

Graphing Using Microsoft Excel

Introduction

A spreadsheet is a table that displays numbers in rows and columns, used for accounting, budgeting, financial analysis, scientific applications, and other work with figures. Spreadsheet tables include row labels and row numbers, and usually contain calculations based on the row numbers. Before the popular use of computers paper spreadsheets were used, but the computerized versions have the advantage of being able to automatically update calculations with changing data. Spreadsheets provide the tools to perform calculations on raw data as well as graphically present the data and results. Modern spreadsheets have the capability of performing everything from simple addition and subtraction to complex statistical analyses. The following tutorial assumes you are using Microsoft Excel™ 97 or 2000. You only need to follow the tutorial if you are unfamiliar with the use of spreadsheets.

Tutorial

You will find the same basic features whether you are using Microsoft Excel™, Corel Quattro Pro™, Lotus 1-2-3™, or any other spreadsheet application. A typical spreadsheet file is comprised of one or more sheets with columns and rows. A blank Excel file begins with 3 sheets (or pages) labeled “sheet1”, “sheet2”, and “sheet3” (labeled at the bottom of the screen). You can choose a particular page by left-clicking on its tab with the mouse, and you can change individual sheet names by right-clicking the tab and selecting the appropriate option. The spreadsheet pages are made up of rectangular boxes arranged in columns labeled A, B, C, etc. and rows labeled 1, 2, 3, etc. These boxes are called cells; each cell is referenced by the column-row coordinates (e.g. A1, C34, D7, etc.). The cell, which is outlined at any time, is called the active cell. By moving the mouse to a particular cell and left-clicking on it, you can select different cells. The active cell is the one into which you can enter data.

PUTTING INFORMATION INTO THE SPREADSHEET

Make B2 the active cell, and type AGE. As you type, notice that the word “AGE” appears in the input line near the top of the screen. If you make a mistake you can use the backspace key to erase backwards, or you can move the pointer onto the input line and click. The cursor will appear wherever you click the mouse on the input line (see Figure 1).

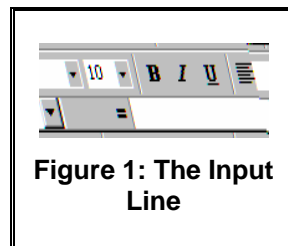
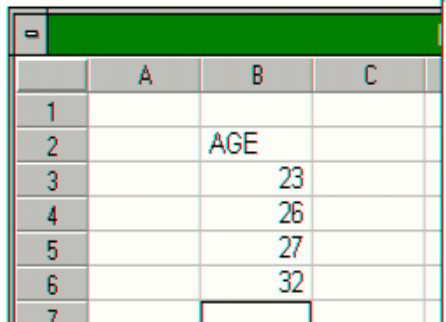


Figure 1: The Input Line

Once you have “AGE” in the input line, you can either press the Enter key or any Arrow key on the keyboard. Pressing the Enter key simply puts the information in the cell and moves the active cell down one (the Down Arrow key pressed achieves the same thing). Since the word AGE is not a number or an instruction that the spreadsheet recognizes, it is “text data”. Numbers are “numeric data”.

Make B3 the active cell. Type in 23; you should see it in the Input Line. Hit the Enter key, and B3 should now have 23 in it, with B4 the new active cell. Now type 26, Enter key, 27, Enter key, 32, Enter key. When you are finished, the spreadsheet should look like Figure 2.



The image shows a screenshot of a Microsoft Excel spreadsheet. The spreadsheet has a grid with columns labeled A, B, and C, and rows labeled 1 through 7. The cell B2 contains the text "AGE". The cells B3, B4, B5, and B6 contain the numbers 23, 26, 27, and 32, respectively. The cell B7 is currently selected and is empty.

	A	B	C
1			
2		AGE	
3		23	
4		26	
5		27	
6		32	
7			

Figure 2: Column with Entered Data

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PERFORMING SIMPLE CALCULATIONS

The Average Function

Now that you have a column of numbers, you can perform simple calculations. For example, you can find the average of these numbers. Spreadsheets have many functions, including a function for finding averages. The numbers must be in a column, row, or block. Since this tutorial assumes you are using MS Excel, you will learn Excel specific function names.

To calculate the average of the numbers, move to cell B8. Click on the "paste function" button on the toolbar near the middle of the screen (see Figure 3). A small screen will appear that contains a list of the function types in the left frame and the spreadsheet functions in the right frame. If you click on the "All" option in the left frame, you will notice that there are a lot of different functions. In this case, we will use the AVERAGE function. Move the mouse to the word AVERAGE in the menu and double-click on it. Look at the input line. It should say "=AVERAGE(B3:B7)" and a box should have appeared on the upper-left portion of the spreadsheet. Excel probably correctly guessed the correct range of cells to average, but you should not always trust the spreadsheet to make the proper decision. With your mouse, click on the "select range" button (see Figure 4), click and hold the left mouse button on cell B3 and drag your mouse down to B7, then click on the "select range" button again. Make sure the formula says "=AVERAGE(B3:B7)" and then click on the "OK" button. The number 27 appears in cell B8. Another way to find the average, instead of using the menu, would be typing the function and range in by hand. This time, make B9 the active cell. Go to the Input Line and type "=average(b3:b7)" and then press Enter. The values in B8 and B9 should be the same. The function names are not case sensitive.



Figure 4: "select range" button

Other spreadsheet functions that you may find useful are (descriptions of all these can be found in the help menu system of Excel):

SIN() ; COS() ; TAN() ; EXP() ; LN() ; LOG10() ; SQRT() ; SUM() ; STDEV() ; SLOPE() ;
INTERCEPT() ; RSQ() ; PI() ; POWER() ; COUNT() ; MIN() ; MAX()

Addition, Subtraction, Multiplication, Division

You can also use spreadsheets to manipulate data with addition, subtraction, multiplication and division. Suppose the numbers you entered were the ages of individuals and you wanted to calculate their year of birth. Since it is 2003, their approximate birth year can be calculated by subtracting their age from 2003. (This calculation is only approximate since you don't know whether or not they have had a birthday this year.) You could do all these calculations and then enter the numbers into the spreadsheet, but the spreadsheet can do the calculations for you.

Move to cell C2 and enter "YEAR OF BIRTH" in that cell. You do this the same way you entered "AGE" in B2. Make cell C3 the active cell, and type "=2003-" then click on cell B3 with your mouse, then hit Enter. If you were successful, the year 1980 should appear in cell C3. Hopefully by now you have noticed that labels and numbers can be entered directly into cells whereas formulas must be preceded by an "=" sign (actually "+" or "-" will also work when appropriate). This is a requirement for Excel; other spreadsheet programs may vary from this, but conceptually they are all organized the same.

You can similarly enter "=2002-B4" in cell C4, "=2002-B5" in cell C5, and "=2002-B6" in cell C6, but it would be easier to copy the formula in cell C3 and use it for the other cells.

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COPYING AND PASTING FORMULAS

Spreadsheets allow users to copy instructions from one cell to the next. In doing so you can successfully fill cells C4, C5, and C6 with the desired formulas. Make cell C3 the active cell. In the input line you should see the instructions you just typed into that cell. With C4 active, pull down the EDIT menu and select COPY by highlighting the word and clicking on the mouse button. If you were successful, the formula in C3 was stored in an area of the computer memory known as the 'clipboard' and the cell was highlighted with dancing hyphens. You now want to paste that instruction into cells C4, C5, and C6. Place the pointer in cell C4, then depress AND HOLD the left mouse button. With the mouse button still held down, move the pointer to cell C6. As you go, you will notice that now all the cells, C4, C5, and C6 are active. Release the mouse button. Now pull down the EDIT menu and select PASTE (by highlighting and clicking in PASTE). If you were successful, C3, C4, C5, and C6 will display the values of 1977, 1976, 1971.

Notice, COPY and PASTE will be very useful when having to type in long columns of repetitive instructions. An easier way to use CUT, COPY, and PASTE is by clicking buttons on the toolbar (see Figure 5). First highlight the cell (or cells) to be copied, then click on the COPY button (the one that has two sheets of paper). Next, highlight the cell (or cells) you want the information copied into, then click the PASTE button (the one with the brown clipboard).

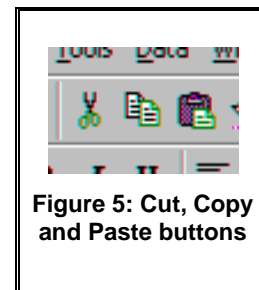


Figure 5: Cut, Copy and Paste buttons

FORMATTING YOUR SPREADSHEET

Formatting numbers

When scientists present numbers in documents (like spreadsheets and reports), they convey information in the number of significant figures that are given for a particular number. If a number is only supposed to carry 2 significant figures (SF's) or 4 SF's, then it should be formatted as such in the spreadsheet. In general, only numbers that represent final answers or calculations need to be formatted for lab reports, not all of the intermediate numbers.

Go to a blank portion of your spreadsheet and type the "12345.6789" in five different cells (expand the column width if necessary). Go to the first instance of the number and right-click on the cell and choose the "Format Cells..." option. Make sure you are on the "Number" page by clicking on the appropriate tab at the top of the dialog box. Click on the "Number" option in the list box on the left and make sure the number of decimal places is set to "3", then click on the "OK" button. The active cell should now read "12345.679" as a result of the formatting and subsequent rounding that occurred. Set the format of the next cell to "Number" with 2 decimal places. In the third cell, set the format to "Scientific" with 2 decimal places. The third cell should read "1.23E+04", which is the way a spreadsheet expresses the " $\times 10^4$ " notation. In the fourth and fifth cells, format the numbers to "Currency" and "Percent", respectively, and observe how this changes the format in which the numbers are displayed.

Superscripts, Subscripts, and Greek characters

One of the often-overlooked formatting features in spreadsheets is superscripting, subscripting, and Greek characters. These formatting features are especially useful in chemistry since chemical formulas and mathematical formulas use these features extensively.

Go to an empty part of your spreadsheet and type "Na₂SO₄" then press Enter. Once the text has been loaded into the cell, double-click on the cell with your mouse. Using your mouse, highlight or select the "2" in "Na₂SO₄", then right-click on the "2". Choose the "Format Cells..." option in the pop up box. When the dialog box appears, put a check in the "Subscript" box and click on the "OK" button. While you are editing the cell, subscript the "4" in "Na₂SO₄" as well, then press Enter. Superscripting is achieved in the same manner if the "Superscript" box is checked instead of the "subscript" box. The displayed cell should now appear as Na₂SO₄.

To get Greek characters, you must change the font of the letter. This can sometimes be tricky since you need to know which letter of the alphabet corresponds to the Greek character you want. Table 1 gives you the alphabet equivalents for the uppercase and lowercase Greek characters in the "Symbol" font. Go to an empty part of your spreadsheet and type "DH_{vap}" and press Enter. (If the "H" gets converted to a lowercase "h" the "AutoCorrect" feature is turned on. You can turn this off by going to the "Tools" menu and choosing "AutoCorrect".) Double-click on the cell and highlight or select the "D" and right-click on the letter and choose "Format Cells..." when the option pops up. In the upper-left part of the dialog box,

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scroll down the "Font:" list and choose "Symbol" then click OK. While you are editing the cell, subscript the "vap" part of the text. When you are done, the cell should display " ΔH_{vap} ".

Table 1. Greek Letters and Their Alphabet Equivalents.

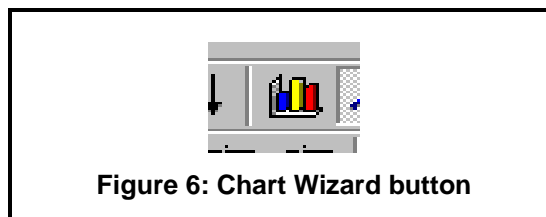
A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
Α	Β	Χ	Δ	Ε	Φ	Γ	Η	Ι	Θ	Κ	Λ	Μ	Ν	Ο	Π	Θ	Ρ	Σ	Τ	Υ	ς	Ω	Ξ	Ψ	Ζ
a	b	c	d	e	f	g	h	i	j	k	l	m	n	o	p	q	r	s	t	u	v	w	x	y	z
α	β	χ	δ	ε	φ	γ	η	ι	φ	κ	λ	μ	ν	ο	π	θ	ρ	σ	τ	υ	ω	ω	ξ	ψ	ζ

GRAPHING

One of the most effective ways to communicate information is through pictures and graphs. Spreadsheets are excellent at converting numerical data into graphical data for the purpose of communicating trends in the data. The three most common types of graphs you will produce for this course and other courses in science are XY (Scatter), Column, and Pie charts. This exercise will show you how to create an XY (Scatter) chart.

Go to a blank spreadsheet and type the data set seen in Table 2. When you are finished with the data, click on the Chart Wizard toolbar button (see Figure 6). Choose the XY (Scatter) chart option and the data points without lines under the "Chart sub-type:" section, then click "Next >". Click on the "select range button" (see Figure 4), select the XY data that you just entered, click the "select range" button again, then click "Next >". Your graph should appear in the preview screen as a series of dots that look linear. If this is correct, then click "Next >". Enter an appropriate chart title and axes labels. Click on the "Gridlines" tab and turn off the Y-axis gridlines and then click "Next >". Choose where you want the chart to go then click "Finish". You have just created a chart.

X	Y
0.1	2.24
0.2	4.52
0.3	6.75
0.4	8.90
0.5	11.94



When selecting your data range, if the columns of data are not next to each other (as in the exercises in the lab) you need to first select the "x" data with the mouse and then hold down the CTRL key and the select the "y" data. This may require a bit of practice. The spreadsheet is also capable of fitting your data to a line and providing you with the linear equation. Make sure the chart you just created is the selected object in the spreadsheet (Does it have eight black squares in the corners?). If not, click on it, then click on the "Chart" menu and choose "Add Trendline...". In the dialog box, choose the "Linear" type and then click on the "Options" tab. Make sure you put a check in the two boxes labeled "Display equation on chart" and "Display R-squared on chart", then click on the "OK" button. Clean up the chart by deleting the legend (click on it and press your Delete key), and get rid of the gray background by double-clicking on it and choosing "None" under the "Area" option.

SAVING THE SPREADSHEET

Up to this point the data and instructions we have entered have only been stored in the memory of the computer. If you were to quit the spreadsheet program your efforts would be lost. You must save what you have done so that if you want the information at some time in the future it will be available to you. In order to save the spreadsheet we must move the pointer to the word FILE on the menu bar, click the mouse button and a menu will appear below the word FILE. Move the mouse so that the pointer is on the words SAVE AS. Provide the dialog box with a name for your spreadsheet (and choose the proper folder or drive if necessary) and click on the SAVE button.

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You now have performed the basic spreadsheet skills that will help you with the following exercises. There is much more to learn, but experimenting with the software is the best way to learn. If you need help, push the "F1" key at any time and the help system of the spreadsheet will appear. Also don't forget the undo button (backward curved arrow) – if you really mess up, just undo your last operation(s). For further help, find someone else in your class or find your instructor.

You do not need to turn in anything up to this point.

Procedure

Parts I-III of this exercise, including all graphs and labeled spreadsheets, are to be turned in to your instructor. Please do each part on a separate sheet in Excel, and label each sheet with its corresponding part number. Graphs/charts can be placed on the same sheet, or put on a separate sheet (please make sure to appropriately label all graph/chart sheets if separate from data). Also make sure all graphs/charts are appropriately labeled so that it is clear what data is being presented. You will need a floppy disk or jump drive to save your work.

Instructions for Part I. Linear Regression

Simple linear regression takes a number of x, y data pairs and tries to fit the data to a linear equation in the form of $y = mx + b$ where y is the variable dependent on the x variable, m is the slope of the line, and b is the y -intercept. Once the values for the slope and intercept have been calculated, predicting the values for y or x becomes possible. For example, if you had measured the electrical conductivity for various concentrations of a salt solution and fit the data to a linear equation, then you would be able to determine the concentration of an unknown solution if you measured its electrical conductivity (assuming this follows a linear trend). Since you would use the y variable for the electrical conductivity (since conductivity is a property that depends on the electrolyte concentration of the solution) and the electrolyte concentration as the x variable (since this is the known value), rearranging the linear equation to solve for the concentration of the unknown solution (the x variable) you would get $x = (y - b) / m$. Substituting the slope and intercept from the regression into this equation and by using the measured conductivity for the unknown (the y value), you could calculate the concentration of the unknown solution. You will use this principle in the worksheet exercises to find the boiling point of Radon.

Instructions for Part II. Making Equations Linear

In Part II of this exercise, you are given some experimental data, and you must determine what form of this data best fits a line. The two equations being considered are given below. In order to answer this question, you will need to put the raw data in the form specified by each equation. These should look familiar to those of you who have learned about kinetics.

$$\ln [A] = \ln [A]_0 - kt \quad \text{Eqn. 1} \qquad \frac{1}{[A]} = \frac{1}{[A]_0} + kt \quad \text{Eqn. 2}$$

First, examine equations 1 and 2 above and try to determine how they are seen as linear equations. Remember, a linear equation has the form $y = mx + b$. If you were to plot y vs. x using the equation $y = mx + b$, m would be the slope of the line and b would be the y -intercept. In Equation 1, if $\ln[A]$ vs. t were plotted on a graph, the slope = $-k$ and $\ln[A]_0$ would be the y -intercept. So, if you were to label each term in equation 1 with the corresponding term in the general linear equation, you would get:

$$\begin{array}{cccc} \ln [A] & = & \ln [A]_0 & - & kt \\ y & & b & & mx \end{array}$$

In the space below the following equation, write the variable from the general linear equation below each of the terms as was done for you in the example above.

$$\frac{1}{[A]} = \frac{1}{[A]_0} + k t$$

If you have done it correctly, you should have labeled them in the order y, b, m, x . Now that you can see how Equations 1 and 2 are linear, you can use experimental data to determine whether that data best fits equation 1 or equation 2. To do

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this for the data from Table 3, you would convert the data to the numbers shown in Table 4 by calculating the natural log of the concentration (and placing those values into column C), and the reciprocal of the concentration (and placing those values into column D).

Table 3: Raw Data

	A	B
1	time (s)	[A] (M)
2	195	0.016
3	604	0.015
4	1246	0.013
5	2180	0.011
6	6210	0.0068

Table 4: Raw Data and Resulting Calculations

	A	B	C	D
1	time (s)	[A] (M)	ln [A]	1/[A]
2	195	0.016	-4.1352	62.5
3	604	0.015	-4.1997	66.66667
4	1246	0.013	-4.3428	76.92308
5	2180	0.011	-4.5099	90.90909
6	6210	0.0068	-4.9908	147.0588

By plotting the data in the form of y vs. x for equations 1 and 2, you can determine whether the experimental data fits equation 1 or 2. Figure 9 and 10 below show the results of this.

By plotting the data in the form of y vs. x for equations 1 and 2, you can determine whether the experimental data fits equation 1 or 2. Figure 9 and 10 below show the results of this.

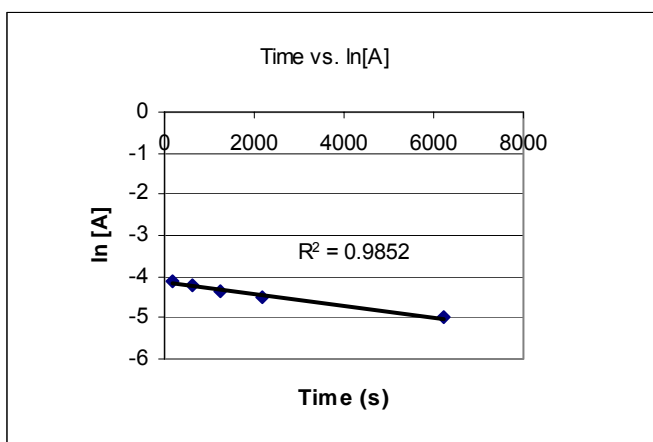


Figure 9: Time vs. ln[A] data

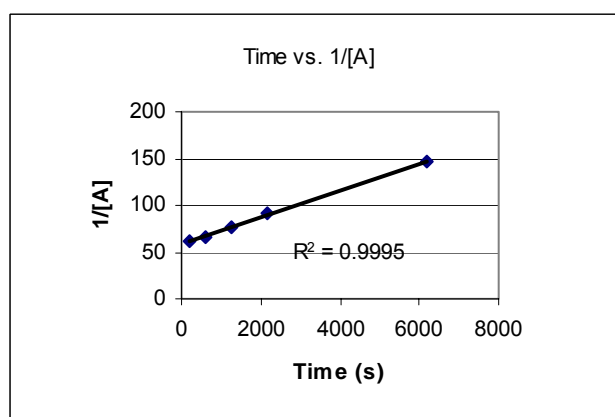


Figure 10: Time vs. 1/[A] data

Hopefully, it is easy to see that the data in Figure 10 fits a line better than the data in Figure 9. However, using the correlation coefficient (R^2 value) gives a statistical tool to help determine this – the more linear the data, the closer this value is to 1 (or -1). Therefore, the experimental data fits Equation 2 better than Equation 1, and the value of k for Equation 2 is 0.0142 for the given data. In the Part II, you will use a spreadsheet to help you determine the order with respect to each reactant and the rate constant k .

SAVE YOUR WORK IN A SPREADSHEET FILE, USING YOUR FIRST INITIAL AND LAST NAME AS THE FILE NAME – YOU MAY BE REQUIRED TO TURN IN THIS FILE AS PART OF THIS ASSIGNMENT PER YOUR INSTRUCTOR'S REQUEST!

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Parts I-III (including all graphs and labeled spreadsheets) may be required by your instructor.

Part I. Linear Regression – Exercise

All the common noble gases are monoatomic and have low boiling points. Using the row number of the Periodic Table, predict the boiling point of Radon (Rn). Assuming boiling points for noble gases follow a linear trend, this is easily done by graphing boiling point vs. row number in a spreadsheet.

- 1) Enter the row number and boiling point data into a blank spreadsheet, putting the row number in column A and the boiling point in column B. In column C, convert all the boiling points to Kelvin by using an equation for each calculation.
- 2) In cell D1 type "slope" and in cell D2 type "y-intercept"
- 3) In cell E1 you will calculate the slope (see the help files for the "slope" function for more assistance)
 - type "=slope(", then use your mouse to select the boiling point data (the numbers in column C)
 - type "," then use your mouse to select the row data (the numbers in column A)
 - type ")" and then hit the "enter" key
- 4) In cell E2 you will calculate the y-intercept (see the help files for the "intercept" function for more assistance)
 - type "=intercept(", then use your mouse to select the boiling point data (the numbers in column C)
 - type "," then use your mouse to select the row data (the numbers in column A)
 - type ")" and then hit the "enter" key
- 5) In cell D4 type "b.p. of Rn", in D5 type "row", and in E5 type "b.p. (K)"
- 6) Use your knowledge of typing spreadsheet formulas to determine the boiling point of Rn

Element	Row number	bp (°C)
Ne	2	-245
Ar	3	-186
Kr	4	-152
Xe	5	-107
Rn	6	?

Slope = _____

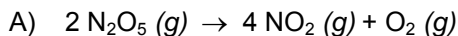
y-intercept = _____

b.p. of Rn = _____

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Part II. Making Equations Linear - Exercise

Determine the rate law for each of the following reactions using the data provided. Make sure you provide the proper units for the rate constant k . If the data fits Equation 1, then the reaction is first order. If the data fits Equation 2, then the reaction is second order. Use your knowledge of kinetics to help you with these exercises, and make sure you report the correct units for k on the spreadsheet.

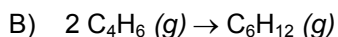


Time (s)	$[\text{N}_2\text{O}_5] \text{ (M)}$
0	0.100
50	0.0707
100	0.0500
200	0.0250
300	0.0125
400	0.00625

Which graph is linear?

Write the rate law:

What is the rate constant?



Time (s)	$[\text{C}_4\text{H}_6] \text{ (M)}$
0	0.0100
1000	0.00625
1800	0.00476
2800	0.00370
3600	0.00313
4400	0.00270
5200	0.00241
6200	0.00208

Which graph is linear?

Write the rate law:

What is the rate constant?

Part III. Formatting Labels and Data - Exercises

On the "Part III" sheet of your Excel file, format the following numbers. Using superscripts, subscripts, and Greek characters, recreate the following chemical formulas and mathematical equations in the "Part III" sheet of your spreadsheet template.

CO_2

C_2H_6

$\text{Na}^+_{(\text{aq})}$

$\text{K}_2\text{Cr}_2\text{O}_7$

$\lambda \text{ (nm)}$

Area = πr^2

ΔH_{vap}

ΔT

β -decay

α -decay