.

| Sample	C_p exp (J/molK) [3] {3}	C_v exp (J/molK) [7]	C_v theo (J/molK) [6]	C_p theo (J/molK) [7]	C_p Error (%) [8]	C_v Error (%) [8]
Gas 1 (N_2)	28.09 ± 0.9	19.78 ± 0.9	20.79	29.10	3.48	4.88
Gas 2 (CO_2)	38.13 ± 2	29.82 ± 2	21.41	29.73	28.3	39.2
Gas 3 (He)	21.82 ± 2	13.51 ± 2	12.47	20.79	4.97	8.28
Gas 4 (CF_3CH_2F)	87.77 ± 8	79.46 ± 8	31.07	39.38	123	156

Now that the initial run has been done. The results and error for the standard heat capacities is determined and can be deemed accurate or inaccurate. As shown in the data above, some gases were fairly accurate to the theoretical values calculated (gases 1 and 3), while others were significant inaccurate (gases 2 and 4). Because of this, it is difficult to prove that the results are in fact accurate to what is being expected. To solve this dilemma, a second confirmation run is performed to see if the trends revealed by the initial run are indeed accurate.

To perform a second run, but receive different values, one of the significant control values must be altered, either temperature or Kundt's Tube Length. Since it is not ideal to crucially change the temperature of the experimental medium, the Kundt's Tube Length is altered. This should result in a large change in the harmonic frequencies of the gases and alter their calibration curves.

Table 6 – Significant values needed for calculation for the confirmation run

Kundt's Tube Length (m)	Temperature (K)
0.4801	294.7

(Note: The temperature was not manually changed. The lab just got slightly colder.)

As done previously, each of the gases are run through the Kundt's Tube apparatus, and the sound wave was run through each gas to receive their harmonic frequencies and construct a calibration curve for each gas.
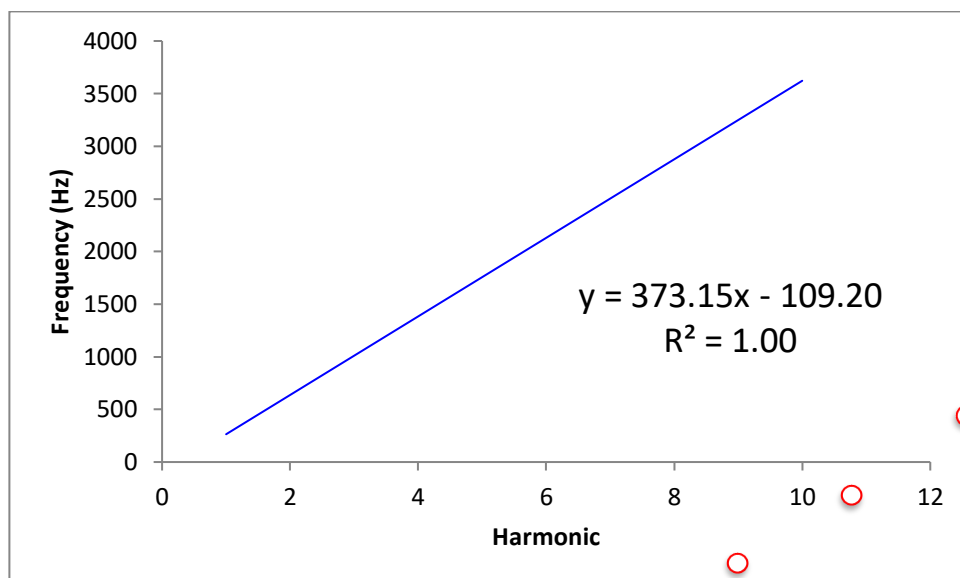
Figure 2 – Calibration curve of the confirmation run of the 1 gas. The axes are plotted harmonic vs frequency. Notice how the slope is different from the initial run of the same gas. This occurs due to the change of the length of the Kundt's Tube.

The calculations up until the heat capacity ratio are done the same as before, but this time, since the gas identities were already hypothesized, the molar masses can just be plugged in believing that the initial hypothesis is true. If the initial hypothesis was correct, the heat capacity ratios should not deviate too much from the ideal heat capacity ratio, 1.666.

Table 7 – Calculative values for the confirmation run of each gas, up until the heat capacity ratio values.				
Sample	Slope (Hz/n)	Speed of Sound (m/s) [1] {1}	γ [2] {2}	Gas Identity
Gas 1	373.1 ± 5	358.3 ± 5	1.468 ± 0.05	N_2
Gas 2	287.6 ± 5	276.2 ± 5	1.370 ± 0.04	CO_2
Gas 3	585.1 ± 10	561.8 ± 10	0.5156 ± 0.02	He
Gas 4	181.8 ± 2	174.5 ± 2	1.269 ± 0.03	CF_3CH_2F

As with the initial run, a couple of the heat capacity ratio values can stray from the ideal value of 1.666. In this case, Gas 3 has the value furthest away from the ideal value. This contrasts with the initial run, as Gas 3 had the most accurate reading. However, when Helium was plugged into the other gas calculations, the received value tends to be even less accurate. In the end, it can be believed that helium is gas 3, and there was just a bit of error with the reading. This is backed up by the fact that the calibration curve does not have quite an accurate fit to the data received from the harmonic readings. (See SF 5)

Regarding every other gas, it can be seen that the heat capacity ratios are much in the same compared between the initial and confirmation runs, so the gas identities are kept the same and presumed that these are the actual gases. This can be further backed up by determining the experimental heat capacities and finding their percent error values. The theoretical values for C_v and C_p do not have to be recalculated.

(4)

Table 8 – Experimental and theoretical values for C_p and C_v, as well as their respective error for the confirmation run.

Sample	C_p exp (J/molK) [3] {3}	C_v exp (J/molK) [3] {3}	C_v theo (J/molK) [6]	C_p theo (J/molK) [7]	C_p Error (%) [8]	C_v Error (%) [8]
Gas 1 (N_2)	26.08 ± 3	17.76 ± 3	20.79	29.10	10.4	14.5
Gas 2 (CO_2)	30.76 ± 4	22.44 ± 4	21.41	29.73	3.66	5.09
Gas 3 (He)	-8.851 ± 0.6	-17.16 ± 0.6	12.47	20.79	143	238
Gas 4 (CF_3CH_2F)	39.26 ± 4	30.94 ± 4	31.07	39.38	0.102	0.130

When looking at the percent error values confirmation run, it is noticed that some gases are more accurate to their theoretical values than others. In this case, gases 2 and 4 are more accurate, and gases 1 and 3 are less accurate. This is the direct inverse of the percent error readings of the initial run, as for that run, gases 1 and 3 were more accurate and gases 2 and 4 were less accurate. In the end, this leaves at least one run for each gas that gives an accurate result to their theoretical values.

Sample Calculations (15 pts)

[1]
$$c = 2Lm$$
$$c_{1I} = 2 \cdot 0.9300 \text{ m} \cdot 190.0 \frac{\text{Hz}}{\text{n}} = 353.3 \frac{\text{m}}{\text{s}}$$

[2]
$$\gamma = \frac{Mc^2}{RT}$$
$$\gamma_{1I} = \frac{\left(0.028014 \frac{\text{kg}}{\text{mol}}\right)\left(353.3 \frac{\text{m}}{\text{s}}\right)^2}{\left(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}}\right)(296.2 \text{ K})} = 1.420$$

[3]
$$C_p = \frac{R\gamma}{\gamma - 1}$$
$$C_{p_{1I}} = \frac{\left(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}}\right) \cdot 1.420}{1.420 - 1} = 28.09 \frac{\text{J}}{\text{mol} \cdot \text{K}}$$

[4]
$$\theta_v = \frac{hC\tilde{v}}{k}$$
$$\theta_{v_{2A}} = \frac{(6.626 \cdot 10^{-34} \text{ J} \cdot \text{s})\left(2.997 \cdot 10^{10} \frac{\text{cm}}{\text{s}}\right)(546.5 \text{ cm}^{-1})}{1.381 \cdot 10^{-23} \frac{\text{J}}{\text{K}}} = 786.3 \text{ K}$$

[5]
$$C_{v \, vib} = \sum \left(\frac{\theta_v}{T}\right)^2 \left(\frac{e^{-\theta_v/T}}{(1 - e^{-\theta_v/T})^2}\right)$$
$$C_{v \, vib_2} = \left(\frac{786.3 \text{ K}}{296.2 \text{ K}}\right)^2 \left(\frac{e^{-(786.3 \text{ K})/(296.2 \text{ K})}}{(1 - e^{-(786.3 \text{ K})/(296.2 \text{ K})})^2}\right) + \left(\frac{1998. \text{ K}}{296.2 \text{ K}}\right)^2 \left(\frac{e^{-(1998.\text{K})/(296.2 \text{ K})}}{(1 - e^{-(1998.\text{K})/(296.2 \text{ K})})^2}\right)$$
$$+ \left(\frac{3348. \text{ K}}{296.2 \text{ K}}\right)^2 \left(\frac{e^{-(3348.\text{K})/(296.2 \text{ K})}}{(1 - e^{-(3348.\text{K})/(296.2 \text{ K})})^2}\right) = 0.6285 \frac{\text{J}}{\text{mol} \cdot \text{K}}$$

[6]
$$C_v = C_{v\,tra} + C_{v\,rot} + C_{v\,vib}$$
$$C_{v_2} = 12.47 \ \frac{J}{mol \cdot K} + 8.314 \ \frac{J}{mol \cdot K} + 0.6285 \ \frac{J}{mol \cdot K} = 21.41 \ \frac{J}{mol \cdot K}$$

[7]
$$C_p = C_v + R$$
$$C_{p_2} = 21.41 \ \frac{J}{mol \cdot K} + 8.314 \ \frac{J}{mol \cdot K} = 29.73 \ \frac{J}{mol \cdot K}$$

[8]
$$\% \ Error \ = \left| \frac{Exp - Theo}{Theo} \right| \cdot 100\%$$
$$\% \ Error_{1I} \ = \left| \frac{28.09 - 29.10}{29.10} \right| \cdot 100\% = 3.48\%$$

{1}
$$\delta c = c \sqrt{\left(\frac{\delta m}{m} \right)^2 + \left(\frac{2\delta L}{2L} \right)^2}$$
$$\delta c_{1I} = 353.3 \ \frac{m}{s} \sqrt{\left(\frac{0.8369 \ \frac{Hz}{n}}{190.0 \ \frac{Hz}{n}} \right)^2 + \left(\frac{2 \cdot 0.00005 \ m}{2 \cdot 0.9300 \ m} \right)^2} = 2 \ \frac{m}{s}$$

{2}
$$\delta \gamma = \gamma \sqrt{\left(2 \cdot \frac{\delta c}{c} \right)^2 + \left(\frac{\delta M}{M} \right)^2 + \left(\frac{\delta R}{R} \right)^2 + \left(\frac{\delta T}{T} \right)^2}$$
$$\delta \gamma_{1I} = 1.420 \sqrt{\left(2 \cdot \frac{2 \ \frac{m}{s}}{353.3 \ \frac{m}{s}} \right)^2 + \left(\frac{5 \cdot 10^{-7} \ \frac{kg}{mol}}{0.028014 \ \frac{kg}{mol}} \right)^2 + \left(\frac{0.0005 \ \frac{J}{mol \cdot K}}{8.314 \ \frac{J}{mol \cdot K}} \right)^2 + \left(\frac{0.05 \ K}{296.2 \ K} \right)^2} = 0.01$$

{3}
$$\delta C_p = C_p \sqrt{\left(\frac{\delta R}{R} \right)^2 + \left(\frac{\delta \gamma}{\gamma} \right)^2 + \left(\frac{\delta \gamma}{\gamma - 1} \right)^2}$$
$$\delta C_{p_{1I}} = 28.09 \ \frac{J}{mol \cdot K} \sqrt{\left(\frac{0.0005 \ \frac{J}{mol \cdot K}}{8.314 \ \frac{J}{mol \cdot K}} \right)^2 + \left(\frac{0.01}{1.420} \right)^2 + \left(\frac{0.01}{1.420 - 1} \right)^2} = 0.9 \ \frac{J}{mol \cdot K}$$

Discussion, 1 (min) − 2 (max) pages, single spaced (35 pts)

Both hypotheses proposed before the experiment was done did not line up with the results given from the experiment. The first hypothesis stated that the speed of sound in the system would correlate to the pressure of the system, as less molecules present in the system would mean less intermolecular interactions and therefore less energy needed to move the molecules. As a whole, this hypothesis ended up being not only inaccurate towards the results, but also not even important in the scheme of the experiment. The pressure of the system was never considered when loading the gases into the Kundt's tube. In the procedure, the gas was just pumped in until the check valve made a noise, which meant that the tube was "full". No pressure is ever determined in the experiment.

The second hypothesis stated that heat capacity would decrease as the molar mass of the gases increased. This was considered thinking that the larger mass would lead to more energy being needed to mobilize the molecules. However, looking at the data, the opposite was found to be true.

Sample	Molar Mass (kg/mol)	C_p exp inital (J/molK) [6]	C_v exp initial (J/molK) [7]	C_p exp confirmation (J/molK) [6]	C_v exp conformation (J/molK) [7]
Gas 3 (He)	0.0040026	21.82 ± 2	13.51 ± 2	-8.851 ± 0.6	-17.16 ± 0.6
Gas 1 (N_2)	0.028014	28.09 ± 0.9	19.78 ± 0.9	26.08 ± 3	17.76 ± 3
Gas 2 (CO_2)	0.044009	38.13 ± 2	29.82 ± 2	30.76 ± 4	22.44 ± 4
Gas 4 (CF_3CH_2F)	0.10203	87.77 ± 8	79.46 ± 8	39.26 ± 4	30.94 ± 4

Table 9 – Comparison of the molar mass of the gases and their experimental heat capacity data, sorted by increasing molar mass.

The data above clearly shows that as the molar mass increased, the heat capacity also increases. Given that this is true for ALL experimental data, it is safe to believe that the initial hypothesis was wrong.

Compared to other calculational values, molar mass tends to be the value that causes the most change in the heat capacity values. This is mainly in part due to the position of the molar mass in the calculation it is used in. [2] In the calculation of the heat capacity ratio, M, the molar mass, is present in the numerator with c^2, whereas T is present in the denominator with R. Since the value for c^2 tends to be a significantly large value (between 25,000 and 1,000,000), a small change in M would cause a more significant change in γ than T, since T only affects R (which has a value of 8.314).
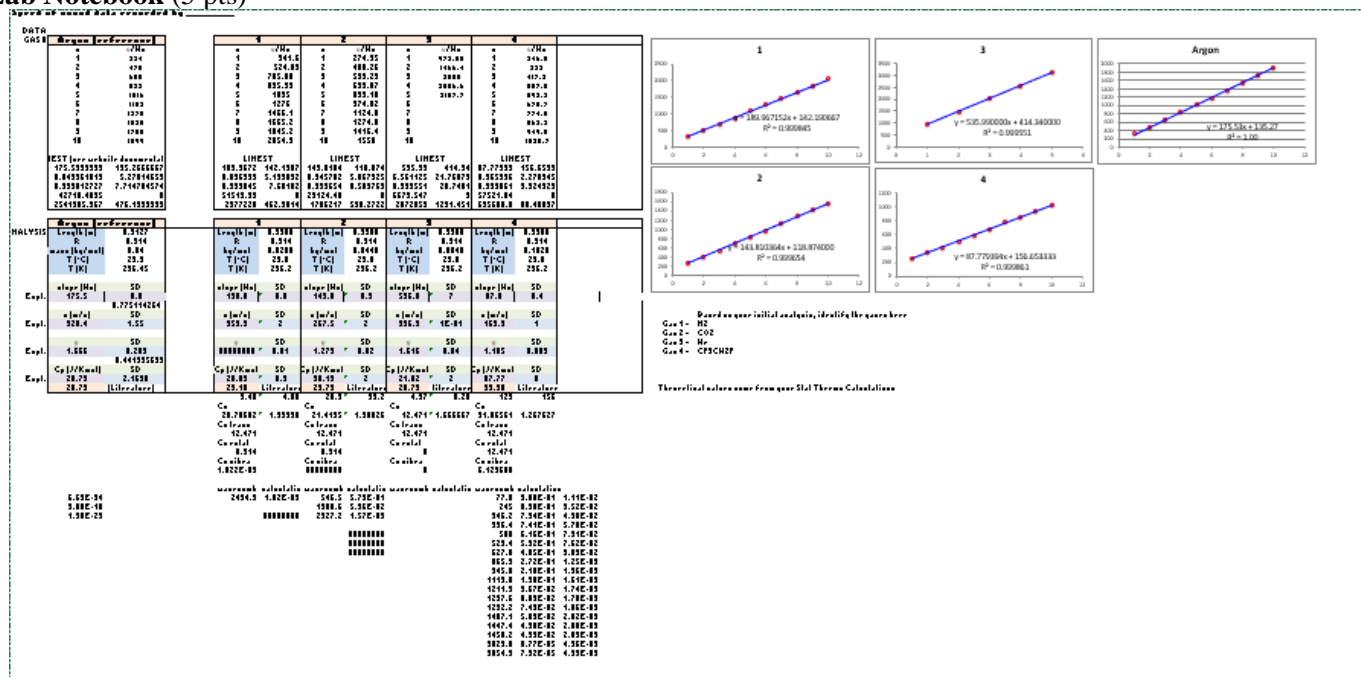
One of the more in-depth calculations done in the experiment was the calculations of the theoretical heat capacities of the gas molecules. So much so that a computational program, Scigress, was utilized in order to make this portion much less problematic overall. The sole problem that arises from this section that makes the use of Scigress intuitive is the vibrational component of the heat capacities, which need to be accounted for to determine the theoretical heat capacities for each gas. Considering it is not ideal to get a IR reading for the gases, the next best option is to computationally receive the value for the vibration component. The use of Scigress also allowed for an easier reading of the IR transmittance peaks, as peaks can be very close to each other, and since the peaks are very sharp, it is not easy to determine the actual axis value of a peak.

Using Scigress gives the numerical values for every peak that shows up for a molecule, which is notably helpful not only for the added accuracy that Scigress provides, but also for the fact that it shows all peaks, even peaks for vibrational modes that are not IR active. In the case of this experiment, N_2 and CO_2 both have a peak for symmetric stretch. In a standard IR reading, these peaks would not show up because symmetric stretching does not change the dipole moment of the molecule and therefore does not give a transmittance value. Scigress accounts for the symmetric stretch, and marks down the wavenumber where it would be present, while also not necessarily giving it a peak.

Despite the vibrational components for the gases needing a computational program to calculate, the values are not very significant to the overall theoretical heat capacities, especially for He and N_2. This comes because the vibrational component of the heat capacity relies on the number of atoms that the molecule has. Even then, if the value of the vibrational component is significant, the individual parts of the vibrational component do not tend to be. This is because of the partition function, and the formula used. [5] For greater values of θ_v, and in turn, $\tilde{v}$, the value for that part of the vibrational component gets closer to zero. Therefore, the IR transitions do not have to be extremely precise, especially at greater wavenumber values.
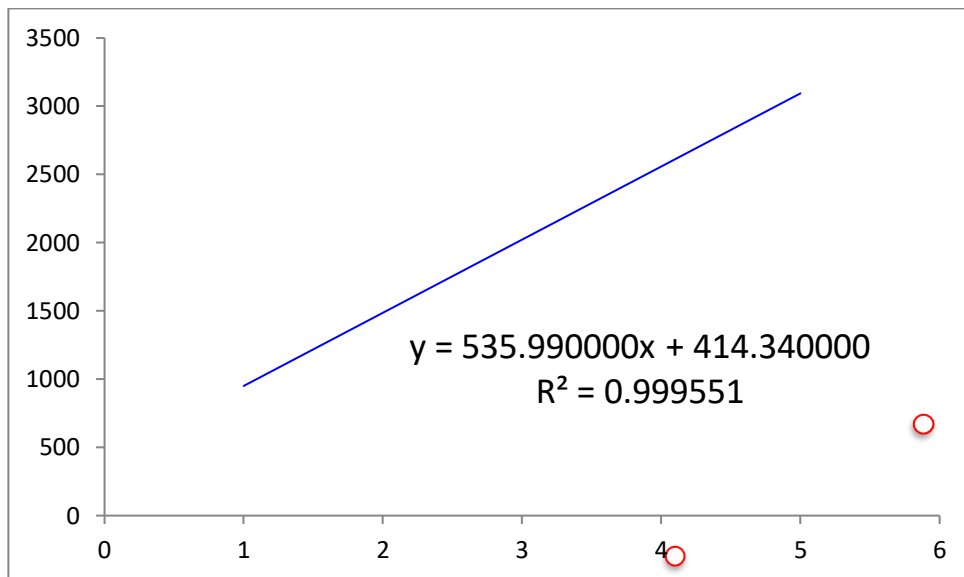
This is also the reason why the electronic component is not considered, as this value tends to be miniscule. The vibrational component seems to be much less intuitive to figure out for multiple different molecules compared to the rotational and translational components, most likely because of where these components stem from. The rotational and transitional components come from the energy stored between molecules, and the vibrational

component comes from the energy inside of molecules. The off chance where the rotational component would not be intuitive is if the molecule is significant polar or asymmetric.

Overall, the data received from the experiment, as well as the numerous calculated values, tend to be accurate with each other. The experimental and theoretical heat capacities for each gas tend to be accurate with each other in at least once instance. The experiment shows that for molecules of greater molar mass, the length L should be made shorter to receive more accurate answers to the theoretical values, and vice versa.

Lab Notebook (5 pts)

Appendix

y = 143.810364x + 118.874000
R² = 0.999654

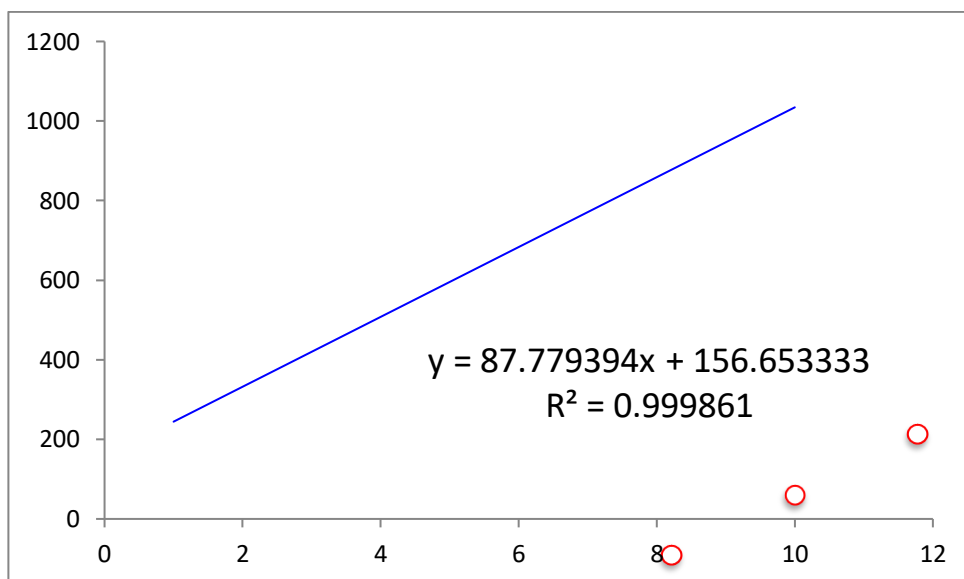**SF 1** – Calibration curve of the initial run of the 2 gas. The axes are plotted harmonic vs frequency.
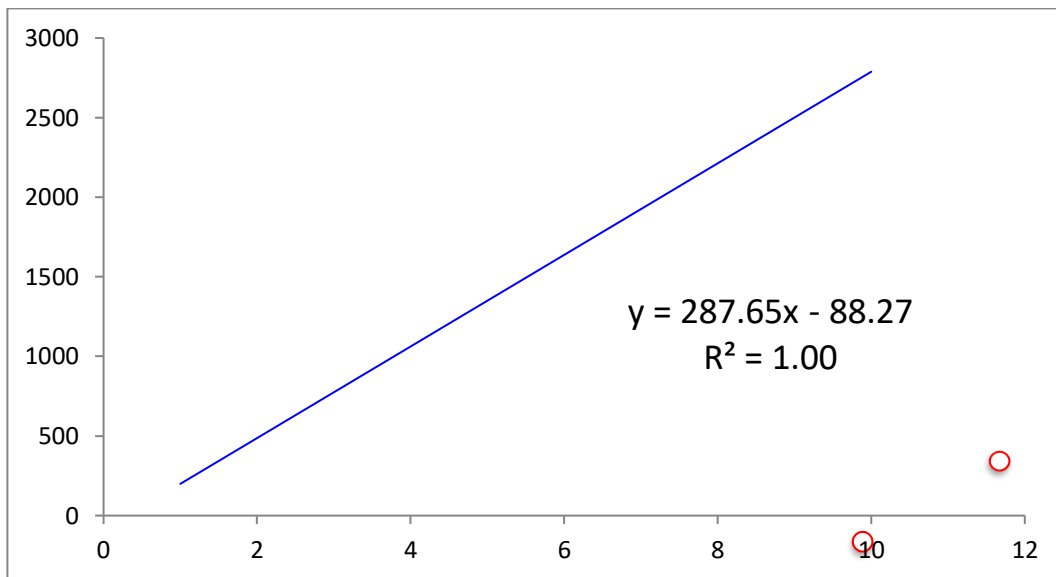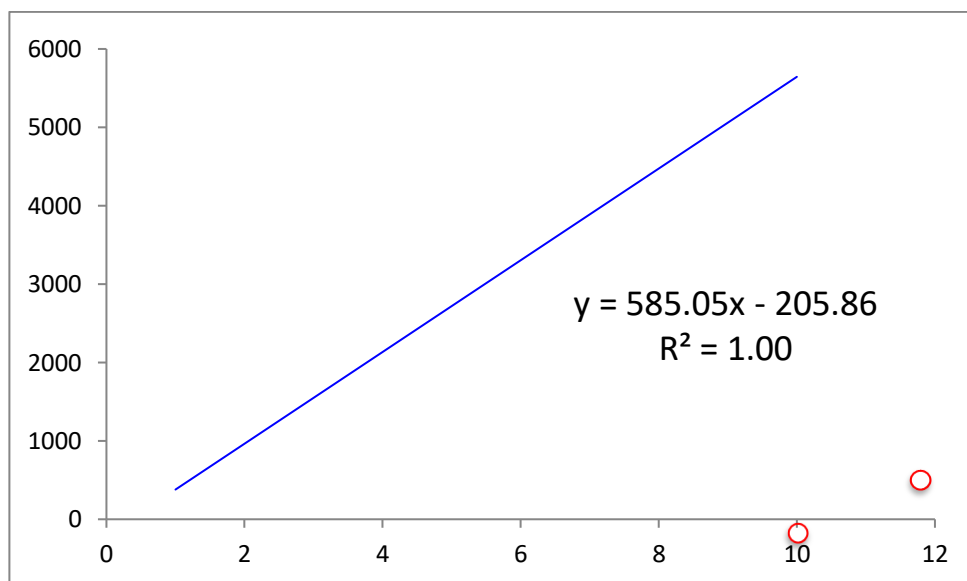
SF 2 – Calibration curve of the initial run of the 3 gas. The axes are plotted harmonic vs frequency.
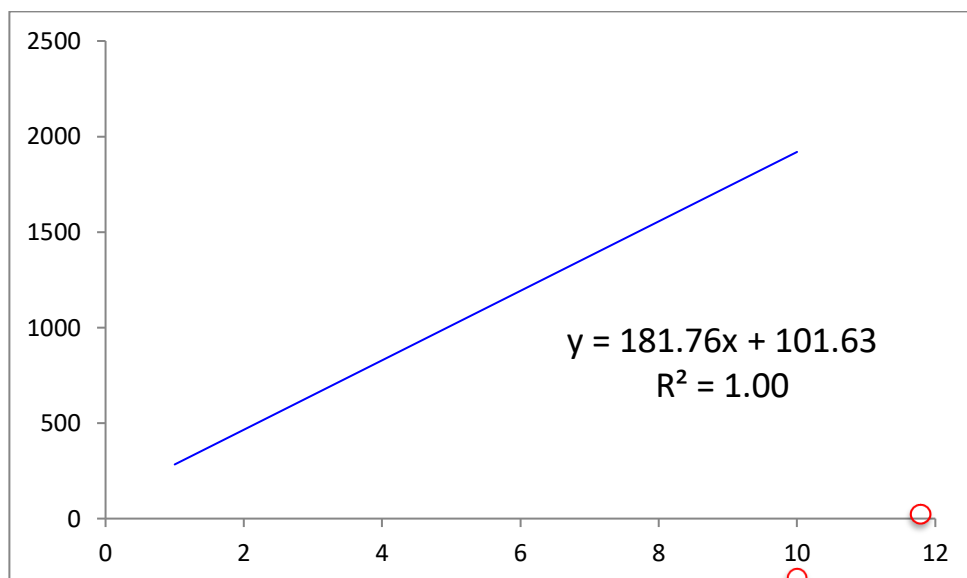

SF 3 – Calibration curve of the initial run of the 4 gas. The axes are plotted harmonic vs frequency.
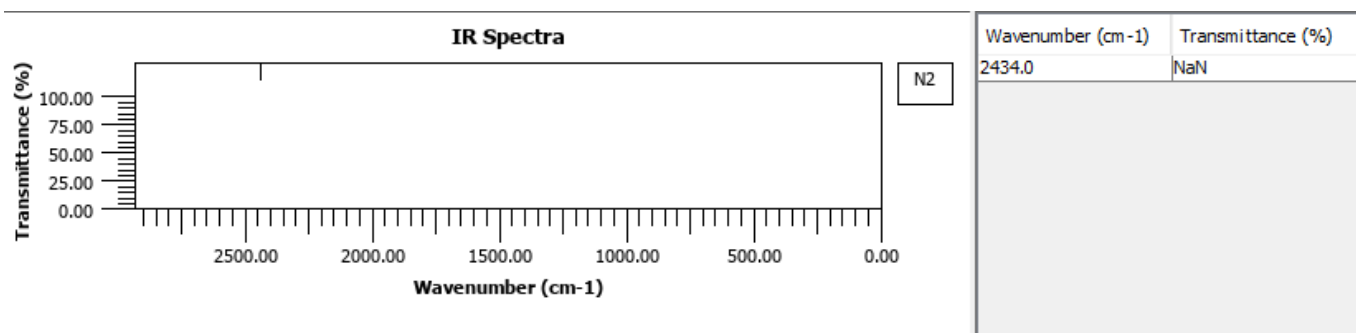
(10)

SF 4 – Calibration curve of the confirmation run of the 2 gas. The axes are plotted harmonic vs frequency.


SF 5 – Calibration curve of the confirmation run of the 3 gas. The axes are plotted harmonic vs frequency.

SF 6 – Calibration curve of the confirmation run of the 4 gas. The axes are plotted harmonic vs frequency.

Wavenumber (cm-1)	Transmittance (%)
2434.0	NaN

SF 7 – IR Spectra data received from Scigress for N_2. Notice how the one data point has no Transmittance data.

Wavenumber (cm-1)	Transmittance (%)
546.5	67.8
546.5	67.8
1388.6	100.0
2327.2	10.0
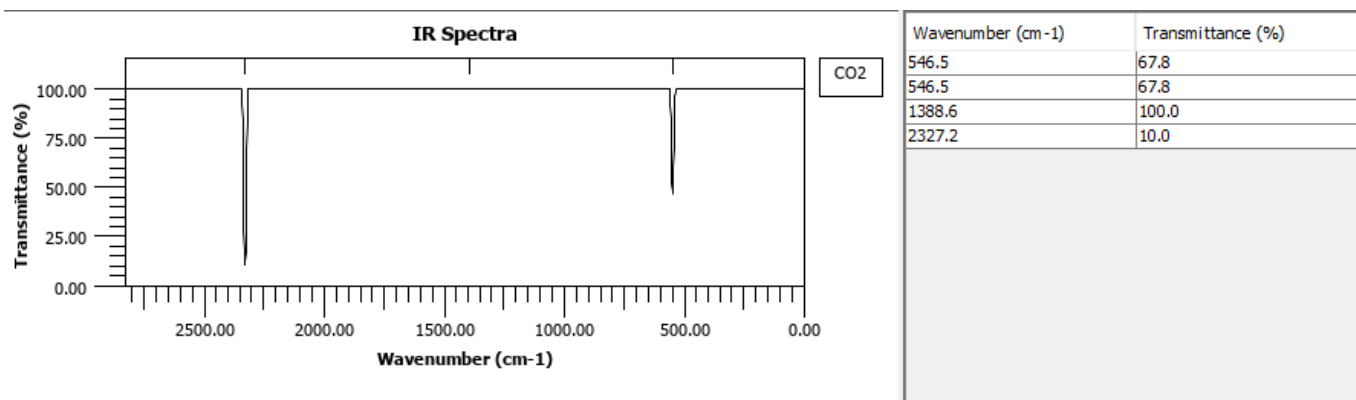
SF 8 – IR Spectra data received from Scigress for CO_2. Notice how there are two different data points for the same wavenumber and transmittance.

IR Spectra
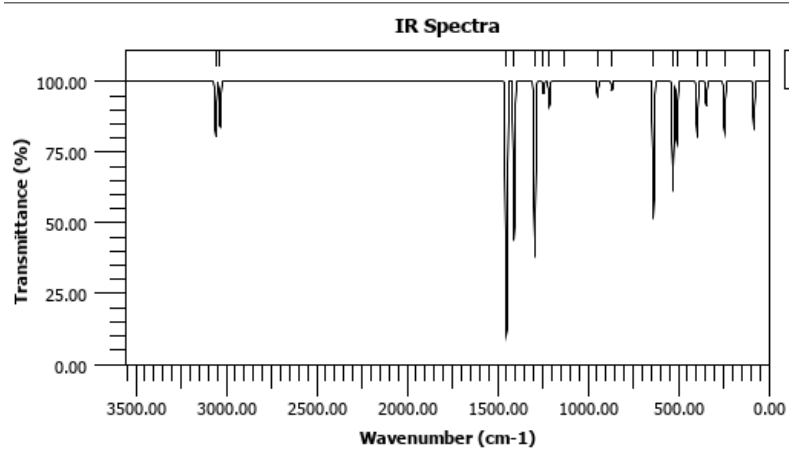
Wavenumber (cm-1)	Transmittance (%)
82.7	70.5
244.9	69.4
346.1	84.0
396.3	66.9
507.6	63.6
529.8	41.0
637.6	29.7
866.1	94.1
946.1	89.6
1129.0	99.5
1212.4	83.9
1244.6	91.5
1292.3	17.2
1407.2	22.4
1447.7	13.6
1450.3	10.0
3030.2	72.4
3054.6	67.1

SF 9 – IR Spectra data received from Scigress for CF_3CH_2F.