Changes in Reaction Rates of Acetone with Iodine: How Rate Coefficients Suggest Reaction Mechanisms

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Academic Honesty Statement

I have read and agree to the terms of the Academic Honesty Statement.

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**Abstract**

The experiment examined how a specific proposed mechanism would predict the reaction rate compared to the literature value for a given temperature. The process used the assumption that I2 is a zeroth order reactant and making the reaction pseudo zeroth order to determine the rate by using the slope of a [I2] vs. time graph and at different [acetone] and [HCl] to determine the rate coefficients of [acetone] and [HCl] and using those values to determine an experimental K value for multiple runs comparing the results with the literature value at the temperature the reaction took place. The experimental K values from runs 1 through 6 in numerical order are as follows: 2.39\*10-5±5.95\*10-6, 1.79\*10-5±5.95\*10-6, 1.61\*10-5±5.95\*10-6, 1.75\*10-5±5.95\*10-6, 1.58\*10-5±5.95\*10-6, 1.89\*10-5±5.95\*10-6; and literature K values of: 2.28\*10-5, 2.30\*10-5, 2.20\*10-5, 2.33\*10-5, 2.30\*10-5, 2.33\*10-5 respectively. All trials but trial 5 fell within the uncertainty range for the literature value meaning the proposed mechanism is a likely candidate for being the actual mechanism.

**Introduction**

This report explores a proposed mechanism for the acid-catalyzed iodination of acetone through the use of changes in reaction rates, due to concentration, to compare the theoretical reaction orders from the proposed mechanism to the experimental results. The overall reaction studied in this report can be seen in Eq. (1).

I2 + C3H6O + H2O 🡪 C3H5OI + H3O+ + I- (1)

And the proposed mechanism studied can be seen in reactions (R1) – (R3).

H3O+ + C3H6O ⇋ C3H7O+ (keto) + H2O (R1)

C3H7O+ (keto) + H2O ⇋ C3H6O (enol) + H3O+  (R2)

I2 + C3H6O (enol) 🡪 C3H5OI + H3O+ + I- (R3)

Where R1 is the acid catalyzed reaction that generates a keto intermediate, R2 is the generation of the enol form of acetone, and R3 is the halogenation (in this case iodination) of the enol form of acetone (Sanders, 2020). This proposed mechanism assumes that reactions (R1) and (R3) are fast reactions and reaction (R2) is the slow reaction (rate determining reaction) (Sanders, 2020). Reaction (R1) uses H3O+ instead of H2O because the acid catalyst (in this case HCl) is a strong acid and completely dissociated in the solution (Sanders, 2020). Due to reaction (R3) being a fast reaction, I2 is assumed to be a zeroth order reactant meaning it has no impact on the reaction rate.

The experiment relies on the comparison of reaction rates (which is the rate at which the reaction proceeds) to determine the rate coefficients of the reactants in the rate law (which is the equation used to determine the reaction rate given concentrations of reactants) (Sanders, 2020). In order to do this, iodine is used to determine the reaction rate by measuring the decrease in its concentration because the reaction is done in with significantly more acetone and acid to make the reaction pseudo zeroth-order (where a reaction is made to functionally be a specific order due to the overwhelming concentration of other reactants, in this case zeroth because the concentration of iodine and acetone are so great that they are functionally constants leaving iodine to determine the rate).

In order to do this, the concentration of iodine can be determined by Eq. (2). Which can be rearranged into Eq. (3)

(2)

(3)

Where this version of the equation was used because concentration [I2] is measured in molarity, and *l* is equal to 1 because the cuvettes used were 1cm in length. The rate can be determined using Eq. (4) and due to the equation being pseudo zeroth order meaning Eq. (5) is true

(4)

(5)

The rates can be determined by the slope of a graph of concentration vs. time of iodine fitted with either a linear fit as seen in Eq. (6) or a quadratic fit as seen in Eq. (7).

(6)

(7)

If the proposed reaction rate is a potentially true, then solving for the rate using Eq. (4) with the exponents solved in figures 4.2 and 4.3 will be similar to the literature value at a given temperature as seen in Eq. (8) and is expected to fall within the range of k .

(8)

**Methods**

ε was determined by measuring absorbance of a solution of known concentration (in this case a solution of 0.0040 M I2 that was made of a 1:10 dilution of given stock solution) at a known wave length (470nm) and solving for it using Eq. (2) (Sanders, 2020). The acetone/HCl solution made following the specifications in table 4.1 was poured into the Erlenmeyer flask with the I­­2/DI water solution following the specifications from the same table and swirled to ensure mixture before absorbance, at the same wavelength as when determining ε, is measured vs. time (Sanders, 2020). This was repeated for every trial and exported as a .txt file using an USB drive.

**Results**

The following figure is an example graph showing the results for run 1

Figure 4.1 From time t=45 to t=300 with the quadratic slope being used as it was a better fit to the points

The following is a figure showing the graph used to determine the coefficient for acetone

Figure 4.2 log of [acetone] vs. the log of the initial rate at three different concentrations

The following is a figure showing the graph used to determine the coefficient for HCl

Figure 4.3 log of [HCl] vs. the log of the initial rate at three different concentrations

The following is a table showing the mixture recipes and data analysis

Table 4.1 Reaction recipes and data analysis

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| reaction mixture recipies and data analysis | | | | | | | | | | | |
| sol # | 100 mL-beaker | | Erlenmeyer flask | | concentration when combined (M) | | | Temp ˚C | rate t=0 | Krun | Literature K |
| mL of acetone | mL of HCl | mL of I2 | mL of DI | [acetone] | [HCl] | [I2] |
| 1 | 5 | 10 | 5.0 | 30 | 0.40 | 0.20 | 0.0040 | 21.9 | 1.92E-06 | 2.39E-05 | 2.27573E-05 |
| 2 | 10 | 10 | 5.0 | 25 | 0.80 | 0.20 | 0.0040 | 22.0 | 2.87E-06 | 1.79E-05 | 2.30095E-05 |
| 3 | 25 | 10 | 5.0 | 10 | 2.0 | 0.20 | 0.0040 | 21.6 | 6.43E-06 | 1.61E-05 | 2.20162E-05 |
| 4 | 5 | 20 | 5.0 | 20 | 0.40 | 0.40 | 0.0040 | 22.1 | 2.79E-06 | 1.75E-05 | 2.32643E-05 |
| 5 | 5 | 30 | 5.0 | 10 | 0.40 | 0.60 | 0.0040 | 22.0 | 3.79E-06 | 1.58E-05 | 2.30095E-05 |
| 6 | 5 | 10 | 5.0 | 30 | 0.40 | 0.20 | 0.0040 | 22.1 | 1.52E-06 | 1.89E-05 | 2.32643E-05 |
|  |  |  |  | average | 0.73 | 0.30 |  | 21.95 | 3.22E-06 | 1.46E-05 | 2.28831E-05 |

Calculation 4.1 sample calculation for run 1 of Krun

Calculation 4.2 sample calculation for literature K for run 1

Calculation 4.3 Uncertainty calculation for Krun

**Discussion**

The orders that were obtained from the slopes from figures 4.2 and 4.3 were rounded up to 1 and all the experimental K values fell within the uncertainty for literature value for K except for run 5 which was likely caused by human error by adding less HCl than was needed. The experimental K values also all fell within the expected range meaning this is definitely a potential mechanism for how the reaction proceeds. However, this does not prove that this is the mechanism as there could be some different, unknown mechanism which may be the true mechanism. It was assumed that reaction (R2) was the rate determining step, and that iodine had a zeroth order for its rate coefficient. The experiment could be improved by taking multiple trials of each solution and averaging the rates generated to minimize any random error.

**References**

Appendix A: Treatment of Data. In *Laboratory Manual for CHM 1220,* 3rd Ed.; Sanders, L.J., Underwood, K. A., Clark, T.B., Dolson, D. A., Aga, R. S.; Van Griner: Cincinnati, OH, 2020; pp 213-220

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Sanders, L.J. (2020). Fundamental equilibrium concepts [PowerPoint slides]. Retrieved from https://pilot.wright.edu/d2l/le/content/529544/viewContent/3062597/View

**Appendix A: Graphs of [I2] change over time**

Figure A.1 From time t=39 to t=300 with the quadratic slope being used as it was a better fit to the points

Figure A.2 From time t=30 to t=300 with the quadratic slope being used as it was a better fit to the points

Figure A.3 From time t=39 to t=300 with the quadratic slope being used as it was a better fit to the points

Figure A.4 From time t=48 to t=300 with the linear slope being used as both slopes fit the points well enough to have little difference

Figure A.5 From time t=36 to t=300 with the quadratic slope being used as it was a better fit to the points

**Appendix B: Calculations**

Calculation B.1 calculation for run 2 of Krun

Calculation B.2 calculation for run 3 of Krun

Calculation B.3 calculation for run 4 of Krun

Calculation B.4 calculation for run 5 of Krun

Calculation B.5 calculation for run 6 of Krun

Calculation B.6 sample calculation for literature K for run 2

Calculation B.7 sample calculation for literature K for run 3

Calculation B.8 sample calculation for literature K for run 4

Calculation B.9 sample calculation for literature K for run 5

Calculation B.10 sample calculation for literature K for run 6