Experiment 2: An “Atomic” Introduction to Conducting Calculations with Excel

(This experiment will be conducted in **Olin-Rice 341**. **Please go there directly.**)

INTRODUCTION

A number of experiments in our chemistry lab sequence require graphing and repetitious calculations involving experimental data. Since the application of a spreadsheet program such as Microsoft Excel® provides a convenient and powerful way to display and manipulate data, we will require that a spreadsheet be used as a laboratory tool throughout this course. The goal of this experiment is to help you obtain a necessary level of proficiency with the Excel skills that you will need to employ in this course. We recognize that each of you brings a different level of Excel experience to this experiment. Some students will have already used Excel extensively, while others may have never used the program. Although this experiment assumes no previous knowledge of Excel, we hope that everyone will benefit from completing these exercises.

LOGISTICS

- **Due to the number of computers in OR 341, not everyone may be able to work independently on this activity. If you work with a partner, try to share the work equally. If one group member has less previous experience with Excel, it would be advantageous for that person to spend more time at the keyboard, even though it will take longer.**
- **If you would like to work on your own laptop, feel free to bring it along, and do so.**
- **Although it is possible to complete these calculations with a handheld calculator, please <u>resist this temptation!</u> A goal of this experiment is that you become sufficiently comfortable with Excel to use it for many laboratory calculations, even those that could be accomplished with a calculator. You will find that Excel, if used properly, is much more powerful, and flexible, than a calculator.**
- **The point of this experiment is to help you to master Excel skills. It will not help you if you race through it. Please take your time, and ask for help from your lab instructor or prefect as needed. The time that you invest today will pay dividends later, when you are carrying out calculations and preparing laboratory reports in this course.**

EXPERIMENTAL PROCEDURE

1. Grab a comfy seat at one of the Chemistry Department’s Mac computers.
2. If the screen is blank, touch any key on the keyboard to “wake up” the system.
3. Start Microsoft Excel® by clicking once on the funky green “×” on the bottom of the screen.

A set of rectangular cells (called a “sheet”) will appear. Each cell provides a potential location for text, numbers, or a set of mathematical instructions. Each cell is “addressed” with a letter and number combination. The vertical columns are labeled with letters and the horizontal rows with numbers. In this way, the fourth cell in the fifth column is labeled E4 while the second cell in the third row is labeled B3. The sheet you are currently looking at is one of three in the “workbook” you are working on. The other two sheets are accessed by clicking on the tabs near the bottom of the screen, labeled “Sheet 2” and “Sheet 3.” If you click on them, you’ll see that they too are blank. Please make sure you are back on “Sheet 1” before proceeding.

Objective I: Analysis of the isotopic distribution of chromium

Let's work with some data of chemical significance! In the periodic table (on the next page), the square for Cr features two numbers: 24, the atomic number, and 51.996, the atomic mass. Where do these numbers come from? To answer these questions, we must consider the different naturally occurring *isotopes* of chromium. The following table provides the number of subatomic particles in the nuclei of the four common isotopes of chromium:

Isotope	Protons	Neutrons	Electrons	% Abundance
Cr-50	24	26	24	4.35
Cr-52	24	28	24	83.79
Cr-53	24	29	24	9.50
Cr-54	24	30	24	2.36

The atomic number indicates the number of protons in the nucleus, and it is 24 for each isotope of Cr. In fact, having 24 protons in the nucleus (and thus an atomic number of 24) is what makes any atom a Cr atom. The number of protons in an atom's nucleus defines its identity, but the number of neutrons in the chromium nucleus can vary. This table indicates the natural abundances for the four chromium isotopes. Approximately 84% of chromium atoms on Earth feature 28 neutrons/nucleus. We'll begin our set of examples using Excel by creating a spreadsheet (including headings) for the data in the table above.

The Periodic Table

1 H 1.0079																	2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.81	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.179
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.69	29 Cu 63.546	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.22	41 Nb 92.906	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	*	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.03	†	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)	111 Rg (272)	112 Uub (285)	113 Uut (284)	114 Uuq (289)	115 Uup (288)			

*	57 *La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
†	89 †Ac 227.03	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

Entering and Formatting Text

4. Make sure that you are working on Sheet 1, and that cell A1 is selected. (The Sheet 1 tab at the bottom of the screen will be bright white, and cell A1 will be highlighted in light blue.)

5. Type the word “Isotope” into cell A1, and hit return or enter. Use the arrow keys or mouse to move to cell B1. Type the word “Protons” into cell B1. *Shortcut: Instead of hitting enter or return when you finish typing, hit the right arrow key or use the mouse to click on the next cell you want to work on. This works great, provided that you are not entering a formula!*. Enter the rest of the headings from the table above (one per cell) into the top row (row 1) of your spreadsheet.
6. After typing in the five headings, select all five cells that they are in, simultaneously, by clicking on cell A1, and with the mouse button held down, moving the mouse to cell E1. (The computer lingo for this is “clicking and dragging” to “select A1:E1”) The five heading cells should now be shaded in light blue, indicating that they are “selected.” You have selected these cells for collective formatting, which will help distinguish the contents of these cells as column headings.
7. Click on the **B** and **U** icons under “▼Font” on the Formatting Palette, which is parked on the right side of your screen. This will boldface and underline the column headings, respectively.
8. Click on the ▶ to the left of “Alignment and Spacing” on the Formatting Palette, which will reveal some text alignment formatting options.
9. Click on the second icon from the left next to “Horizontal:” to center the headings in their cells.
10. You will see that the last column isn’t quite wide enough to accommodate the “% Abundance” heading. To remedy this, move your mouse to the grey row of cell column letters at the top of your sheet, onto the line dividing the E and F cells. If you are in the right spot, your mouse pointer will change from a hollow ✚ or arrow to a symbol that looks vaguely like this: ←|→. Double-click on the mouse to automatically adjust the width of the column to accommodate the widest entry in the column (the heading!), or click and drag to manually adjust the column width.

Entering and Formatting Data

11. Copy the data from the chromium isotope table into the spreadsheet: Start in cell A2, and put the entry “Cr-50” there. Enter the remainder of the data from the table into the appropriate cells. As you attempt to do this, Excel may interrupt you with an offer to "help you" by opening something called the "List Manager." The List Manager is actually the great-grandmother of all evil, and you should not only reply with a stern NO!, but also click the box that says "Don't ask me this again".
12. Once you have all of the data in place, simultaneously highlight the four rows of cells with data in them by clicking cell A2, holding the mouse button down, and dragging the mouse to cell E5. (Remember, the shorthand for this is “clicking and dragging” to “select A2:E5.”) We could reformat these cells using the Formatting Template, as we did in steps 7 and 8, but we’ll show you a few other ways to do it instead – after that, you can keep using whichever one you like the best!
13. At the very top of your screen, click on “Format”, then click on “Cells…” (The computer shorthand for this is “Format:Cells…”, and it indicates that the menu item “Cells…” should be selected from the Format menu.)
14. Click on “Alignment” from the menu at the top of the “Format Cells” window.
15. Under “Horizontal:” click the squarish blue button next to the box that currently has the entry “General” in it. This will reveal a “pull-down menu” of horizontal alignment options, from which you should select “Center”.
16. Click “OK”, and you should find your data is now neatly centered under your column headings.

Excel will display the % Abundance value for ^{53}Cr as “9.5” instead of “9.50”. Since we are scientists, the number of significant figures is critical, and “9.5” is incorrect! Here’s how to rectify this situation:

17. Select and highlight all the % Abundance data. (Click and drag to select E2:E5.)
18. We need to format these cells, and we have learned two ways to do so already: we could use the Formatting Palette, or we could Format:Cells…, but you may have noticed the symbol “⌘1” next

to “Cells…” on the menu when you did the latter. That’s actually the keyboard shortcut for that command: so just holding down the ⌘ key on the keyboard and pressing “1” will do exactly the same thing as selecting the menu item Format:Cells…, and get you to the same endpoint. Try it! The “Format Cells” window should pop up.

19. Click on “Number” from the menu at the top of the window, then choose “Number” from the “Category:” list that appears. Ensure that the number of decimal places is set to 2, then click “OK”. The *scientifically correct* % Abundance value, “9.50”, [which is shorthand for 9.50 ± 0.01] should now be displayed for ^{53}Cr. [9.5 indicated that the value was ± 0.1, which it isn’t!]

There’s another, more subtle significant figure correction we need to make as well. The number of electrons, protons, and neutrons in each isotope is *exact*, which is why these numbers are underlined in the table in this handout. The Cr-52 nucleus doesn’t contain 24 ± 1 protons, it contains *exactly* 24 protons. This is indicated by underlining the number. You should update your table to reflect this:

20. Click and drag over the elementary particle counts in your table. (Select cells B2:D5.)
21. Underline these items using the keyboard shortcut ⌘U.

Well, golly, that wasn’t so bad. Now that you’ve reproduced the table as presented in these instructions, let’s put Excel to work on it. We’ll start by sorting the table by % Abundance:

Sorting the Table

22. Click and drag over the table to select all the cells that comprise it, including the headings. (Click and drag to select cells A1:E5.)
23. Select Data:Sort… (Remember, that’s shorthand for clicking on “Data” on the menu at the very top of your screen, then clicking on the “Sort…” option that appears on its sub-menu.)
24. Because Excel assumes that your table has a header row (notice the little circle [it’s called a “radio button”] in front of “Header row” has a dot in it, at the bottom of the “Sort” window), click the square button next to the box that currently has the entry “Isotope” in it in order to choose to sort your table by % Abundance (remember, this is called a “pull-down menu”). Let’s have the table present the isotopes in order of decreasing abundance: select the radio button in front of “Descending”, right next to where you selected % Abundance from the pull-down menu. Click OK, and check it out! Your table has been re-sorted!

A common term associated with atoms is the “mass number.” The mass number of an atom is the sum of the number of protons and the number of neutrons in its nucleus. Let’s use Excel to calculate the mass number for each of the four naturally occurring isotopes of chromium. Excel provides a way to set up each calculation only once, rather than having to deal with each one separately and repeatedly (as you would need to do with a calculator). The ability to perform such repeated calculations conveniently is one of the most useful features of Excel. A convenient place to list the mass numbers is in between the “Neutrons” and “Electrons” columns. Let’s insert a column between these two table entries, and then carry out the calculation required to correctly fill in the new column:

Inserting a Column

25. Select D1, the cell containing the heading “Electrons”.
26. From the menu at the top of the screen, select Insert:Columns. A new, blank column should appear between the “Neutrons” and “Electrons” columns.
27. Label this column “Mass Number”. Excel will assume it too is a heading, and format this heading like the others! You’ll need to adjust the column width slightly to make it fit. (See step 10!)

Carrying out Calculations

28. Select cell D2 in the spreadsheet.

29. The mass number for ^{52}Cr is the sum of the number of protons (in cell B2) plus the number of neutrons (in cell C2). To conduct this calculation, first type an “=” sign. Then, click on cell B2. (The “formula entry window” near the top of your screen will now show “=B2”.) Next, type a “+”, and finally click on cell C2. When you hit return or enter, the entry in cell D2 should automatically change to show the correct mass number for ^{52}Cr, 52. If you move your selection cursor back onto cell D2, you’ll see that the formula entry window shows the formula for this calculation is “=B2+C2”. You could have just typed that in directly, but generally it is easier to use the mouse to “point” to the cells you want to use as you put together a formula.
30. Because the mass number is the sum of two exact values, it too is *exact*. If Excel didn't already do it, select cell D2 and underline its contents (⌘U) to indicate that this numerical result is *exact*.

The mass number is used to specify which isotope is being considered. In the table you have prepared, the mass number is incorporated into the name of the isotope. Note that the ‘=’ communicates to Excel that the cell contains mathematical instructions. A wide variety of mathematical operations can be carried out in this fashion. The standard symbols include + (addition), - (subtraction), * (multiplication), and / (division), as well as ^ (raised to a power). To represent a number in scientific notation, use the letter e in a number to represent 10 raised to a power. For example, 6.02e23 is interpreted by Excel to mean 6.02×10^{23}. What about the other mass numbers for our new column? You could repeat the process above for each isotope, but this isn’t necessary! There’s a much easier way:

31. Select cell D2, which contains the formula for the first mass number.
32. You’ll note that there’s a small square in the lower right hand corner of the blue shading around cell D2. Move your mouse over it, and the pointer will change into a thin, non-hollow **+** symbol. Once your mouse pointer has transformed, click and drag (click, then move the mouse while holding down the mouse button) through the three empty cells below. When you release the mouse button, you should see the other mass numbers automatically appear!

By clicking and dragging that little blue square, you have copied the formula in cell D2 into the cells below it. Excel modifies the formula as it copies it, so that the same calculation is conducted in each cell, but using the corresponding data from each row. Spreadsheet applications are extremely useful when working with repeated calculations or large quantities of data, because they have been designed to make it easy to manipulate formulas in this way.

Next, we will calculate the mass of a single atom of each isotope. As you might expect, an excellent approximation for the atomic mass should be the sum of the masses of the component subatomic particles. The atomic mass unit (amu) is typically associated with masses of this magnitude. 1 amu = 1.66054×10^{-24} grams. Our goal now is to calculate the approximate atomic mass of each isotope efficiently, without re-typing the necessary conversion factors four times. To this end,

33. Type “Proton mass =” in cell A7, type “1.00727” in cell B7, and type “amu” in cell C7.
34. Type “Neutron mass =” in cell A8, type “1.00866” in cell B8, and type “amu” in cell C8.
35. Type “Electron mass =” in cell A9, type “5.4858e-4” in cell B9, and type “amu” in cell C9.
36. Column A will not be quite wide enough to hold some of these entries: if you don’t remember how to fix this, refer back to what you did in step 10! Adjust the column width to accommodate A7:A9. Also, format those cells such that they are aligned against the right edge of each cell. To do this, set the horizontal alignment to “right”, (the third icon over) using the formatting palette.

In an attempt to help you out, Excel will underline the proton and neutron masses to make it look like the other numbers you’ve put in. Thanks, E, but no thanks! These masses are not exact! So, to fix it:

37. Select B7:C7, then click on the **U** icon at the top of the screen, or use the keyboard shortcut ⌘U.

Excel will also not display the mass of the electron with the correct number of significant digits. (*&@%! Alas, Excel is clearly rather clueless about significant figures!) Here's how to remedy this:

38. Select cell B9, then use your favorite trick to get to a formatting window or palette.
39. You'll note that the "Number" format has already (automatically) been changed to "Scientific". To correct the number of significant figures, adjust the number of decimal places until the value in the sample window has the correct number of significant digits. If you are using the formatting palette, click the light blue arrows next to .00 and .0 next to "Decimal:" under "Number".

We need to do a little more formatting now, to prepare a new table for the data we are about to calculate. Our new table will involve the same isotopes as does the table at the top of the spreadsheet. We could easily transfer the appropriate heading and entries from the table above by copying and pasting them, but let's learn another potentially useful way to do essentially the same thing. The advantage of this approach is that if you make any changes in the top table, the bottom table will automatically change to reflect them:

40. In cell A14, type "=A1". That's right, we've entered a simple formula that involves *text*, which is not only possible, but often handy when working in a spreadsheet! You'll see A14 now contains the contents of cell A1.
41. Copy the formula in cell A14 into A15:A18, either by using the copy and paste commands, or by clicking and dragging the blue square on the selection box.
42. Now we need to format these new entries. There is an easy way to do this, since we have already generated other headings and data, and formatted them as we would like them to appear, up at the top of the sheet. On the "toolbar" near the top of the screen, just below the menu, there's a small paintbrush with deep blue paint on it, called the "Format Painter." To quickly copy the formatting of the table above, select A1:A5., then click the Format Painter paintbrush icon, and finally click and drag over A14:A18. Neat, huh? You can quickly format entire tables this way, if you like.
43. Create a new column heading, "Mass of Component Particles (amu)" in B14, and use the Format Paintbrush to format it to make it like the other column headings: select A14, click on the Format Paintbrush icon, and then click on B14. Whoa, too wide, huh? And here, if we adjust the column width to make this monster fit, our other table will get all wacky…what to do? Well, click on cell B14 again, and then click between the words "Component" and "Particles" in the formula entry window at the top of your screen. Now, hold down the control and ⌘ keys at the same time, and while still holding them down, hit return. You'll see that a "line break" has been added to the heading text in the formula window. Hit return all by itself, and you'll see this forces the cell to grow upward, rather than outward, to accommodate the verbosity of its contents.
44. At this point, if Excel is set to start in the Page Layout view, the page break in the middle of your table may really start to annoy. If so, use View:Normal to fix it.

Ok, the table is now ready and waiting, and we are in position to set up the calculation:

45. Enter the following formula into cell B15: "= B2*B$7 + C2*B$8 + E2*B$9". The $ characters in the formula indicate that we plan to use these values as *constants* in subsequent calculations: when Excel copies this formula, it will not dynamically update the values with $ signs in front of them.
46. The mass of 24 protons + 28 neutrons + 24 electrons, 52.43013 amu, should (sort of) appear in cell B15. Center the contents of this cell. Excel will again mess up the significant figures, of course! How many should this entry have? Think about it carefully: the number of protons, neutrons, and electrons in each isotope are *exact*, but the component masses have a finite number of significant figures. Change the numeric format to "Number" and adjust the number of decimal places so that the calculation result has the correct number of significant figures.

47. Select cell B15, and then choose “Edit:Copy” from the program menu (or, just use the keyboard shortcut, ⌘C). A box with an animated black dashed line should appear around the contents of cell B15, indicating that it is ready to be copied.
48. Select cells B16:B18. Choose “Edit:Paste” from the program menu (or, use the keyboard shortcut ⌘V). Very nifty! This is an alternative to clicking and dragging the little blue box at the bottom of a selection: it accomplishes the same thing, but also works when the cells you want to copy to are not adjacent to the source cells, or not in a simple row or column. Inspecting cells A16 through A18, you’ll see that the formula in each has been changed to use the correct number of protons, neutrons, and electrons for each isotope (by referencing the appropriate cells in the table at the top of the spreadsheet), but the references to the component masses in cells B7:B9 have not changed. This is because of the $ signs in the formula!

If the constants weren’t indicated via the $ characters, Excel would have used data in B8, B9, and B10 to calculate the mass in cell B16. The $ characters “lock in” the constants so that the same cell is referenced in each calculation. The process of adding the $ characters establishes an “absolute cell reference.” Note that the cell row references without $’s *were* updated as you copied down!

The numbers in this new column are in the vicinity of the 51.996 amu listed in the periodic table for chromium, but none of the numbers match this value within their uncertainty windows. The atomic mass in the periodic table is the *average of the masses of the naturally occurring isotopes weighted according to their abundances*. Let’s conduct this calculation using Excel!

49. Enter “Average Component Mass =” in B11 and format the text so that the equal sign sits at the right edge of cell B11. (This is the same format used for the elementary particle masses, so you could also just copy that format with the format paintbrush, if you prefer.)
50. Enter “amu” in D11.

To calculate the *abundance weighted* average of the various isotopes' component masses, we need to express each abundance value in decimal form. Then, we will multiply this value by the component mass sum for each isotope in order to obtain the average component mass value:

51. Add the heading “Abundance” to cell G1.
52. In cell G2, enter the formula “=F2/100”. Format the result correctly (centered, and with the correct number of significant figures), and copy it to cells G3:G5.
53. Select cells G2:G5, then change the numeric format of these cells to “Percentage” using Format:Cells… or the Formatting Palette. Note that the numbers now appear with a % symbol after them, which means something numeric to Excel! The values stored in those cells are still less than one!
54. Add the heading “Component mass contribution (amu)” to cell C14. You could use the control-⌘-return key combination to add a line break, so that this heading doesn’t overflow the column, but since you did that already, it’s enough to simply use the Format Painter to copy the formatting of the heading in cell B14: when you do, the line break characteristics will be copied as well.
55. In cell C15, enter the formula “=B15*G2”. Copy this formula into cells C16:C18.
56. Format the entries in C15:C18 so that they are centered (like other data), and have the correct number of significant figures. *Be careful here! Not every entry in this column deserves to have the same number of significant figures (though they may have the same number of decimal places)! Think through the sig figs of the numbers involved in the calculation that leads to the result shown in each cell, and make sure that the result has the correct number of significant figures. Get in the habit of doing this, because Excel doesn’t do it for you!* ***You will often be graded on getting this right!***

57. The sum of the component values in C15:C18 is the weighted average component mass we need in cell C11. While we'll learn a more elegant way to do this shortly, for now, calculate this sum by entering the formula "=C15+C16+C17+C18" into cell C11.

Why is this value larger than the average atomic mass reported for chromium in the Periodic Table? Are the abundances incorrect? If you got 52.49 amu, the abundances are right…but an assumption we are making is wrong! Would you believe that the mass of a single Cr-52 atom is actually less than 52.4301 amu? It's actual mass is 51.94 amu! How is it possible that an atom's mass doesn't equal the sum of the mass of its component subatomic particles? It turns out that another fascinating factor is at work here that we haven't yet considered. When atoms are created from subatomic particles (in stars), a portion of the masses of the subatomic particles is converted to energy. The energy equivalent of this lost mass (called the "mass defect") can be calculated using Einstein's famous equation $E = mc^2$ (where c is the speed of light). Although we won't conduct this calculation today, it is the reason that our estimated average molar masses come out too high when we simply add up the mass of the component particles.

Alrighty, so let's enter the actual mass of each isotope, taking the mass defect into account, and see if that sets things right:

58. Enter "Actual atomic mass (amu)' in D14 and "Mass discrepancy (amu)" in E14. Using the Format Paintbrush tool, format the headings in these cells like the entry in cell B14.
59. Enter the actual masses for Cr-52 (51.94), Cr-53 (52.94), Cr-50 (49.95), and Cr-54 (53.94) into the cells below the Actual atomic mass heading. These masses take into account the mass defect phenomenon. Format this data appropriately.
60. Below the Mass discrepancy heading, enter formulas that calculate the difference between the mass of the component particles and the actual atomic mass. (Subtract the smaller value from the larger value.) Format the results so that they have the correct number of significant figures. (You may have to reduce the width of the column, if it is automatically increased by Excel.)
61. Type "Average atomic mass =" into cell B12, and format it like B11. Put "amu" in D12.
62. Add and format the heading "Actual mass contribution (amu)" to cell F14.
63. In F15:18, set up a formula analogous to that in C15:C18, which calculates the product of the actual atomic mass and the abundance of each specific isotope. Format these results correctly.
64. Calculate the weighted average of the actual atomic masses by setting up a formula that determines the sum of F15:F18 in C12. Make sure your result has the correct number of significant figures.

At last, your average atomic mass result should match the value given for chromium in the periodic table! Keep in mind that no chromium atoms of mass 52.00 amu actually exist – this is only an average value based on the abundances of the naturally occurring isotopes!

The Function Wizard

In addition to the mathematical operations that can be performed within cells, Excel has the capability to perform a wide range of calculations using the "Function Wizard." This wizard can be activated by selecting the button labeled f_x in the toolbar at the top of the screen, or by selecting Insert:Function… from the pull-down menu at the very top of the screen. Let's use the Function Wizard to carry out some sample calculations on our data, to demonstrate its capabilities.

Let's calculate the sum of the abundances for our four isotopes, and store it in cell F6:

65. If you have activated the Function Wizard, hit ESC or click cancel to close it.
66. Enter "Total (%) Abundance =" in E6 and align this entry on the right edge of cell E6 by selecting the third icon next to "Horizontal" under "Text Alignment" in the Formatting Palette.

67. Move to cell F6 and activate the Function Wizard using one of the two methods outlined in the paragraph at the start of this section. A window entitled “Paste Function” should appear.
68. Select “Math & Trig” from the “Function category” list.
69. Select “SUM” from the list of Function names, and then click “OK”.
70. Type F2:F5 in the box adjacent to “Number 1” in the “SUM” box, and then click on “OK”.
71. Format the result in F6 so that it is centered, and verify that it has the correct number of sig figs.

To illustrate an important difference between the data in column F and the data in column G, let’s determine the sum of the abundance values in column G. We’ve already set up a function that calculates the sum of cells F2:F5, so simply copying it to a cell one column to the right should produce the analogous result for column G:

72. With cell F6 selected, select Edit:Copy, or use the shortcut, ⌘C.
73. Move to cell G6, and select Edit:Paste, or use the keyboard shortcut, ⌘V.

Note that the sum of the abundances in column G is 1.0000 (you'll need to correct the significant figures, but Excel should get this numerical value), because “83.79%” actually means 0.8379: “%” is simply shorthand for “× 0.01!” This is actually the best way to store and use percent data in a spreadsheet, because multiplying such values by the value of a whole gives the number of that type, as when you used the data in column G to determine the mass contributions in C15:C18 and F15:F18.

Excel provides multiple ways to enter data into a function. To illustrate another method, let’s calculate the average of the mass discrepancies, and store it in cell F8:

74. First, type “Average mass discrepancy =” in E8 and format it as you did cell E6.
75. With cell F8 selected, activate the Function Wizard. Select the “AVERAGE” function from the “Statistical” subset of Excel functions, and click “OK”.
76. Click the ≐ icon next to the “Number 1” box. The whole spreadsheet should be displayed.
77. Select cells E15:E18 by clicking and dragging over them, and then hit return. You’ll see that E15:E18 is now entered next to “Number 1” in the data entry box for the Average function.
78. Click on “OK”, and you should find that the (non-weighted) average of the mass discrepancies for the four isotopes now appears in cell F8. It has units, so be sure to put them in cell G8. Also, averaging is a mathematical operation, but a familiar one, so figure out how many significant figures the result in cell F8 should have, and format it appropriately!

Once you learn the names of the most-commonly used functions, you can bypass the function wizard altogether, and enter them by hand, if you like. For example, the result in cell F8 could have been attained by typing “=AVERAGE(E15:E18)” directly into the cell, or by typing “=AVERAGE(“ and then clicking and dragging to select cells E15:E18.

The Chart Wizard

Now, let’s learn how to use Excel’s Chart Wizard. We’re going to make a bar graph with our chromium isotope abundance data. Excel calls a bar graph with vertical bars a “column graph.” The easiest way to use the Chart Wizard is to start by selecting the data you want to graph. Doing this correctly makes things go much more smoothly later on, and there are some tricks to learn! Here goes:

79. We will want to plot the abundance values in cells G2:G5, so start by selecting them. These values will provide our y-axis data.
80. However, we also need x-axis data! What do these abundances describe? Well, they are the abundances of the four isotopes in column A. So our x-axis data is that in A2:A5. If we were to click and drag on those normally, we’d lose our selection of cells G2:G5, but here we want to tell

the chart wizard that our x data is in A2:A5, *and* that our y-axis data is in G2:G5. To do that, we need to select both sets of values, *simultaneously*. How to do it? Hold down the ⌘ key while clicking and dragging over A2:A5! Once you have A2:A5 *and* G2:G5 highlighted in light blue, you have all your x-axis and y-axis data selected, and are ready to activate the chart wizard!

81. Activate the Chart Wizard by selecting Insert:Chart from the main menu, or by clicking on the Chart Wizard icon on the toolbar at the top of the screen. The Chart Wizard icon is a tiny column graph, and is located three icons to the right of the Function Wizard icon.
82. The long list of possible graph types is listed under “Standard Types”. Select “Column”, and the standard sub-type (“Clustered Column”) in the upper-left-hand corner of the available options.
83. To preview the general appearance of your graph, click on “Press and Hold to View Sample”.
84. Click on “Next >” twice, as we started out with the correct “data ranges” already selected, and Excel is actually smart enough to figure out that the numbers are the y-axis data in this case!
85. In the “Chart Wizard – Step 3 of 4 – Chart Options” window, you’ll want to add an *appropriate* title and axis labels to your graph. A good chart title says what the chart is *for*, or what it *represents*, rather than simply stating the obvious, that y is plotted against x. Please avoid the temptation of generating the title of your plots by simply combining the x- and y-axis labels!
86. Select the “Titles” tab and then:
87. Enter “Terrestrial Abundance of Chromium Isotopes” in the “Chart title” entry box.
88. Label the Category (x) axis “Isotope”
89. Label the Value (y) axis “Natural Abundance”
90. Select the “Legend” tab and uncheck the “Show Legend” box. (It’s not helpful in this case!)
91. Click on “Next”. You’ll see that you have the option of placing your plot on a separate sheet in the workbook, or of inserting it as an object in the current sheet. Generally, in order to save paper, we’d prefer that you keep your data and charts on the same page. The exception to this would be cases where there isn’t enough room on the sheet to print the chart at a useful and legible size: in those cases, a separate sheet for the plot is appropriate. In this case we have room to spare, and this chart need not be very large to do its job: so make sure that the radio button in front of “As object in:” is selected, and click “Finish”. Your graph should appear in your spreadsheet.
92. Move the graph to the left edge of the sheet and slightly below the data by clicking on an “empty” portion of the chart (one of the corners of the white space should work) and dragging. If you move only one element of the chart by mistake, you can undo whatever you did by hitting ⌘Z, which is the keyboard shortcut for the very handy (“Ooops!” reversal) command Edit:Undo.

That’s it! We’re done with our work on chromium isotopes. So, it’s time to save and print out what we’ve done. First, let’s save our work (something that you should get in the habit of doing often!):

93. Select File:Save As… from the main menu. In the “Save As:” box, type “Chem 115 Expt 2 – XXX”, replacing the XXX with your initials. Make sure that “Where:” is set to “Desktop”, and that “Append File Extension” is checked. Then click on “Save”.

One more procedural step – we want to make sure that it’s clear this is your work! So, let’s insert a few lines at the top of your spreadsheet, and use them to identify you and the objective of this spreadsheet!

94. Select A1:A2. (Cells A1 and A2 should have a thick, light blue line around them.)
95. Select Insert:Rows from the main menu. Two empty rows should appear.
96. Enter the following in (now empty) cell A1, replacing the *Names* below with your actual name(s): ”Chemistry 115 Experiment 1 – *Name 1* and *Name 2*”

Please get in the habit of including your name and the experiment number at the top of all of your spreadsheets! Okay, now, let's print out what we've done. In order to make our printed page come out nicely formatted, to make good use of the space available on the page, and to keep our printout to the minimum number of sheets, there are a few tricks we want you to learn here, too:

97. Make sure that you have a cell in the spreadsheet selected, not the chart, or the following steps will operate on the chart only, rather than the entire spreadsheet!
98. Select File:Print Preview from the main menu. If you click on the bright green arrow at the top of the resulting view, you'll see that your document currently spills across two pages. That not only makes it very hard to read, but it wastes paper – so here's an easy way to fix it!
99. Click the "Setup" button on the Print Preview toolbar. On the Page tab, select the radio button in front of "Fit to:", and set the document to print to 1 page wide by 1 page tall. Then click OK.

You should now see that the bright green arrow is dimmed out, and that your entire spreadsheet is showing up on a single page in the Print Preview window! Handy, huh? However, we can still do better. You'll see that there is a lot of empty white space in the bottom right corner of the page – space that could be put to good use making the plot bigger and easier to read! Here's how to do that:

100. Click on the words "Page Break Preview" on the toolbar.

As Excel will tell you, in this view you can change the spreadsheet and see the impact the changes have on the page breaks, that is, the way the spreadsheet will print on paper. Because we have told Excel to keep our spreadsheet on one page, it will automatically move the page breaks (the dark blue lines) for us. But in other cases it can be very handy to move the page breaks yourself.

101. Click on an empty corner inside your chart to select it. (It will have a dark line around it.)
102. Use the mouse to move your pointer over the black box in the lower right corner of the box around the plot. This is called a "handle." Click and drag the handle down and to the right while holding down the shift key: this will resize the plot while maintaining its aspect ratio. Extend the plot's lower right corner so that it ends at the right edge of Column G: this will cause it to print large enough to fill the page. You'll see that the blue page break line is automatically moved so as to keep the entire spreadsheet on a single page.
103. Return to the Print Preview screen by selecting File:Print Preview. Remember that you need to select a cell in the spreadsheet if you want to print or work with the entire spreadsheet! If you are seeing only the chart, it's because you had it selected when you went to Print Preview. (Close and click on a cell somewhere in the spreadsheet to de-select the plot, then go to Print Preview again!)
104. Provided the Print Preview looks good, print your spreadsheet by clicking on the printer icon, just to the right of "Setup" on the Print Preview toolbar. The default options here should all be good, just click on "Print" to print *one* copy of this spreadsheet. You don't need two!
105. To return to the normal view, select View:Normal from the main menu.

Because we are going to add to the work we have done so far, we will label what we have done on this "sheet" of the "workbook" (the collection of "sheets" in our spreadsheet program) before we proceed:

106. At the bottom of the screen you will see three "tabs," labeled "Sheet 1", "Sheet 2", and "Sheet 3". If you double-click on "Sheet 1", you should see that the name of the tab becomes blue, and you will now be able to rename (the tab of) the top sheet. Change the name to "Chromium Isotopes".
107. Next, click on the tab labeled "Sheet 2" to bring up a blank sheet, which you will use in the next part of this experiment –where you'll learn how to use scatter plots and trendlines!
108. You'll probably want to set View:Normal here, as well, so you don't see the page breaks.

Objective II: Calculation of the Atomic Spectrum of Hydrogen

We will now turn our attention to the electronic structure of the hydrogen atom, so:

109. Double-click on “Sheet 2”, on the tab at the bottom of the worksheet. It should turn light blue, and you can then change it to read “Atomic Spectrum”. Hit enter to save your changes.

This will put you in cell A1, at the top of a fresh sheet. As we learned above, we want to label each sheet with your name and the experiment number, as we did on the first sheet. Since we have already done this on the first sheet, the easiest thing to do is to copy what we did there:

110. The tab attached to the Chromium Isotopes sheet may have scrolled off of your screen. To get it back, click on the ◄ symbol in the bottom left corner of the screen. Then click on the Chromium Isotope tab, to bring up the sheet with the Chromium Isotopes analysis. If it is still tiny, select View:Normal to get out of Page Preview mode.
111. Select and copy the contents of A1, where your name and the experiment number are stored.
112. Click on the tab labeled “Atomic Spectrum” to return to that sheet, and then paste into cell A1.

One of the things we hope you take away from this course is an understanding of the “electronic structure of atoms.” What does this mean? The key concept is that the electrons have wavelike properties that restrict them to possessing only very specific, “allowed” energies. You may have already heard about electron “shells” or perhaps even “orbitals” as part of your pre-Macalester chemistry experiences. The “shell” or “orbital” designation for an electron provides some information about its energy. The objective of this Excel activity is to introduce you to some key ideas regarding possible energies of electrons in the hydrogen atom.

When a hydrogen molecule is subjected to a very high voltage, the single bond holding its two constituent atoms together breaks, and the two hydrogen atoms separate. The high voltage then causes the single electron in each hydrogen atom to become “electronically excited.” An “excited” electron is one that possesses a higher energy than the minimum for an electron in hydrogen. We say that an electron in hydrogen at the minimum energy possible is in the “ground state.” The ground state energy level is labeled $n = 1$. An excited electron could be described as occupying an energy level with an n value from 2 to any integer value approaching infinity. Each level corresponds to a specific energy.

An electron is most stable in the ground state ($n = 1$) and there is a natural tendency for excited electrons ($n = 2$ or greater) to release energy to ultimately arrive in the ground state. The released energy can be in the form of a photon of x-ray, ultraviolet, infrared, or visible radiation, depending on the difference in energy between the energy levels occupied by the electron before and after the change. Consequently, if we can measure the energy of the photon released when an electron moves from one level to another, we have determined the difference in energy between the energy level occupied by the electron before the transition, and the energy of the level it fell into. This concept of energy levels and released energy is portrayed diagrammatically in Figure 1, on the following page. Please note that this figure is only representative, and the energies shown don’t correspond to those in any real atom.

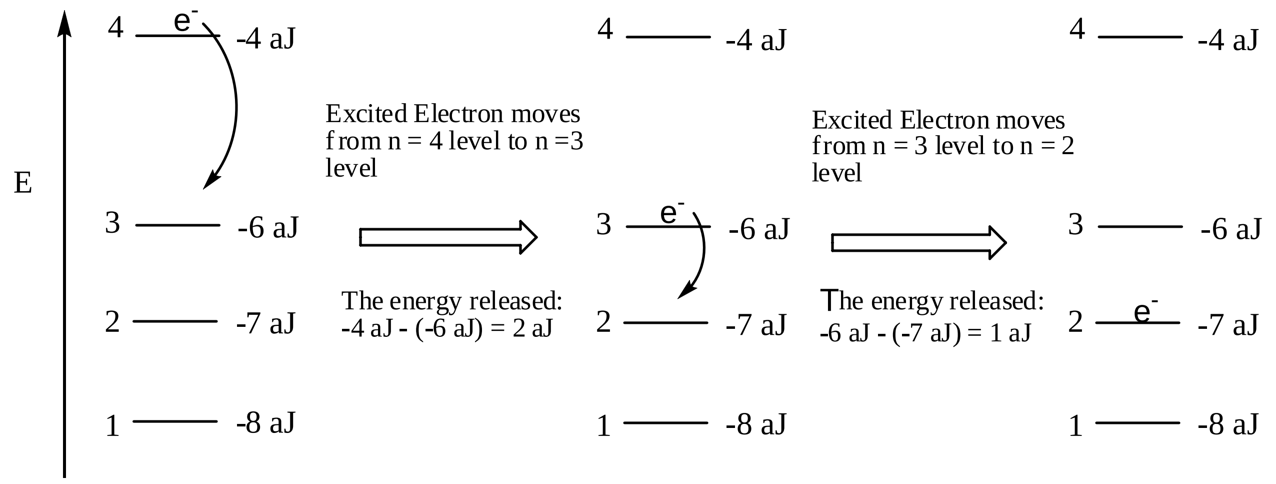


Figure 1: The Relationship between Released Energy and the Difference in Energy Between Levels

In this representation, the excited electron starts in the $n = 4$ level with an energy of -4 aJ. The Joule (J) is the SI unit for energy, and 1 aJ ≡ 10^{-18} J. The electron moves from the $n = 4$ level to the $n = 3$ level, and thus lowers its energy to -6 aJ. The difference in energy between the two levels (2 aJ) is released (or emitted) as a photon. In the next step in Figure 1, the electron jumps to the $n = 2$ level and emits a photon with 1 aJ of energy. Note that excited electrons aren't limited to jumping between adjacent levels (as the electron is shown doing in Figure 1). It would certainly be possible for an electron to jump directly from $n = 4$ to $n = 1$. In that case, a 4 aJ photon would be emitted. Intermediate jumps, for example from $n = 4$ to $n = 2$, and then from $n = 2$ to $n = 1$, are also possible.

The main point is that a measurement of the emitted photon's energy provides information about the separation between the energy levels. As mentioned earlier, the energy released when an excited electron drops to a lower level is emitted as either x-ray, ultraviolet, infrared, or visible radiation.

The next part of this experiment will provide you with a glimpse of the photons emitted by excited hydrogen atoms (the excitation occurring as a result of subjecting hydrogen molecules at low pressure to a very high voltage). You will find that the overall (visible) color of the light emitted by the excited hydrogen atoms is perceived by your eyes as pink; this indicates that some visible radiation is emitted as excited electrons drop into lower levels. We can use a diffraction grating to separate the pink color into its component colors - each component color will correspond to the energy difference between two hydrogen atom energy levels.

Go to where the hydrogen spectrum tube has been set up and examine these colors (often referred to as the atomic spectrum of hydrogen)! Notify your lab assistant or lab instructor when you are ready to look at the spectrum. Take care when moving near the hydrogen sample, since the device that contains it generates a very high voltage, well in excess of 10,000 Volts.

If all went well, the pink color of the excited hydrogen atoms should have separated into three (possibly four) visible lines upon employment of the diffraction grating: violet, blue-green, and red. To find the energy level separations that correspond to these colors, we must convert these colors to energies. We'll use Excel and material from Chapter 1 of Jones and Atkins/Chapter 15 of Oxtoby/Chapter 7 of Silberberg to conduct these calculations. These topics will be discussed in class very soon, so don't worry if some of the steps seem nebulous at the moment.

You may have heard of the "wave-particle duality" before; applied to photons, it means that they simultaneously exhibit properties of both particles and waves. The color of light is determined by its characteristic wavelength. Each color of the visible spectrum has a unique wavelength. A common unit for wavelength, the distance between any point on a wave and the corresponding point on the next wave, is nanometers. One nanometer is one billionth of a meter, or 10^{-9} m.

It turns out that all of the *visible* radiation emitted from excited hydrogen atoms is the result of electrons moving from higher levels to the $n = 2$ level. Transitions to the ground ($n = 1$) level emit ultraviolet light, which our human eyes cannot detect. If you have ever tanned at a tanning salon, you have been bombarded with ultraviolet radiation from mercury (Hg) atoms that were excited with a very high voltage, just as the hydrogen atoms were in the tube today. In fact, the fluorescent lamps in the ceiling above you also contain mercury vapo(u)r, but they are coated with a fluorescent material that absorbs the ultraviolet light and converts it to visible light. (Because mercury is toxic, it is very important to avoid breaking fluorescent light tubes, and to recycle them properly!)

Alright, let's get back to the atomic spectrum of hydrogen! The table below quantifies some important information about the lines you should have seen in the atomic spectrum of hydrogen. While there is some uncertainty in the wavelength measurements (specifically, ± 0.1 nm), the *n* values in the table are *exact*. Thus, they are underlined, to indicate they have no uncertainty. (Were they not underlined, they would each be understood, in light of their significant figures, to be ± 1.)

Spectral Emission Data for the Hydrogen Atom

Emitted Color	Wavelength (nm)	Initial n	Final n
(near) Ultraviolet	410.2	6	2
Violet	434.0	5	2
Blue-green	486.1	4	2
Red	656.3	3	2

113. Copy the table above into the first four columns of your new spreadsheet. Be sure to format the headings at the top of each column so that they can be read, and are clearly differentiated from the data. (You can copy the formatting from the Chromium Isotopes sheet, if you like.) Also, be sure that the contents of your spreadsheet indicate the correct number of significant figures. (This includes ensuring that the *n* values are underlined, to indicate that they are exact!)

Our initial objective is to convert the wavelength values in the table above into their associated energies. For the sake of unit consistency, we will convert our nanometer wavelengths to meters before conducting this calculation. Let's use Excel to our full advantage to accomplish this objective. Start by setting up the constant $\underline{1}$ nanometer ≡ $\underline{1 \times 10^{-9}}$ meters, as follows:

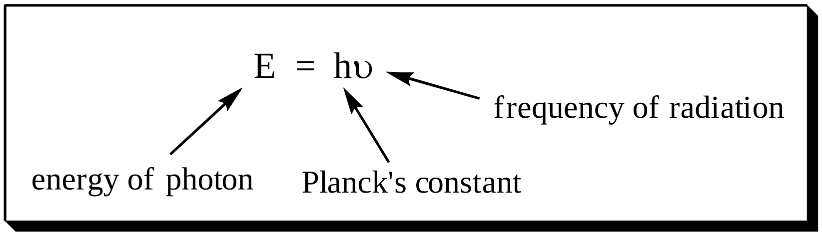
114. Move to column A, in a cell just below your table. Enter and format "1 nanometer =" in the A cell, "1e-9" in the B cell of the same row, and the units, "meters" in the C cell. One nanometer is *exactly* $\underline{1 \times 10^{-9}}$ meters (by definition), so format it as scientific, with zero decimal places, and underline it (to indicate that it is exact).
115. Add a new column to the right side of your table, with the heading "Wavelength (m)". Populate the column with an equation that uses the constant prepared in the previous step (as a locked constant – use $ in that cell reference) to calculate the wavelength of each color of light in nanometers. Format the results in scientific notation with the correct number of significant figures.

The wavelength of electromagnetic radiation such as light is related to its frequency (the number of cycles the wave undergoes per second) by the following equation:

$$\text{frequency} = \frac{\text{speed of light (m/s)}}{\text{wavelength(m)}} \; [=] \; {}^{1}\!/_{s} \; [=] \; \text{Hertz(Hz)} \qquad \text{- or, symbolically -} \qquad \nu = \frac{c}{\lambda}$$

116. Just below your nanometer to meter conversion factor, set another constant. This will be the "Speed of light", which is 3.00×10^{8} meters per second (and IS NOT EXACT).
117. Use the formula given above, along with the constant you just created, to add another heading to your table, "Frequency (1/s)", and calculate values for it. Be sure to use a locked constant ($), and ensure that your results show the correct number of significant figures.

The energy of a photon is related to its frequency by Planck's Law:



A "photon" is a "packet" of energy. The wave-particle duality of light means that the blue radiation emitted by excited hydrogen atoms can be *simultaneously* considered to consist of waves with a wavelength of 434.0 nm and as a stream of photons, each possessing exactly the same amount of energy, with the amount of energy tied to the wavelength and given by Planck's Law.

Let's calculate the photon energy that corresponds to each color that you observed. You'll want to start by adding Planck's constant, 6.626×10^{-34} J·s, to your spreadsheet, as a constant:

118. Below the speed of light, define Planck's constant in your spreadsheet.
119. Our first table is getting about as wide as the screen, so start a new table, below your constants. In the leftmost column, copy the heading and contents of the first column of the table above (emitted colors). Give the next column to the right the heading "Photon Energy (J)". Use Planck's constant and Planck's Law to calculate the data for this column.

A famous equation was developed to calculate the energy difference between any two energy levels in a hydrogen atom, if the initial and final values of *n* are known:

$$\mathrm{E_{photon}} = \Delta\mathrm{E_{electron}} = \mathrm{R_H}\left(\frac{1}{n^2_{\text{final}}} - \frac{1}{n^2_{\text{initial}}}\right)$$

In this expression, $\mathrm{R_H}$ is called the Rydberg constant, and it is the same for any pair of *n* values. We can find the Rydberg constant by manipulating this equation and then graphing our data appropriately. The equation above can be *linearized* – made to match the equation of a line, $y = \mathrm{m}x + \mathrm{b}$ – because our data all has the same n_{final} value, 2. As a result:

$$\mathrm{E_{photon}} = \mathrm{R_H}\left(\frac{1}{n^2_{\text{final}}} - \frac{1}{n^2_{\text{initial}}}\right) = \mathrm{R_H}\left(\frac{1}{n^2_{\text{final}}}\right) - \mathrm{R_H}\left(\frac{1}{n^2_{\text{initial}}}\right) = \left(\frac{\mathrm{R_H}}{2^2}\right) - \mathrm{R_H}\left(\frac{1}{n^2_{\text{initial}}}\right)$$

$$\mathrm{E_{photon}} = -\,\mathrm{R_H}\left(\frac{1}{n^2_{\text{initial}}}\right) + \left(\frac{\mathrm{R_H}}{4}\right) \quad \Leftrightarrow \quad y = \mathrm{m}x + \mathrm{b}$$

$$\text{where} \qquad y = \mathrm{E_{photon}}, \quad x = \left(\frac{1}{n^2_{\text{initial}}}\right), \quad \mathrm{m} = -\mathrm{R_H}, \quad \text{and} \quad \mathrm{b} = \left(\frac{\mathrm{R_H}}{4}\right)$$

Consequently, a plot of the energy of the various photons versus $1/n^2_{\text{initial}}$ should yield a linear relationship, with the slope of the line (m) equal to $-\mathrm{R_H}$ and the *y*-intercept equal to ¼ of $\mathrm{R_H}$.

Okay, let’s set up the data we have for graphing, in accordance with this insight:

120. Continue adding to your second table. The third heading should be $1/n^2_{\text{initial}}$. Believe it or not, you really can enter this into Excel – the trick is to highlight specific elements and then format them individually. Start by typing “1/n2initial” into the cell. Then use your mouse to highlight *just* the letter n. Next, choose Format:Cells from the menu at the top of the screen, or just use the keyboard shortcut, ⌘1. Change the font style of the letter n to “Italic”. Next, select just the number 2. Use Format:Cells or ⌘1 again, and this time check “Superscript” under “Effects”. The same trick will allow you to subscript the entire word ‘initial’ – just select and format it all at once.
121. Calculate values for $1/n^2_{\text{initial}}$, and thereby fill in the column. Note carefully that because each n value is exact, $1/n^2$ is also an exact number, and should be underlined. In order to show these values correctly, with no rounding, set their numeric format to “Fraction – Up to two digits.”

You have just prepared a column containing the *x*-axis data for the plot we want to prepare. The last column of your second table should contain the data for the *y*-axis of your plot to determine R_H.

122. Set up and populate that column, keeping significant figures in mind.
123. Next, select the *x*- and *y*-axis data in the table (do not include the column headings in your selection), and activate the Chart Wizard.

Scatter Plots and Linear Regression

Every experiment in this course that requires the use of a spreadsheet to plot data involves the generation of what Excel calls “XY (Scatter)” plots. These plots differ in a critical way from the column chart you prepared in the Chromium exercise, in that the *numerical values* of the entries for the x-axis are important. *(In a column chart, and indeed in most Excel chart types, the x-axis data is always treated as text: if you use a chart like this to plot x-y numerical data, the x-axis data will always be treated as a linear series, like 1, 2, 3, etc., no matter what it actually is! The correct value for each data point can be made to appear under the relevant point on the x-axis, but the equation of the best-fit line in the chart will still be incorrect. This is a common source of confusion, frustration, and error, so please learn to do this right, here and now!)* The take-home message in this exercise is that from now on, you should use only the “XY (Scatter)” chart type in science! Here’s your first opportunity:

124. Select the “XY (Scatter) category from the Chart type heading in the Chart Wizard. Choose the default chart sub-type, the one with no lines on it, and click the “Next >” button.

Important note: A key decision here is which column should be designated as the x-axis data, and which should be the y-axis data. Should the graph plot “$1/n^2$” (y) versus “E_{photon}” (x), or should it be of “E_{photon}” (y) versus “$1/n^2$” (x)? Well, generally, the correct variable to put on the *y*-axis should be *dependent*, while the *x*-axis data is called *independent*. The *dependent* variable is determined *experimentally*. The *independent* variable is the one known by the experimentalist before the value of the *dependent* variable is measured, and it is usually under his or her control. That’s not so helpful here, because we didn’t actually let you measure the data in the tables. However, the photon wavelengths were the “measurement,” and they led to the E_{photon} values, so those would be the *dependent* values in this instance. However, here we are *linearizing* an equation, so the considerations just described are trumped by the need to plot the data in accordance with the linearized equation. As discussed above, we should get a linear plot with slope $-R_H$ if (and only if) we put E_{photon} on the *y*-axis, and $1/n^2$ on the *x*.

125. Excel should plot the data correctly in this case, so just click “Next >” again to move on to step 3.
126. Provide an appropriate title and axis labels for the plot. (You will not be able to add italics or super/subscript formatting at this point, but you can go back and add it once the chart has been created, using the technique you just learned for formatting cell entries.) Remove the “Major

gridlines" from the *y*-axis, by unchecking the appropriate box on the Gridlines tab. Choose to not show the legend (on the legend tab). Then click on "Finish".

Now, we want to add a linear trendline, and its equation, to the chart, along with the R^2 value of the regression analysis (the mathematical operation that leads to the trendline):

127. With the chart selected (with a dark black line around it), choose Chart:Add Trendline… from the menu at the top of the page. (If the chart is not selected, the Chart menu item won't be there!)
128. Choose the (default) linear regression on the "Type" tab, then click over to the "Options" tab.
129. Click the checkboxes in front of "Display equation on chart" and "Display R-squared value on chart". Then click on "OK".

The resulting plot should show all of your data falling on the trendline, and have an R^2 value of 1. However, you'll note that the nice little plot that emerges from this process, makes rather poor use of the chart space. This can't just be left as it is! We need to remedy this shortcoming to get a good plot:

130. Double-click on the numbers that make up the y-axis, currently ranging from 0 to 6×10^{-19}. This should bring up a "Format Axis" window. Click on the "Scale" tab. Looking at the data we are plotting, we see that it is all between 3 and 5×10^{-19} Joules. Excel's automatic selections for chart axis limits tend to be far too coarse for the production of useful scientific plots.
131. Change the "Minimum" value to 3e-19, the "Maximum" to 5e-19, then click "OK". There are no "right" values for these limits, but you should always adjust your plot axes so that your data occupies the majority of your chart's area, and is not shunted off into a corner.

In this case, we don't need to do the same thing for the x-axis, but generally, be prepared to manually rescale *both* axes when generating a plot in Excel, such that the data fills the chart area reasonably well.

Another important issue worth considering is how many significant figures should be included in the equation of the line. Remember, Excel is clueless about this, so you have to do the thinking, and format the equation of the line appropriately. Excel is currently displaying the slope with one significant figure. How many should it have? Well, slope results from a combination average and division operation. It's hard to know just how much uncertainty to give it. We will ask you to use the following guidelines:

- Slope is defined as rise over run, or change in *y* over change in *x*. Each change is a difference, but they vary in size, and may have different numbers of sig figs. What to do?
- Use the biggest difference on each axis: that is, consider the difference between the largest and the smallest *x*-values, and determine how many significant figures that difference has. In this case, the *x*-axis values are exact, so their difference has an infinite number of significant figures. In contrast, the *y*-axis values range from 3.03×10^{-19} to 4.85×10^{-19} Joules. The difference between these is 1.82×10^{-19} Joules, which has three significant figures.
- The slope is calculated by dividing rise by run. This means that the number of significant figures in the slope should be the *lesser* of the two sig fig counts you just calculated: the number of significant figures in the difference of the largest and smallest x-values, and the number in the y-axis range.

(Note: With large amounts of very accurate data, slopes can actually be appreciably more reliable than this estimation method suggests.) In order to get the equation of the trendline to show the correct number of significant figures in the slope:

132. Double-click on the equation of the trendline. This will bring up a "Format Data Labels" window.
133. Click to the "Number" tab, and change the "Category" to "Scientific". Adjust the number of "Decimal places" to ***one less*** than the number of significant figures that the slope should have.
134. Verify that the value shown in the "Sample" box has the correct number of significant figures (the same number that the slope should have), then click "OK"

You'll notice that the y-intercept ("b value") and R^2 value both change to the numeric format of the slope. This may not be the correct number of significant figures for each of these, but we will usually only worry about getting the significant figures of the slope to show up correctly. We'll tell you if any exceptions arise; otherwise, always just make sure that the sig figs in your slopes are correct.

The slope of your graph should equal $-R_H$, the Rydberg Constant ($2.18 * 10^{-18}$ J). The *y*-intercept (b) should be equal to one fourth of the same value. Because our data here is exceptionally good, these two estimates of R_H agree perfectly. However, what if they didn't? (That's entirely possible, because measured scientific data has some uncertainty in it!) Well, slopes are generally more resilient in the face of bad data than are intercepts, so if these two estimates did not agree, the slope-derived R_H value would be the one to go with. It would be more accurate, less susceptible to the effect of (random) error.

The R^2 value measures the strength of the linear association between the variables, and is sometimes called the correlation coefficient. It can range from 0 to 1. A correlation coefficient (R^2 value) of exactly 1 indicates a perfect linear relationship, and a perfect fit - all points lie exactly on the trendline. That's very rare in science, but it can happen in cases (such as this one) where the data and the theory are both very good. (In truth, our R^2 value here isn't *exactly* one, but it rounds off to that value, at least out to the third decimal place!) More often, R^2 values of less than one are obtained, indicating that the data points don't fall exactly on the line. R^2 gets smaller as the discrepancies grow larger, and determining the *reason* for such discrepancies is a key challenge in science. There are two types of deviation from a linearization model, and it is important to understand the difference:

- *Random* deviations from linearity generally reflect shortcomings in one's equipment and methodologies, rather than an inadequacy in the theory. These are most common.
- *Systematic* deviations from linearity can be caused by calculation errors, systematic errors in the laboratory, or by a failure of the theory that is being applied. If you see a systematic error, be careful! Try to ensure that it isn't the result of a calculation error.

It is important to realize that an R^2 value can't really tell you if you have a "good fit!" It can tell you if you have a perfect fit, but that is very rare indeed. When $R^2 < 0.95$ or so, you really have to look at your data and determine if the deviation from linearity is *random* or *systematic*. If the deviation is *random*, the R^2 value is probably a very good indicator of the quality of your data and the applicability of your theory. If the error is *systematic*, on the other hand, you may not have a "good fit!" R^2 assumes your error is random. R^2 can be used to compare the relative quality of two different curve fits (two different theories), but one R^2 value winning out over another does not preclude the possibility that yet another fit (another theory) fits the data better still, and is actually the valid one.

Alright, we now have a plot that should allow us to work backwards to an initial *n* value from the energy of a photon released as an electron in a hydrogen atom drops down to $n = 2$. Because the fit is so good, it should be reliable even out to energies outside the data range that makes up the plot. So, our objective will be to use the equation of the line in the plot to determine what electronic transition in a hydrogen atom leads to the generation of a photon with a wavelength of 389.1 nm. A purely graphical method can be used to make this determination, but the equation of the trendline we have generated provides a better way. Here's how to get a better estimate, with the correct number of significant figures:

135. Move your plot out of the center of the screen, clearing up a region of your spreadsheet for some new calculations. Remember, you have to click on an "empty" part of the plot to move the whole thing: if you click on any specific element, you'll move that instead!
136. Create a new heading, "Calculation of Initial Electronic Level"
137. Under this heading, create an entry, "Photon wavelength:". In the first complete empty cell to the right of this entry, enter the value "389.1", and then put the units, "nm", in the next cell over.

138. On the next row, create another entry, “Photon energy:”. Put in a formula to calculate the energy of the photon with the wavelength above, and put the units (please use J) in the next cell to the right. If you want to add a row that determines the wavelength in meters, that’s cool with us. Make sure that your calculated photon energy shows the correct number of significant figures.
139. Now, below the photon energy, create an entry called “Calculated $1/n^2_{\text{initial}}$:”.

We want to calculate the “x” in the equation of the trendline (the one on the chart), given the y value. The most direct way to do so is to use a little algebra, and solve this equation for x:

$$(-2.18\times10^{-18})x + 5.45\times10^{-19} = y$$

(Subtract 5.45×10^{-19} from each side)

$$(-2.18\times10^{-18})x = y - 5.45\times10^{-19}$$

(divide both sides by -2.18×10^{-18})

$$x = \frac{y}{-2.18\times10^{-18}} - \frac{-5.45\times10^{-19}}{-2.18\times10^{-18}}$$

$$x = -4.58_7\times10^{17}y + \tfrac{1}{4}$$

In an empty cell to the right of your last entry, type in the formula above, starting with the = sign, replacing the “y” in the formula with a reference to the cell with the photon energy in it. You should also “show your work,” by showing the formula you used here in plain text on the spreadsheet, both symbolically and numerically, in a cell adjacent to where the calculation was carried out:

140. To get an equation to show up as text rather than have Excel (try to) calculate it, you need to enter a single quote (‘) at the start. So, to enter the equation above symbolically, you would type “’= (photon energy)/slope – (y-intercept)/slope”. The numerical line would read “’= [insert your photon energy here, with units]/-2.18E-18 J – (-5.45E-19 J)/(-2.18E-18 J)” This is the Excel equivalent of “showing your work,” and it is very important to do so whenever you derive a formula and use it in a spreadsheet.

In order to extract n_{initial}, you’ll need to carry out one more calculcation, on the next line.

You should end up with $n_{\text{initial}} = 7.990197476$, reasonably close to a possible whole number, 8. This result has way too many sig figs, though, and that should be fixed:

141. Correct the number of sig figs in the calculation result, so that it is consistent with the calculation.
142. Use the print preview function (File:Print Preview) to arrange and re-size the plot on the sheet so that everything fits on a single printed page, and the plot fills the page well.
143. Save your work (File:Save). Print a copy of this sheet (File:Print).
144. Select and copy the contents of cell A1.
145. Click on the third tab, currently labeled “Sheet 3”
146. Paste into cell A1, labeling this new sheet with your name(s) and the experiment number.

You’ll be doing two exercises on your own, to practice what you have learned, so that it sticks! That means we’ll need two blank sheets, not just the one we have. Here’s how to get one more:

147. Holding down the **option** key, click and drag the Sheet 3 tab into the empty space just to the right of it. You should see a small “+” sign and a sheet icon, and when to release the mouse, a new tab called “Sheet 3 (2)” should appear. You’re ready to show us you understand this stuff!

SELF-GUIDED EXCEL EXERCISES

Now that you have become an Excel Master, you must avoid the temptations of the Dark Side (using Excel's pivot tables as an employee of a management consulting firm) and instead put your knowledge to good use! Please use Excel to complete the following two additional exercises.

Your report for this experiment will consist of four printed spreadsheets: the two from the chromium isotopes and atomic spectrum work above, and a page each for the following two exercises. Each of these self-guided exercises should be put on a separate electronic sheet in your spreadsheet, and an appropriate name added to each tab. In some labs, you will also hand in your spreadsheet electronically.

Take care to generate spreadsheets that are easy to read, with formatting similar to that presented earlier in this activity (*i.e.*, headings should be differentiated from data in some way; data should be clearly presented in tabular form, with units; conversion factors should be shown with labels and units; and conversion factors should be "locked" during calculations). Be sure to put titles and axis labels on all charts. Include a title at the top of each spreadsheet, explaining what it is for and who prepared it, and remember to save your work (File:Save or ⌘S) as you go along!

These will be the spreadsheet expectations whenever Excel is used in chemistry!

Barium Sulfate Yield Determination

One of the reactions that you will carry out this semester is that between sulfuric acid and barium nitrate. The result is the precipitation of barium sulfate:

$$H_2SO_{4(aq)} \;+\; Ba(NO_3)_{2(aq)} \;\rightarrow\; 2\;\; HNO_{3(aq)} \;+\; BaSO_{4(s)} \qquad (1)$$

A student mixed aqueous solutions containing 1.10 moles of sulfuric acid and 2.00 moles of barium nitrate. She subsequently collected the barium sulfate precipitate via filtration, and determined the mass of the solid. The student repeated this experiment seven times, obtaining the following data:

Trial #	Mass of $BaSO_{4(s)}$ [g]
1	235.1
2	220.4
3	250.6
4	246.5
5	224.0
6	228.5
7	243.5

In theory, the mass obtained in the experiment described here should be the same every time. However, that's clearly not what actually happened – and to the extent that it isn't, *random error* is to blame.

Organize the data in the table above in a blank spreadsheet, and calculate the average and standard deviation of the seven mass results. These are both functions listed under "Statistical" in the Function Wizard. (Use the sample standard deviation, not the population standard deviation STDEVP, which would only apply if we somehow had every possible result. STDEVP is almost never appropriate in chemistry.) Format the standard deviation so that it has two significant figures. This is (a lower bound on) the *uncertainty* in the average. Format the average so that it has the correct number of significant figures, as indicated by this value. You may have to use the *scientific* number format to pull that off!

Organize the data in the table above in a blank spreadsheet, and calculate the average and standard deviation of the seven mass results. These are both functions listed under "Statistical" in the Function Wizard. Format the standard deviation so that it has two significant figures. This is (a lower bound on) the *uncertainty* in the average. Format the average so that it has the correct number of significant figures, as indicated by this value. You may have to use the *scientific* number format to pull that off!

The theoretical yield of barium sulfate is 257 grams in each of these reactions. Use Excel to calculate the experimental yield (on a mass basis) for each trial, in a column adjacent to the masses. Use 257 grams as a "locked" constant (use an absolute cell reference to a cell containing this value) for these calculations. Yield by mass is defined as the mass of $BaSO_4$ actually obtained, divided by the theoretical yield. Format the result of carrying out this calculation with the "percentage" number format, and the correct number of significant figures.

Systematic error is to blame for some of the discrepancy between the actual yield values and the theoretical yield – as you can see, there was a substantial amount of systematic error in this experiment, because the yield came out consistently low! (If the yield was as often above 100% as it was below, the error would probably all be random.) The take-home lesson from this: you can readily see and quantify *random* error if you do *replicates* (take repeated measurements). But *systematic* error is much harder to detect – and you really need to have an "expected" result in order to find it! But it can be as large as or larger than random error, and you can't just average it away…so don't forget to consider the possibility of systematic error when analyzing the validity of your experimental results in science.

Chemical Kinetics

One topic of interest in chemistry is chemical kinetics, the study of the rates of chemical reactions and the factors that influence these rates. Suppose that the chemical kinetics of the reaction

$$\mathrm{A} \rightarrow \mathrm{B}$$

were studied by measuring how the concentration of A changed with time. A chemist collected the following data:

Time Elapsed (seconds)	Reactant Concentration (M)
0.	5.0_0
10.	4.7_0
20.	4.3_8
30.	4.0_1
40.	3.7_8
50.	3.3_8
60.	3.0_8

1. Display these data in a spreadsheet with appropriate column headings. Be careful with significant figures! You may have to use the "scientific" number format to correctly indicate the number of significant figures in some of this data.
2. Use the Chart Wizard to create a graph that clearly and accurately communicates the decrease in concentration of the reactant with time. Provide your graph with appropriate titles and axis labels.
3. Think carefully about which variable belongs on which axis, and be sure you plot them correctly.
4. Fit a trendline to the data, and display its equation and R^2 value on the chart (don't do it by hand!).
5. Use the equation of the trendline to predict what the reactant concentration will be at 80 seconds. Carry out the calculation on the spreadsheet: do not use a calculator, except perhaps to check your work. Make sure that your result makes sense in light of the data given above. (For example, 4.05 M would *not* make sense…nor would a negative concentration, like, say, -12.16 M!) Also, please show your calculations symbolically, in text, on the spreadsheet. (Show your equations!)

Remember to print out your two self-guided exercises, and save your work.

Saving Your Work to Your Account

It's often really nice to be able to take your electronic work "with you"…and you can! You have a network account where you can keep files, and you can access it from any web browser. Here's how to use it to store your work from this lab:

- Start a web browser program, whichever one you like best
- Go to the following web address: http://webfile.macalester.edu
- Type in your Macalester username and password when prompted
- Click on the Home@MACALESTER folder in the left-side panel
- Click the small underlined blue word "File", and select "Upload…"
- Click on "Browse…", then on "Desktop", and finally double-click on the name of your file.
- Click the "Upload" button, and your file will be saved to your account!
- Check the board for possible additional instructions on submitting your work electronically.