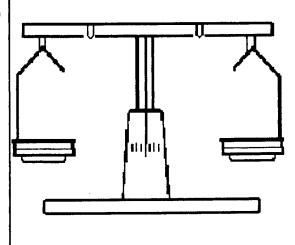


Mathematical Relationships in Chemistry

Summary of Electrical Usage

Month	Avg. temp(°F)	Energy usage(KWH)
January	30.0	2400
February	20.0	2850
March	46.0	1800
April	55.0	1000
May	58.0	800.0
June	64.0	900.0
July	65.0	950.0
August	69.0	900.0
September	68.0	950.0
October	52.0	900.0
November	45.0	1600
December	32.0	2400



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Unit 2: Mathematical Relationships in Chemistry

I. Quantitative vs Qualitative

Physical and chemical properties of matter, and the changes that it undergoes, can be described in two different ways. **Qualitative** observations relate the general appearances and behaviors of the matter in descriptive terms. Characteristics, such as color, odor, texture, or phase of matter are qualitative. **Quantitative** observations involve measurements and calculations that give more specific information, such as mass, volume or density. All quantitative measurements are comparisons to some standard unit of measurement that always has the same value. The measurement **must** have BOTH a <u>numerical value</u> and a <u>unit value</u>. For scientific measurements, the metric (SI) system is preferred, because every unit in the system is 10 times the size of the next smaller unit, and the names of every unit are derived from using a prefix with the base unit name. Study the chart of the most frequently used units and prefixes below:

Prefix	abbreviation	Power of 10	Mass unit	Length unit	Volume unit
*mega-	М	10 ⁶ o r 1,000,000	megagram, Mg	megameter, Mm	megaliter, ML
kilo-	k	10 ³ or 1000	kilogram, kg	kilometer, km	kiloliter, kL
hecto-	h	10 ² or 100	hectogram, hg	hectometer, hm	hectoliter, hL
deka-	da	10 ¹ or 10	dekagram, dag	dekameter, dam	dekaliter, daL
base unit		10 ⁰ or 1	gram	meter	liter
deci-	d	10 ⁻¹ or 0.1	decigram, dg	decimeter, dm	deciliter, dL
centi-	С	10 ⁻² or 0.01	centigram, cg	centimeter, cm	centiliter, cL
milli-	m	10 ⁻³ or 0.001	milligram, mg	millimeter, mm	milliliter, mL
*micro-	μ	10 ⁻⁶ or 0.000001	microgram, <i>µ</i> g	micrometer, μm	microliter, μL

*Note that these units are more than a power of 10 difference from the previous units. The following phrase might help you remember these common prefixes and their relative values:

Many // kids have dropped over dead converting metric // units! Mega // kilo hecto deka base unit deci centi milli // micro(μ) Changing a measured value from one metric unit to another involves simply moving the decimal point location in the number. If the units get larger in value, then the decimal point is moved to the left to make the number smaller by an equal power of 10. If the units get smaller in value, then the decimal point is moved to the right to make the number larger by an equal power of 10.

Example: 3.42 meters = 0.00342 kilometers = 342. centimeters

Problems:

Determine the numerical value for the following metric-metric conversions:

 $1.04 \text{ Mg} = ____g \quad 0.893 \text{ cm} = ____m \text{m} \quad 45 \text{ daL} = ___k \text{L}$

7.6 μ L = _____dL 2.175 hg = _____cg 9307 mm = _____km

All of the basic units are interrelated in that 1 gram of water(at 4°C) has a volume of exactly 1 cm³ or a capacity of 1 mL. (Also, 1 kg water = 1000 cm³ = 1000 mL = 1 liter = 1 dm³)

Principal English System-Metric System Conversion Factors:1 inch = 2.54 cm1 m = 39.37 inches1 ft. = 30.5 cm1 km = 0.62 mile1 lb. = 453.6 g1 kg = 2.20 lbs.1 liter = 1.06 qts.1 mL = 1 cm³1 a.m.u.(atomic mass unit) = 1.660 x 10⁻²⁴ g

II. Dimensional Analysis and Unit Conversions

Many problems in chemistry require changing a measurement with given units to an equivalent value with different units. The simplest way to solve this type of problem is to use the appropriate conversion factor to change the units. A **conversion factor** is an equivalent or proportional relationship that can be expressed as the quotient of the two units. For example, since 1 meter = 100 centimeters, this relationship can be written as a conversion factor in one of two ways: <u>1 meter</u> or <u>100 centimeters</u> 1 meter

Density (mass / volume) is another useful relationship that can be expressed as a conversion factor. Since the density of aluminum metal is 2.70 g/cm³, this proportion can be written as shown below: 2.70 g or 1 cm^3 2.70 g

Sample Problem 1:

What will be the mass in grams of a pile of pennies that has a volume of 25 cm^3 and a density of 8.96 g/cm³?

Step 1: Determine what is the "unknown" quantity that you are trying to find and set it equal to the "given" quantity(other than the conversion factor) in the problem.

 $x \text{ grams} = 25 \text{ cm}^3$

Step 2: Multiply the "given" quantity by the appropriate conversion factor(s) that will cancel the "given" units and leave only the units of the "unknown" quantity.

x grams = $25 \text{ cm}^3 \text{ x} (8.96 \text{ grams}) = 25 \text{ x} (8.96 \text{ grams}) = 224 \text{ grams}$ (1 cm³) 1 Sample Problem 2: How many miles will a marathon runner travel in 2 hours if her speed is 15 kilometers/hour? Step 1: x miles = 2 hours

Step 2: x miles = 2 hours x (15 kilometers) x (0.62 miles) = (1 hour) (1 kilometer)

x miles = 2 x (15) x (0.62 miles) = 18.6 miles

Note that <u>two</u> conversion factors were needed to first convert the given units of "hours" into "kilometers", then change "kilometers" into "miles". An unlimited number of conversion factors can be used together in a series to solve a particular problem.

Problem 1:

How many cm^3 of pennies will you have if their mass is 3.75 kg with a density of 8.96 g/cm³?

answer: 419 cm^3

Problem 2:

If a weight lifter can bench press 250. pounds, how many kilograms can he lift?

answer: 114 kg

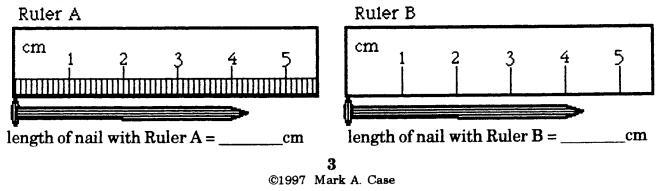
Problem 3:

How many pounds of the atmosphere's weight are pressing down on you if your body has a surface area of 1.25 square meters and the pressure of the atmosphere is 14.7 pounds per square inch(psi)?

answer: 28500 lbs

III. Accuracy, Precision and Significant Figures

All measured quantities will have some degree of uncertainty due to the limitations of the measuring tools or the ability of the person to use them correctly. Anytime a measurement is recorded, all digits that are certain plus one uncertain (estimated) digit are included. These digits that help to express the value of the measurement are called **significant figures**. Two identical nails are placed next to different centimeter rulers below. Record the length values you can obtain from reading each of these rulers, using as many significant figures as possible.



Since Ruler A has smaller divisions (0.1 cm), there is less uncertainty in the measured value. The length is greater than 4.3cm, but less than 4.4cm. By estimating between the divisions, a possible length could be 4.37cm, with the 7 digit being doubtful. This measurement has 3 significant figures. Student answers could range between 4.34cm to 4.40cm, which means the uncertainty is ± 0.03 cm. With Ruler B having larger divisions of 1 cm each, the length of the nail appears to be less than 4.5cm, but it can only be estimated to be either 4.3cm or 4.4cm. The uncertainty is at least ± 0.1 cm. There are only 2 significant figures in this value, which makes it less precise. **Precision** refers to the uncertainty in a measurement. The less the uncertainty, the higher the precision and easier it is to reproduce the measured value again and again. The ± 0.1 cm difference when using Ruler B might seem trivial, but this would be a huge error if you were measuring a smaller distance, such as the thickness of a piece of paper.

A better reflection of uncertainty is **relative uncertainty** (also called **relative precision** or **relative error**). The uncertainty is divided by the total amount measured. For the measurements with the two rulers:

relative uncertainty Ruler A = $\underbrace{0.03 \text{ cm}}_{4.37 \text{ cm}}$ = 0.00686 or 0.686% uncertainty relative uncertainty Ruler B = $\underbrace{0.1 \text{ cm}}_{4.4 \text{ cm}}$ = 0.0227 or 2.27% uncertainty

If the uncertainty of a measured value becomes too large, then its value cannot be determined accurately. As an example, a piece of paper has a actual thickness of approximately 0.0160cm. Therefore, with Ruler B the

relative uncertainty for paper = 0.1cm = 6.25 or 625% uncertainty 0.0160cm

The paper thickness measurement has no reliability of being correct using Ruler B.

The **accuracy** of a measurement is how close it comes to the actual or accepted value. A micrometer determines the actual length of the nails to be 4.3800 with an uncertainty of ± 0.0001 cm. The accuracy of the measurement from Ruler A is calculated as a percent error which indicates how far away the measured value is from the actual (or accepted) value. The general formula to find percent error for a measurement is:

> percent error = <u>measured value - actual value</u> x 100 actual value % error = <u>4.37cm - 4.3800cm</u> x 100 = -0.228%

> > 4.3800cm

Problem:

Calculate the relative uncertainty for the micrometer measurement and the percent error for the measurement from Ruler B.

Exact numbers have an infinite number of significant figures. For example, there is no uncertainty in the number of centimeters in 1 meter. However, in any recorded observation it is necessary to know the number of significant figures. Sometimes zeros are used solely for spacing the decimal point and are not part of the actual measurement. If a recorded distance is 100 meters, you need to know if the person recording the data counted by 1, 10 or 100 m increments. The Atlantic-Pacific rule can be used to determine which digits in a recorded value are significant.

If the decimal point is **present**, start from the **Pacific** side of the number and move right to the first nonzero digit. This digit, and every one to its right, is significant.

If the decimal point is **absent**, start from the **Atlantic** side of the number and move left to the first nonzero digit. This digit, and every one to its left, is significant.

The significant figures are underlined in the examples below:

Pacific Side: decimal P	resent	Atlantic Side: decimal A	bsent
0.00 <u>19</u> 65.01	2 SF 4 SF	<u>802</u> 00 400000	3 SF 1 SF
0.0 <u>300</u> 700.	4 SF 3 SF 3 SF	<u>32105</u> 700	5 SF 1 SF

Problems:

Underline the significant digits in the following numbers:									
0.3080	5600	0.00007	900.000001	428	160.	2003	9.00000		

The number of significant figures in a calculated value will be limited by the least precise number used in its calculation. When <u>multiplying or dividing</u> numbers, the answer contains the same number of significant figures as the measurement with the least number of significant figures.

Examples:	31.8 cm x 24 cm 3 SF 2 SF	$n = 763.2 \text{ cm}^2$ 4 SF	2 rounding off to 2 SF it becomes 760 cm 2
	8.340g / 4.27mL 4 SF 3 SF	= 1.9532g/mL 5 SF	rounding off to 3 SF it becomes 1.95g/mL

When <u>adding or subtracting</u> numbers, the answer contains the same number of <u>decimal</u> <u>places</u> as the measurement with the least number of <u>decimal places</u>.

Examples: 49.1g I decimal place	+	8.001g = 3 decimal places	57.101g 3 decimal places	rounding to 1 decimal place = 57.1g
240m to 10s place	-	71.3m = 1 decimal place	168.7m 1 decimal place	rounding to the 10s place = 170 m

If the number to be rounded is followed by a number greater than 5, then the digit is rounded up. If it is followed by exactly 5, then the number is rounded up only if it is an odd number. With any other possibilities, the number to be rounded is unchanged. Examples: The following numbers are rounded to 3 significant figures:

2359 rounds to 2360	0.7244 rounds to 0.724	9.575 rounds to 9.58
9.58500 rounds to 9.58	0.0105 rounds to 0.0105	69980 rounds to 70000

*Note the line drawn over the 100s place zero to show it is a significant digit in 70000.

Problems:

Solve the following problems and round your answers to the correct number of significant figures:

A) 29.01m x 75m = _____(calculated) = _____(rounded) B) 510km / 5 hours = _____(calculated) = _____(rounded) C) 0.2934L + 0.9L + 12.07L = _____(calculated) = _____(rounded) D) 33dg - 6.81dg = _____(calculated) = _____(rounded) E) (7.23g - 2.8g) / 145mL = _____(calculated) = _____(rounded)

Note: In multiple step problems, such as Problem E above, do not round off calculated intermediate values. Round *only* the final answer to the correct number of significant figures.

IV. Scientific (Exponential) Notation

Scientists deal with numerical extremes ranging from small-sized atoms to the vastness of the universe. Scientific notation makes it easier to deal with these numbers by expressing them in the form $M \ge 10^n$, where M is an integer from 1 to 10 and n is a positive or negative whole number exponent. All of the digits in M are significant and zeros as decimal place holders are not needed. Consider the examples below:

To write 17500 in scientific notation, move the decimal point 4 places to the left to determine the M value and increase the exponent, n, by 4.

$$17500 = 1.75 \times 10^4$$

To write 0.0000302 in scientific notation, move the decimal point 5 places to the right to determine the M value and decrease the exponent, n, by 5.

 $0.0000302 = 3.02 \times 10^{-5}$

One very large number, 6.02×10^{23} , appears in chemistry many times. This value (called Avogadro's Number) is the number of atoms of an element present in a mass equal to its atomic weight. The pH scale is another example of chemical measurements having a range in values covering fourteen powers of 10. Examine the chart below:

pH value 3 4 5 6 7 8 9 12 14 1 2 10 11 13 $10^{-1} \ 10^{-2} \ 10^{-3} \ 10^{-4} \ 10^{-5} \ 10^{-6} \ 10^{-7} \ 10^{-8} \ 10^{-9} \ 10^{-10} \ 10^{-11} \ 10^{-12} \ 10^{-13} \ 10^{-14}$ Concentration of H+ ions in moles / liter strong base strong acid neutral

Problems :

Convert the following numbers into scientific notation or express them in long form:

303008 =	6.4 x 10 ⁻³ =	0.0090 =	
$5.01 \times 106 =$	7000000 =	$8 \ge 10^2 =$	

6 ©1997 Mark A. Case When performing mathematical operations with numbers in scientific notation, the rules for exponents apply. The following is a summary of those rules:

- 1. For multiplication, multiply the M's and add the n's.
- 2. For division, divide the M's and subtract the n's (numerator denominator)
- 3. For addition or subtraction, all numbers must be changed to have the same value of n. Then add or subtract the M's and attach the common value of n.

Sample Problem 1: $(5.2 \times 10^3)(3.75 \times 10^{-2}) = (5.2 \times 3.75)(10^{(3 + -2)}) = 19.5 \times 10^1 = 20 \times 10^1 = 2.0 \times 10^2$ (2 SF)

Sample Problem 2: $\frac{(1.08 \times 10^5)}{(6 \times 10^{-3})} = \frac{(1.08)}{(6 \times 10^{-3})} \times (10^{(5 - (-3))}) = 0.18 \times 10^8 = 0.2 \times 10^8 = 2 \times 10^7 \text{ (1 SF)}$

Sample Problem 3: $(6.3 \times 10^4) + (2 \times 10^6) = (6.3 \times 10^4) + (200 \times 10^4) = (6.3 + 200) \times 10^4 = 206.3 \times 10^4$ $= 2 \times 10^6 (1 \text{ SF})$

Problems :

Solve the following problems and round your answers to the correct number of significant figures:

- A) $(1.9 \times 10^{-8})(4 \times 10^{-2}) =$
- B) $(\underline{3.3 \times 10^3}) = (6.1 \times 10^3)$
- C) $(8.03 \times 10^{-7}) (3.5 \times 10^{-6}) =$
- $D)\left(\frac{5.9 \times 10^5}{(2.89 \times 10^4)}\right) =$

V. Graphical Analysis of Data

The purpose of most experimentation is to try to find "cause and effect" relationships between an independent variable and a dependent variable. Whether a relationship or pattern exists may not be obvious by simple examination of the data, and graphing the results will help this search for some sort of trend or consistency.

Examine the following set of experimental data comparing the mass of pennies versus the number of pennies used:

Mass in g	3.16	6.29	9.44	11.87	15.01
# of pennies	1	2	3	4	5

A general tendency for mass to increase when the number of pennies used increases can be easily observed, but is the change in mass proportional to the number of pennies used? Prepare a graph to answer this question, using the following steps:

- 1. The independent variable (number of pennies) is plotted on the horizontal (x) axis and the dependent variable (mass in g) is plotted on the vertical (y) axis.
- 2. Spread the data out over the entire piece of graph paper. This is done by determining the scale to be used when plotting each variable. The origin of the graph does NOT have to start at 0. Calculate the range of numbers for the x variable (largest smallest x value), then divide by the number of blocks on the horizontal axis of the graph paper. Round this value up to the nearest unit that

will produce a convenient scale. Repeat this process for the y variable.

Example: The number of pennies (x) has a range of 4 pennies (5-1) and there are 54 blocks on the horizontal axis. 4 pennies / 54 blocks = 0.08 penny / block Rounding up to 0.1 penny / block means that every 10 blocks would represent 1 penny. Label the x axis from 0 to 5, with 10 blocks per 1 penny. For the y variable (mass), the range = 15.01g - 3.16g = 11.85g. Divide this value by 34 blocks on the vertical axis to get 0.35g / block. If this is rounded up to

0.4g / block , then every 5 blocks would equal 2 grams. Label the y axis. 3. Clearly label the axes and give the graph a descriptive title.

- 4. Carefully locate each pair of data on the graph with an x or a dot with a circle around it.
- 5. Draw a smooth curve or straight line to represent the general tendency of the data points.

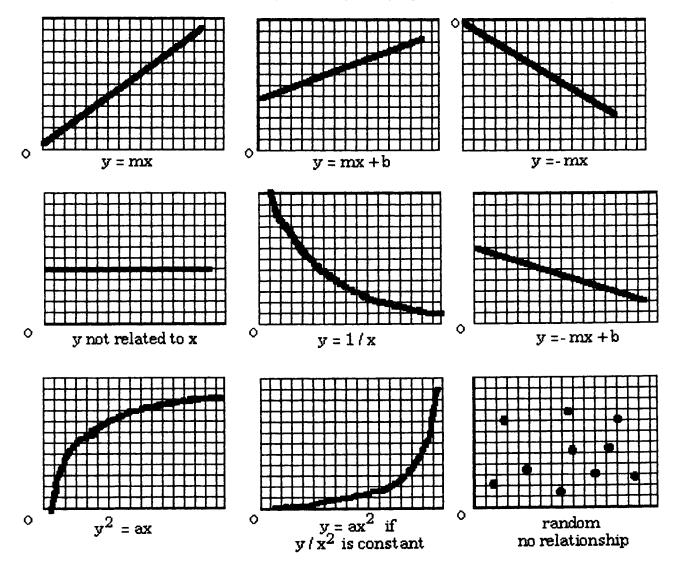
	Mass vs # of Pennies		
		(5.0, 15.0)	
15			
13-			
11		· · · · · · · · · · · · · · · · · · ·	· · · · · · ·
Mass			
in 9			
			· · · · · · ·
7	slope(m) = 15.0 - 5.	$\underline{0} = \underline{10.0} = 2.9 \text{ g}/1$	penny
	5.0 - 1.4		· · · · · · ·
5 . 	(1.6, 5.0)	· · · · · · · · · · · · · · · · · · ·	· · · · · · · ·
	·	· · · · · · · · · · · · · · · · · · ·	· · · · · · ·
3	······		
I	Number of pennie	<u>+</u>	· · · · · · ·

If the points on the graph had appeared scattered, then there may be no cause and effect relationship between the variables. In this case a smooth line connect the points, indicating a cause and effect relationship. The equation form for this linear relationship is y = mx + b, where "m" is the slope of the line and "b" is the y-intercept (the value of y when x = 0). The slope (m) is calculated by selecting two data points that lie on the line, then divide the change in the y variable by the change in the x variable. The b value for this experiment = 0, because zero pennies has zero mass.

The equation for the line is: y = 2.9x

Mathematically, the b value could be calculated by selecting any data point on the line, substituting the x and y coordinate values of this data point into the equation, then solving for b. In this example, the mass of 3 pennies seems to be closer to 9.0 grams based on the best-fitting line, rather than the measured mass of 9.44 g. Experimental error in measurement could account for this discrepancy, and it is usually better to use the value based on the graph, which tends to "average out" high and low measurements. Substitute the 3 for "x" and the 9 for "y" in the equation (y = 2.9x + b): 9 = 2.9(3) + b Solve for the value of b: 9 = 8.7 + b........ b = 9 - 8.7 = 0.3

Other common relationships are expressed by the graphs below:



Problem:

Take a piece of paper and fold it in quarters. Using a watch with a second hand as a timer, make as many pencil dots as you can in 2 seconds in the first quadrant. Count the number of dots and record the value. In the second quadrant, make as many dots as you can in 4 seconds. Record the number of dots. Repeat this process in the remaining quadrants (front and back of the paper), doubling the amount of time used for each successive trial. You will have results for additional time periods of 8s, 16s, 32s, 64s and 128s. Prepare a full-page graph of your data and determine what mathematical relationship, if any, exists between the number of dots made versus time.

VI. Statistical Analysis of Data

For some types of data the methods of graphical analysis are insufficient or not applicable, and analysis using statistics is more appropriate. Usually statistics focus on two characteristics of the data: central tendencies and dispersion (spread) of the data.

Central tendencies indicate the degree of sameness within a group of data by using one value that is a "summary" of the data in the group. The **median** is the middle value for a group of data that has been arranged from lowest to highest values. The **mode** is the value that occurs most often and the **mean** is simply the average value (calculated by obtaining the sum of all the values (x) in a set of data, then dividing by the number (n) of values in the set). Using all 3 central tendencies gives a better representation of the data than any single tendencies.

Sample Problem:

You want to conduct a research experiment to determine the effects of temperature on the rate of a chemical reaction. So as the control, you run 10 trials at 20°C and time when each reaction is complete. You then run 10 trials at 40°C as your experimental group and record the times for complete reactions to occur. The sets of data were listed in order of increasing numerical value and summarized in the chart below:

Times at 20°C	22s	24s	24s	24s	24s	28s	29s	30s	31s	34s
Times at 40°C	19s	20s	21s	21s	21s	22s	22s	24s	25s	25s

The median at 20°C is between 24s and 28s, which is <u>26s</u>. At 40°C, it is between 21s and 22s, or <u>21.5s</u>.

The <u>mode</u> at 20°C is <u>24s</u> which occurs four times, and at 40°C it is <u>21s</u> which occurs three times.

The <u>mean</u> (average) for each set is calculated by adding all the time values, then dividing by the number of trials, which is 10. The mean at 20°C is <u>27s</u> and at 40°C it is <u>22s</u>. Just one unusally high or low value can produce a mean value that is misleading. For example, if you wanted to determine the average salary of ten people in America, and Bill Gates was one of your group, you would think everyone was a millionaire! The mean is most accurate as a representative of a set of data that is evenly or symmetrically distributed.

The amount of **dispersion** indicates how closely the values of a given set of data agree with each other. This spread can be shown simply as the **range** between the highest value and the lowest value in the set. The <u>range</u> at 20°C is the difference between 34s -22s = 12s. The <u>range</u> at 40°C is 25s - 19s = 6s. The data for reaction times at 40°C has less variation, which makes it more precise.

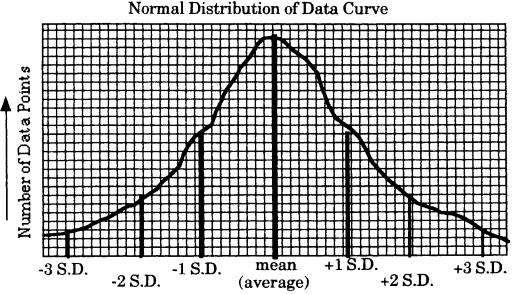
Another way of indicating dispersion is by calculating the **standard deviation** for the data set. This can be thought of as an indication of the "average" of individual data differences from the mean value of a set of data. Standard deviation is calculated by 4

easy steps:

- 1. Subtract each value in a data set from the mean. These differences are called deviations.
- 2. Square the deviations.
- 3. Add all of the squared deviations together, then divide this sum by 1 less than the total number of values in the data set (n-1).
- 4. Take the square root of this number.

For the reaction times data at 20°C, the standard deviation is calculated to be 4°C, whereas the data at 40°C has only a 2°C standard deviation. The 40°C data has twice the precision of the 20°C data.

For a normal distribution of data, 68% of the measurements will fall within a range equal to the mean \pm 1S.D.(standard deviation), 95% within the mean \pm 2S.D. and 99% within the mean \pm 3S.D.



More advanced statistical analysis can be done to confirm that differences in experimental results are due to the variation in conditions, and not merely caused by chance.

Problem:

Seven lab groups experimentally determined the density (g/cm^3) of aluminum metal, and their results are summarized in the table below:

und unon i		outilitud 100	u in uno van	10 0010		and the second sec	
Group #	1	2	3	4	5	6	7
Density	2.8	2.6	2.9	3.2	2.7	3.0	2.6

Determine the mean, median, mode, and standard deviation for this data. The accepted value for the density of aluminum is 2.70 g/cm^3 . Calculate the percent error based on the mean value. What can be said about the precision and accuracy of this set of data?

Ans: mean = 2.83 g/cm^3

Ans: median = 2.8

Ans: mode = 2.6

Ans: S.D. = 0.22

Ans: % error = 4.8

Unit 2 Objectives

Having studied the unit notes and done the problems, you should be able to:

- 1. Distinguish between quantitative and qualitative characteristics.
- 2. List and define the basic SI units and prefixes with their categories of measurement.
- 3. Demonstrate a logical approach to solving a problem and making SI conversions, using dimensional analysis.
- 4. Define density and perform calculations using the math relationship among density, mass, and volume. Be able to determine either density, mass or volume given any two of the three variables.
- 5. Differentiate between precision and accuracy.
- 6. Estimate the precision possible for any instrument that is used in the laboratory.
- 7. Determine the relative uncertainty, percentage uncertainty and percent error of a measurement made in the laboratory.
- 8. Define significant digits and determine the number of significant figures in a measurement.
- 9. Express the results of addition, subtraction, multiplication and division problems in the correct number of significant digits.
- 10. Convert numbers from decimal notation to scientific notation and vice-versa, and perform calculations using scientific notation.
- 11. Prepare a graph from a table of data. The graph must contain all the information needed for a person to interpret it.
- 12. Determine the mathematical relationship between two variables from a graph representing a proportional relationship.