Handling Data: Communicating Precision & Accuracy

1. **Handling Data: Communicating Precision & Accuracy**
    1.1. Physical vs. Chemical Changes
    1.2. Best fit lines (interpolations)
        1.2.1. Gathering data
        1.2.2. Plotting graphs
        1.2.3. Standard deviation and relative standard deviation
        1.2.4. Relative percent error (co-variance)
    1.3. Measurements of precision
    1.4. Measurements of accuracy
    1.5. Discussion of error propagation for context

2. **Learning Objectives**
    2.1. Identify three unknown chemicals based on a combination of their physical and chemical properties.
    2.2. Explain the logic in making your determination of each chemical.
    2.3. Enter data into an Excel sheet.
    2.4. Create a scatter chart in Excel.
    2.5. Add axis labels and a title to an Excel chart.
    2.6. Add a linear trendline and equation to an Excel chart.
    2.7. Interpret data from a linear trendline on an Excel chart.
    2.8. Demonstrate the use of Microsoft Excel to perform simple data analysis comparing three different data sets of penny masses.
    2.9. Interpret the data obtained from the measuring of water in two different pieces of glassware to determine precision and accuracy.

3. **Equipment**
    3.1. Computer
    3.2. Spreadsheet software
    3.3. (Excel, Google Sheets, etc.)

4. **Chemicals**
    4.1. DI water (obtained from the plastic faucet in the laboratory)
    4.2. Hexanes
    4.3. Acetone
    4.4. Isopropyl alcohol
    4.5. Unknown A
    4.6. Unknown B
    4.7. Unknown C

5. **Additional Resources**
    5.1. Measurements in Chemistry from OpenStax Chemistry
    5.2. Uncertainty, Accuracy, and Precision from OpenStax Chemistry
    5.3. Conversions from OpenStax Chemistry

6. **Introduction**
    6.1. **Physical vs. Chemical Changes**

All substances are defined by a series of unique chemical and physical properties. These properties are often measured by observing a chemical or physical change. **Physical properties** are characteristics that matter shows by itself, without changing into or interacting with another substance. A **physical change** occurs when a substance alters its physical properties, not its composition. An example of this occurs when water melts from a solid to a liquid. The physical properties that changed were the water's hardness, its density, and its viscosity. The substance itself never changed during this process, always remaining the same water. **Chemical properties** are characteristics a substance shows as it changes into or interacts with another substance or substances. A **chemical change (or reaction)** occurs when a substance is converted into a different substance. An example of this type of observation can be shown in the electrolysis of water. The chemical property observed here is the ability of water to break apart into hydrogen and oxygen when a current is allowed to flow through the sample. In this example, the water molecule is split into two new compounds.

In this experiment, you are going to look at various physical and chemical properties to identify three unknown liquids. The physical properties you are going to observe are: solubility in water, solubility in cyclohexane, smell, color, viscosity, density, freezing point, and boiling point. The chemical property that you will observe is the flammability of each compound. Some of these observations will be qualitative and others will be quantitative. A qualitative observation is one that does not have any numbers associated with the data. A quantitative observation is defined by having numbers associated with the data. Both types of data are important and valid.

Often, a chemist can perform simple qualitative observations to help refined future quantitative observations. For example, if we set up three cold baths at certain temperatures, we can refine the freezing point range for a substance and possibly identify that substance without the need to use quantitative equipment.

6.2. Graphing with Spreadsheets

Graphical representation of laboratory data is often used to interpret the results of laboratory experiments. Microsoft Excel and other spreadsheet software can provide many ways to graphically represent data for a laboratory experiment. Spreadsheet software makes it easy to organize the data, to produce graphs and to carry out basic analyses of the data.

Graphs can be prepared by hand or by computer. While you may want to do a quick sketch of your data in graphical form to get a first impression of any relationships or trends, you will want to produce your final, working graph using graphing software. General instructions are provided here that work for both Excel and Google Sheets using data provided below. Note that spreadsheet software refers to a graph as a "chart."

Organized data is the very first step to being able to understand and analyze what we have. Spreadsheets are designed for organizing data. Spreadsheets have a lot of functionality including the ability to enter in equations. Those equations can take data from specific locations, called cells, to make the calculations. The locations are specified based on a cartesian coordinate grid where one axis is labeled numerically and the other alphabetically. Excel has the rows run numerically and the columns run alphabetically. Most spreadsheets use this convention. For this lab, you will use some built in functions to evaluate the precision and accuracy of your data. You will also do a scatter plot; plotting individual data points without any sort of "best-fit" line.

Data measurement is often the easy part of any experiment. The hard part comes when it is time to analyze the data to determine if it is viable to build conclusions on. One of the first methods of data analysis is to determine the accuracy and precision of the data. **Accuracy** determines how close a value is to the true value. You will be verifying this in the last part of this experiment by determining the volume of water in a 10 mL volumetric pipet using the mass of water and the density. Precision is defined as the measure of how close a value is to the rest of the data set. **Precision** is easily measured by calculating the mean and standard deviation of a data set. If the standard deviation is low (less than 5 %), then the data is considered to have good precision. The mean (average) of a data set can be calculated using Equation DA.1, where xi is each individual data point, and n is the total number of data points. The standard deviation can be calculated using Equation DA.2. average =

$$\text{average} = \frac{\Sigma(x_i)}{n}$$ (Equation DA.1)

$$\text{standard deviation} = \sqrt{\frac{\Sigma(x_i - \text{average})^2}{(n-1)}}$$ (Equation DA.2)

When measuring data, it is important to be aware of possible sources of error in the data. In science, an error is defined differently from a simple mistake. A **mistake** is blunder or unintentional action that results in undesirable data. Examples of mistakes include not allowing the balance to equilibrate before adding or taking away chemicals or reading the ruler starting at 1.00 mm instead of 0.00 mm. Mistakes are usually easily corrected in an experiment. **Error** accounts for a range of values obtained from successive measurements of the same quantity, even though no mistakes were made in the measurement. There are two sources of error in a chemistry lab: systemic and random. **Systemic error** is inherent to the measuring device and its use these errors bias the data away from the "true" value. Systemic errors always produce results that reduce the accuracy of the data. **Systemic errors** arise from measuring devices that are not properly calibrated, using the wrong device for the measurement, or using the proper measuring device improperly. It is important to know which measuring devices to use, how to properly calibrate them if needed, and how to properly operate the device. **Random error** arises from multiple measurements on the same measuring device. Random errors reduce the precision of a measuring device. There is not much you can do at this point in your chemical education to reduce random error. The best way to test for random error is to perform a Q test on each data point within a set and remove outliers to improve precision. Random error is the primary reason we, as scientists, repeat measurements and experiments multiple times.

$$s_{\text{pooled}} = \sqrt{\frac{s_1^2(n_1-1) + s_2^2(n_2-1)}{n_1+n_2-2}}$$ (Equation DA.3)

Many times, a scientist is given different sets of data that may or may not be combined into one larger data set. In order to determine if this is possible, the scientist must determine whether individual data sets are statistically different or similar. This is easily done using the Student's t-test. In this test, you must first calculate the standard deviation of the pooled data sets (s-pooled), using Equation DA.3. In Equation DA.3, $s1$ is the standard deviation of the first data set, $n1$ is the number of data points in the first set, $s2$ is the standard deviation of the second data set, and $n2$ is the number of data points in the second set.

$$t_{calc} = \frac{|\text{average}_1 - \text{average}_2|}{s_{\text{pooled}}} \times \sqrt{\frac{n_1 n_2}{n_1+n_2}}$$ (Equation DA.4)

This number is then used to calculate $tcalc$, given as Equation DA.4. In Equation DA.4, average1 is the mean of the first data set, and average2 is the mean of the second data set. The value obtained for $tcalc$ is then compared to a given t value for a specific number of data points in each set at the 95 % confidence level. A list of t values is given in Table DA.1. Two sets of data are statistically different if $tcalc$ is greater than t listed in the table. If $tcalc$ is less than t listed in the table, then the two data sets are statistically similar and can be combined to form one larger data set.

Table DA.1: *t* values at 95% Confidence

n	95%	n	95%	n	95%	n	95%
1	12.71	11	2.201	21	2.080	40	2.021
2	4.303	12	2.179	22	2.074	50	2.009
3	3.182	13	2.160	23	2.069	60	2.000
4	2.776	14	2.145	24	2.064	80	1.990
5	2.571	15	2.131	25	2.060	100	1.984
6	2.447	16	2.120	26	2.056	120	1.980
7	2.365	17	2.110	27	2.052		
8	2.306	18	2.101	28	2.048		
9	2.262	19	2.093	29	2.045		
10	2.228	20	2.086	30	2.042		

6.3. Measuring Tools

In chemistry, it is important that our measuring tools be both accurate and precise as possible. For this semester, much of the accuracy and precision will be inherent to the tool you are using to measure your reagents and products. For solid reagents and products, the balance that is provided to you has a certain level of accuracy and precision built into the equipment that we cannot change. For this equipment, the data will be reported back to you with a typical accuracy of four decimal places. The precision of these measurements will depend on how good you are at placing the solid on the balance consistently. This will become easier with practice and by the second or third experiment this semester, you will become very precise in your balance measurements.

Figure DA.1: Meniscus of liquid in glassware

For liquid reagents and products, precision and accuracy is based on the type of glassware you are using to measure your liquid. In general, beakers are the least accurate and least precise tool to use for measuring liquids. Volumetric pipettes and volumetric flasks are generally the most accurate and most precise glassware to use to measure liquid volumes. This level of accuracy is useful for more advanced measurements. A good piece of glassware that should give a moderate level of accuracy and precision is the graduated cylinder. For this class, the focus of your experiments is to teach you how to use the basics of the chemistry laboratory. Therefore, a moderate level of accuracy and precision is sufficient for the experiments you will perform, so the majority of the experiments will utilize graduated cylinders for measuring out reagents and products.

When using glassware to measure the volume of a liquid, it is important to know how to read the volume of your liquid. Figure DA.1 shows a slightly colored liquid in a piece of glassware. You will notice that the liquid in the glassware does not lay flat, but instead curves up the sides of the container. This creates what is called a meniscus on the liquid, which is the case of the liquid in Figure DA.1 is at the very bottom of the curvature of the liquid. Most liquids in glass will form a meniscus of this type. When measuring the volume of a liquid, you need to measure at the meniscus. For this glassware, the volume markings increase as you move from the top of the glassware to the bottom. The photo is zoomed in on the picture to show the markings at 21 milliliters and 22 milliliters. Between these markings, are several smaller markings at 0.1 mL each. Since the meniscus lays between the first and second smaller markings, we know that our liquid is somewhere between 21.1 milliliters and 21.2 milliliters. At this point, we need to make and educated estimate of the actual volume marking. Since the meniscus is slightly above halfway between 21.1 and 21.2, I can say that our volume is 21.14 milliliters.

$$\text{density} = \frac{\text{mass}}{\text{volume}}$$

(Equation DA.5)

For this experiment, your precision will be based on how well you place the meniscus at the same point in your glassware between each measurement. The accuracy of your measurements will be tested by verifying the volume of the water by mass, using the density given in Equation DA.5. The value for the density of your water is given in the Procedure.

To observe the level of precision, you will take the standard deviation of your density measurements for each of the six or seven samples. To observe the accuracy of your density measurements, the known densities of the knowns will be provided in the lab. The scatter plots provide a visualization of the data. Visualized data provides other means of analyzing quantitative information. It can be easier to make connections with the right visualization whether it is a graph, a chart, or a scientific illustration .

7. Procedure

7.1. Chemical and Physical Properties

7.1.1. Preparation

7.1.1.1. Obtain approximately 20 mL of each of the following liquids in labeled 50 mL beakers.

7.1.2. Qualitative Observations: Sensory and Appearance

7.1.2.1. On your Data file, record the color and viscosity of each liquid sample.

7.1.2.2. Using your hand, gently waft the liquid samples and record any observations about the odor.

7.1.3. Qualitative Observations: Solubility in Water

7.1.3.1. Obtain and clean 6 small test tubes from your Station drawer. Label these for your liquid samples.

7.1.3.2. Place approximately one inch of liquid sample in each test tube.

7.1.3.3. Add 2 mL of DI water to each test tube and gently mix the two liquids.

7.1.3.4. If the liquids mix, write “yes” on your datasheet for this section. If the liquids do not write, type “no” on your datasheet.

7.1.3.5. Discard the liquid mixtures in the appropriate waste container.

7.1.4. Qualitative Observations: Solubility in Hexanes

7.1.4.1. Place approximately one inch of liquid sample in each test tube.

7.1.4.2. Add 2 mL of hexanes to each test tube and gently mix the two liquids.

7.1.4.3. If the liquids mix, write “yes” on your datasheet for this section. If the liquids do not mix, write “no” on your datasheet.

7.1.4.4. Discard the liquid mixtures in the appropriate waste container.

7.1.5. Qualitative Observations: Flammability

7.1.5.1. Obtain an evaporating dish from your Station drawer.

7.1.5.2. Place a very small amount (less than 1 mL) of DI water in the evaporating dish.

7.1.5.3. Obtain some matches. When you are ready to test the flammability, ignite a match. Once the match is aflame, immediately drop it in the liquid in your evaporating dish.

7.1.5.4. Record your observation on the flammability of the liquid in your evaporating dish in your datasheet.

7.1.5.5. If the liquid sample ignites, allow the sample to completely burn away before continuing to the next step. If the liquid sample does not ignite, discard in the proper waste container and wipe the evaporating dish with a paper towel.

7.1.5.6. Repeat Steps 3-6 of this section with the remaining liquid samples.

7.2. Spreadsheet Instructions

7.2.1. Graphs can be prepared by hand or by computer. While you may want to do a quick sketch of your data in graphical form to get a first impression of any relationships or trends, you will want to produce your final, working graph using graphing software. General instructions are provided here that work for both Excel and Google Sheets using data provided below. Note that spreadsheet software refers to a graph as a “chart.”

7.2.2. Creating a Chart

7.2.2.1. Open the spreadsheet software.

7.2.2.2. Enter the paired data from Table EX.1 in the spreadsheet. Be sure to label the columns with informative titles such as those provided in the headers on the table. Include units in the title where applicable but not in the same cells as the data.

Table EX.1: Practice Data

Pb level, micrograms per liter	IQ	Pb level, micrograms per liter	IQ
1	119	15	93
2	120	17	103
3	105	22	93
7	110	28	73
8	88	33	79
9	100	44	90
11	95	50	85
12	98		

7.2.3. Using Excel to Graph Data

7.2.3.1. Insert a scatter plot and select the data for the x and y values as shown in the video. Set the Pb levels as the x values and IQ as the y values.

7.2.3.2. Format the chart to change the title and to add labels to both axes, following the example in the video.

7.2.3.3. Fit your data to a linear trendline and to display the equation and R-squared value on the chart.

7.2.3.4. Double click on the equation to change the "y" and "x" to "IQ" and "(Lead Levels)" respectively.

7.2.3.5. If needed, this page of the workbook can be printed; both the data and the graph will be on one page. Alternatively, by clicking on the graph and then printing, you will obtain a full-page chart.

7.3. Determination of Water Volume Accuracy

7.3.1. Obtain approximately 600 mL of DI water.

7.3.2. Record the temperature of the DI water in the cells provided in the provided Excel file.

7.3.3. Determine the water's density using Table DA.1 and record that density in the labeled cells in the provided Excel file.

7.3.4. Record the mass of an empty 50 mL beaker in the provided cells of the Excel file, picking up the beaker and setting it back down on the balance each time.

7.3.5. **Using the beaker only,**

7.3.5.1. measure out 10 mL of water and record the mass of the beaker and water in the labeled cells.

7.3.5.2. Dispose of the water and dry out the beaker.

7.3.5.3. Repeat Step 5 three more times recording each subsequent mass in the cells provided.

7.3.5.4. Record the mass of an empty 25 mL graduated cylinder in labeled cells provided.

7.3.6. **Using the graduated cylinder only,**

7.3.6.1. measure out 10 mL of water and record the mass of the cylinder and water in the provided cell.

7.3.6.2. Dispose of the water and dry out the cylinder.

7.3.6.3. Repeat Step 8 three more times recording each subsequent mass in cells provided.

7.4. *Water Volume Analysis*

7.4.1. *Calculating the Volume of Water*

7.4.1.1. In the cell labeled for volume, type the following formula: =”cell(beaker+water)”-“cell(beaker), using the cell locations based on the column letter and row number.

7.4.1.2. In cell labeled for density, type the following formula: =”cell(water mass)”/”cell(water density at temp)”.

7.4.1.3. Repeat Steps 1 and 2 for replicates.

7.5. Determination of Densities for Knowns and Unknowns

7.5.1. Record the mass of an empty 50 mL beaker in the provided cells of the Excel file, picking up the beaker and setting it back down on the balance each time.

7.5.2. *Using the beaker only,*

7.5.2.1. measure out 10 mL of the sample and record the mass of the beaker and the sample in the labeled cells.

7.5.2.2. Dispose of the sample into a waste beaker at your workspace.

7.5.2.3. Dry out the beaker.

7.5.2.4. Repeat Step 5 three more times recording each subsequent mass in the cells provided.

7.5.2.5. Record the mass of an empty 25 mL graduated cylinder in labeled cells provided.

7.5.3. *Using the graduated cylinder only,*

7.5.3.1. measure out 10 mL of the sample and record the mass of the cylinder and the sample in the provided cell.

7.5.3.2. Dispose of the sample and dry out the cylinder.

7.5.3.3. Repeat Step 8 three more times recording each subsequent mass in cells provided.

7.5.4. *Calculating the Density of the Sample*

7.5.4.1. In the cell labeled for volume, type the following formula: =”cell(beaker+sample)”-“cell(beaker), using the cell locations based on the column letter and row number.

7.5.4.2. In cell labeled for density, type the following formula: =”cell(sample mass)”/”cell(sample volume)”.

7.5.4.3. Repeat Steps 1 and 2 for replicates.

7.6. Calculating Average and Standard Deviation

7.6.1. For each measurement, type the following formula: =AVERAGE(RangeStart:RangeEnd), the range should encompass all of the cells for the replicates of that measurement.

7.6.2. In cell L10, type the following formula: =STDEV(RangeStart:RangeEnd), the range should encompass all of the cells for the replicates of that measurement.

7.7. Drawing the scatter plots

7.7.1. Prepare a hand-drawn plot of the two variables, mass and volume, using the grid sheet at the end of the document or other graph paper.

7.7.2. Include a title, axis labels (with units), and label groupings of datapoints for each sample.

7.7.3. Submit a copy of this graph.

7.8. Creating the scatter plot in Excel

7.8.1. For the known samples, create a scatter plot:

7.8.1.1. Using the columns labels, create a scatter plot.

7.8.1.1.1. Include a title for the plot.

7.8.1.1.2. Include units in the axis titles.

7.8.1.1.3. Give each sample an identifying color and/or shape to label them.

7.8.1.1.4. Add a legend to the plot.

7.8.2. For the unknown samples, create a scatter plot:

7.8.2.1. Using the columns labels, create a scatter plot.

7.8.2.1.1. Include a title for the plot.

7.8.2.1.2. Include units in the axis titles.

7.8.2.1.3. Give each sample an identifying color and/or shape to label them.

7.8.2.1.3.1. Hint: use different identifiers from the previous plot.

7.8.2.1.4. Add a legend to the plot.

7.8.3. For the known and unknown samples together, create a scatter plot:

7.8.3.1. Using the columns labels, create a scatter plot.

7.8.3.1.1. Include a title for the plot.

7.8.3.1.2. Include units in the axis titles.

7.8.3.1.3. Give each sample an identifying color and/or shape to label them.

7.8.3.1.3.1. Hint: keep the identifiers for the known and unknown samples the same as they were in the previous two plots so that the similarities visually pop.

7.8.3.1.4. Add a legend to the plot.

7.8. Identifying the Unknowns

7.8.1. Use all your recorded data to identify Unknown A, B, and C as DI water, acetone, hexanes, or isopropyl alcohol.

7.8.2. If you have contradicting data from your observations, use your best judgment in identifying your unknowns. The Post-lab Question for this experiment will give you the opportunity to explain possible reasons for any contradictions in your data.