

You may complete the following individually, or with one (1) partner. You may use your textbook and notes, but may not receive assistance from your classmates or anyone other than Dr. Lamp. This signed sheet must accompany the completed assignment. By signing below, you certify that you completed the problems in accordance with these rules. No credit will be given to unsigned papers.

Signature \_\_\_\_\_ Date \_\_\_\_\_

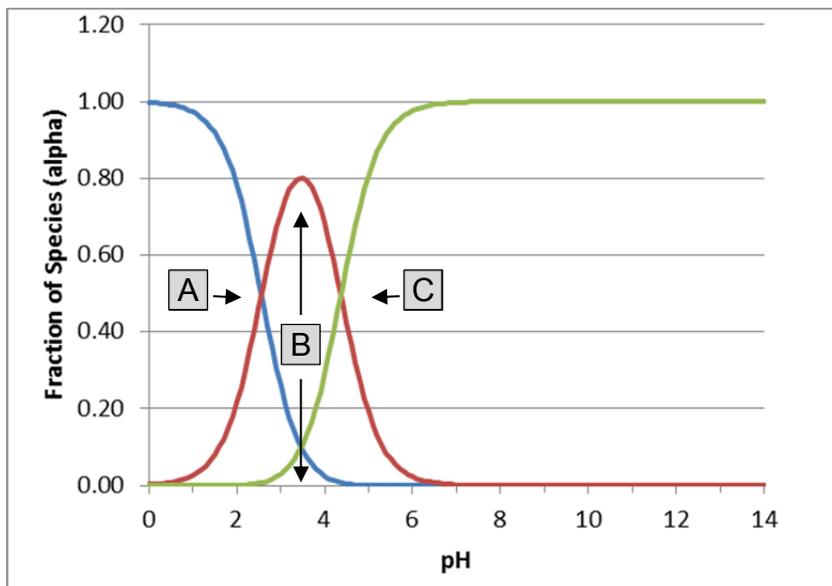
To complete this portion of the exam, prepare a *generic* spreadsheet program that will allow you to calculate a curve for the titration of a weak diprotic acid with a strong base. The spreadsheet should allow you to enter **pK<sub>a</sub>'s for each dissociation**, and **concentration and volume of analyte and concentration of titrant** used and must output two plots: **(1) a plot of the fraction of dissociation of the acid as a function of pH** (see Figure 9-4 as an example), and **(2) a plot of the titration curve, using at least 100 points**. Section 10-10 introduces one approach to this challenge. To demonstrate the utility of your spreadsheet, use it to complete the following tasks:

1. Model the titration of 20.00 mL of a 75.0 mM solution of *oxobutanedioic acid* with 0.100 M KOH. For oxobutanedioic acid,  $\text{pK}_{\text{a}1} = 2.56$  and  $\text{pK}_{\text{a}2} = 4.37$ .
2. Model the titration of your unknown acid from the  $K_{\text{a}}$  experiment. Use your experimental conditions and your best guess for the identity of your acid. If your unknown was triprotic, you only need to consider the first two  $K_{\text{a}}$ 's. If your acid was monoprotic, use a value of 20 for  $\text{pK}_{\text{a}2}$ . (If you are working with a partner, you need only model one of your unknowns.)
3. Using the results from the model created in Task 2, above, plot the experimental data from your  $K_{\text{a}}$  experiment on the same axes as the theoretical curve and provide a brief discussion of the similarities and differences in the data and whether the simulation supports your identification of the unknown acid. (If you are working with a partner, you need only plot and analyze one of your unknown data sets.)

**Requirements:** Submit both a hardcopy of your spreadsheet plots for each task, as well as an electronic copy of the spreadsheet file itself, with the data corresponding to Task 1 above. The spreadsheet file must be uploaded to the "Exam 5 Part III" assignment on our Blackboard course page. Your hardcopy must include (a) this signed sheet, (b) two plots from Task 1, (c) two plots from Task 2, and (d) one plot and a discussion from Task 3. *If you work with a partner, you only need to submit one electronic version and one hardcopy of the assignment.*

**Grading Criteria:** As I grade your spreadsheets, I will be comparing your results to those of a simulation that I have prepared (20 points). I will also input data for a third titration and examine the flexibility of your approach (5 points) and evaluate your comparison to experimental data in Task 3 (5 points).

## Task 1

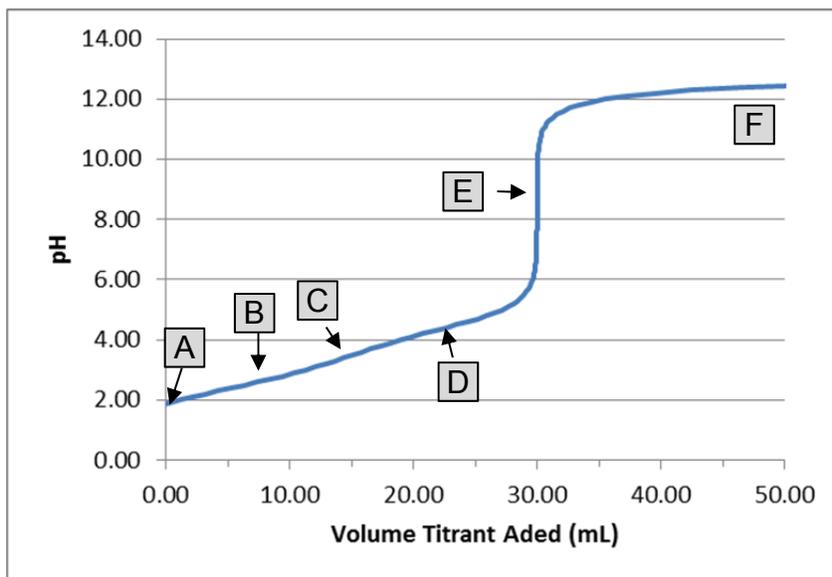


Key Characteristics:

Point A: At pH = 2.56,  $\alpha_{\text{H}_2\text{A}} = \alpha_{\text{HA}^-} = 0.5$

Point B: At pH = 3.47,  $\alpha_{\text{HA}^-}$  is maximized at about 0.80 and  $\alpha_{\text{H}_2\text{A}} \approx \alpha_{\text{A}_2^-} \approx 0.10$

Point C: At pH = 4.37,  $\alpha_{\text{HA}^-} = \alpha_{\text{A}_2^-} = 0.5$



Key Characteristics:

Point A: At  $v = 0$  mL,  $\text{pH} \approx 1.9$

Point B: At  $v = 7.5$  mL,  $\text{pH} = \text{p}K_{\text{a}1} = 2.56$ .

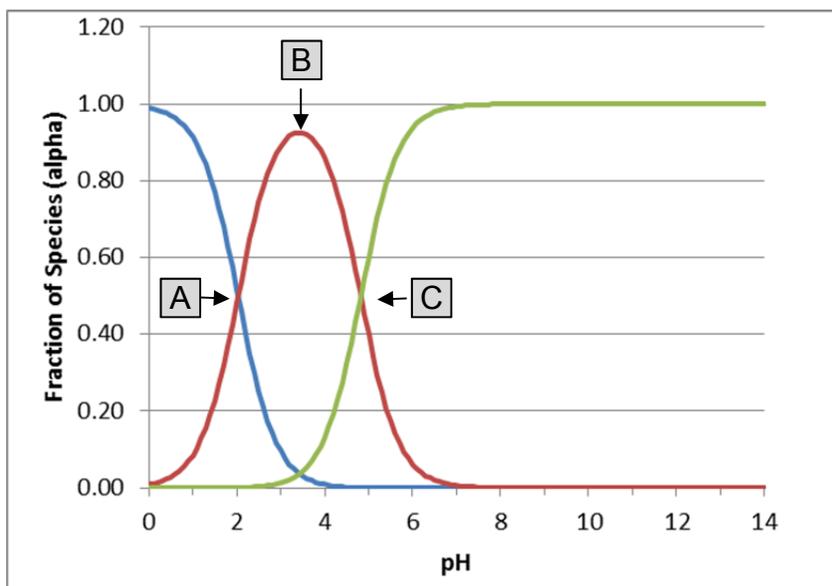
Point C: At  $v = 15.0$  mL (1<sup>st</sup> equivalence point),  $\text{pH} = \frac{1}{2}(\text{p}K_{\text{a}1} + \text{p}K_{\text{a}2}) = 3.47$

Point D: At  $v = 22.5$  mL,  $\text{pH} = \text{p}K_{\text{a}2} = 4.37$

Point E: At  $v = 30.0$  mL (2<sup>nd</sup> equivalence point),  $\text{pH} = 8.5$

Point F: Maximum pH = 13.0 (pH of 0.100 M NaOH) occurs at large volumes

**Task 2:** I input into your spreadsheet parameters for the titration of 25.0 mL a 0.100M diprotic weak acid ( $pK_{a1} = 2.03$ ,  $pK_{a2} = 4.82$ ) with 0.200M NaOH.

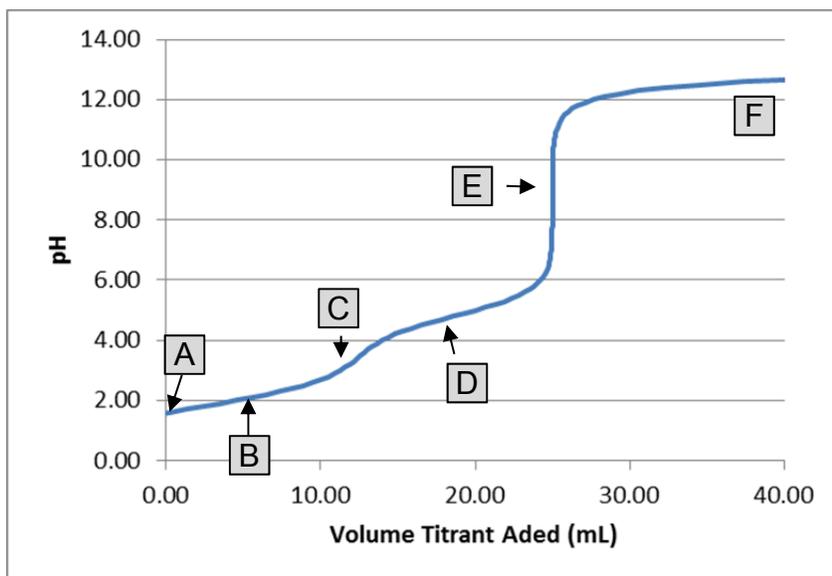


Key Characteristics:

Point A: At  $pH = 2.03$ ,  $\alpha_{H_2A} = \alpha_{HA^-} = 0.5$

Point B: At  $pH = 3.4$ ,  $\alpha_{HA^-}$  is maximized at about 0.93 and  $\alpha_{H_2A} \approx \alpha_{A^{2-}} \approx 0.035$

Point C: At  $pH = 4.82$ ,  $\alpha_{HA^-} = \alpha_{A^{2-}} = 0.5$



Key Characteristics:

Point A: At  $v = 0$  mL,  $pH \approx 1.6$

Point B: At  $v = 6.25$  mL,  $pH \approx pK_{a1} \approx 2.03$ .

Point C: At  $v = 12.5$  mL (1<sup>st</sup> equivalence point),  $pH = \frac{1}{2}(pK_{a1} + pK_{a2}) \approx 3.4$

Point D: At  $v = 18.75$  mL,  $pH \approx pK_{a2} \approx 4.82$

Point E: At  $v = 25.0$  mL (2<sup>nd</sup> equivalence point),  $pH \approx 10.2$

Point F: Maximum  $pH = 13.3$  ( $pH$  of 0.200 M NaOH) occurs at large volumes

**Task 3:**

Your score is based upon plotting your data and your discussion comparing your experimental data to the curve predicted by your spreadsheet model.