

Spectroscopic Study of Wine

OBJECTIVE

To determine the concentration of ethanol in a wine sample.

INTRODUCTION

Earlier this semester you experienced spectroscopic techniques. In the “Spectroscopy and Conductivity of CuSO₄ Solutions” experiment, you observed a linear relationship between absorbance and concentration and used this relationship to determine the concentration of an unknown CuSO₄ solution. This linear relationship is known as Beer’s Law:

$$A = \epsilon \ell c \quad \text{or} \quad A = (\epsilon \ell) c + 0 \quad \text{Equation 1}$$

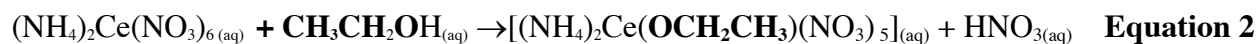
Written in the form of the equation for a line, the slope is the product of the extinction coefficient (ϵ), also called molar absorptivity, and the path length (ℓ), the distance the light travels through the sample. Both the path length and the extinction coefficient are constants. This constant is primarily a function of the identity of the absorbing species, however the extinction coefficient is dependent on the temperature and the solvent. Therefore, it is a constant only at the stated conditions. Restated, for you to get the same extinction coefficient as your neighbor the data must be collected in the same solvent and at the same temperature.

In this experiment, you will use Beer’s Law to determine the % ethanol in wine.

Looking back at your previous experiment, the Beer’s Law data was collected at one wavelength with the spectrometer. This wavelength was chosen for you, and you might not have questioned why that particular wavelength was chosen. In this experiment, you will have to *propose* an appropriate wavelength to collect data that will result in a Beer’s Law relationship.

The first conclusion you should reach is that the chemical species you want to measure *must* absorb light in a region where the spectrometer operates. Typically, but not always, this means the solution will have color. Determining the ethanol content in wine appears to fit this requirement, since most wines range from a pale yellow to a deep red. However, the wine color is not a result of the concentration of ethanol, so it cannot be determined by simply placing wine solutions in the spectrometer and measuring the absorbance. In fact, ethanol is a colorless liquid. So, we have researched and found a chemical that will react with ethanol to form a colored complex of known composition in solution.

Aqueous ammonium hexanitrate cerium(IV), (NH₄)₂Ce(NO₃)₆, will react with ethanol (Equation 2) to form a red ethoxy-cerium(IV) complex in solution. An example of the experiment can be seen in **Figure 1**.



Orange/Yellow

Colorless

Red Intermediate

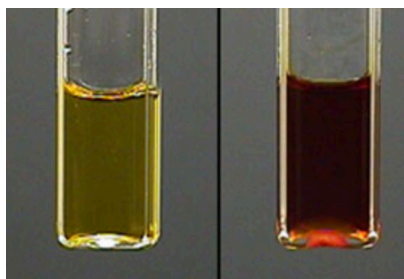
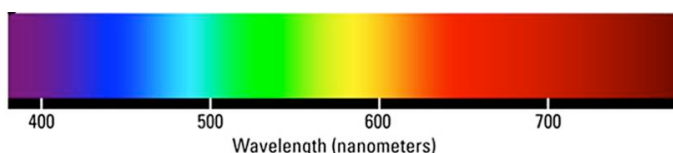
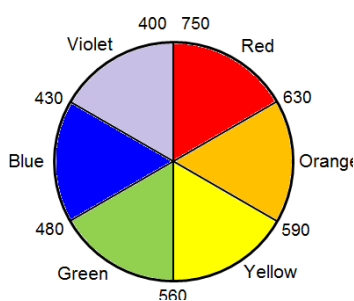


Figure 1: Aqueous ammonium hexanitrate cerium(IV) (left) and red ethoxy-cerium(IV) complex (right)

Since the reaction stoichiometry is 1:1, the concentration of ethoxy-Ce(IV) is equal to the original concentration of ethanol as long as *ethanol is the limiting reagent*.

The brackets around the new complex indicate that this product is an intermediate in a reaction that is not finished. Often, intermediates exist for very short time periods, but this complex is stable for a few hours. This stability allows us to measure the absorbance of the ethoxy-cerium(IV) complex. This technique is called an “indirect analysis” since the amount of ethoxy-cerium(IV) complex is measured, rather than the ethanol directly.

Part A – Picking a Wavelength for Wine Analysis



As mentioned before the red ethoxy-cerium(IV) complex appears dark red in color as shown in **Figure 1**. Using the color wheel and the visible spectrum answer the following two questions.

1. The cerium (IV) solution used in this experiment is orange/yellow. What wavelength of light does it transmit the most? What wavelength does it absorb the most (2 pts)
2. The reaction of cerium (IV) with ethanol forms a deep red ethanol-cerium complex solution. What wavelength of light does it transmit the most? What wavelength of light would you use to measure the maximum absorbance? (2 pts)

Part B – Colorimetric Analysis of Wine

Standard Solutions

Calculate the volumes needed to prepare 10.00mL of four standard ethanol solutions; 1.00%, 3.00%, 5.00%, and 8.00% ethanol in water from a 10.0% (v/v) alcohol in water stock solution. (2 pt)

Table 1: Volumes of stock solution and of deionized water to prepare 10.00mL of standard solutions.

Ethanol Concentration (%)	Volume of Stock Solution	Volume of Deionized water
1.00		
3.00		
5.00		
8.00		

Wine Solution

Note: Because most wines range between 10% and 20% alcohol which will be outside the standard range of the sample data. The value given for the wine sample will be after it was diluted to half its actual concentration.

Cerium Solutions

- A total of 7 solutions were prepared and labelled 0, 1, 3, 5, 8, 10, and W (for wine).
- To the solution labelled (0) just deionized water + cerium were added. This solution was used as your 0% standard and as the “blank” solution during calibration of the spectrophotometer.
- To the other cuvettes (1% through 10%) and the *diluted wine sample*, each were filled with the corresponding solution and cerium solution was added to form the red ethoxy-cerium complex.
- Figure 2 shows a schematic representation of the results

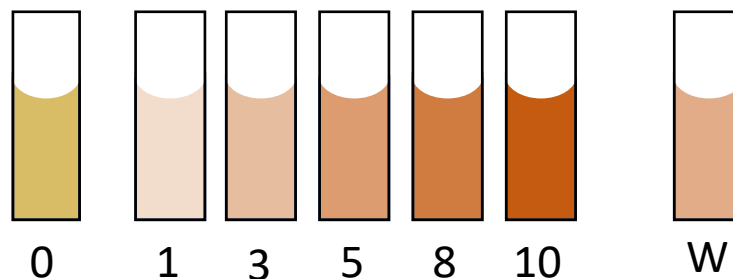


Figure 2: Schematic representation of solutions obtained after adding cerium solution (0.00%, 1.00%, 3.00%, 5.00%, 8.00%, 10.00% standard solutions and for the unknown wine sample).

Measuring the Absorbance of Cerium-Ethanol Solutions

- The spectrophotometer was calibrated using the 0% solution as blank to ensure a 0.00 absorbance value for a 0% alcohol solution.
- The maximum wavelength was set to the one you determined in part A.
- Absorbance was measured for all standard solutions
- The absorbance unknown wine was also measured.
- A sample of the results are shown in Table 2.

Table 2: Sample of results obtained for absorbance of cerium-ethanol solutions.

Ethanol Concentration (%)	Absorbance
0.00	0.000
1.00	0.056
3.00	0.175
5.00	0.345
8.00	0.545
10.00	0.667
W	0.448

DATA ANALYSIS

1. Plot the sample data in **Table 2** in Excel according to Beer's Law. Make sure to include a (0, 0) point. Perform a linear regression and display the equation for the line and R^2 value on the graph. (5 pts)
2. Using the equation of your line, calculate the concentration of ethanol in your wine sample. **Remember that the actual wine sample was diluted to half its original concentration with water.** (2pts)
3. Calculate the percent error for % ethanol of wine sample. The accepted value for the wine sample is 12.5% as shown in **Figure 3**. (1 pt)

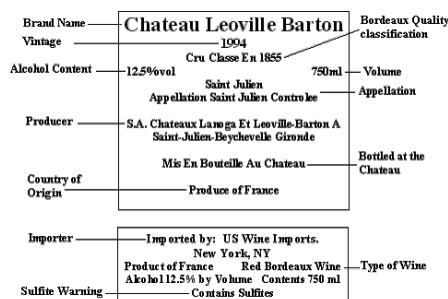


Figure 3: Label from the Wine sample showing the accepted alcohol concentration.

POST LAB QUESTIONS

The following questions will apply to the Beer's Law graph you created in Part B of the experiment to determine the percent alcohol content of the wine.

1. What is the general relationship between the variables for this graph? (1 pt)
2. Write the numerical value of the slope with appropriate units. (1 pt)
3. Write the numerical value for the y-intercept with appropriate units? (1 pt)
4. What is the scientific meaning of the slope? (1 pt)
5. What is the scientific meaning of the y-intercept? (1 pt)
6. The **general equation** for a line is $y = mx + b$. Write the **specific equation** for this line substituting appropriate variables for x and y, and using your numerical values for the slope and the y-intercept. (1 pt)
7. Using your equation of the best fit line, calculate the absorbance for a solution containing 24% alcohol. (1 pt)
8. Using your equation of the best fit line, calculate the percent alcohol for a solution with an absorbance of 1.90. (1 pt)