

Experiment 1:

Measurement and Expression of the Experimental Data

Instructor Notes and Lab Preparation

Each fall and spring semester a week after school starts, things are hectic, students are still registering for classes, and some sort of holiday interrupts the first week of labs. This allows the instructors only to check in the labs but then have an off week before the students are able to start performing experiments. Rather than allow the students to waste a full week of lab time, assigning this math and graphing review as the first experiment of the semester is a great way to refresh their minds and get them back into the swing of things. Part A is designed for the first semester, and Part B is designed for the second semester of general chemistry.

As the check-in process is generally quick, at the end of the check-in day, I have each of my teaching assistants give a short lecture on the math involved.

Particular Points to Stress

Scientific or exponential notation is used so often in scientific literature and calculation; it seems we sometimes forget how confusing it can be to someone dealing with it for the first time. I always stress that students should look at the values they calculate to make sure they make sense. For example, one of the most common mistakes students make when dealing with exponents is when they must change an exponent to add or subtract two exponential values. The process requires students “move the decimal” in the correct direction to “match up” the exponents. The most common mistake is the movement of the decimal in the wrong direction. So ask the students to check and make sure that the number resulting after the move still makes sense, that is, does it have the same value it did before the move? Simply plugging it into a calculator should do the trick.

Another sticky point with many students is an overall lack of graphing skills. I have placed a brief Excel® tutorial at the end of the manual to encourage students to use this program or one similar to it to complete the graphing exercises. If you choose to have your students complete the graphs by hand, I understand the reasoning, but I would encourage you to consider asking for the graphs in both styles. The reality of the world today is that computers are everywhere. Skillful use of technical programs like Excel® is a must for scientific analysis.

The most common mistakes that should be discussed with respect to graphing are (1) attempts to fit straight lines to data that do not fit $y = mx + b$ and (2) irregular spacing of values on an axis. I often see graphs with axes that are marked at regular intervals with the values given as part of the problem. Markings of this sort always generate perfectly straight lines, which thrill the students, but give me migraines.

Last but not least, the discussion we have about logarithms and the proper use of significant figures in logarithms is generally the first exposure students will have to the subject. Special attention should be paid to the introduction of this material.

Lab Report Key

Exercises 1A

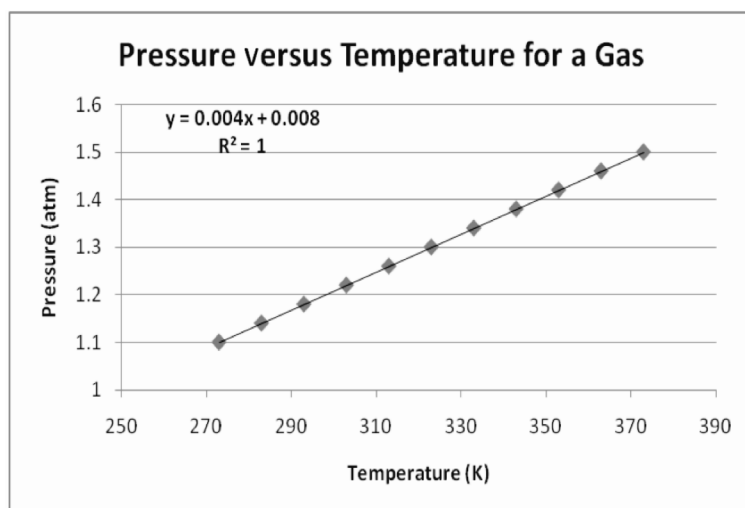
- 1) Indicate how many significant figures are present in each of the following:
 - (a) 01.501×10^3 **4**
 - (b) 700.01 **5**
 - (c) 193005 **6**
 - (d) 6.010×10^{-4} **4**
 - (e) 0.070 **2**
- 2) Round the following to three significant figures (put in scientific notation where necessary):
 - (a) 151626 **$1.52\text{e} + 05$**
 - (b) 0.00844 **$8.44\text{e} - 03$**
 - (c) 0.000010350 **$1.04\text{e} - 05$**
 - (d) 1255 **$1.26\text{e} + 03$**
 - (e) 33.353 **33.4**
- 3) Perform the following mathematical operations:
 - (a) $(6.49 \times 10^5/2) - 45.38 =$ **$3\text{e} + 05$**
 - (b) $5.32 \times 10^{-15} \times 2.447 \times 10^{16} =$ **$1.30\text{e} + 02$**
 - (c) $(3.15 \times 10^{-1} - 9.7 \times 10^{-3}) \times [(4.7 \times 10^{-2})/(2.33 \times 10^{-3})] =$ **6.2**
 - (d) $1.62 \times 10^{-3} + 8.1 \times 10^{-4} =$ **$2.43\text{e} - 03$**
 - (e) $(0.45 + 167.6)/1.6 \times 10^{-2} =$ **$1.1\text{e} + 04$**
- 4) Express the following using scientific notation:
 - (a) The Bohr radius: 0.0000000000529189379 m **$5.29189379\text{e} - 11 \text{ m}$**
 - (b) The speed of light: 299792458 m/s **$2.99792458\text{e} + 08 \text{ m/s}$**
 - (c) Charge of a proton: 0.0000000000000000001602176487C **$1.602176487\text{e} - 19 \text{ C}$**
 - (d) Rydberg constant: 10973731 m^{-1} **$1.0973731 \text{e} + 07 \text{ m}^{-1}$**
- 5) Calculate the following and round to the proper number of significant figures:
 - (a) Antilog 0.485 = **3.05**
 - (b) $\ln 60 =$ **4.09**
 - (c) $e^{-1.41} =$ **2.4E-01**
 - (d) $\log 3.975 \times 10^{-2} =$ **-1.4007**
 - (e) Antilog 6.86 = **$7.2\text{e} + 06$**
 - (f) $\log 8.74 =$ **0.942**
- 6) Calculate the average and standard deviation for the following set of calibration data:
3.8842, 3.8611, 3.8263, 3.8191, 3.8945, 3.8916, 3.8511, 3.8651

average = 3.8616

STDev = 0.0285

7) Graph the following data and answer the questions about the resulting line.

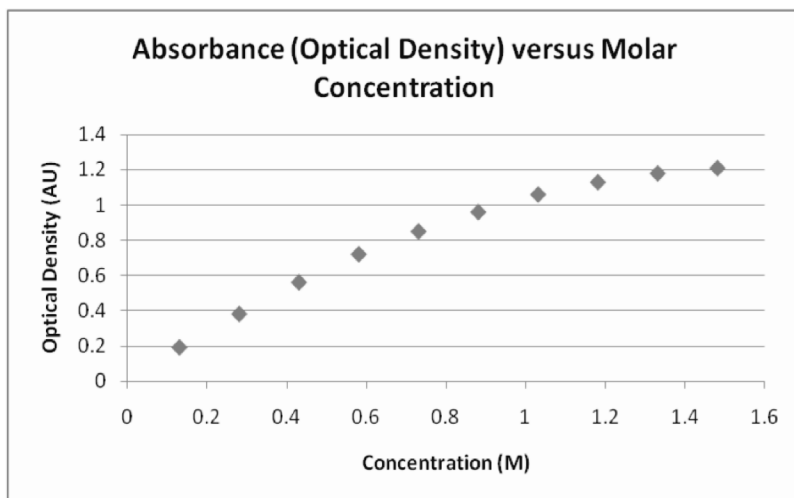
Temperature (K)	Pressure (atm)
273	1.10
283	1.14
293	1.18
303	1.22
313	1.26
323	1.30
333	1.34
343	1.38
353	1.42
363	1.46
373	1.50



Q1: According to the graph, how would you describe the relationship between temperature and pressure (linear or nonlinear)? **linear**

8) Create a graph of the absorbance (optical density) versus molar concentration and answer the questions about the resulting line.

Concentration (M)	Optical Density (AU)
0.13	0.19
0.28	0.38
0.43	0.56
0.58	0.72
0.73	0.85
0.88	0.96
1.03	1.06
1.18	1.13
1.33	1.18
1.48	1.21



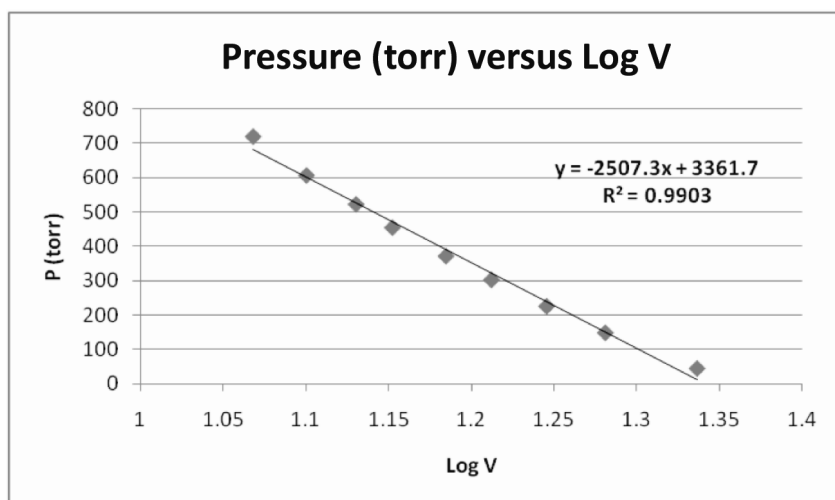
NOTE: The absorbance, or optical density, of a solution for a particular wavelength of light is given by $\log(I_0/I)$, where I_0 is the incident light on a sample and I is the transmitted light. Beer's law states that the optical density of a substance in solution is directly proportional to its concentration (i.e., it has a linear relationship). Not all substances follow Beer's law, but a calibration graph of optical density versus concentration can still be used to measure concentrations of unknown solutions. Because optical density is a ratio, it does not have any units; the expression *absorbance units* is sometimes used.

Q1: Does the solution in your graph follow Beer's law? **no**

Q2: What is the concentration of a solution that has an optical density of 0.28? **0.20 M**

Q3: What is the concentration of a solution that has an optical density of 1.01? **0.95 M**

9) Using the same data as above, calculate the logarithm of the volume. Graph the pressure versus the \log_{10} volume and answer the questions about the resulting line.



Q1: If this graph is a straight line, then it is of the form $P = m\text{Log}_{10}V + b$, in which m is the slope, and b is the y -intercept. Is the graph a straight line or a curved line (nonlinear variation)? **straight line with some slight deviation; see fit below**

Q2: If possible, calculate the equation of the line for the graph. Show your work.

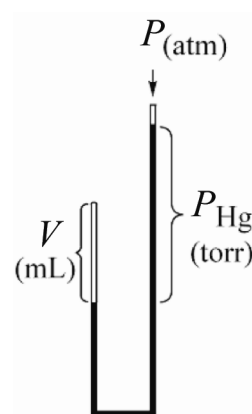
$$P = -2507.3\text{Log}V + 3361.7 \quad R^2 = 0.9903$$

Q3: Using the resulting equation from question 2, what would be the volume of a system that had a pressure of 5.4 atm? **0.51 mL**

10) Robert Boyle used an open-end barometer (similar to that in the figure) for the experiments, which led to the discovery of Boyle's law, which describes mathematically the effect of pressure on the volume of a gas. He determined the nature of the law by graphing his data. The law states that $PV = \text{constant}$, where P is the total pressure, which is the sum of $P_{\text{atm}} + P_{\text{Hg}}$. The pressure can be measured in torr, which corresponds to the height of the mercury column in millimeters.

The following table contains some data in an experiment similar to that of Boyle's, though the open-end manometer is considerably larger. The volume of the gas in the closed end of the tube is measured in milliliters, and the pressure recorded is P_{Hg} , the height of the column, not the total pressure.

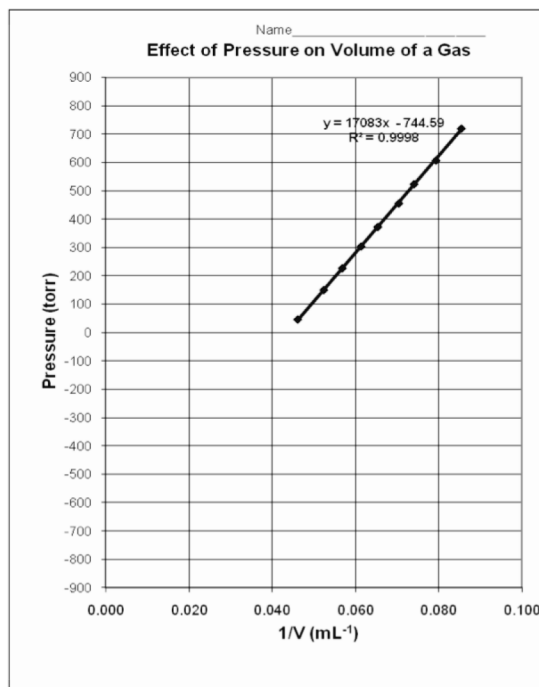
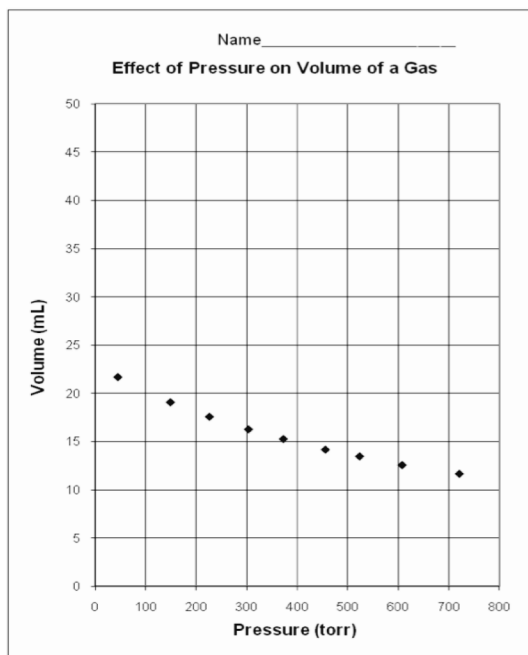
Pressure (torr)	Volume (mL)
45	21.7
149	19.1
226	17.6
303	16.3
372	15.3
455	14.2
523	13.5
607	12.6
720	11.7



You are to analyze this data by graphing it, discovering that a direct graph (V vs. P) gives a curved line. Scientists often try manipulating data to give a straight line, and when the data is regraphed as P vs $1/V$, you will see that a straight line is produced, revealing the nature of Boyle's law (that pressure and volume are reciprocally related). Further analysis of this straight line will also reveal the atmospheric pressure at which the measurement is made. Since

$$\begin{aligned}
 P_{\text{total}}V &= \text{constant} \\
 P_{\text{total}} &= \text{constant}(1/V) \\
 P_{\text{atm}} + P_{\text{Hg}} &= \text{constant}(1/V) \\
 P_{\text{Hg}} &= \text{constant}(1/V) - P_{\text{atm}}
 \end{aligned}$$

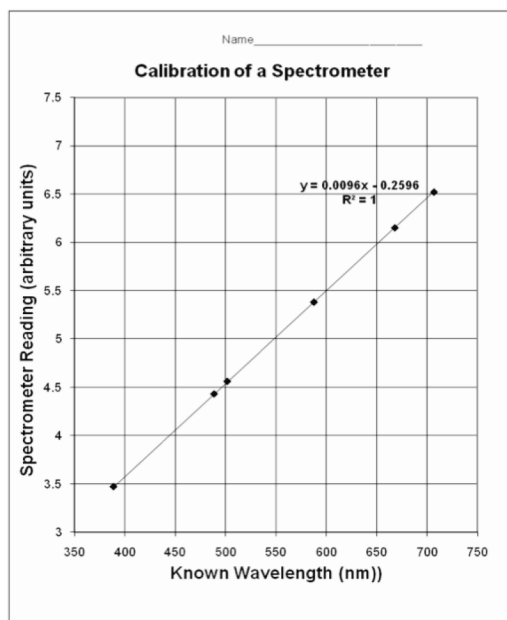
the graph is of the form $y = mx + b$, where the slope, m , gives the value of the constant, and the P -intercept is the negative of the atmospheric pressure.



Q1: What is the slope of the line (i.e., the constant in the Boyle's law equation)? Give units in your answer. **1.70E + 04 torr•mL**

Q2: What is P_{atm} (i.e., the negative of the P -intercept)? Give units in your answer. **7.40e + 02 torr**

11) The following data was used to calibrate a spectrometer. Graph the data and answer the questions regarding the resulting line.



Known Wavelength (nm)	Spectrometer Reading (absorbance units)
388.9	3.47
488.6	4.43
501.6	4.56
587.6	5.38
667.8	6.15
706.5	6.52

Q1: Add a best-fit line and calculate the equation for that line.

$$y = 0.0096x - 0.2596$$
$$R^2 = 1$$

Q2: You have collected some more data using the above spectrometer. Use either the graph or the equation of the line to “correct” the data you have collected.

Experimental Spectrometer Reading (absorbance units)	Corrected Wavelength (nm)
5.82	633
4.27	472
4.00	444
6.18	671

Exercises 1B

1) Consider the following experiment in which you wish to determine the molarity of the concentrated HCl in your new bottle of reagent. You carefully measure out 100.0 mL of the concentrated acid and dilute it to 1.000 L (in a 1 L volumetric flask). You then use a 5.00 mL volumetric pipette to remove 7 aliquots for titration with 0.1045 M sodium hydroxide solution. The following are the volumes of base needed for each sample.

59.0 mL, 58.8 mL, 59.2 mL, 58.9 mL, 58.9 mL, 59.1 mL, 57.9 mL

Calculate Q_{exp} for both the maximum and minimum values in this data.

- (a) Q_{exp} for 59.2 mL = **0.077**
- (b) Q_{exp} for 57.9 mL = **0.692**
- (c) Can you reject 59.2 mL with 90% confidence? **no**
- (d) Can you reject 59.2 mL with 95% confidence? **no**
- (e) Can you reject 59.2 mL with 99% confidence? **no**
- (f) Can you reject 57.9 mL with 90% confidence? **yes**
- (g) Can you reject 57.9 mL with 95% confidence? **yes**
- (h) Can you reject 57.9 mL with 99% confidence? **yes**

Average your measurements (throwing out the outlier if justified with 90% confidence) and calculate the molarity of the original concentrated HCl solution. **12.3 M**

2) You are asked to calibrate a 10 mL volumetric pipette by weighing to the nearest 0.1 mg the mass of water delivered by the pipette. You weigh six samples of water delivered by the pipette and convert the mass of each to volume by dividing by the density of water at 25 °C (0.997048 g/mL). Following are your measurements:

9.9690 mL, 9.9700 mL, 10.0360 mL, 9.9650 mL, 10.0150 mL, 10.0200 mL

Calculate the following statistical measures for this data:

Mean (\bar{x}) = **9.9958** Standard deviation (s) = **0.03131**

Variance (s^2) = **9.9958** Standard error of the mean (s_{mean}) = **0.01278**

90% confidence interval = 9.9958 ± 0.0258

(The “true value” of the volume will lie within this interval 90% of the time.)

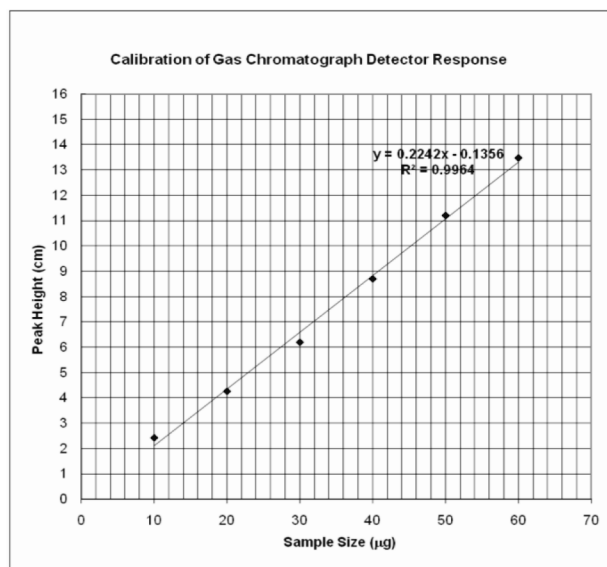
95% confidence interval = 9.9958 ± 0.0329

(The “true value” of the volume will lie within this interval 95% of the time.)

99% confidence interval = 9.9958 ± 0.0515

(The “true value” of the volume will lie within this interval 99% of the time.)

3) The table below shows some data in which the peak height of triplicate samples of a substance is listed as a function of the quantity of material injected. You would like to know first how good the precision of the method is by determining the standard deviations and confidence intervals of each set of triplicate samples. Then you would like to know whether the means of the triplicate samples show a linear relationship with sample size, and the equation for this relationship.



Gas Chromatograph Calibration			
Sample Mass μg	Peak Height (cm)		
	Trial 1	Trial 2	Trial 3
10	2.6	2.3	2.4
20	3.8	4.2	4.8
30	6.2	6.5	5.9
40	9.0	8.7	8.4
50	11.3	10.9	11.4
60	13.7	13.0	13.7

Q1. Using Excel or another similar spreadsheet program, graph the average peak height versus sample mass. Apply a best-fit line to the resulting graph.

Q2. Again using the spreadsheet program, calculate *sample mean*, *variance*, *standard deviation*, *standard error of the mean*, and *confidence intervals* for the data above.

Q3. Answer the following questions:

- For the 60 μg sample, what is the sample standard deviation and 90% confidence interval of the three peak height measurements? **standard deviation = 0.404; confidence interval = 0.681**
- Excel gives the best straight line fit to the data as an equation $y = mx + b$. What are the slope and intercepts of this line? (Be sure to include units.) **$m = 0.224 \mu\text{g/cm}$; $b = -0.1356 \mu\text{g}$**

4) The table below contains data that were collected to create a calibration curve in which the absorbance of a substance is plotted versus samples of known concentration. Graph this data.

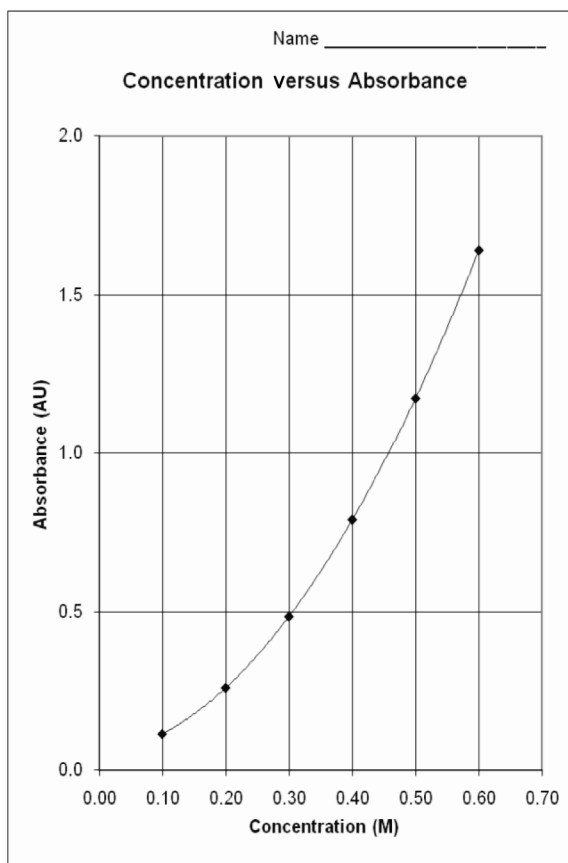
Known Concentration (M)	Absorbance (AU)
0.10	0.115
0.20	0.260
0.30	0.485
0.40	0.790
0.50	1.175
0.60	1.640

Determine from your graph the concentrations of the following unknown solutions. (Give units.)

Solution A: 0.163 AU: **0.14 M**

Solution B: 0.658 AU: **0.36 M**

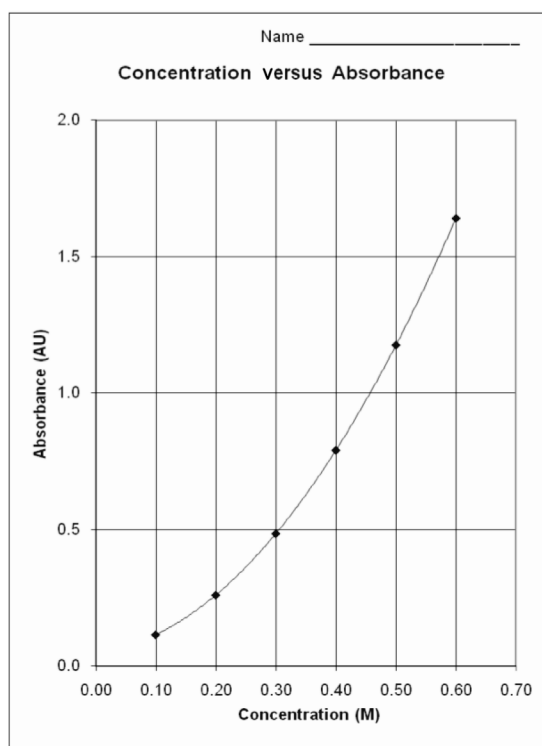
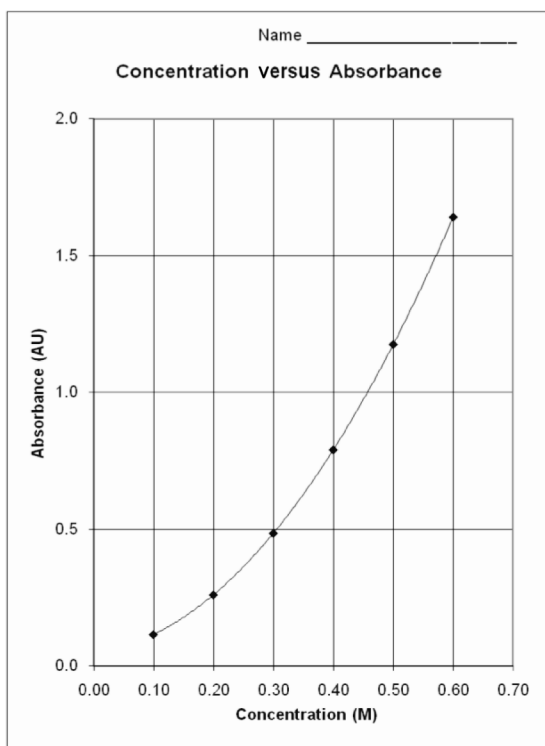
Solution C: 1.444 AU: **0.56 M**



5) The table below contains some initial reaction rate data for reaction of substances **A** and **B** at the indicated initial concentrations. The rate law for this reaction follows the form **rate** = $k[A]^a[B]^b$, where **a** and **b** are the **reaction orders** for **A** and **B**, respectively.

Experiment	Initial Conc. (M)	Initial Conc. (M)	Initial Rate (M/s)
	[A]	[B]	
Trial 1	2.0×10^{-2}	4.3×10^{-3}	2.2×10^{-3}
Trial 2	4.0×10^{-2}	4.3×10^{-3}	8.9×10^{-3}
Trial 3	6.0×10^{-2}	4.3×10^{-3}	2.0×10^{-2}
Trial 4	2.0×10^{-2}	8.6×10^{-3}	4.5×10^{-3}
Trial 5	2.0×10^{-2}	1.3×10^{-2}	6.7×10^{-3}

Q1. Plotting log rate versus log [A] at constant [B] will give **a** as the slope, and plotting log rate versus log [B] at constant [A] will give **b** as the slope. Use a spreadsheet to determine these values. Calculate the logarithm of the concentration and rate data to enter in the spreadsheet. Use trials 1, 2, and 3 for the log rate versus log [A] plot, and trials 1, 4, and 5 for the log rate versus log [B] plot. Add trend lines to the resulting graphs and determine the slopes of the lines.



(a) What is the reaction order for reactant A? **2**

(b) What is the reaction order for reactant B? **1**

Q2. The reaction rate constant (k) can be determined from the rearranged rate equation $k = [(rate)/([A]^a[B]^b)]$ using data from any of the trials. The units of k will depend on the **overall order** of the reaction, which in this case will be $a + b$. (The units of k must be such that the units of the rate become **M/s**.) The following table gives the units for different overall orders.

Overall Reaction Order ($a + b$)	Units of k
0	$M s^{-1}$
1	s^{-1}
2	$M^{-1} s^{-1}$
3	$M^{-2} s^{-1}$
4	$M^{-3} s^{-1}$

What is the rate constant for the above reaction? (Include units.) $1.3E + 03 \text{ m}^{-2}\text{s}^{-1}$