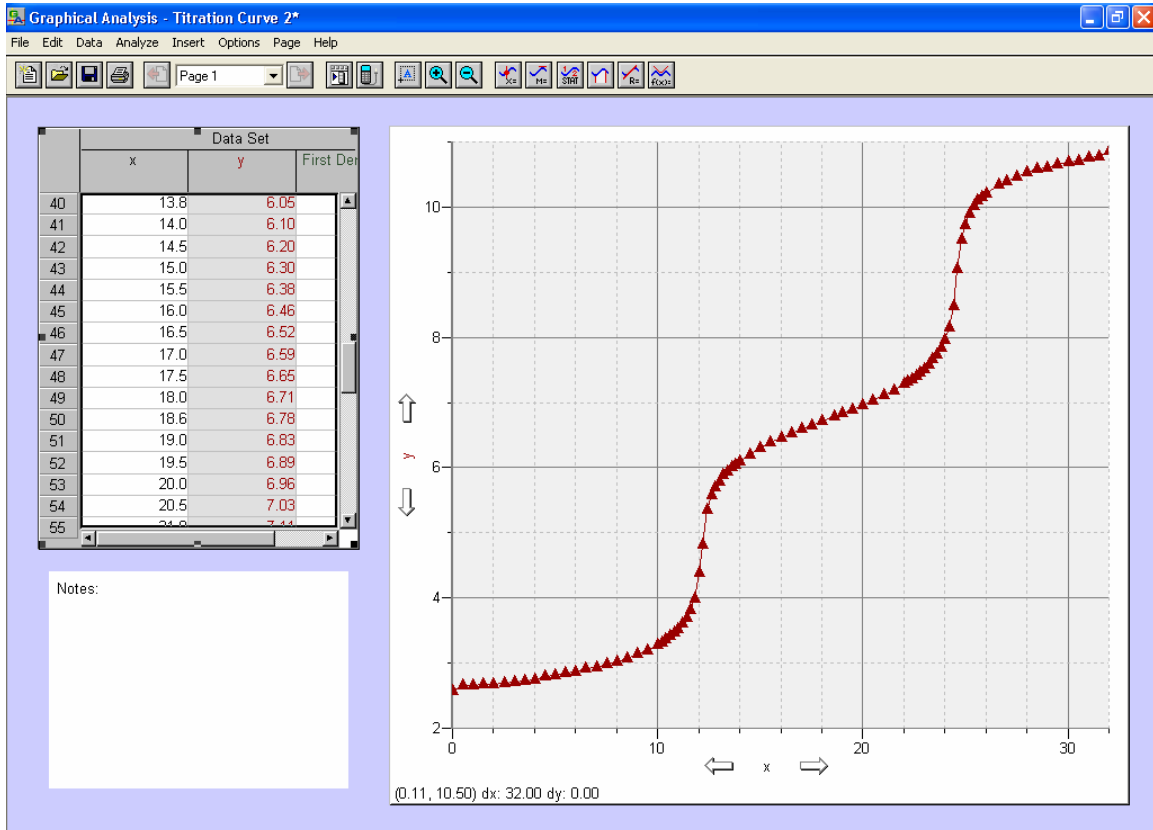


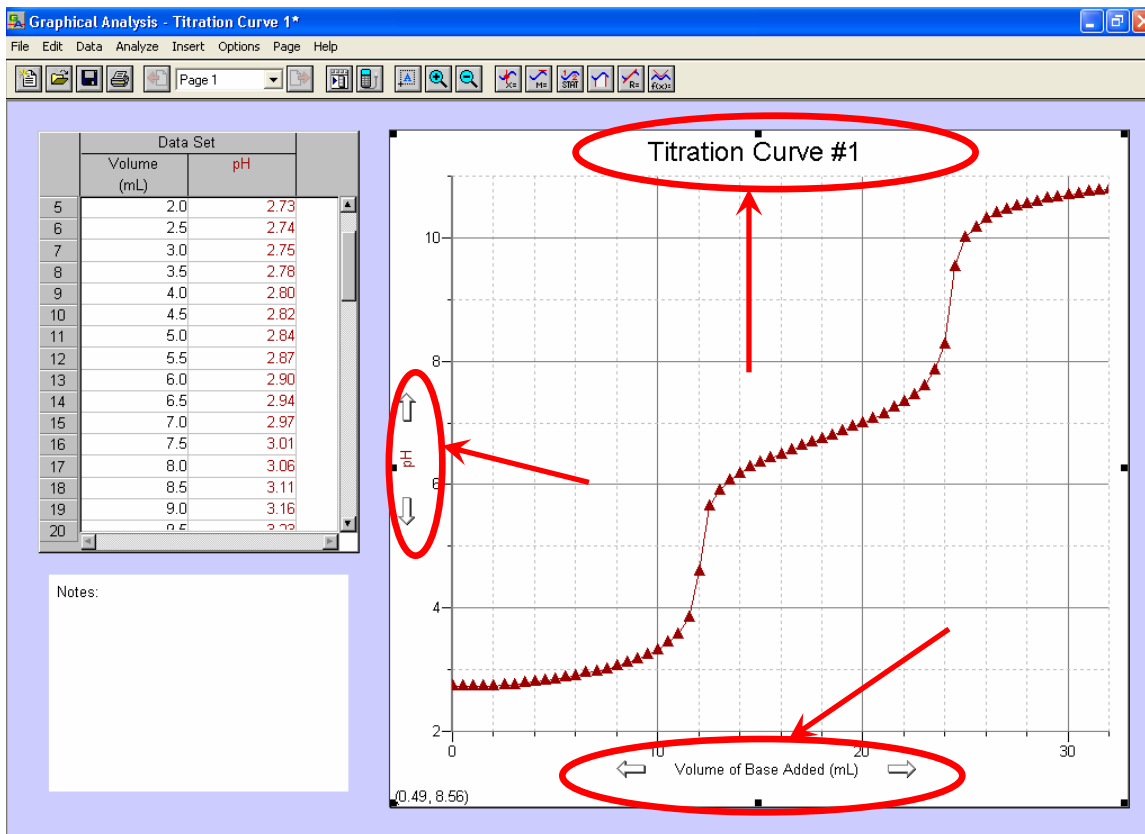
# Using Graphical Analysis for Titration Curves

1. Click **File...Import...from File**. And select your data file. You will get a basic graph as shown below

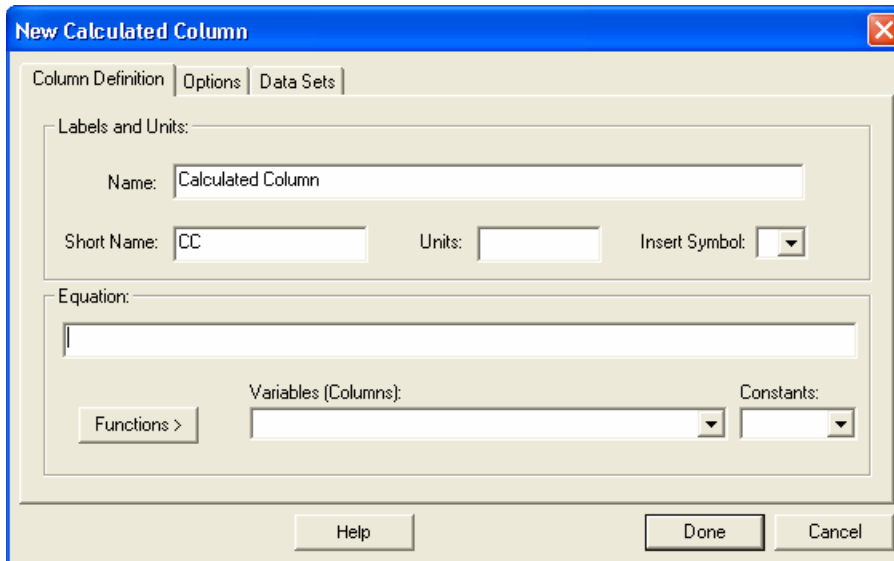


**Be sure to print off each of the various graphs to show how you calculated these values. Also be sure to record all of these values before printing.**

2. Fill out X and Y and title as shown below by clicking on the appropriate axis.



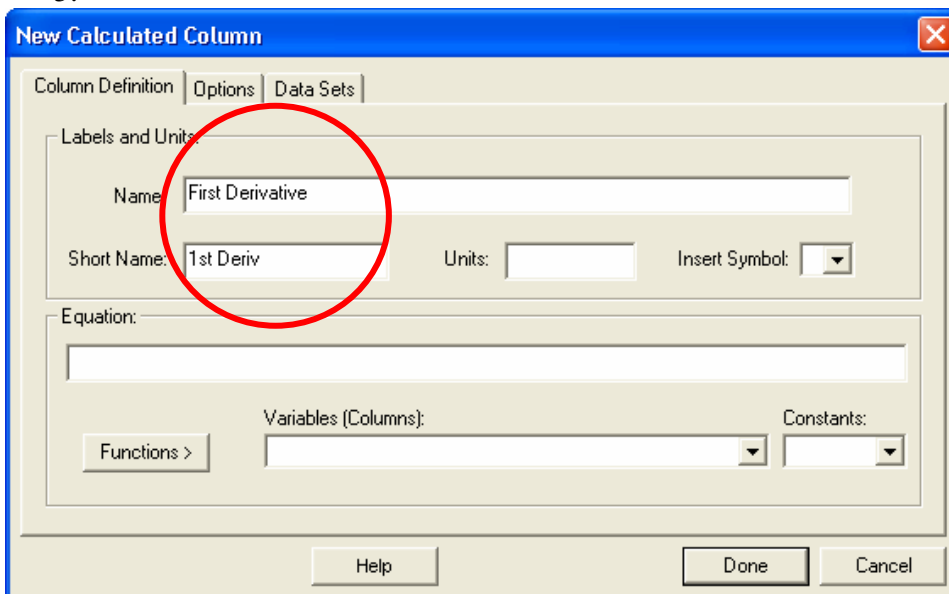
3. To Get 1<sup>st</sup> order derivative. *Click Data....New calculated column.* The following screen will pop up



The screenshot shows the 'New Calculated Column' dialog box with the following fields:

- Column Definition | Options | Data Sets
- Labels and Units:
  - Name: Calculated Column
  - Short Name: CC
  - Units: [empty]
  - Insert Symbol: [dropdown]
- Equation: [empty text box]
- Variables (Columns): [dropdown]
- Constants: [dropdown]
- Buttons: Functions >, Help, Done, Cancel

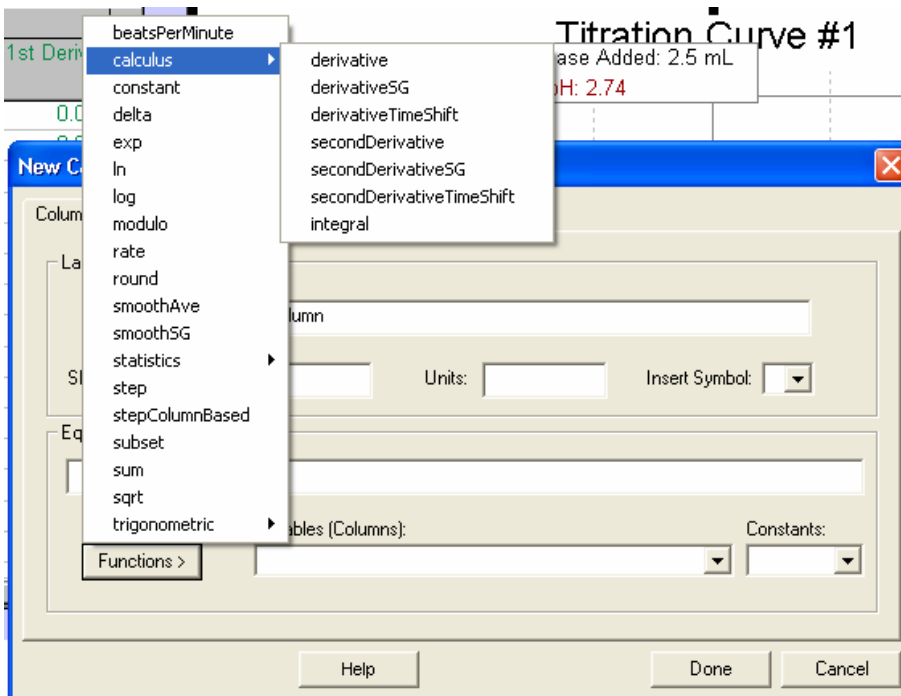
4. Fill in information such as **Name (First Derivative)** and **Short Name (1<sup>st</sup> Deriv)**
- 5.



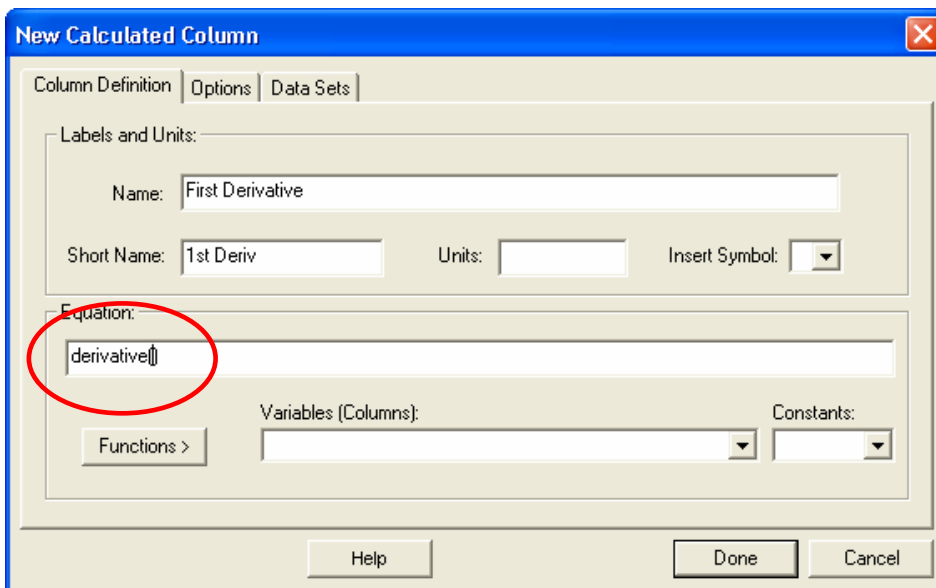
The screenshot shows the 'New Calculated Column' dialog box with the following fields:

- Column Definition | Options | Data Sets
- Labels and Units:
  - Name: First Derivative
  - Short Name: 1st Deriv
  - Units: [empty]
  - Insert Symbol: [dropdown]
- Equation: [empty text box]
- Variables (Columns): [dropdown]
- Constants: [dropdown]
- Buttons: Functions >, Help, Done, Cancel

5. Click **Functions...Calculus .....Derivative**



**The Derivative function will appear in the Equation box**



6. Make sure cursor is in the brackets () and click down arrow for **Variables** and select the Y column (**pH**)

**New Calculated Column**

Column Definition | Options | Data Sets

Labels and Units:

Name: First Derivative

Short Name: 1st Deriv Units: Insert Symbol: ▾

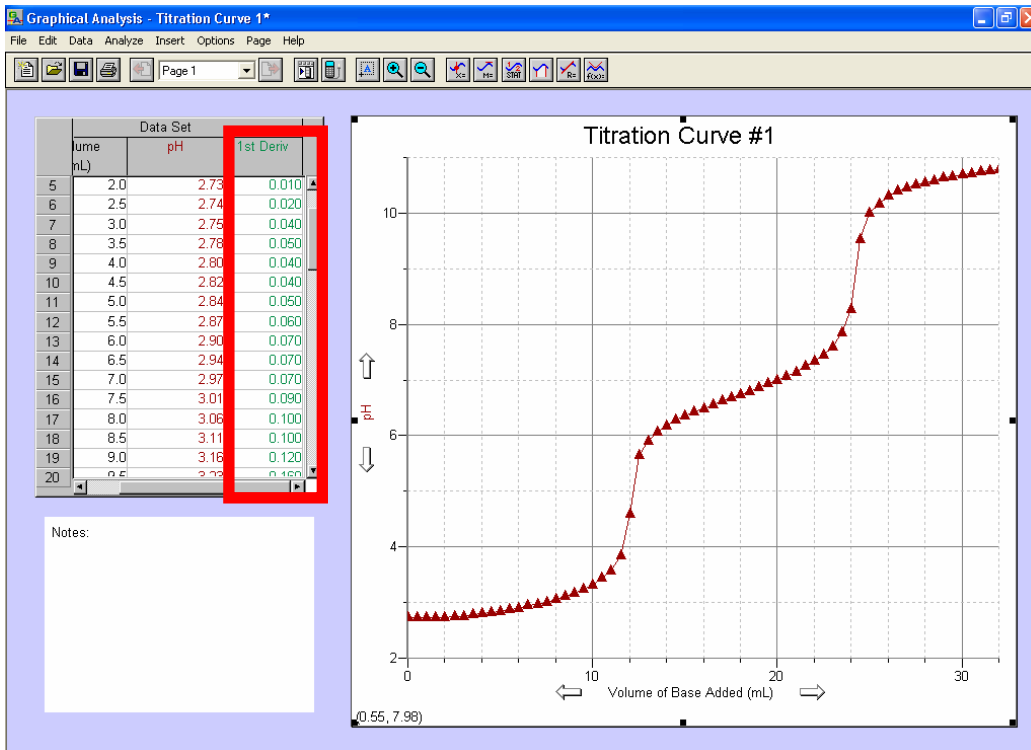
Equation:

derivative("pH")

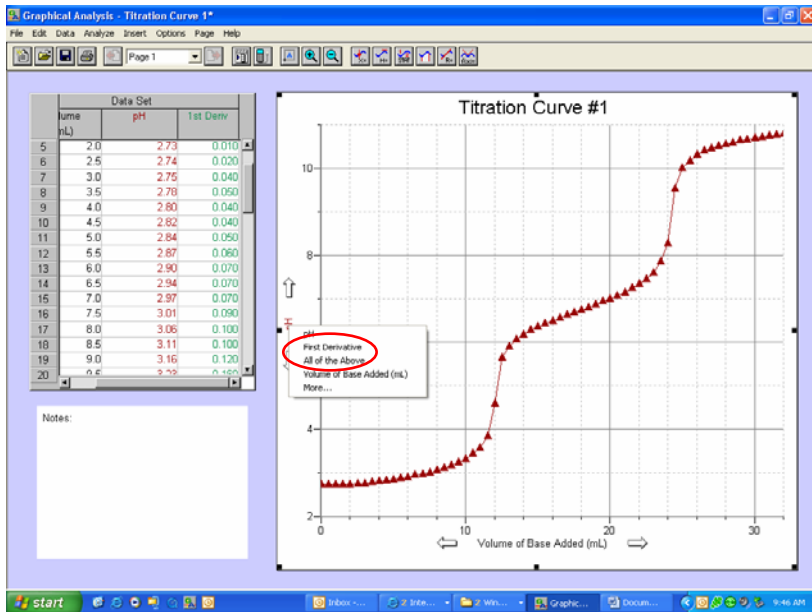
Functions > Variables (Columns): Constants:

Help Done Cancel

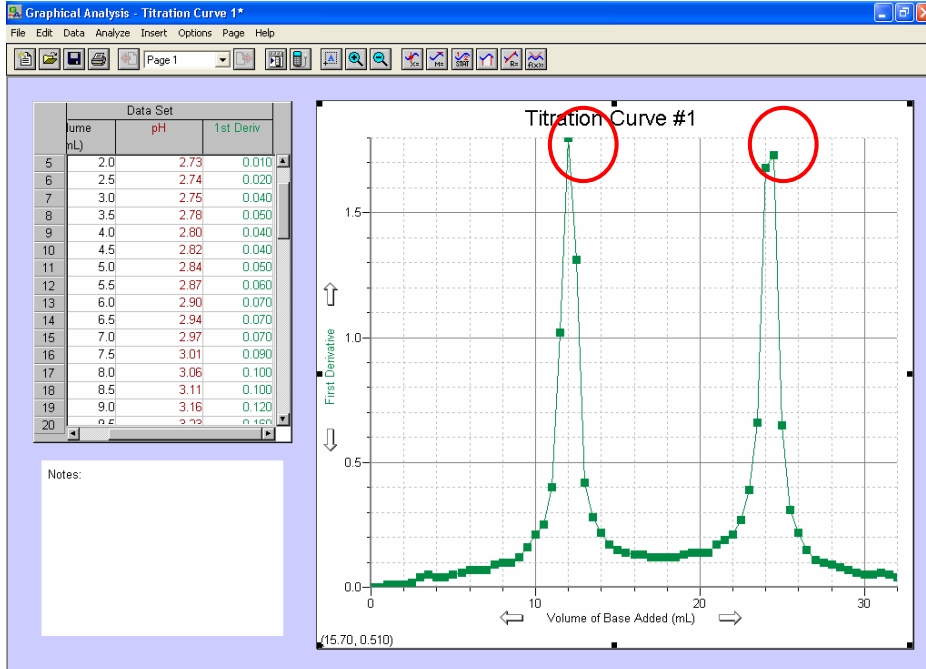
Click **Done** and column will appear next to the Y (pH) column as shown below (SAVE YOUR WORK)



7. Next place your mouse over the pH legend of the graph and *click*. You will get a pop up box with the various selections available for graphing. Select **First Derivative**

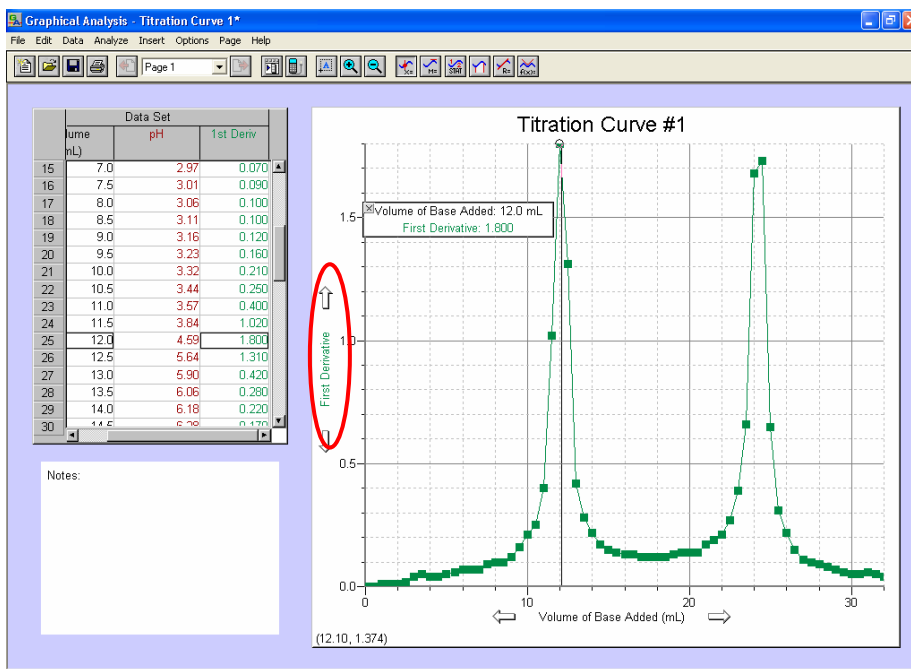


You will then get the 1<sup>st</sup> order derivative of the plot

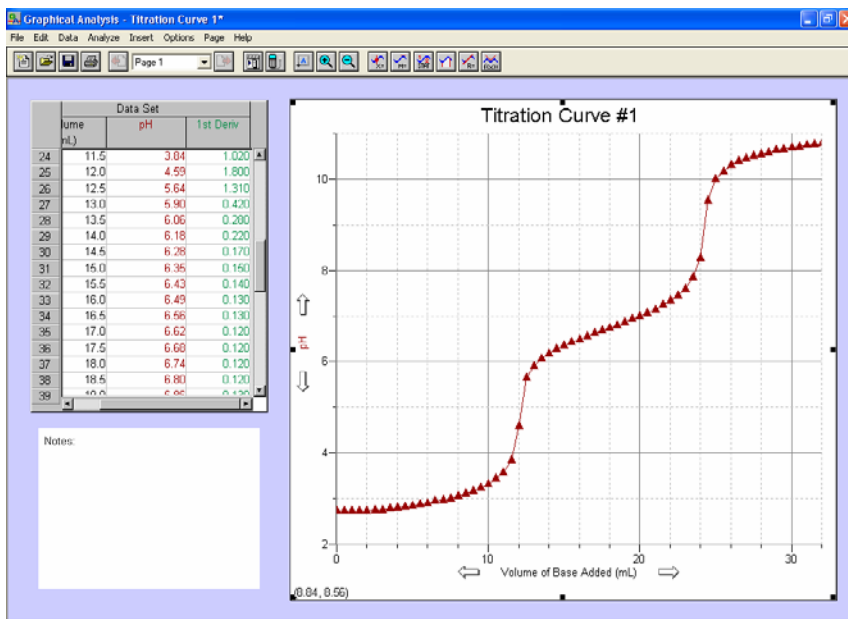


The top of the two peaks are the first and second equivalence points

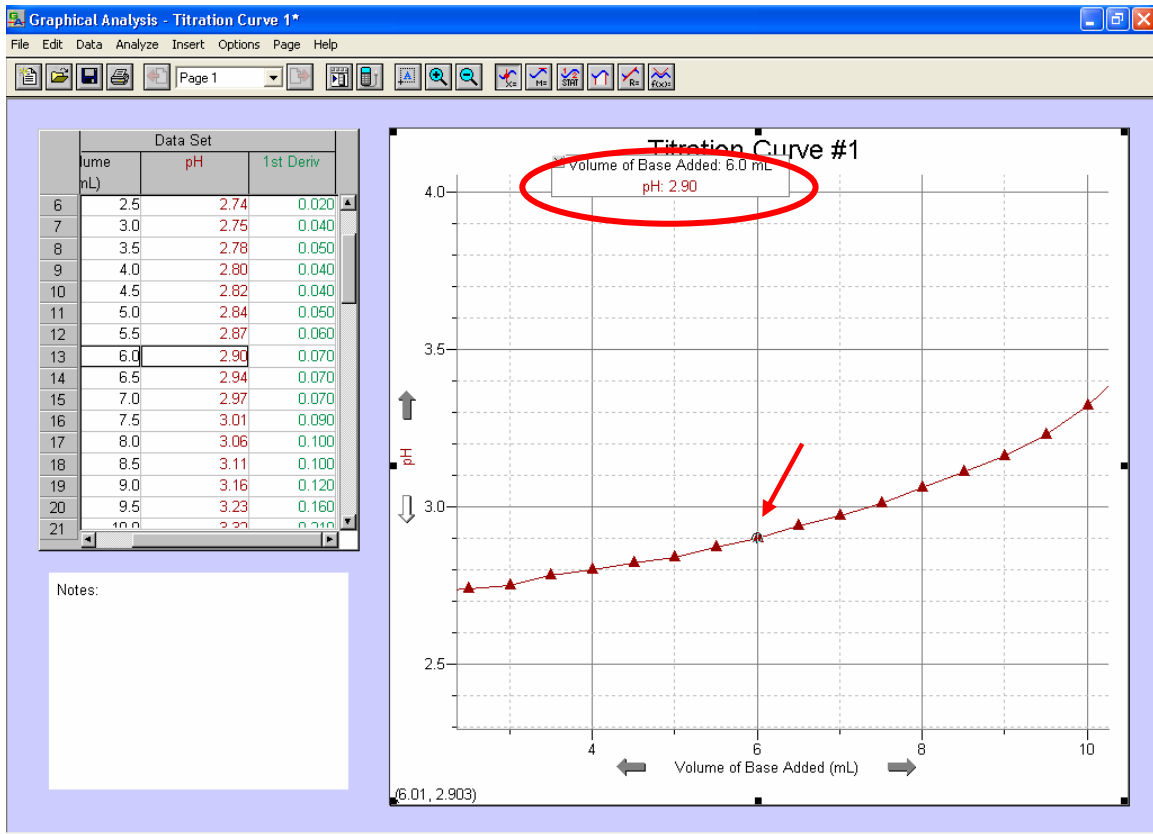
8. Click **Analyze** than **Examine** to point to the two points and get the volume of base for the equivalence points. Record these two values (**a** and **b**) as you will need them to extrapolate the pKa values.



Change the graph back to pH by *clicking* on the **y axis box** and selecting **pH**. You will get the original plot back (shown below)



9. To find  $a/2$  and  $(a+b)/2$  simply take the volume value for  $a$  (i.e. 12.0mL) and calculate  $a/2$  (in this example 6.0mL) than zoom into that area of the graph and *click* on the volume value to extrapolate the pH (in this case  $pK_{a1}$ )



In this example the  $pK_{a1}$  is 2.90

Do the same for  $pK_{a2}$  ( $(a+b)/2$ )

**Again, Be sure to print off each of the various graphs to show how you calculated these values. Also be sure to record all of these values before printing.**