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| Experiment 4: Inversion of Sucrose |
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# Abstract

In this experiment, the optical properties of the molecules involved in the acidic decomposition of sucrose reaction were used to estimate the rate of reaction using 2.0 N solutions of HCl, sulfuric acid, and acetic acid. The optical rotation of each reaction solution was measured in regular intervals using a polarimeter, and, assuming the reaction was first order in the concentration of the acid, a plot was calculated to recover the rate constant. The rate constants in each solution were calculated to be 0.0351 min-1, 0.0153 min-1, and 1.69E-19 min-1 for HCl, sulfuric acid, and acetic acid, respectively. As these numbers do not represent true rate constants, as the rate constant should not change, but more a rate of reaction for each solution, a relationship between these constants and hydrogen ion concentration was set up. With this relationship, the concentration of [H+] ions in the sulfuric acid solution was calculated to be 0.871 M. The calculation for acetic acid was not applicable due to no observed reaction activity in the polarimeter.

# Introduction

Chiral molecules rotate plane polarized light according to a specific rotation, where the total rotation is a function of the specific rotation of a chiral molecule, its mass concentration, and the path length of the light that travels through the solution. When there are multiple chiral molecules in solution, the effect is additive.

In the acid catalyzed conversion of sucrose to glucose and fructose according to equation 1, the reaction solution will contain three chiral molecules: sucrose, glucose, and fructose. As each of these molecules have a specific rotation, the rotation light by the reaction solution will change as the reaction progresses. Assuming the reaction is first order, this gives us the following equations.

Equation 1: Acid Catalyzed Reaction of Sucrose

Equation 2: Derivation of Rate Constant as a Function of Rotation Angle

Where S, G, and F represent sucrose, glucose, and fructose, respectively, representes the optical rotation of the reaction solution with the reaction in final equilibrium, represents the optical rotation of the reaction solution initially, k represents the rate constant, and t represents time. The theoretical rotations of the solution at the beginning and at the end are as follows.

Equation 3: Expressions of Expected Rotation Angle at Beginning and End of Acid-Catalyzed Sucrose Reaction

Where L is the path length in dm, and M is the molecular weight. Furthermore, assuming that the rate of the equation is proportional to the concentration of [H+], it is also possible to find the concentration of acid that the experiment was run in given a baseline.

Therefore, if the angle of rotation is measured by a polarimeter as the reaction progresses at different time points, a plot can be recovered, and an appropriate rate constant can be derived from Equation 2.

# Experimental

To begin, a 10 cm sample cell was obtained for the polarimeter, and 100 mL of 0.25 M sucrose solution was prepared from dissolving the appropriate amount of sucrose in a 100 mL volumetric flask.

Next, the polarimeter was calibrated by setting it to read at 589 nm and loading the sample cell in the polarimeter with water.

Then, three 30 mL solutions of three different acids were prepared. The solutions were a 4.0 N (4.0 M) solution of HCl, a 4.0 N (2.0 M) solution of sulfuric acid, and a 4.0 N (4.0 M) solution of acetic acid. 25 mL of each of these solutions were aliquoted to a graduated cylinder.

Then, 25 mL of the sucrose solution was added to a beaker, followed by 25 mL of 4.0 N HCl. The time when half the HCl was added was recorded to signify the beginning of the experiment. Then, the mixture was stirred thoroughly. The sample cell was then filled with a sample of the mixture and was measured with the polarimeter. This was repeated a minute later with sucrose and the acetic acid solution, and another minute later with the sucrose and sulfuric acid solution.

This process of measuring the angle of rotation was repeated every 5 minutes for 60 minutes, except for the acetic acid solution, which was measured only once every 10 minutes, and the angle of rotation was recorded. Finally, at the end of the experiment, the temperature of the room was recorded.

# Results

To begin with the calculation of the rate constant, the values for and must be calculated. Given known values for the specific rotations for sucrose, glucose, and fructose as 66.5, 52.7, and -92.7 degrees cm3 dm-1 g-1 respectively, and with the known concentration of sucrose in each reaction solution as 0.125 M, each value can be calculated as seen in Equation 4.

Equation 4: Calculation of Reaction Optical Rotation Values

This value for the initial rotation matches up nicely to the experimental value measured from the polarimeter of 2.83 degrees. After the rotations are measured at each time period, using the values calculated from equation 4, the right side of equation 2 was calculated with the given data points, and the results are seen in the table attached in the appendix. An example table is shown below.

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| **Time (min)** | **Optical Rotation HCl (°)** | **Log Value HCl** |
| 0 |  |  |
| 5 | 2.27 | 0.167068562 |
| 10 | 1.79 | 0.331593417 |
| 15 | 1.33 | 0.519588839 |
| 20 | 0.96 | 0.701544435 |
| 25 | 0.66 | 0.878050325 |
| 30 | 0.41 | 1.053437435 |
| 35 | 0.2 | 1.229022839 |
| 40 | 0.04 | 1.387131369 |
| 45 | -0.12 | 1.575020365 |
| 50 | -0.25 | 1.758875166 |
| 55 | -0.35 | 1.927604567 |
| 60 | -0.45 | 2.13070013 |

Table : Measured Optical Rotation and Log Value Table for HCl Reaction Solution

Then, to calculate k from equation 2, a scatter plot was calculated with time on the x-axis and the expression on the y axis, so linear regressions will allow the slope, k, to be calculated. This is shown in figure 1.

Figure 1: Scatter Plot and Regression to Calculate Rate Constant of Inversion of Sucrose Reactions

The rate constants can be taken from the slopes of the equations on the graphs as 0.0351, 0.0153, and 1.69E-19 for HCl, sulfuric acid, and acetic acid, respectively. Assuming this reaction is first order in the concentration of the acid, the units of this rate constant are min-1.

# Discussion

In this experiment, an interesting observation is the apparent changing of the rate constant k with different initial concentration of acids. However, this is a simplification of the idea of a rate constant that does not conflict with the original definition of a first-order reaction. Given that the rate of a first order reaction is expressed as kr[A], and that the reaction is assumed to the first order in the concentration of the acid, the rate of this reaction can be expressed as kr[H+]. Furthermore, it is important to recall that given the different pKa’s of the acids used, the initial concentration of the acids vary on magnitudes of 10. Thus, the rate of reaction of the HCl reaction will be very different from the rate of reaction of the sulfuric acid, due to the hydrogen ion concentration term of the first order rate equation being different values. The overall kr of the reaction does not change between the reaction solutions.

Thus, we can represent the k values calculated by the slopes in figure 1 as an adjusted rate value, and substitute this as the rate in the first order rate equation. Given this representation, substitution and rearrangement leads to the following representation.

Equation 5: Derivation of Relationship Between Rate Constant and Hydrogen Ion Concentration

Thus, we derive a direct relationship between the measured “rate constants” and the concentration of hydrogen ions in solution. With the known concentration of 2.0 M H+ in the first HCl solution, the concentration can be estimated in the other solutions. An example calculation has been done in equation 6.

Equation : Estimation of Hydrogen Ion Concentration in Sulfuric Acid Solution

Using this same equation, the concentration of hydrogen ions in the acetic acid solution was calculated to be 9.63E-18 M.

Although the estimation for the concentration of the hydrogen ion in the sulfuric acid solution may be accurate, the estimation of the ion concentration in the acetic acid solution cannot be correct, as it is lower than the constant for the autoionization of water. This inaccuracy is likely due to the experimental data. The pKa of acetic acid, at 4.71, is much lower than that of stronger acids such as HCl and sulfuric acid, and thus, there was no observed angle change and therefore, no observable reaction in this experiment. This makes sense, as sulfuric acid, with a pKa1 less than zero and a pKa2 of about 2, this is still more than 2 magnitudes more strong than acetic acid. Thus, the reaction rate as measured by the polarimeter is effectively zero, and the true acid concentration will not be accurate.

# Appendix

1. Excel spreadsheet of experiment data 