EXCEL WORKSHOP
(A "Computer Lab" period for Chemistry 14BL)

EXCEL is a very popular spreadsheet software that allows the user to perform all sorts of statistical analyses on the data. It can also perform a variety of mathematical calculations. In addition, ***EXCEL*** can also plot the data in a variety of formats. During the workshop, each of you will have a chance to duplicate the graphs *(using the PC version of* ***EXCEL***) that I generated on the lecture guide. The goal of the workshop is to familiarize you with the ***EXCEL*** software so that you can use it to write your reports (not just in chemistry!) in the near future.

You will work in groups of **TWO** (*may be THREE if needed*) for the rest of the lab period. Go to "**START**" (located at the bottom left corner of the screen) and select "**PROGRAMS**". Click on "**Microsoft EXCEL**".

NOTE: There is NO NEED to save any files during the workshop period. If you do decide to save the files, you will need to save them on a high-density 3.5" disk or in the "My Document" folder.

Before you start, take out your titration lecture guide (the one with the sample titration graphs and data tables), you will need it during the workshop.

There are, in general, three different steps when working with ***EXCEL***.

Step (I) Data Entry – you will first enter the raw data for the titration of 1.0M acetic acid with 0.5M NaOH (**refer to page 5**). Follow the instructions below to enter the data.

On the spreadsheet, notice that the columns in ***EXCEL*** are labeled as A, B, C … etc. The rows of the spreadsheet are labeled as 1, 2,3 …etc. Each cell (i.e. a rectangular box) is defined by the location of the row and column in ***EXCEL***. For example, the very first cell located on the upper left corner has an address of ***A1*** in ***EXCEL***.

Before you start entering the data, you may want to increase the width of the columns. For example, if you want to increase the width of column A, point the cursor to the letter A and click on the left button of the mouse. The entire column A should now be highlighted. Go to the menu bar and click on "**FORMAT**". Select "**COLUMN**" and then select "**WIDTH**". A dialog box will appear. Type in a number that is greater than the original number shown to increase the width of the column. To decrease the width of the column, type in a smaller number. You can always go back and increase the column width anytime even after you enter the data. Let's go ahead and start entering the data.

Move the cursor (or cross) to the cell with an address *A1* (i.e. the very first cell in the spreadsheet). Type "**ml of NaOH**". Move the cursor to cell *B1* and type "**pH**". These are the labels or titles for each of the columns. Now go to cell *A2* and start entering the volume into each cell. When you are done entering the data for the volume of NaOH, enter the data for the pH (starting from cell *B2*). Your spreadsheet at this point should look like the one on page 5. You are now almost ready to ask ***EXCEL*** to do some simple calculations (follow step (II) below). But before you can generate the data for column C (average volume), and column D ((pH2-pH1)/(V2-V1)), you should type in the headings "**(V2+V1)/2**" into cell *C1* and "**(pH2-pH1)/(V2-V1)**" into cell *D1*.

Step (II) Data Analysis – This is where you will find how valuable a spreadsheet program is. Now let's use the program to calculate the average volumes (column C) and the derivatives (column D).

Locate the cell that you want to place the *FIRST* entry of the average volume. This should be cell **C3** (NOT C2! Leave cell C2 empty). To calculate the average volumes, you will need to type in a simple equation so that ***EXCEL*** knows what you want it to do. Let's suppose V1 is located at cell A2 and V2 is located at cell A3. Go to cell C3 and type **=(A2+A3)/2**. Make sure you include the equal sign; otherwise, ***EXCEL*** will think you are typing a label. A number should appear in cell C3 *(check your number with the one on the lecture guide. They should be similar*). You are now ready to finish the rest of the data in column C. Move the cursor to the number you just calculated (i.e. cell C3). Go to the menu bar and click on "**EDIT**"; select "**COPY**". The cell C3 should now be highlighted with a dotted line. Now use your mouse and highlight the rest of the column C by holding down the left mouse button and drag the cursor down the column C until it reaches the location for the last data point in the column C. You can easily tell where the last data point for column C is by looking at the location of the last data point for column A. Release the mouse button and part of the column C should now be highlighted in black. Go to the menu bar again, click on "**EDIT**" and select "**PASTE**". You just finished generating the average volume data for column C. Check your numbers with the ones on the lecture guide and make sure they agree. If they do, go on and finish the calculations in column D by using the equation **=(B3-B2)/(A3-A2***) (you should double check to make sure that the cell addresses are correct in this equation*). If you have trouble generating the data, ask your TA for assistance.

We are almost there. All you need now is to learn how to plot graphs on ***EXCEL***.

Step (III) Graphs – you are now ready to generate or reproduce the graphs on the lecture guide.

NOTE: Before you try to plot the graphs, make sure that the X axis data is always located adjacent to and ***LEFT*** of the Y axis data when using ***EXCEL***.

Let's plot the full titration graph and the expanded titration graph (see lecture guide) from the raw data. If you follow step (I) and (II) correctly, the volume of NaOH should be located in column A and the pH should be located in column B. To generate the full titration graph, hold down the left mouse button and highlight all the data in both column A & B (ONLY!!) by dragging the cursor to the desired point. Release the mouse button. All the data in column A & B should now be highlighted. Go to the menu bar and click on "**EDIT**"; select "**COPY**". Now go to the menu bar again and choose "**INSERT**". Select "**CHART**". A box appears (*CHART WIZARD*) on the screen which gives you all the different choices for graphs. You should select "**XY (Scatter)".** Click on "**NEXT**". A little tiny graph should appear on the screen. This is the "pre-view" of the graph. Click on "**NEXT**" again. You now see a table with five different options. All you need to modify are the titles and the gridlines. Click on "**TITLES**". Type in the title of the graph and also the labels for the axes. Click on "**GRIDLINES**" and activate all the major and minor gridlines for both the X & Y-axis. Click on "**NEXT**". There is one last thing that ***EXCEL*** needs to know before it can generate the graph. It wants to know where you want to put the graph. Click on "**AS NEW SHEET**". This means you want ***EXCEL*** to plot the graph on a separate sheet of paper; otherwise, ***EXCEL*** will plot the graph and the print the data on the same piece of paper.

Congratulation, you have just finished plotting the full titration graph using ***EXCEL***. You should see a huge graph on the screen with the X-axis scale from 0 to 20. Go ahead and double click on any one of the numbers on the X-axis. A dialog box will pop up. Click on "**SCALE**". Now change the minimum value to "14" and change the maximum value to "15.6". Also change the major unit to "0.2" and the minor unit to "0.04*" (scale for the minor unit should always be less than that of the major unit*). If you are curious, try not to modify the major and minor unit and see what happens to the expanded titration graph. Click "**OK**". A new graph will show up on the screen. This is the expanded titration graph (see lecture guide) showing just the equivalence point region of the titration.

You just completed both the full titration graph and the expanded titration graph. Now go ahead and work on your own to plot the first derivative graph (i.e. *column C & D*). To do this, you will first need to go back to your spreadsheet. Take a look at the bottom of the screen, click on "**SHEET 1**". This should bring you back to the raw data. From what you have just learned, now plot the first derivative graph from the data in column C & D.

Once you have finished plotting all three different graphs for the titration of 1.0M acetic acid with NaOH, repeat Step(I) – Step (III) and plot the three different graphs again for the titration data of acetate buffer with 0.5M HCl and 0.5M NaOH (see page 6 of this handout). Make sure each group member has a chance to work on the EXCEL. Use the lecture guide as a reference.

Before you start working on the buffer data, follow the instructions on the next page to construct the buffer data spreadsheet.

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Data Entry for the Buffer Data Spreadsheet

Although the procedures for entering data into ***EXCEL*** for any data set are the same, there is however a little "trick" that you need to be aware of when entering the buffer data (unlike the ones you just finished).

In order to plot the buffer titration graphs, you will need to ***combine*** both the HCl data and the NaOH data onto ***two new*** *columns (see the fifth and sixth columns of the data table on your lecture guide*). To do this, first enter all the data on page 6 of this handout onto the ***EXCEL*** spreadsheet (use a NEW spreadsheet if you want to). Once you finish that, highlight *(by dragging the mouse and holding the left button of the mouse at the same time*) the entire HCl volume and pH data (**data ONLY - do not highlight the titles**) on your spreadsheet. Release the mouse button and go to the menu bar and select "**EDIT**". Select "**COPY**". Now highlight the **EXACT same number of cells** as there were in the previous step (i.e. the copy step) on **TWO NEW** columns by dragging the mouse and holding the left button of the mouse at the same time. Release the mouse button and select "**EDIT**". Select "**PASTE**". All the HCl data should now be copied onto the new columns. Notice that on the lecture guide, the HCl data (the top part of the fifth column) are "flipped" with negative signs on all the HCl volume. To do this, highlight all the data you just copied to the new columns. Go to the menu bar and select "**DATA**". Select "**SORT**". A table will pop up and ask you how you want the data to be sorted. You will sort the data in the **ascending** order from the **HCl pH data**. Select the column from the table that corresponds to the HCl pH column. Click "**OK**". All the data should now be "flipped" except for the negative signs. You can now manually add the negative signs to the HCl volume data. Once you finish that, copy the NaOH volume & pH data to the same columns as the HCl data (refer to lecture guide). There is one more thing you need to check before you can go on further. Take a look at the data table you just finished, there may be **TWO identical entries** on the spreadsheet (i.e. the 0 ml; 4.76 pH entry). You need to eliminate one of them; otherwise, it will affect the calculation steps. Highlight one set of the duplicate entry (both the pH and the volume). Go to the menu bar and select "**EDIT**". Click on "**DELETE**". A window will pop up and by default, ***EXCEL*** will ask you if you want to ***SHIFT THE CELLS UP***. This is what you want; click on "**OK**". ***EXCEL*** will erase the duplicate entry and move all the data in those two columns up one row. Now go ahead and finish the rest of the calculations as before (see the last two columns of the data table on the lecture guide). You are now ready to plot the graphs (follow instructions from before on how to plot the graphs on ***EXCEL***).

One final note: for your post-lab reports, you should connect the data points by drawing smooth curves (i.e. best fit curves) through them by hands. DO NOT ask EXCEL to connect the data points for you. It doesn't know how to draw best fit curves through non-linear data points

Sample data for the titration of 1.0M acetic acid with 0.5M NaOH

ml of NaOH	pH
0.03	2.59
3.02	4.03
6.17	4.46
9.63	4.82
12.04	5.29
12.59	5.39
12.99	5.53
13.91	5.92
14.04	5.99
14.13	6.09
14.15	6.14
14.20	6.21
14.25	6.28
14.33	6.37
14.36	6.47
14.41	6.59
14.43	6.78
14.52	7.09
14.55	8.21
14.58	10.36
14.63	10.91
14.70	11.17
14.75	11.32
14.81	11.44
14.89	11.53
15.00	11.66
15.51	11.97
16.08	12.16
17.21	12.35
19.31	12.55

Sample data for the titration of acetate buffer with 0.5M HCl and 0.5M NaOH

Vol HCl (ml)	pH	Vol NaOH (ml)	pH
0.00	4.76	0.00	4.76
0.52	4.69	0.51	4.85
1.01	4.64	1.00	4.92
1.50	4.58	1.50	4.99
2.03	4.52	2.01	5.05
2.51	4.46	2.51	5.12
3.02	4.39	3.02	5.22
3.52	4.34	3.51	5.31
4.02	4.27	4.03	5.43
4.52	4.2	4.51	5.57
5.01	4.15	5.02	5.82
5.52	4.06	5.70	6.03
6.01	3.99	5.81	6.09
6.52	3.89	5.91	6.14
7.01	3.81	6.01	6.21
7.51	3.69	6.21	6.28
8.01	3.53	6.33	6.37
8.52	3.41	6.35	6.47
9.02	3.23	6.42	6.59
9.51	2.69	6.45	6.78
		6.51	7.09
		6.55	8.2
		6.61	10.4
		6.65	10.9
		6.70	11.2
		6.75	11.3
		6.81	11.4
		6.91	11.5