Math 145 - Calculus I Name________________________

Titration Lab - Lab 11 [1]

Titration is a method of chemical analysis in which a reactive substance is slowly added to another substance, and some property of the combined substance is measured. This procedure is taught in CHM 116, General Chemistry II.

We will be looking at an example of acid-base titration. Specifically, 25 mL of an unknown monoprotic weak acid is titrated against 0.105M NaOH (which is a strong base). This means we are adding the base to the acid using a burette in a slow and precisely controlled manner. We measure the pH after each addition. (A pH of less than 7 is an acid, and a pH of more than 7 is a base.)

1. Open the titration spreadsheet file (found on Moodle). Explain in words what the point $(13, 3.41)$ means.

2. Create a scatter plot of the data. Do not connect the points. Sketch your plot below.

3. Imagine a smooth function $P(x)$ connecting the data points. What are the variables P and x (including units)?

4. How would you describe the function $P(x)$ in mathematical terms? (Consider terms like positive, negative, increasing, decreasing, concave up, concave down, maximum, minimum, etc.)

[1] This example was created with the help of Chemistry professor Joan Kunz. Thank you, Joan!

5. Create a new column and calculate the rate of change between each pair of points. Put the first computed value into cell C4. What observations can you make of your rate of change results? List a few things.

6. In titration we are interested in the *equivalence point*. Chemically this is when enough of the base has been added to completely neutralize the acid. Graphically this is when the *reaction rate begins to decrease*. How do we determine the equivalence point from P? Next, how do we determine the equivalence point from P'? What does the data suggest? Estimate the equivalence point with these two approaches using your data and graph.

7. Suppose we have a formula for the titration function $P(x)$. What calculation would we want to do to find the equivalence point? What is our mathematical name for that type of point?

8. Go back to your spreadsheet and calculate estimates of the second derivative. Put the first computed value into cell D5. How many times does the second derivative change sign? What does that tell us about the concavity of $P(x)$? How would we determine the equivalence point from P''? What does the data suggest?

9. We are interested in when the second derivative is equal to zero. This actually happens a few times with our data set, but there is only one equivalence point. With our data there are a number of consecutive places early on where the second derivative is zero. To figure out why this happens, suppose we have a function whose second derivative is always zero. So we have $\dfrac{d^2y}{dx^2} = 0$. What is $\dfrac{dy}{dx}$ for this function?

10. With that derivative, what kind of function must y be? Conclusion: If $f(x)$ is a __________________ function on an interval, then $f''(x) =$ _____ on that interval.

11. We are not interested in the places where the titration curve is linear, we are interested in where the concavity of the curve changes, specifically where it changes from concave up to concave down. Between what two data points does that happen? What is the concavity before and after the change?

    Between $x =$______ and $x =$______ the second derivative changes from _______ to _______.

12. What is your best guess of the equivalence point for this titration? (Your answer should be the mL of NaOH at the desired point.)

13. The spreadsheet has a second page with more precise data near the equivalence point. Redo the scatter plot, and the first and second derivative calculations.

    Between $x =$______ and $x =$______ the second derivative changes from _______ to _______.

    What is your new estimate of the equivalence point?

14. If we know the equivalence point, we can find K_a, the *acid dissociation constant* for the acid in question. This constant shows how completely the acid ionizes, and can be used to identify the acid. The relationship is that the pH at **half** of the equivalence value is equal to 'pK_a', defined as $-\log_{10}(K_a)$, which means pH $= -\log_{10}(K_a)$. So, since the equivalence point is _______, half of that is _______, and from our measured data the pH there is about _______.

    Now solve for the value of K_a.

15. Here's a list of common acids:

Acid	Use	K_a
benzoic acid	food preservative	6.5×10^{-5}
formic acid	ant bite sting	1.7×10^{-4}
acetylsalicylic acid	aspirin	3.0×10^{-4}
acetic acid	vinegar	1.8×10^{-5}
hydrofluoric acid	glass etching	7.1×10^{-4}

Which acid do you believe was used in our titration?