Determining the Acid Dissociation Constant for an Organic Dye

One of the simplest ways to estimate a solution's pH is to add a small amount of an organic dye and observe the solution's color. For example, a solution of bromothymol blue—one of several sulfonophthalein dyes—is yellow when the pH is less than 6 and blue when the pH is greater than 8. Figure 1 shows the structure of bromothymol blue in its weak acid and weak base forms. When the pH of a solution of bromothymol blues is adjusted from 6 to 8, its color transitions from yellow to blue by passing through various shades of yellow-green, green, and green-blue, each of which correlates to within a few tenths of a pH unit.

Figure 1: Structure of bromothymol blue in its weak acid form (left) and its weak base form (right); modified from https://commons.wikimedia.org/wiki/File:Bromothymol blue protolysis.svg.

This relationship between the change in color and pH, is easy to appreciate from the basics of mixing color. Less obvious is the mathematical relationship between absorbance and pH

$$\log\left(\frac{A - A_{\text{In}}}{A_{\text{HIn}} - A}\right) = pK_a - pH$$

where A is the absorbance at a particular pH and $A_{\rm In}$ and $A_{\rm HIn}$ are the absorbance values for the weak base and weak acid forms, respectively. Note that this equation suggests it is possible to determine a dye's p K_a by monitoring its absorbance as a function of pH. The purpose of this two-week, open-ended project is to design and carry out suitable experiments that can provide the p K_a value for two organic dyes: bromocresol green and neutral red.

Preparing for Lab

Planning for this lab is critical to your success. Read the following paper as it provides useful information for determining the pK_a values for organic dyes; a copy of the paper is in your group's Dropbox folder.

Patterson, G. S. "A Simplified Method for Finding the pK_a of an Acid–Base Indicator by Spectrophotometry," J. Chem. Educ. 1999, 76, 395-398.

Be sure to complete the relevant sections of your notebook before each week's lab session. As you develop strategies for determining the pK_a values for these dyes, keep the following in mind:

- The paper provides complete experimental details for determining the pK_a of bromophenol blue and sufficient information to help you design a procedure for determining the pK_a of bromocresol green. You will need to adapt the procedure to determine the pK_a for neutral red.
- The work described in the paper uses a different instrument for acquiring absorbance spectra and for measuring absorbance; you will need to modify the published procedure to take advantage of the spectrometer available to you.
- One shortcoming of the paper is that the author did not verify Beer's law, which means they provide
 no evidence that absorbance is a linear function of concentration. Review how you did this in an earlier
 lab and adapt that approach to this lab.

- You will need to complete some research on each dye. Among the information you may find useful are structures, the expected color of the weak acid and weak base forms, and approximate pK_a values.
- Any experimentally determined values should be compared to their expected theoretical values.

Procedure

During the first week you should plan to work on determining the pK_a value for bromocresol green. During second week you will determine the pK_a for neutral red.

Cautions

There are no cautions for this lab other than the normal respect for chemicals and hot solutions.

Waste Disposal

You may dispose of all solutions by rinsing them down the drain with copious amounts of water.

Lab Report

Remember to switch roles for this lab.

Role	Final Product	Responsibilities
Manager	formal report	organizes all aspects of the group's work both in and out of lab; makes all final decisions on experimental design; determines when sufficient work is complete
Chemist Technician	short report oral report	prepares solutions; weighs out samples; carries out the experiment sets up, calibrates, and optimizes the group's equipment; maintains the group's electronic laboratory notebook

All group members must contribute to planning the experiment and to the analysis of data, and are responsible for understanding how to convert the experiment's data into results. Here are some details on the different types of reports:

- For the **formal** report you will present the results of your experimental work in the form of a journal article. For more details on the format of formal reports, review the document "Some Guidelines for Preparing a Formal Report," "Sample Report," and "Rubric for Evaluating Formal Reports" available at the course website. Although I will not formally review a draft of your report, I do encourage you to bring a draft of your report to my office with specific questions you wish to discuss. This report is due Thursday, May 4th.
- For the **short** report you will receive a set of data that is similar to that collected in lab along with some specific questions to answer using this data. This report is due Friday, April 28th.
- For the **oral** report we will meet to discuss your group's work on this experiment. To prepare for this meeting, review your group's experimental plan, your group's data, and your group's analysis of that data. When you are ready, schedule a 30 minute meeting with me. This meeting should take place after your group has finished analyzing the data, but no later than Friday, April 28th.