In Class Activity: Modeling a Weak Acid Titration Curve using Excel

The following is an Excel based, guided inquiry activity to help in understanding acid-base titrations and alpha fractions. Answer each question carefully, and organize your data neatly!

Getting Started

I. Open the Excel document entitled “Model_titration.xls”. Familiarize yourself quickly with the spreadsheet. Certain information you will have to input into selected cells where called out. Information in the columns needs to be generated with the appropriate equation and iterated down the column.

II. The ‘drops’ column has already been filled in for you. There are more drops than needed to reach the end point. There is no reason to extend this column. The information bulleted below needs to be used to generate the remaining columns.

- There are approximately 20.00 drops in a 1.000 mL during the titration.
- We are using 0.1000 Molar NaOH to titrate 50.00 mL of solution at the start. Solution is made by diluting 0.1000 gram of weak acid with water.

Data/Calculations

Part One

I. Make up a fictitious $K_a$ for a weak acid and record the number in cell $G2$. This number should be confirmed with the instructor or learning assistant as being reasonable. You can access your textbook’s appendix if you wish.

II. If we have 0.1000 grams of weak acid (assume the molar mass is 95.00 g/mole), determine the analytical concentration (molarity) of the weak acid at the start of the titration (record in cell $F9$).

III. As you begin adding drops of base, what happens to the ‘volume of titrant’ column? Assure that the column accurately reflects an increase in the amount of titrant added as the drops increase, (i.e. adjust the “titrant mL” column accordingly). You obviously need to keep a ‘running total’ of the titrant added.

IV. While you are titrating the acid solution, the total volume of the solution is changing with each drop added. Again, assure that the column labeled ‘total volume (mL)’ reflects this change.

Assume the reaction of the strong base with the weak acid is complete to address the questions below.

$$HA + OH^- \rightarrow H_2O + A^-$$
Upon addition of base, what two major, relevant species are left in the solution (water is not one of them)?

_____________ & _______________

V. Use the results just completed to fill in the columns for ‘moles OH\(^{-}\) added’, [HA] and [A\(^{-}\)]. The [HA] and [A\(^{-}\)] concentrations will be considered analytical concentrations. You can use the equilibrium expression (1) or the Henderson-Hasselbalch equation (2) to determine [H\(^{+}\)] and pH.

\[
K_a = \frac{[H^{+}][A^{-}]}{[HA]} \quad (1)
\]

\[
pH = pK_a + \log \frac{[A^{-}]}{[HA]} \quad (2)
\]

VI. Find out where your endpoint is and note this somehow on our spreadsheet. The pH after this point is no longer determined by the weak acid and its conjugate base. Rather the pH is determined by what?

Knowing this, determine the pH beyond the endpoint. Next, plot your titration curve as “pH vs. volume base (mL)” added.
**Questions.**

**Question 1** – How did you express the analytical concentrations of [HA] and [A⁻] in your spreadsheet?

**Question 2** – Vary the value for the $K_a$ term by making it an order of magnitude higher or lower from your original value. How does this affect the graphing of the titration curve?

**Question 3** – As learned in class, the pH of a weak acid solution (before any base is added) is equal to $[H^+] = \sqrt{k_a C_{HA}}$

Given your $K_a$ value and your initial analytical concentration for the weak acid, calculate the $[H^+]$ and the resulting pH of that solution. Compare this value of the pH with a pH value close to the starting point from your Excel spreadsheet. Is there a significant difference in the pH values – remember that pH differences are differences in orders of magnitude!? If so, discuss with your neighbor, instructor, or learning assistant what may be going on here.

**Question 4** – What do you think would happen if the $K_a$ value was $10^{-7}$ or lower in value? How concerns would a person have about calculating the pH for this kind of acid?

**Question 5** – Generate on the spreadsheet the first and second derivatives of the pH as a function of base added. Plot these graphs.

$$1st \ derivative = \frac{\Delta \ pH}{\Delta \ titrant \ added}$$

$$2nd \ derivative = \frac{\Delta 1st \ derivative}{\Delta \ titrant \ added}$$

**Part Two (Alpha Fractions)**

Alpha plots show differences in parent acid and conjugate base composition as a function of solution pH. Alpha values are unitless and are normally presented as a function of $[H^+]$ and associated $K$ values for a given system at equilibrium (see below). Alpha-0 ($\alpha_0$) represents the
fully protonated fraction, while \( \alpha_1 \) represents the deprotonated form of the acid. Both fractions must add up to 1.00.

\[
\alpha_0 = \frac{[H^+]}{[H^+] + K_a} \quad \alpha_1 = \frac{K_a}{[H^+] + K_a}
\]

**Calculations.**

I. Make columns for \( \alpha_0 \) and \( \alpha_1 \) in your Excel spreadsheet.

II. Using your \([H^+]\) and \(K_a\) value, fill-in numbers in for your alpha values in the columns created in step I. You need to find the expression for alpha values from your book or notes!

III. Make a plot of both your alpha value columns in a graph of Fractional composition vs. pH.

IV. Make a plot of both your alpha value columns in a graph of Fractional composition vs. Volume of base added (titrant mL).