Chemistry 1211
IDENTIFICATION OF AN ORGANIC ACID
Plotting titration data with Excel to determine the pKa

These instructions were developed using Microsoft Office Excel 2007. A different version of Excel may require slightly different menu selections and commands, but you should still be able to follow along In the instructions below, items you click and commands or formulas you type are in **bold**. Also, there is more than one way to analyze titration data using a spreadsheet. These instructions just outline how I happen to to do it while writing this web page.

Assume you have carried out a titration of your unknown organic acid with your NaOH using a pH meter. You have collected the following data.

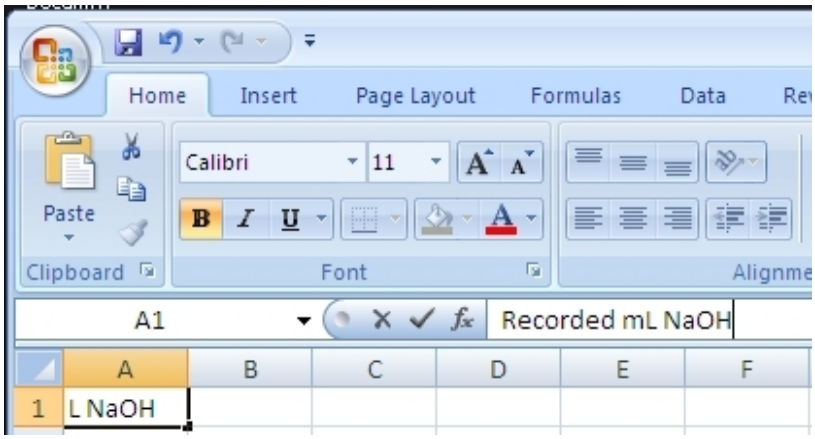
mL NaOH buret reading	**pH**		**mL NaOH buret reading**	**pH**
0.72	3.31		20.42	6.55
1.72	3.69		20.54	6.81
3.72	3.98		20.62	7.09
5.72	4.22		20.72	7.69
7.72	4.43		20.78	8.91
9.72	4.61		20.82	9.61
10.72	4.69		20.86	9.96
11.72	4.77		21.02	10.52
12.72	4.87		21.6	11.14
13.72	4.96		22.9	11.54
15.72	5.14		23.72	11.81
17.72	5.43		25.72	12.06
18.72	5.63		27.72	12.21
19.22	5.77		30.72	12.39
19.85	6.04		31.72	12.42

Note: The volumes above are the buret readings. In this example the initial buret reading is 0.72 mL. This 0.72 mL needs to be subtracted from each recorded reading to obtain the actual volume of NaOH delivered at each pH reading during the titration. We will let Excel do the arithmetic for us.

Enter the raw data in to Excel

Click on cell **A1** and give column A a heading

You can make the font **bold**, and **Format** the cell to turn on **Wrap text** and set **Number** to 2 **Decimal places**.



Now give column **B** a heading

Enter your data in the appropriate columns.

You should have something similar to this.

	A	B
1	**Recorded mL NaOH**	**pH**
2	0.72	3.31
3	1.72	3.69
4	3.72	3.98
5	5.72	4.22
6	7.72	4.43

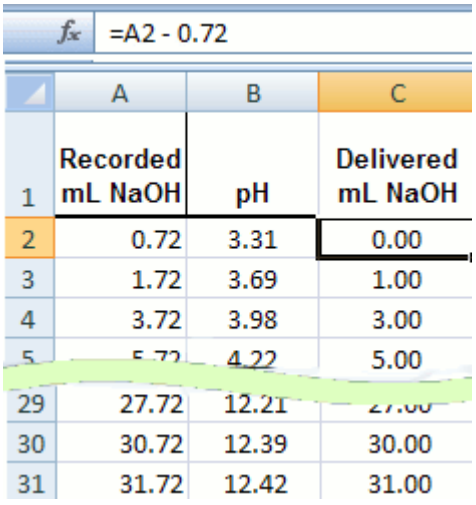
We will use Column C for the volume of NaOH delivered from the buret.

Give column **C** a heading

Click on cell **C2** and type **=A2 - 0.72** then hit **Enter** (*of course you should use your starting volume, not 0.72*)

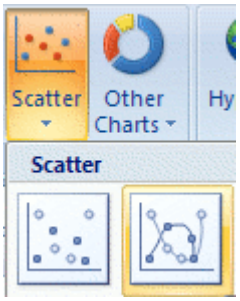
You should see 0.00 in C2

Now **Copy** cell C2 and **Paste** in to cells C3 to as many as you need for you data.



Now we will graph the data

Click on **Insert** => **Scatter** =>
Scatter with Smooth Lines and Markers

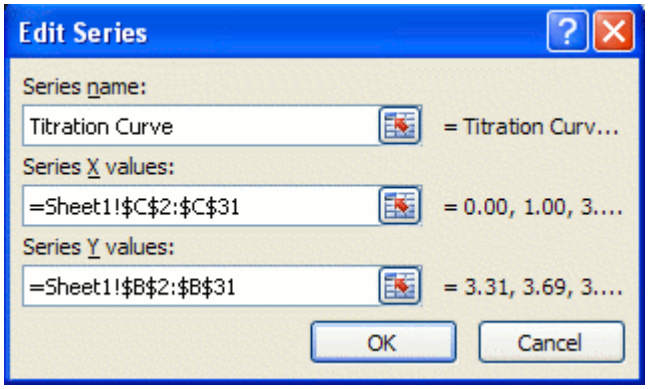


You should see a blank "chart".
Right-click on the blank chart and select **Select Data**.

Under Legend Entries (Series) Click **Add**.
Type something appropriate such as **Titration Curve** for **Series name**.

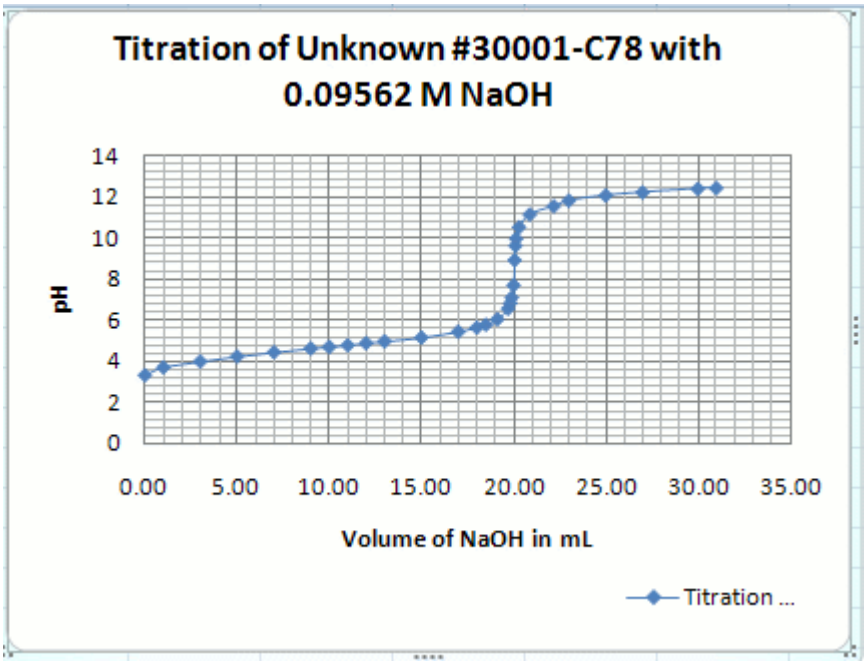
Click on the **Series X values** icon, and select your delivered volumes of NaOH from column C.

Click on to go back.



Do the same for the **Series Y values** icon and select the pH vales from column B.

Click **OK**



You can experiment with different **Chart Layouts**.
You can Right-click on various parts of the Chart to do things such as **Format Axis** and **Format Major Grid Lines** and provide a descriptive title to make a nice graph.
You should have a title, labels and units on the axises, a legend, and reasonable grid lines

The endpoint of the titration is at the inflection point. The slope of the titration curve at any given point is just the change in pH over the change in volume. The Greek letter *Delta*, Δ signifies "change in". So "Δ pH" means "change in pH". As you move along the titration curve from left to right the slope of the curve increases before the inflection point, reaches a maximum at the inflection point and decreases after the inflection point. The endpoint of the titration occurs at the inflection point on the titration curve. Sometimes this can be difficult to determine by looking at the titration curve. However, if we make a plot of how the slope changes during the titration we should be able to find the maximum slope and thus the inflection point which gives us our endpoint volume.

A plot of ΔpH/ΔV verses average volume for each point is a first derivative plot.

Now we will calculate the first derivative of the titration curve.

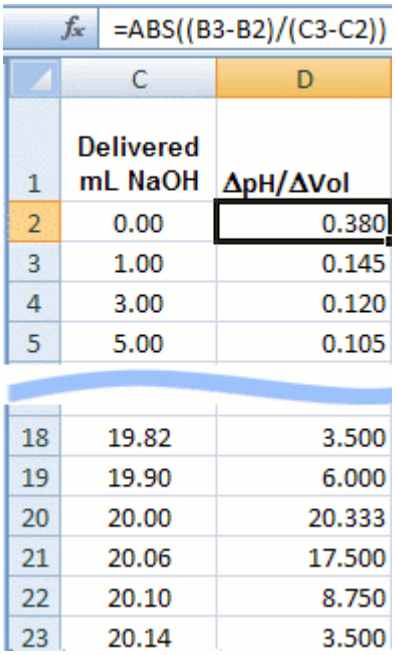
Select another column such as **D** for the ΔpH/ΔV values.

Give it a nice heading.

In Cell **D2** type the formula **=ABS((B3-B2)/(C3-C2))**.
The "ABS()" calculates the absolute value of the expression.

Copy D2 and **Paste** it in to as many other cells in column D to fit your data.

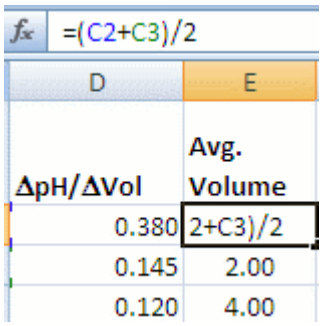
You can Right-click on **Column D** and **Format Cells** to set **Number** to 3 **Decimal places**.



In column **E** we will calculate the average or mean volume for each (ΔpH/ΔV).
So give column **E** an appropriate heading.

In Cell **E2** type the formula **=(C2+C3)/2**.

Copy and **Paste** to fill in the rest of **Column E** to fit your data.



Note: You will have one less data point in each of columns D and E because of the equation (C2_C3)/2

Plot the first derivative on the same chart as the titration curve.

Right-click on your titration curve chart and choose **Select Data**. Under Legend Entries (Series) Click **Add**.
Type something appropriate such as **First Derivative** for **Series name**.

Click on the **Series X values** icon, and select your average volumes of NaOH from column E.

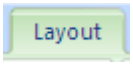
Click on to go back.

Do the same for the **Series Y values** icon and select the ⊗pH/⊗V vales in column D.

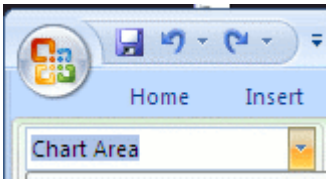
Click **OK**

To make the first derivative curve look better right-click on it and select **Format Data Series** then click on **Line Style** and reduce the **Width**.

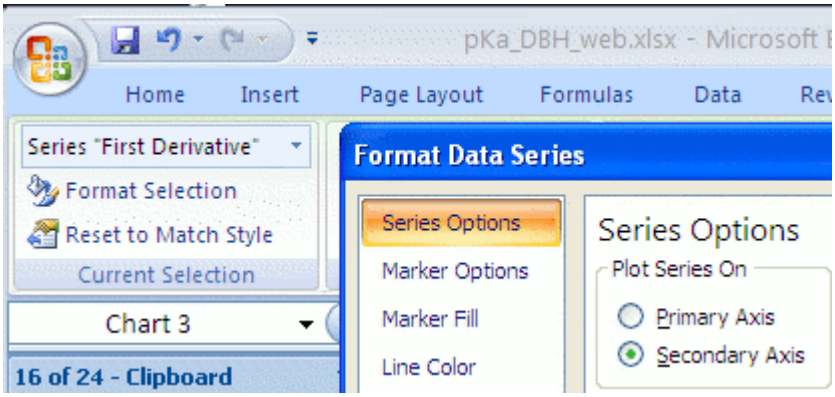
You may have noticed that the Y axis has changed to reflect the new ΔpH/ΔV values. But a pH above 14 does not make sense in water. So we will make a new axis for the ΔpH/ΔV values and put it on the right.

Click on the **Layout** tab. 

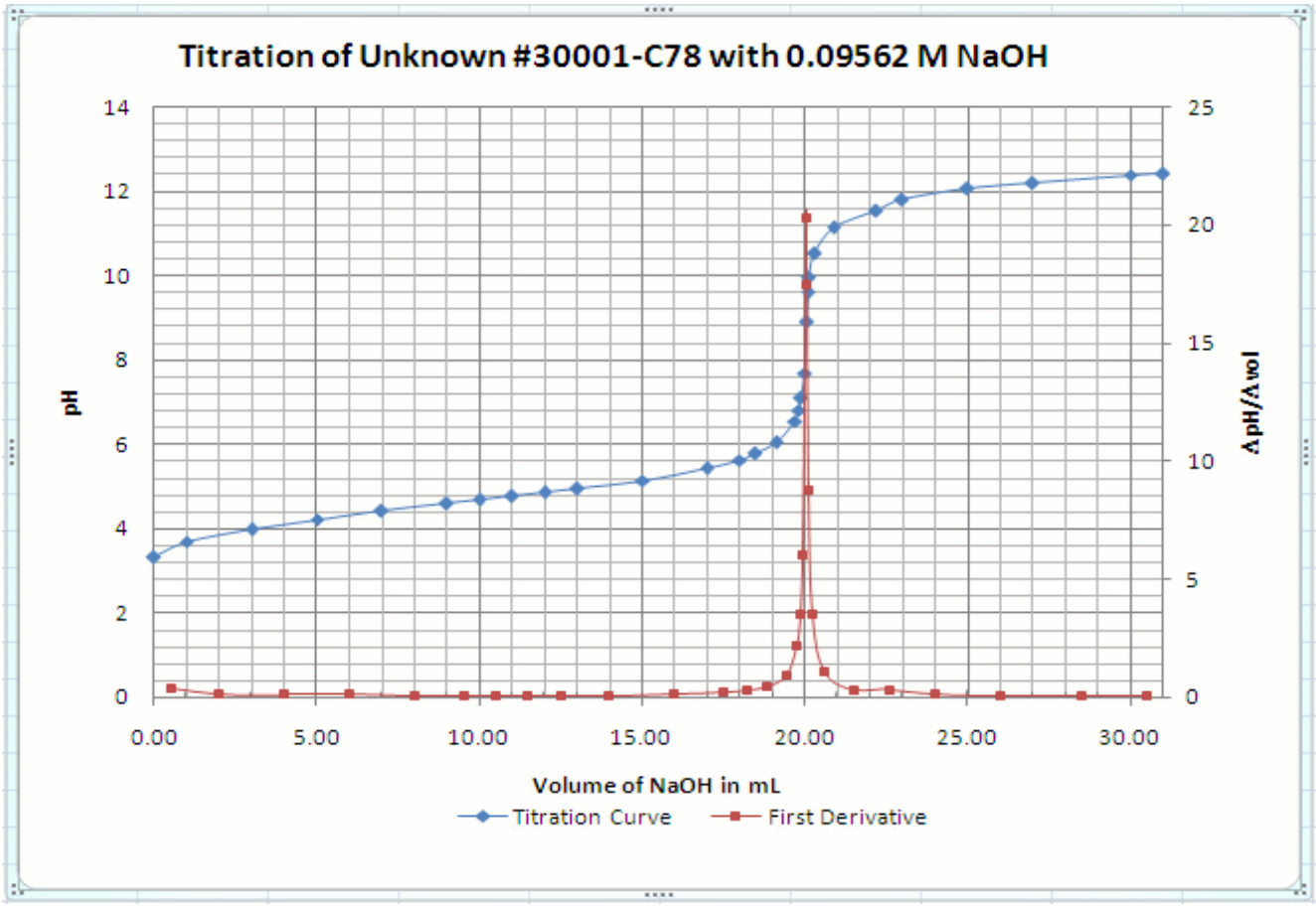
Click on **Chart Area** (should be in the top right coroner of the Excel window).



Select **Series "First Derivative"**.
Click on **Format Selection**
Under **Series Options** click **Secondary Axis**.
Click **Close**

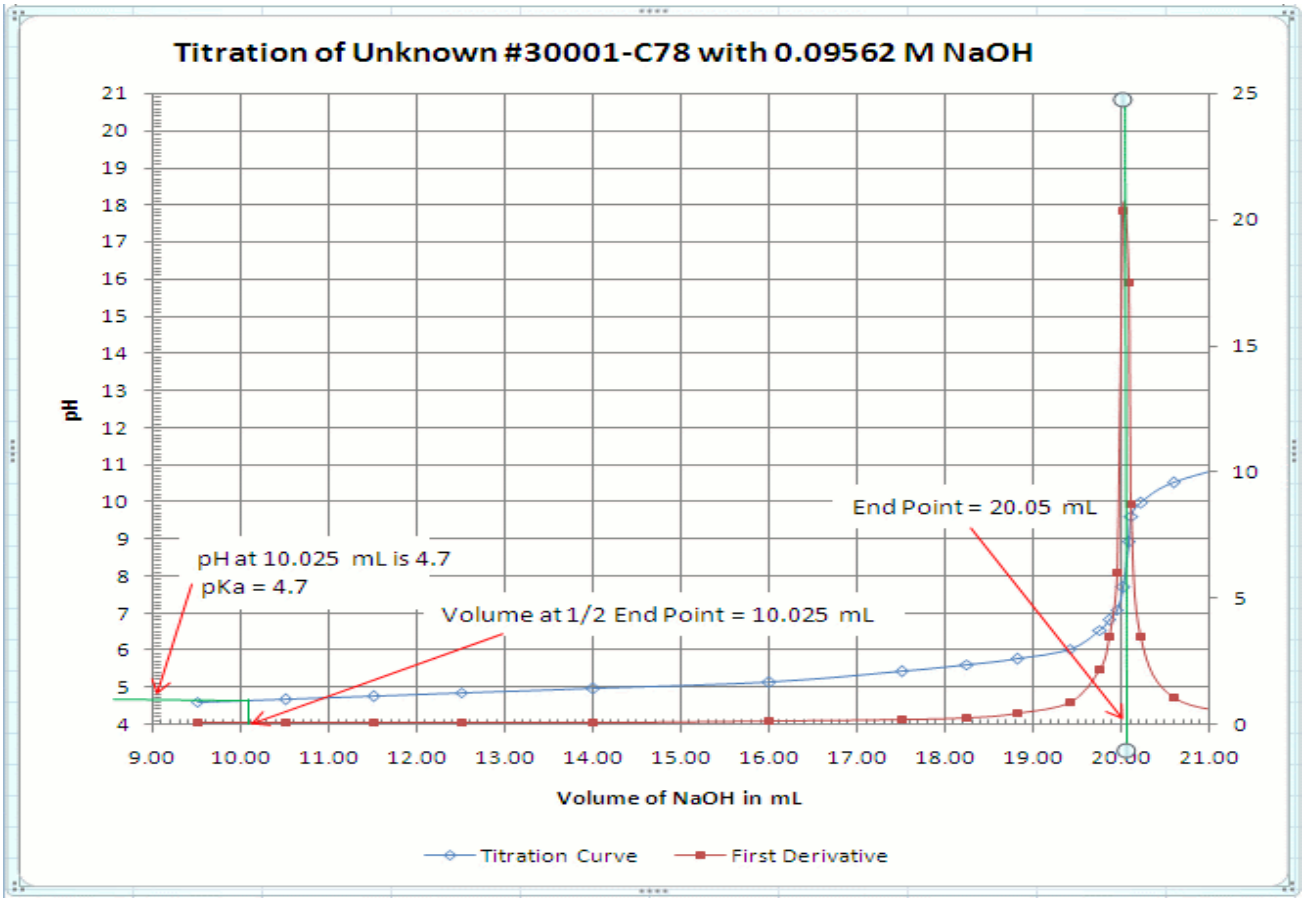


Soon you should have a nice graph of your titration data.



Be sure to make the graph fit the data and include reasonable grid lines, labels, units, and a legend

To accurately determine the end point volume you should enlarge the graph or make another chart of just the data very close to the endpoint. By now now you have enough knowledge of Excel to do this on your own. Drop a vertical line from the apex of the first derivative plot to the X axis. Where this vertical line meets the X axis is the end point volume.



Since your data has the volume to 1/100th of a mL you should determine the endpoint volume to 1/100th of a mL