Acid Catalyzed Iodination of Acetone

1: Introduction

This investigation aims to investigate the effect of the concentration of Hydrochloric Acid, Iodine and Acetone on the rate of Iodination of Acetone in the presence of a Hydrochloric Acid catalyst. The balanced chemical equation of the Iodination of Acetone is seen below:

$$CH_3COCH_3 + I_2 \xrightarrow{[H+]} CH_3COCH_2I + H^+ + I^-$$

The reactants of the reaction are Acetone and Iodine, and the products of the reaction are Iodoacetone, Hydrogen cations and Iodine anions. Even though the Hydrochloric Acid is only present as a catalyst, but due to the multi-step nature of the reaction, the concentration of the Hydrochloric Acid will also affect the overall rate of the reaction.

1.1: Research Question

To what extent does the effect of the volume of 2.75 Molarity Acetone (0.50 mL, 1.00 mL, 1.50 mL, 2.00 mL, 2.50 mL), 1 Molarity Hydrochloric Acid (0.50 mL, 1.00 mL, 1.50 mL, 2.00 mL, 2.50 mL) and 0.005 Molarity Iodine (1.00 mL, 1.50 mL, 2.00 mL, 2.50 mL, 3.00 mL) affect the overall rate of reaction.

2: Variables

2.1: Independent Variable

The independent variable of the investigation is the concentration of the two reactants: Acetone and Iodine, as well as the Hydrochloric Catalyst.

2.1: Dependent Variable

The dependent variable of the investigation is the overall rate of the iodination of Acetone given as the concentration of Acetone Iodinated over a given period of time.

2.1: Controlled Variable

2.1.1: Concentration of Non-Altered Reactants

Each trial of the experiment will alter the concentration of either one of the reactants or the catalyst. Therefore, the concentrations of the other reactants should be kept constant to ensure that the rate change occurred from the concentration of the independent variable rather than the other reactants or catalyst.

2.1.2: Volume of Water

The volume of water within the experiment is used to keep the concentration of the independent variable consistent throughout all the trials. If the volume of water was kept constant when the concentration of the independent variable increased, then the concentration will not be the same as if the water has been decreased accordingly.

2.1.3: Calibration of Photo-Spectrometer

The Photo-Spectrometer used to determine the absorbance of the resulting solution must be calibrated using the same blank solution with the following composition: 1.50 ml of 2.72 Molarity Acetone, 1.50 mL of 1 Molarity Hydrochloric Acid, 4.00 mL of Distilled Water and 0 ml of 0.005 Molarity Acetone. This ensures that the collected absorbance levels for all the trails remain constant and does not fluctuate.

3: Experimental Procedure

3.1: Materials

The material as well as chemical required to execute this experiment is listed below:

1. 2.72 M Acetone
2. 1 M Hydrochloric Acid
3. 0.005 M Iodine
4. Distilled Water
5. Spectrophotometer
6. Cuvettes
7. 10 mL Pipettes
8. PI Pumps
9. Test Tube Rack
10. Aluminum Foil Wrap

11. Stopwatch

12. Lens Paper

3.2: Experimental Procedure

The experimental method to determine the rate of the reaction was to measure the concentration of Iodine displaced over a certain period of time through the use of a Photo-Spectrometer observing the 400 nm wavelength. The time taken to reach the lowest absorbance value measured by the spectrometer will be the time to iodinate the Iodine.

1. The Photo-Spectrometer is connected to a computer with downloaded Sparkvue software through the use of either the Bluetooth Feature or an USB cable.

2. The "Blank Solution" can be created by mixing 1.50 mL of 2.72 M Acetone with 1.50 L of 1 M HCl and 4.00 mL of Distilled water within a beaker.

3. The Photo-Spectrometer can be calibrated to observe the absorbance of Iodine at 400 nm by setting the base value to be the value recorded with the "Blank Solution".

4. Measure stoichiometrically matching proportions of Hydrochloric Acid and Acetone through the use of a 10 mL pipette and pour the solution into a beaker.

5. Add the matching volume of Iodine to the beaker and begin to time on a stopwatch.

6. Through the use of a pipette, transfer a significant portion of the solution from the beaker into the cuvette and place the cuvette within the Photo-Spectrometer.

7. Each time the Photo-Spectrometer outputs a value lower than the previously recorded lowest value, record the time on the stopwatch using the lap feature.

8. When the absorbance stabilizes or once the absorbance value discontinues its decrease, stop the timer and record the final value.

9. Repeat steps 4-8 for all trials and record the values for each trial in a well-organized table.

10. Dispose of the final solution in an organic waste bin instead of pouring it down the drain.

4: Data Collection

4.1: Raw Data Collection

The collected raw data for all five altercations of the three independent variables can be seen in the tables below.

Table 1: Effect of Acetone Concentration on the Rate of Reaction

	Rate of Absorbance (± 1 s)			
Acetone (± 0.1 mL)	*Trial 1*	*Trail 2*	*Trail 3*	*Average*
0.50	280	200	290	257
1.00	142	264	-	203
1.50	190	180	120	163
2.00	52	105	-	79
2.50	41	39	70	50

Table 2: Effect of Hydrochloric Acid Concentration on the Rate of Reaction

	Rate of Absorbance (± 1 s)			
Hydrochloric Acid (± 0.1 mL)	*Trial 1*	*Trail 2*	*Trail 3*	*Average*
0.50	357	-	262	310
1.00	272	105	222	200
1.50	216	130	166	171
2.00	195	85	101	127
2.50	184	60	91	112

Table 3: Effect of Iodine Concentration on the Rate of Reaction

	Rate of Absorbance (± 1 s)			
Iodine (± 0.1 mL)	*Trial 1*	*Trail 2*	*Trail 3*	*Average*
1.00	101	70	44	72
1.50	64	79	60	68
2.00	-	72	50	61
2.50	49	90	72	70
3.00	93	101	92	95

4.2: Data Processing

The collected raw data above can be used to find the concentration of the Iodine through the use of Beer Lamber's Law given by the following equation where A is the absorbance value measured by the Pasco-Spectrophotometer and L is the wavelength in centimeters. From this equation and utilizing the literature absorption coefficient of Iodine α at 440 nm, the concentration can be determined by isolating the c value.

$$A = \alpha L\ c$$

The final concentration value of Iodine in the solution can be determined from the above equation. To measure the change in concentration, change of Iodine, the initial concentration value can be subtracted from the final concentration value.

$$\Delta I = I_{final} - I_{initial}$$

After the change in Iodine concentration has been determined, the rate of rection can be calculated by dividing the concentration of Iodine by the change in time. The rate of reaction can then be determined indicated by the following equation:

$$Rate = \frac{[I_2]}{\Delta t}$$

The concentration of the Acetone, Hydrochloric Acid and Iodine within each of the trail can be determined by multiplying the molarity of the solution by the volume within each of the trails and divided by the total volume of all the trials of 7 mL.

4.3: Sample Calculation

A sample calculation involving the data collected in trial one in the effects of Acetone on rate of reaction graph. The measured absorption value by the spectrophotometer (A) was 0.014 AU and was measuring at a wavelength of 440nm. Through the use of the literature value of the absorptivity constant of Iodine measured at 440 nm being 557 dm^3/mol cm (Kazantseva, Ernepesova, Khodjamamedov, Geldyev, Krumgalz, 2002), the final concentration of Iodine can be calculated determined as follows:

$$c = \frac{A}{\alpha L}$$
$$= \frac{0.014\ AU}{557\ dm^3/mol\ cm\ \times 4.4 \times 10^{-5}\ cm} \times 10^{-3}$$
$$= 5.7 \times 10^{-4}\ mol/dm^3$$

After the final concentration of Iodine has been determined, the change in Iodine concentration from before and after the reaction can be calculated to be the difference between the initial and final concentration values given as follows:

$$\Delta I = I_{final} - I_{initial}$$
$$= 5.0\ \times 10^{-3}\ mol/dm^3 - 5.7\ \times 10^{-4}\ mol/dm^3$$
$$= 4.43 \times 10^{-3}\ mol/dm^3$$

The determined concentration change value can then be used to calculate the rate of reaction by dividing the concentration change over the observed time period.

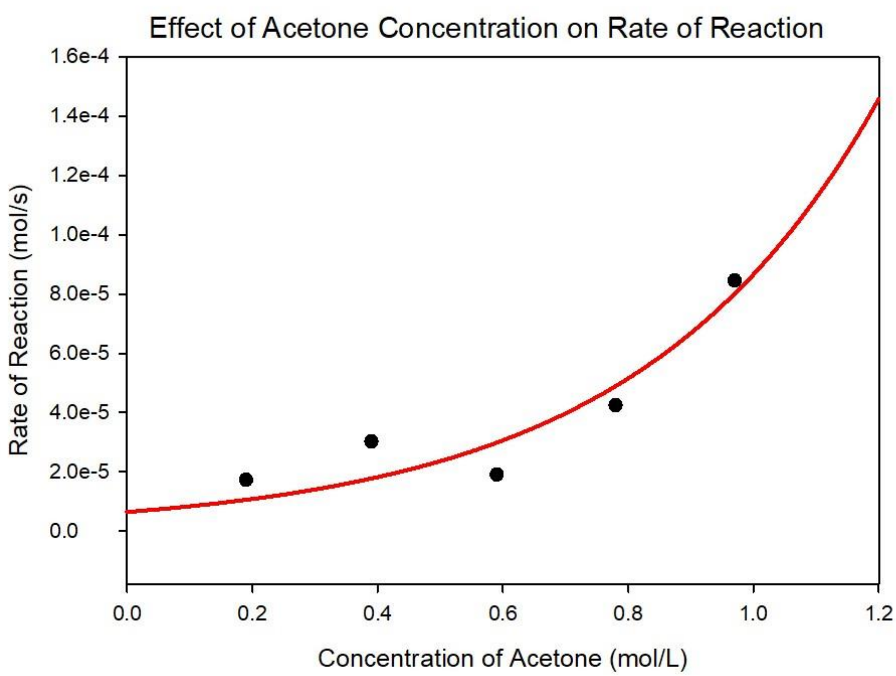
$$Rate = \frac{[I_2]}{\Delta t}$$
$$= \frac{4.43\ \times 10^{-3} mol/dm^3}{280\ s}$$
$$= 1.58\ \times 10^{-5}\ mol/dm^3\ s$$

This process can be repeated for all the trials to determine the following data.

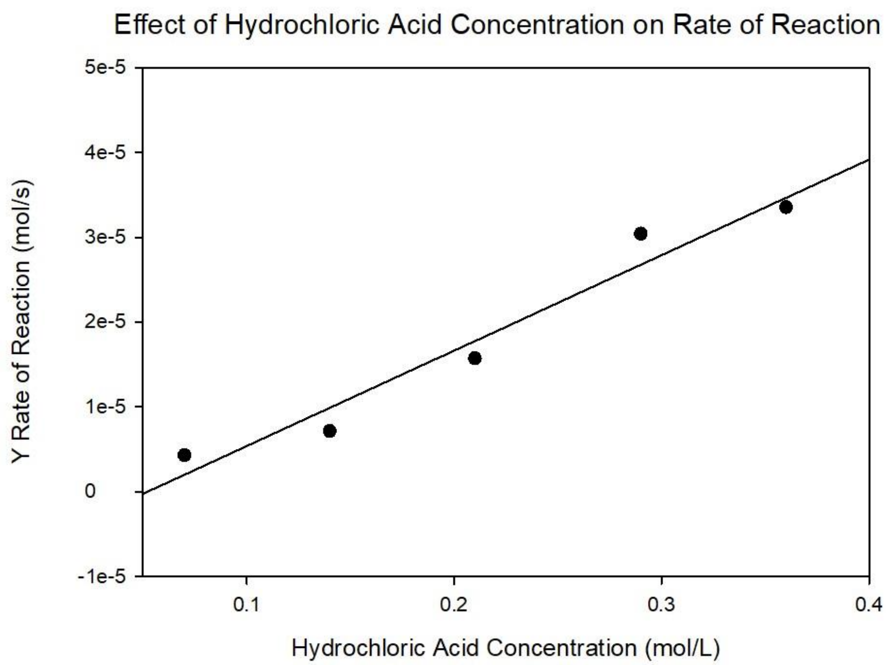
4.4: Processed Data

The processed data can be shown in the following series of graphs where the concentration of the independent variable was graphed to the rate of reaction. From the graphs below, the order of the individual reactants can be determined based on the shape of the graphs. If the graph is linear with a slope that is not equal to one, then the order of the reactant would be first order and if the graph takes the form of a polynomial function, then it would be a second order reaction.

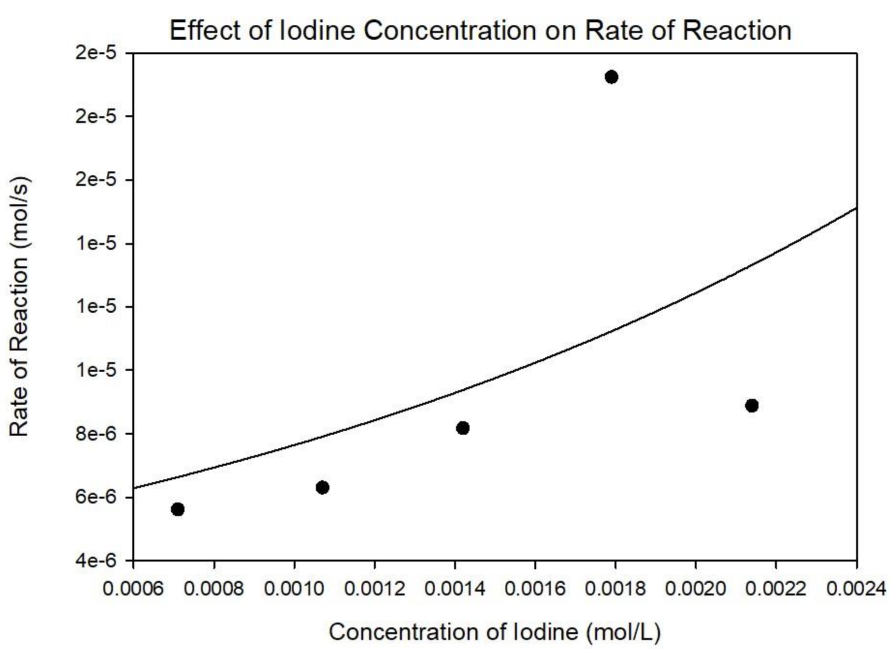
Graph 1: Effect of Acetone Concentration on Rate of Reaction



Graph 2: Effect of Hydrochloric Acid Concentration on Rate of Reaction



Graph 3: Effect of Iodine Concentration on Rate of Reaction



Based on the graphs above, the Acetone can be determined to be a second order reactant while both Hydrochloric Acid and Iodine are first order reactant. Therefore, the rate law of the reaction can be given as follows:

$$r = k[CH_3COCH_3]^2[I_2][HCl]$$

To determine the k value of the rate law, the rate of the reaction as well as the concentration of the reactants for an individual trial can be used. Taking trial one of the acetone concentrations change table, the rate of the rate of the reaction is given as 1.58×10^{-5} mol/s and the concentration of CH_3COCH_3 is 0.194 mol/L, the concentration of I_2 is 2.14×10^{-3} mol/L and the concentration of the Hydrochloric acid is 0.214 mol/L. Therefore, the rate constant can be given as follows:

$$\begin{aligned} k &= \frac{r}{[CH_3COCH_3]^2[I_2][HCl]} \\ &= \frac{1.58 \times 10^{-5}\ mol/s}{(0.194\, mol/L)^2(2.14 \times 10^{-3}\, mol/L)\,(0.214\, mol/L)} \\ &= 0.917 \end{aligned}$$

Hence the final rate law for the iodination of acetone can be given as follows:

$$r = 0.917[CH_3COCH_3]^2[I_2][HCl]$$

5: Conclusion

This investigation explored the effect of the changing concentrations of the two reactants, Acetone and Iodine as well as the concentration of the catalyst Hydrochloric Acid on the rate of the overall reaction. The data was collected using a spectrophotometer and was graphed to determine the order of the individual reactants. This consequently produced the rate law of the reaction, and the rate constant was calculated.

6: Citations

Kazantseva, N.N. & Ernepesova, A. & Khodjamamedov, A. & Geldyev, O.A. & Krumgalz, Boris. (2002). Spectrophotometric analysis of iodide oxidation by chlorine in highly mineralized solutions. Analytica Chimica Acta. 456. 105-119. 10.1016/S0003-2670(01)01625-7.